Mathematical Methods for Physics using Microsoft Excel

Shinil Cho

CRC Press
Taylor & Francis Group

Mathematical Methods for Physics using Microsoft Excel

In *Mathematical Methods for Physics using Microsoft Excel*, readers will investigate topics from classical to quantum mechanics, which are often omitted from the course work. Some of these topics include rocket propulsion, Rutherford scattering, precession and nutation of a top under gravity, parametric oscillation, relativistic Doppler effect, concepts of entropy, kinematics of wave packets, and boundary value problems and associated special functions as orthonormal bases. Recent topics such as the Lagrange point of the James Webb Space Telescope, a muon detector in relation to Cherenkov's radiation, and information entropy and H-function are also discussed and analyzed. Additional interdisciplinary topics, such as self-avoiding random walks for polymer length and population dynamics, are also described. This book will allow readers to reproduce and replicate the data and experiments often found in physics textbooks, with a stronger foundation of knowledge. While investigating these subjects, readers will follow a step-by-step introduction to computational algorithms for solving differential equations for which analytical solutions are often challenging to find. For computational analysis, features of Microsoft Excel® including AutoFill, Iterative Calculation, and Visual Basic for Applications are useful to conduct hands-on projects. For the visualization of computed outcomes, the Chart output feature can be readily used. There are several first-time attempts on various topics introduced in this book such as 3D-like graphics using Euler's angle and the behavior of wave functions of harmonic oscillators and hydrogen atoms near the true eigenvalues.

Shinil Cho completed his graduate studies at the Seoul National University (MS) and the Ohio State University (PhD). He has conducted research in statistical physics and cryogenic magnetic resonance spectroscopy. Currently he is a Professor at La Roche University. His current research interests include quantum computation and biometric authentication.

Taylor & Francis
Taylor & Francis Group
http://taylorandfrancis.com

Mathematical Methods for Physics using Microsoft Excel

Shinil Cho

CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

Designed cover image: Shutterstock_1145743310

First edition published 2025
by CRC Press
2385 NW Executive Center Drive, Suite 320, Boca Raton FL 33431

and by CRC Press
4 Park Square, Milton Park, Abingdon, Oxon, OX14 4RN

CRC Press is an imprint of Taylor & Francis Group, LLC

ISBN: 9781032844541 (hbk)
ISBN: 9781032850634 (pbk)
ISBN: 9781003516347 (ebk)

DOI: 10.1201/9781003516347

Typeset in Minion
by Deanta Global Publishing Services, Chennai, India

Contents

Preface

"I OFTEN SAY THAT WHEN you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot express it in numbers, your knowledge is of a meager and unsatisfactory kind; it may be beginning of knowledge, but you have scarcely in your thoughts advanced to the stage of Science."

William Thomson (Lord Kelvin)
1824–1907

Mathematics is the queen of physics. Without it, physics cannot make quantitative arguments. Although there are many books on mathematical physics, books of concise descriptions of advanced topics with an easy-to-read guide of computation and visualization are few. This book aims to demonstrate how to study the subjects of physics with numerical analysis as supplemental material for self-study. This book also aims to give you tips on computational algorithms. For number crunching, we use Microsoft Excel®. Its *AutoFill* and macro (Visual Basic for Applications) features are useful for conducting hands-on computational projects. For the visualization of computed results, we use the *Chart* output feature.

There is a wide spectrum of topics covered by this book, from classical mechanics to quantum mechanics. Chapter 1 demonstrates graphical representations of the dynamics of a projectile with air resistance, rocket propulsion, and three-body problems including the Lagrange points, Rutherford scattering, and motions of a top. In Chapter 2, you analyze oscillations with external damping and driving forces, parametric oscillations, and coupled oscillation. Chapter 3 describes wave properties including the relativistic Doppler effect and foundation of wave optics such as the Fourier transform, Huygens's principle, and diffractions. Chapter 4 describes electromagnetic potentials and EM waves derived from Maxwell's equations. The main theme of Chapter 5 is entropy, from its thermodynamical definition to that of information. Chapter 6 guides special functions that we apply to boundary value problems. The concept of orthonormal basis is the main theme and shows series expansions using various special functions. Chapter 7 discusses the kinematics of wave packets and how eigenfunctions and eigenvalues are determined by the boundary condition of a particle in a box, a harmonic oscillator, and a hydrogen atom using a shooting method. In Chapter 8, we discuss polymer properties such as elasticity and length determined by self-avoiding walks. Several models of population dynamics are also introduced in this chapter to learn how to establish a model and visualize their outcomes.

It is the author's wish that readers enjoy the journey of analyzing these topics and feel them on their computers.

CHAPTER 1

Classical Mechanics

Topics of classical mechanics are the foundation of physics. The mathematics of differential equations in classical mechanics can be applied to other areas of physics. Computational algorithms for numerical solutions of differential equations are useful when analytical solutions are difficult to find. We demonstrate numerical solutions of topics in classical mechanics which we often skip in lectures, including projectile motions with air resistance, rocket propulsion, Rutherford scattering, three-body problems, and motions of a top.

1.1 PROJECTILE MOTION WITH AIR RESISTANCE

In general physics, we usually assume no air resistance for projectile motions, introducing only terminal velocity. Let us analyze the projectile motion with air resistance in both the horizontal and vertical directions. The equations of motion including the air resistance are

$$\begin{cases} m\dfrac{dv_x}{dt} = -kv_x \\ m\dfrac{dv_y}{dt} = -mg - kv_x \end{cases} \tag{1.1}$$

where the terms $-kv_x$ and $-kv_y$ are the air resistances proportional to the speed of the object and the coefficient k is the proportional constant. With the initial conditions, $x_0 = y_0 = 0$, $v_{x0} = v_0\cos\theta_0$, and $v_{y0} = v_0\sin\theta_0$, where θ_0 is the initial projection angle, the analytical solution is given by

$$\begin{cases} v_x(t) = v_0\cos\theta_0 e^{-at},\; x(t) = \dfrac{v_{x0}}{a}\left(1-e^{-at}\right) \\ v_y(t) = -\dfrac{g}{a} + De^{-at},\; y(t) = \dfrac{D}{a}\left(1-e^{-at}\right) - -\dfrac{g}{a}t \end{cases} \tag{1.2}$$

where $a = k/m$ and $D = v_{y0}+g/a$.

DOI: 10.1201/9781003516347-1

For the numerical solutions, we apply the Euler method of solving differential equations to Equation 1.1. Refer to Appendix A2 for the Euler method. Figure 1.1 shows the VBA code assuming `g = 1, a = 0.5, v0 = 5`. The time increment is `dt = 0.08`.

Figure 1.2 shows the computed trajectories with the initial angle from 75° to 5° by 10° step. With the air resistance, the maximum range is not attained with the initial angle of approximately 45° but approximately 30° with a detailed analysis.

```
Sub Projectile()
Cells(1, 1) = "Projectile motion with air -resistance using Euler's method"
Dim x(100)
Dim y(100)
Dim vx(100)
Dim vy(100)
Dim theta(8)                            'Initial angle from 5 to 75 degrees
Pi=3.1415927
'Initialization:
   For i = 0 To 99
      x(i) = 0
      y(i) = 0
      vx(i) = 0
      vy(i) = 0
   Next i
      g = 1                             'Gravitational acceleration
      a = 0.5                           'Coefficient of air resistance
      v0 = 5                            'Initial speed
      dt = 0.08                         'Time increment
         Cells(2, 3) = "g=": Cells(2, 4) = g
         Cells(2, 6) = "alpha=": Cells(2, 7) = a
         Cells(2, 9) = "v0=": Cells(2, 10) = v0
'Calculate x, y, vx, vy for a given initial angle theta.
   Radangle = Pi / 180 'Angle unit conversion from degree to radian.
      For i = 5 To 75 Step 10
         'Make integers from 1 to 8:
           ii = (i + 5) / 10
           theta(ii) = i * Radangle            'Initial angle in radian
      'Initial velocities:
           vx(0) = v0 * Cos(theta(ii))
           vy(0) = v0 * Sin(theta(ii))
           RowNum = 100 * (ii - 1)
              Cells(3 + RowNum, 1) = "Angle=": Cells(3 +  RowNum, 2) = i
              Cells(3 + RowNum, 3) = "degrees"
              Cells(4 + RowNum, 3) = "time"
              Cells(4 + RowNum, 4) = "x"
              Cells(4 + RowNum, 5) = "y"
              Cells(4 + RowNum, 6) = "vx"
              Cells(4 + RowNum, 7) = "vy"
           For j = 0 To 97
              jj = j + 1
              Alphax = -a * vx(j)
              Alphay = -g - a * vy(j)
              vx(jj) = vx(j) + Alphax *  dt
              x(jj) = x(j) + vx(j) *  dt
              vy(jj) = vy(j) + Alphay *  dt
              y(jj) = y(j) + vy(j) *  dt
                 Cells(5 + RowNum + j, 3) = j * dt
                 Cells(5 + RowNum + j, 4) = x(j)
                 Cells(5 + RowNum + j, 5) = y(j)
                 Cells(5 + RowNum + j, 6) = vx(j)
                 Cells(5 + RowNum + j, 7) = vy(j)
           Next j
      Next i
End Sub
```

FIGURE 1.1 VBA code for the projectile motion with air resistance.

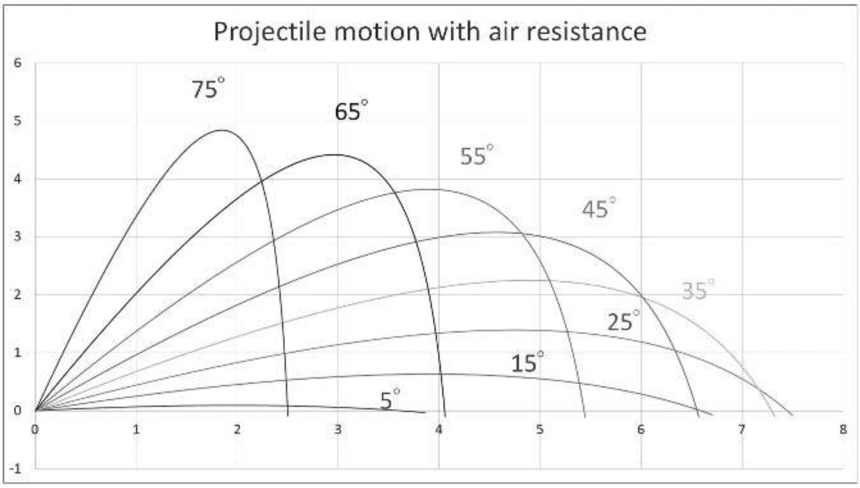


FIGURE 1.2 Trajectories with different initial angles of projectile motion with air resistance.

Note: ***Why does the air resistance depend on the object speed?***

Imagine that a board of cross-sectional area A is moving at speed V through air as shown in Figure 1.3. Here, we assume that V is slower than the average speed of air "particles" v. These particles hit the board from both the front and back sides of the moving board.

Consider the change in momentum of a single particle hitting from the backside is given by

$$\Delta p_1 = m(v - V) - m(-(v - V)) = 2m(v - V), \tag{1.3}$$

and the change in momentum of a single particle hitting from the front side is given by

$$\Delta p_2 = -m(v + V) - m(v + V) = -2m(v + V). \tag{1.4}$$

Suppose the numbers of air particles from the backside and the front side per unit time are I_1 and I_2, respectively, the net force exerted on the board, which is the air resistance, is given by

$$F = (\Delta p_1)I_1 + (\Delta p_2)I_2. \tag{1.5}$$

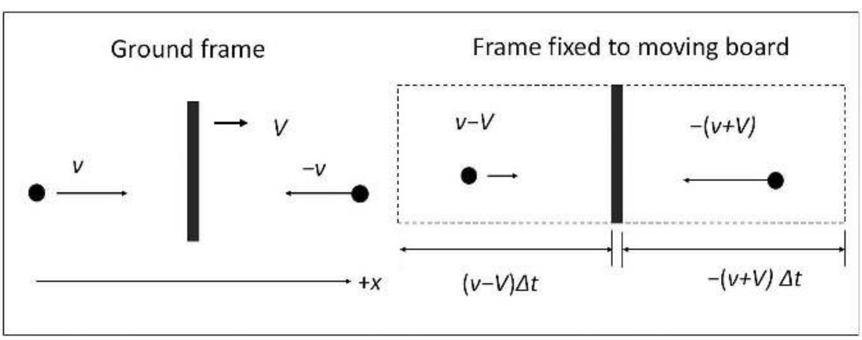


FIGURE 1.3 A plate moving at speed V to $+x$-direction.

Let the mass density of the air be ρ. In the frame of reference fixed to the moving board, in a time interval Δt, all air particles in the volume $(v-V)\bullet\Delta t\bullet A$ at the backside collide with the board to have

$$I_1 = \rho A\left(v - V\right). \tag{1.6}$$

Similarly, all air particles in the volume $(v+V)\bullet\Delta t\bullet A$ at the backside collide with the board per unit time to have

$$I_2 = \rho A\left(v + V\right). \tag{1.7}$$

Therefore, the air resistance is proportional to the speed of the moving board V,

$$F = (\Delta p_1)I_1 + (\Delta p_2)I_2 = 2m\left(v - V\right)\rho A\left(v - V\right) - 2m\left(v + V\right)\rho A\left(v + V\right) = -8m\rho A v V. \tag{1.8}$$

1.2 ROCKET PROPULSION

Rockets are propelled by the momentum produced by the exhausted gas particles. Because rockets lose their masses as the fuel burns, the equations of motion of rockets involve time-varying mass. Assume a rocket projected vertically upward in a uniform gravity field, having velocity $v(t)$, mass $m(t)$ at time t; let the initial velocity and the initial altitude of the rocket be both zero; assume the exhaust gas velocity is $-v_f$ relative to the rocket and a constant rate of expending the fuel is ε per unit time. At time $t + dt$, the rocket velocity becomes $v + dv$, and the rocket mass is reduced to $m - dm$ by burning the fuel dm to produce the high-speed gas of exhaust velocity $-v_f$. The rocket mass at time t should be given by $m(t) = m_0 - \varepsilon t$, where m_0 is the initial rocket mass (i.e., the rocket body + the loaded fuel). For example, numerical data of Saturn V are m_0=2.8 × 10^6 kg, ε = 20 × 10^3 kg, and v_f = 2.40 × 10^3 m/s. These data are cited from NASA's web page [1].

The changing rate of the momentum of the rocket gives the external force exerted on the rocket.

$$\frac{(m - dm)(v + dv) + dm(v + dv - v_f) - mv}{dt} = -mg \tag{1.9}$$

From Equation 1.9, the acceleration of the rocket is

$$\frac{dv}{dt} - v_f \frac{1}{m}\frac{dm}{dt} = -g \tag{1.10}$$

where $dm/dt = \varepsilon$ because $m(t) = m_0 - \varepsilon t$. Solving Equation 1.10, the velocity is given by

$$v(t) = gt - v_f \ln\left|1 - \frac{\varepsilon}{m}t\right|, \tag{1.11}$$

and the altitude of the rocket is

$$h(t) = \int_0^t v(t)dt = -\frac{1}{2}gt^2 + \frac{v_f m_0}{\varepsilon}\left[\left(1 - \frac{\varepsilon}{m_0}t\right)\ln\left|1 - \frac{\varepsilon}{m_0}t\right| + \frac{\varepsilon}{m_0}t\right]. \tag{1.12}$$

```
Sub Rocket()
Cells(1, 1) = "Launching Saturn V using Euler's method"
Dim a(140)
Dim v(140)
Dim h(140)
Dim M(140)
Dim Vtheory(140)
Dim Ytheory(140)
Dim Mtheory(140)
For i = 0 To 139
   a(i) = 0
   v(i) = 0
   y(i) = 0
   M(i) = 0
Next i
   g = 9.8 / 1000            'Gravitational Acceleration in km/sec^2
   vf = 2.4                  'Exhaust speed in km/s.
   t = 0
   dt = 1                    'Time increment in second.
   dM = 20                   'Burning rate of fuel in ton/sec
   M(0) = 2800               'Initial rocket mass with fuel in ton.
   Cells(2, 1) = "Payload": Cells(3, 1) = M(0): Cells(2, 2) = "vf": Cells(3, 2) = vf
   Cells(2, 3) = "dt": Cells(3, 3) = dt
   Cells(5, 2) = "Numerical"
   Cells(6, 1) = "Time": Cells(6, 2) = "Speed": Cells(6, 3) = "Altitude": Cells(6, 4) = "Mass"
   Cells(5, 6) = "Theory"
   Cells(6, 6) = "Speed": Cells(6, 7) = "Altitude": Cells(6, 8) = "Mass"
For i = 0 To 130
   t = i * dt
   a(i) = -g + vf / ((M(0) / dM)  - t)
'Euler's method
   v(i + 1) = v(i) + a(i) * dt                    Use the average velocity
   h(i + 1) = h(i) + (v(i) + v(i + 1)) * dt / 2   between t and t+dt.
   M(i + 1) = M(i) - dM * dt
      Cells(7 + i, 1) = i * dt
      Cells(7 + i, 2) = v(i)
      Cells(7 + i, 3) = h(i)
      Cells(7 + i, 4) = M(i)
'Theoretical calculation
    Epsilon = Abs(1 - t * dM / M(0))
    Vtheory(i) = -g * t - vf * Log(Epsilon)
    Ytheory(i) = -g * t ^ 2 / 2 + (vf * M(0) / dM) * (Epsilon * Lo g(Epsilon) + 1 - Epsilon)
    Mtheory(i) = M(0) - dM * t
      Cells(7 + i, 6) = Vtheory(i)
      Cells(7 + i, 7) = Htheory(i)
      Cells(7 + i, 8) = Mtheory(i)
Next i
End Sub
```

FIGURE 1.4 VBA code of the rocket propulsion.

Figure 1.4 shows the VBA code of launching Saturn V. Because one may expect that the accelerated motion is smooth in time, we apply Euler's method (Appendix A2) for obtaining numerical solutions of $v(t)$ and $h(t)$. In this code, we also calculate the theoretical values using Equations 1.11 and 1.12. Because the initial velocity and the initial altitude of the rocket are both zero, the altitude of the next instance needs to have a non-zero velocity for Euler's method. For this reason, one may use the average velocity between two successive times to calculate the altitude.

Figure 1.5 shows the time dependence of the altitude, the velocity, and the mass of Saturn V. The solid lines are the computed curves and the broken lines are theoretical curves. The theoretical and numerical calculations are in good agreement. For 120 s after launching the rocket, the altitude reaches approximately 120 km, and the rocket mass becomes only about 14% of the initial mass!

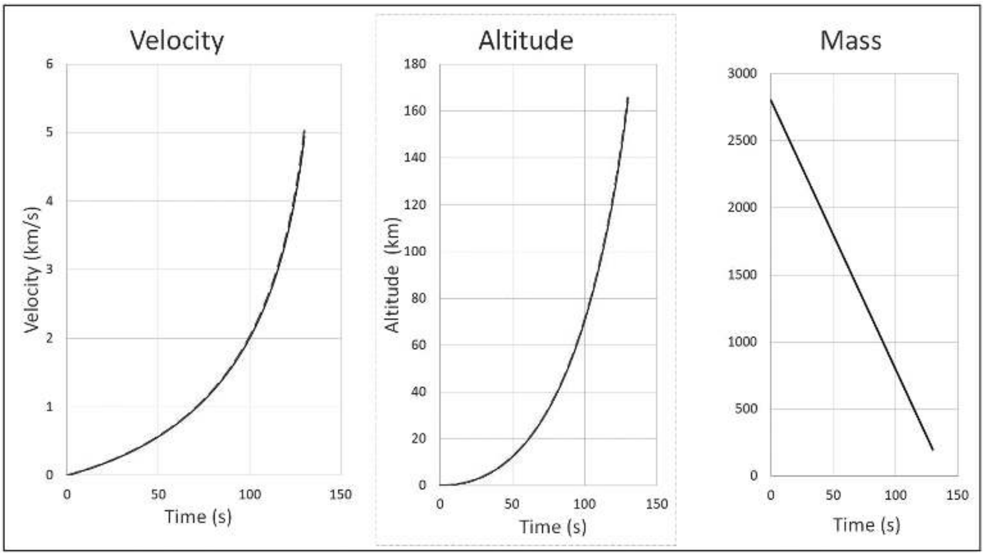


FIGURE 1.5 Time dependence of payload of Saturn V.

1.3 TWO- AND THREE-BODY PROBLEMS OF UNIVERSAL GRAVITY

1.3.1 Two-Body System (Sun-Earth)

Before we analyze three-body systems, we analyze a two-body system such as the Earth around the Sun to demonstrate how planetary motions are computed. For this analysis, we may consider that the Sun is fixed in space. Suppose position (x_e, y_e) and velocity (u_e, v_e) of the Earth are given by equations of motion,

$$\begin{cases} \dfrac{dx_e}{dt} = u_e \\ \dfrac{dy_e}{dt} = v_e \end{cases} \text{and} \begin{cases} \dfrac{du_e}{dt} = -GM_s \dfrac{x_e}{R_e^3} \\ \dfrac{dv_e}{dt} = -GM_s \dfrac{y_e}{R_e^3} \end{cases} \tag{1.13}$$

where G is the universal gravitational constant and Ms is the mass of the Sun. For the numerical calculation, we use the astronomical unit, AU. One AU is the average distance between the Sun and the Earth, denoted as Re. With the AU unit, $GM_s = 4\pi^2$ AU^3/yr^2 [2]. The computational algorithm used here is the Runge-Kutta method. Refer to Appendix A3 for the Runge-Kutta method. Figure 1.6 lists the VBA code for this calculation, and Figure 1.7 shows the orbit of the Earth assuming that the Earth starts moving at $v_{y0} = 2\pi$ AU/year from the initial position (1 AU, 0). The orbit is nearly a circle as expected.

1.3.2 Three-Body System (Sun-Earth-Moon)

Figure 1.8 is a schematic diagram of a three-body, e.g., Sun-Earth-Moon, system. We again assume that the Sun is at the origin of a fixed coordinate frame. Because the orbits of the Earth and the Moon are nearly on the same plane, we may assume their motions are two-dimensional.

```
Sub Earth()
Cells(1,1)="Orbit of Earth"
PI=3.141592654
Cells(2,1)="GM": GM=4*PI^2: Cells(2,2)=GM: Cells(2,3)="AU^3/yr^3"
'Initial conditions:
   Cells(3, 2) = "Initial t": t=0: Cells(4, 2) = t
   Cells(3, 3) = "Initial x": x=1: Cells(4, 3) = x
   Cells(3, 4) = "Initial y": y=0: Cells(4, 4) = y
   Cells(3, 5) = "Initial vx": vx=0: Cells(4, 5) = vx
   Cells(3, 6) = "Initial vy": vy=2*PI: Cells(4, 6) = vy
   Cells(3, 7) = "delta t": h=0.02: Cells(4, 7) = h
'Parmeter names:
   Cells(10, 2) = "t"
   Cells(10, 3) = "x"
   Cells(10, 4) = "y"
   Cells(10, 5) = "vx"
   Cells(10, 6) = "vy"
'Runge-Kutter method:
  n=1000   'number of iterations
  For i = 0 To n
    Cells(i + 11, 2) = t
    Cells(i + 11, 3) = x
    Cells(i + 11, 4) = y
    Cells(i + 11, 5) = vx
    Cells(i + 11, 6) = vy
   lx1 = gx(GM, t, x, y)
   ly1 = gy(GM, t, x, y)
   kx1 = fx(t, x, y, vx, vy)
   ky1 = fy(t, x, y, vx, vy)
   lx2 = gx(GM, t + h / 2, x + h * kx1 / 2, y + h * ky1 / 2)
   ly2 = gy(GM, t + h / 2, x + h * kx1 / 2, y + h * ky1  / 2)
   kx2 = fx(t + h / 2, x + h * kx1 / 2, y + h * ky1 / 2, vx + h * lx1 / 2, vy + h * ly1 / 2)
   ky2 = fy(t + h / 2, x + h * kx1 / 2, y + h * ky1 / 2, vx + h * lx1 / 2, vy + h * ly1 / 2)
   lx3 = gx(GM, t + h / 2, x + h * kx2 / 2, y + h * ky2 / 2)
   ly3 = gy(GM, t + h / 2, x + h * kx2 / 2, y + h * ky2 / 2)
   kx3 = fx(t + h / 2, x + h * kx2 / 2, y + h * ky2 / 2, vx + h * lx2 / 2, vy + h * ly2 / 2)
   ky3 = fy(t + h / 2, x + h * kx2 / 2, y + h * ky2 / 2, vx + h * lx2 / 2,  vy + h * ly2 / 2)
   lx4 = gx(GM, t + h, x + h * kx3, y + h * ky3)
   ly4 = gy(GM, t + h, x + h * kx3, y + h * ky3)
   kx4 = fx(t + h, x + h * kx3, y + h * ky3, vx + h * lx3, vy + h * ly3)
   ky4 = fy(t + h, x + h * kx3, y + h * ky3, vx +  h * lx3, vy + h * ly3)
     vx = vx + h * (lx1 + 2 * lx2 + 2 * lx3 + lx4) / 6
     vy = vy + h * (ly1 + 2 * ly2 + 2 * ly3 + ly4) / 6
     x = x + h * (kx1 + 2 * kx2 + 2 * kx3 + kx4) / 6
     y = y + h * (ky1 + 2 * ky2 + 2 * ky3  + ky4) / 6
    t = t + h
   Next i
End Sub
______________________________________________________________________________
Function gx(GM, t, x, y)
'dvx/dt=gx
     gx = -GM * x / ((x ^ 2 + y ^ 2) ^ 1.5)
End Function
______________________________________________________________________________
Function gy(GM, t, x, y)
'dvy/dt=gy
     gy = -GM * y / ((x ^ 2 + y ^ 2) ^ 1.5)
End Function
______________________________________________________________________________
Function fx(t, x, y, vx, vy)
'vx=dx/dt
     fx = vx
End Function
______________________________________________________________________________
Function fy(t, x, y, vx, vy)
'vy=dy/dt
     fy = vy
End Function
```

FIGURE 1.6 VBA code for the Earth orbit.

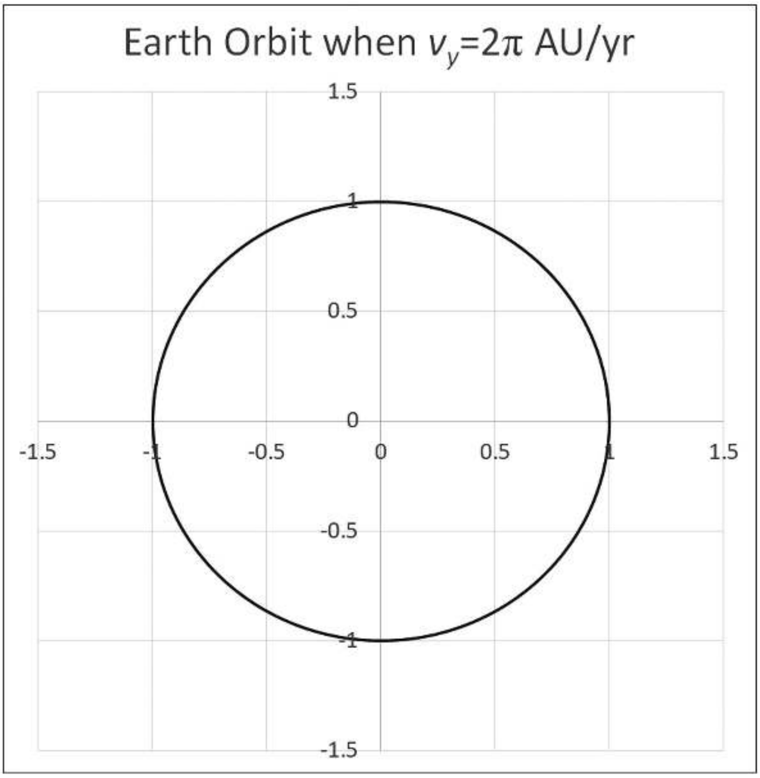


FIGURE 1.7 Earth orbit using the AU unit.

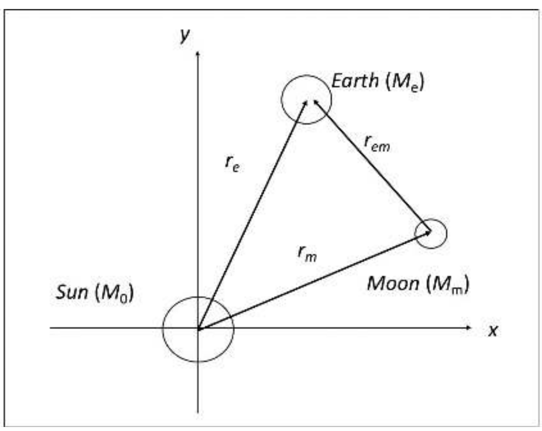


FIGURE 1.8 Positions of Sun-Earth-Moon.

Equations of motions are

$$\begin{cases} \dfrac{dx_e}{dt} = u_e \\ \dfrac{dy_e}{dt} = v_e \end{cases} \text{and} \begin{cases} \dfrac{du_e}{dt} = -GM_s \dfrac{x_e}{r_e^3} + GM_m \dfrac{x_m - x_e}{r_{em}^3} \\ \dfrac{dv_e}{dt} = -GM_s \dfrac{y_e}{r_e^3} + GM_m \dfrac{y_m - y_e}{r_{em}^3} \end{cases} \tag{1.14}$$

for the Earth, and

$$\begin{cases} \dfrac{dx_m}{dt} = u_m \\ \dfrac{dy_m}{dt} = v_m \end{cases} \text{and} \begin{cases} \dfrac{du_m}{dt} = -GM_s \dfrac{x_m}{r_e^3} + GM_e \dfrac{x_e - x_m}{r_{em}^3} \\ \dfrac{dv_e}{dt} = -GM_s \dfrac{y_e}{r_e^3} + GM_e \dfrac{y_e - y_m}{r_{em}^3} \end{cases} \tag{1.15}$$

for the Moon, where $r_{em} = \sqrt{(x_e - x_m)^2 + (y_e - y_m)^2}$.

Because the actual scaled orbiting radii are difficult to draw on paper, the initial positions of the Earth and the Moon are changed to (10 AU, 0) and (10.1 AU, 0), respectively. The initial velocity of the Earth is (0, 2.0) and that of the Moon is (0, 1.5). While the actual mass ratios are $K_m = M_m/M_s = 0.037\times10^{-6}$ and $K_e = M_e/M_s = 3.00 \times 10^{-6}$, we assume $K_e = 5.0 \times 10^{-4}$ and $K_m = 1.0\times10^{-5}$ to show the orbits clearly on a graph. The equations of motion are now

$$\begin{cases} \dfrac{du_e}{dt} = -4\pi^2 \dfrac{x_e}{r_e^3} + 4\pi^2 k_m \dfrac{x_m - x_e}{r_{em}^3} \\ \dfrac{dv_e}{dt} = -4\pi^2 \dfrac{y_e}{r_e^3} + 4\pi^2 k_m \dfrac{y_m - y_e}{r_{em}^3} \end{cases} \text{and} \begin{cases} \dfrac{du_m}{dt} = -4\pi^2 \dfrac{x_m}{r_e^3} + 4\pi^2 K_e \dfrac{x_e - x_m}{r_{em}^3} \\ \dfrac{dv_m}{dt} = -4\pi^2 \dfrac{y_m}{r_e^3} + 4\pi^2 K_e \dfrac{y_e - y_m}{r_{em}^3} \end{cases} \tag{1.16}$$

For analyzing the planetary problems, it is better to apply the Runge-Kutta method (Appendix A3). Figure 1.9 lists the VBA code for the three-body system, and Figure 1.10 shows the computed orbits of Earth and the Moon. The actual mass ratios are very small, and we adjusted the ratios in computation to accentuate the orbit of the Moon.

1.3.3 Euler's Satellite

In the three-body problem, assume the mass of the third object, m, is much smaller than the two fixed-in-space objects M_1 and M_2. Let M_1 be at the origin and M_2 is at $(d, 0)$. The position of the third object is the coordinate (x, y). What is the two-dimensional orbit of the third object as the inter-planetary distance between M_1 and M_2 is changed?

The equation of motion for the third object is given by

$$\begin{cases} \dfrac{dx}{dt} = u \\ \dfrac{dy}{dt} = v \end{cases} \text{and} \begin{cases} \dfrac{du}{dt} = -4\pi^2 \dfrac{x}{\left(x^2 + y^2\right)^{3/2}} + 4\pi^2 K \dfrac{x - d}{\left((x-d)^2 + y^2\right)^{3/2}} \\ \dfrac{dv}{dt} = -4\pi^2 \dfrac{y}{\left(x^2 + y^2\right)^{3/2}} + 4\pi^2 K \dfrac{y}{\left((x-d)^2 + y^2\right)^{3/2}} \end{cases} \tag{1.17}$$

where GM_1 is scaled to be 1 and the mass ratio $M_{12} = M_1/M_2 = 0.5$.

The VBA code for the motion of the third object m is very much similar to the previous three-body problem. Figure 1.11 shows the orbits of the Euler satellite for different distances between M_1 and M_2. Depending on the distance between M_1 and M_2, the satellite exhibits quite different orbits.

```
Sub SunEarthMoon()
Cells(1, 1) = "Sun-Earth-Moon"
    GM = 39.478                 'GM =4*pai^2 is the astronomical unit (AU).
    KE = 0.0005                 'KE=GM(earth), actual value = 3.00E-6
    KM = 0.00001                'KM=G(moon), actual value=0.037E-6
'Writing labels and initial value:
  'Labels:
    Cells(3, 2) = "Initial t": t = 0: Cells(4, 2) = t
    Cells(3, 3) = "Initial xE": xE = 10: Cells(4, 3) = xE
    Cells(3, 4) = "Initial yE": yE = 0: Cells(4, 4) = yE
    Cells(3, 5) = "Initial vxE": vxE = 0: Cells(4, 5) = vxE
    Cells(3, 6) = "Initial vyE": vyE = 2: Cells(4, 6) = vyE
    Cells(3, 7) = "Initial xM": xM = 10.1: Cells(4, 7) = xM
    Cells(3, 8) = "Initial yM": yM = 0: Ce lls(4, 8) = yM
    Cells(3, 9) = "Initial vxM": vxM = 0: Cells(4, 9) = vxM
    Cells(3, 10) = "Initial vyM": vyM = 1.5: Cells(4, 10) = vyM
    Cells(3, 11) = "delta t": h = 0.04: Cells(4, 11) = h          'Time increment
  'Parmeter names:
    Cells(6, 2) = "t"
    Cells(6, 3) = "E-x"
    Cells(6, 4) = "E-y"
    Cells(6, 5) = "E-vx"
    Cells(6, 6) = "E-vy"
    Cells(6, 7) = "M-x"
    Cells(6, 8) = "M-y"
    Cells(6, 9) = "M-vx"
    Cells(6, 10) = "M-vy"
'Runge-Kutter method:
 n = 1000    ' iteration #
 For i = 0 To n
     Cells(i + 7, 2) = t
     Cells(i + 7, 3) = xE
     Cells(i + 7, 4) = yE
     Cells(i + 7, 5) = vxE
     Cells(i + 7, 6) = vyE
     Cells(i + 7, 7) = xM
     Cells(i + 7, 8) = yM
     Cells(i + 7, 9) = vxM
     Cells(i + 7, 10) = vyM
 lxE1 = gxE(GM, KM, xE, yE, xM, yM)
 lyE1 = gyE(GM, KM, xE, yE, xM, yM)
 kxE1 = fxE(xM, yM, vxE, vyE)
 kyE1 = fyE(xM, yM, vxE, vyE)
 lxM1 = gxM(GM, KE, xE, yE, xM, yM)
 lyM1 = gyM(GM, KE, xE, yE, xM, yM)
 kxM1 = fxM(xM, yM, vxM, vyM)
 kyM1 = fyM(xM, yM, vxM, vyM)
 lxE2 = gxE(GM, KM, xE + h * kxE1 / 2, yE + h * kyE1 / 2, xM + h * kxM1 / 2, yM + h * kyM1 / 2)
 lyE2 = gyE(GM, KM, xE + h * kxE1 / 2, yE + h * kyE1 / 2, xM + h * kxM1 / 2, yM + h * kyM 1 / 2)
 kxE2 = fxE(xE + h * kxE1 / 2, yE + h * kyE1 / 2, vxE + h * lxE1 / 2, vyE + h * lyE1 / 2)
 kyE2 = fyE(xE + h * kxE1 / 2, yE + h * kEy1 / 2, vxE + h * lxE1 / 2, vyE + h * lyE1 / 2)
 lxM2 = gxM(GM, KE, xE + h * kxE1 / 2, yE + h * kyE1 / 2, xM + h * kx M1 / 2, yM + h * kyM1 / 2)
 lyM2 = gyM(GM, KE, xE + h * kxE1 / 2, yE + h * kyE1 / 2, xM + h * kxM1 / 2, yM + h * kyM1 / 2)
 kxM2 = fxM(xM + h * kxM1 / 2, yM + h * kyM1 / 2, vxM + h * lxM1 / 2, vyM + h * lyM1 / 2)
 kyM2 = fyM(xM + h * kxM1 / 2, yM + h * kyM 1 / 2, vxM + h * lxM1 / 2, vyM + h * lyM1 / 2)
 lxE3 = gxE(GM, KM, xE + h * kxE2 / 2, yE + h * kyE2 / 2, xM + h * kxM2 / 2, yM + h * kyM2 / 2)
 lyE3 = gyE(GM, KM, xE + h * kxE2 / 2, yE + h * kyE2 / 2, xM + h * kxM2 / 2, yM + h * kyM2 / 2)
 kxE3 = fxE(xE + h * kxE2 / 2, yE + h * kyE2 / 2, vxE + h * lxE2 / 2, vyE + h * lyE2 / 2)
 kyE3 = fyE(xE + h * kxE2 / 2, yE + h * kyE2 / 2, vxE + h * lxE2 / 2, vyE + h * lyE2 / 2)
 lxM3 = gxM(GM, KE, xE + h * kxE2 / 2, yE + h * kyE2 / 2, xM + h * kxM2 / 2, yM + h * kyM2 /  2)
 lyM3 = gyM(GM, KE, xE + h * kxE2 / 2, yE + h * kyE2 / 2, xM + h * kxM2 / 2, yM + h * kyM2 / 2)
 kxM3 = fxM(xM + h * kxM2 / 2, yM + h * kyM2 / 2, vxM + h * lxM2 / 2, vyM + h * lyM2 / 2)
 kyM3 = fyM(xM + h * kxM2 / 2, yM + h * kyM2 / 2, vxM + h * lxM2 /  2, vyM + h * lyM2 / 2)
```

FIGURE 1.9 VBA code for the Sun-Planet-Satellite system.

```
 lxE4 = gxE(GM, KM, xE + h * kxE3, yE + h * kyE3, xM + h * kxM3, yM + h * kyM3)
 lyE4 = gyE(GM, KM, xE + h * kxE3, yE + h * kyE3, xM + h * kxM3, yM + h * kyM3)
 kxE4 = fxE(xE + h * kxE3, yE + h * kyE3, vxE + h * lxE3, vyE + h * lyE3)
 kyE4 = fyE(xE + h * kxE3, yE + h * kyE3, vxE + h * lxE3, vyE + h * lyE3)
 lxM4 = gxM(GM, KE, xE + h * kxE3, yE + h * kyE3, xM + h * kxM3, yM + h * kyM3)
 lyM4 = gyM(GM, KE, xE + h * kxE3, yE + h * kyE3, xM + h * kxM3, yM + h * kyM3)
 kxM4 = fxM(xM + h * kxM3, yM + h * kyM3, vxM + h * lxM3, vyM + h * lyM3)
 kyM4 = fyM(xM + h * kxM3, yM + h * kyM3, vxE + h * lxM3, vyM + h * lyM3)
     vxE = vxE + h * (lxE1 + 2 * lxE2 + 2 * lxE3 + lxE4) / 6
     vyE = vyE + h * (lyE1 + 2 * lyE2 + 2 * lyE3 + lyE4) / 6
     xE = xE + h * (kxE1 + 2 * kxE2 + 2 * kxE3 + kxE4) / 6
     yE = yE + h * (kyE1 + 2 * kyE2 + 2 * kyE3 + kyE4) / 6
     vxM = vxM + h * (lxM1 + 2 * lxM2 + 2 * lxM3 + lxM4) / 6
     vyM = vyM + h * (lyM1 + 2 * lyM2 + 2 * lyM3 + lyM4) / 6
     xM = xM + h * (kxM1 + 2 * kxM2 + 2 * kxM3 + kxM4) / 6
     yM = yM + h * (kyM1 + 2 * kyM2 + 2 * kyM3 + kyM4) / 6
   t = t + h
  Next i
End Sub
_______________________________________________________________________
Function gxE(GM, KM, xE, yE, xM, yM)
    'dvxE/dt=gxE
       gxE = -GM * xE / ((xE ^ 2 + yE ^ 2) ^ 1.5) - GM * KM * (xE - xM) / (((xM - xE) ^ 2 + (yM - yE) ^ 2) ^ 1.5)
End Function
_______________________________________________________________________
Function gyE(GM, KM, xE, yE, xM, yM)
    'dvyE/dt=gEy
       gyE = -GM * yE / ((xE ^ 2 + yE ^ 2) ^ 1.5) - GM * KM * (yE - yM) / (((xM - xE) ^ 2 + (yM - yE) ^ 2) ^ 1.5)
End Function
_______________________________________________________________________
Function gxM(GM, KE, xE, yE, xM, yM)
    'dvxM/dt=gxM
       gxM = -GM * xM / ((xM ^ 2 + yM ^ 2) ^ 1.5) + GM * KE * (xE - xM) / (((xM - xE) ^ 2 + (yM - yE) ^ 2) ^ 1.5)
End Function
_______________________________________________________________________
Function gyM(GM, KE, xE, yE, xM, yM)
    'dvyM/dt=gyM
       gyM = -GM * yM / ((xM ^ 2 + yM ^ 2) ^ 1.5) + GM * KE * (yE - yM) / (((xM - xE) ^ 2 + (yM - yE) ^ 2) ^ 1.5)
End Function
_______________________________________________________________________
Function fxE(xE, yE, vxE, vyE)
    'vxE=dxE/dt
       fxE = vxE
End Function
_______________________________________________________________________
Function fyE(Ex, Ey, vxE, vyE)
    'vyE=dyE/dt
       fyE = vyE
End Function
_______________________________________________________________________
Function fxM(xM, yM, vxM, vyM)
    'vxM=dxM/dt
       fxM = vxM
End Function
_______________________________________________________________________
Function fyM(xM, yM, vxM, vyM)
    'vyM=dyM/dt
       fyM = vyM
End Function
```

FIGURE 1.9 Continued.

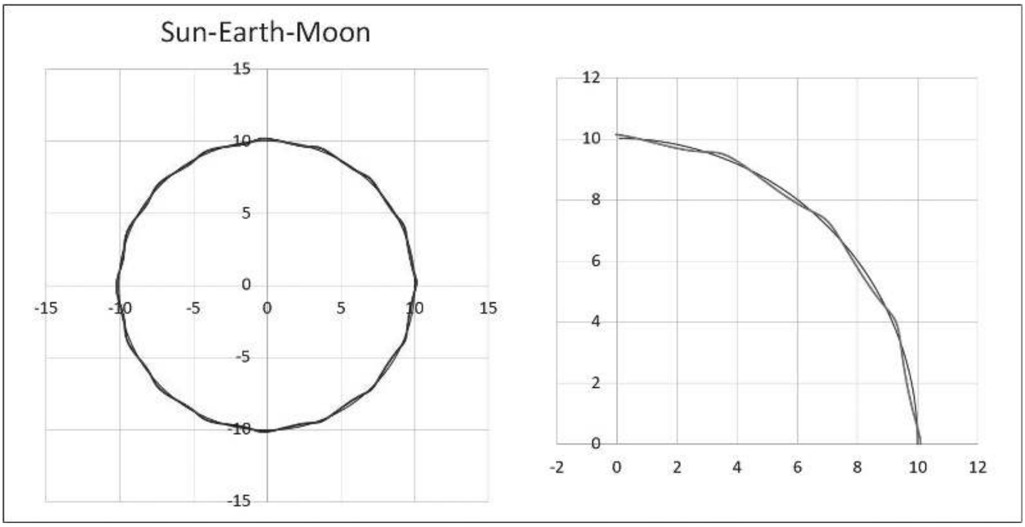


FIGURE 1.10 Orbits of a planet and its satellite plane around the Sun.

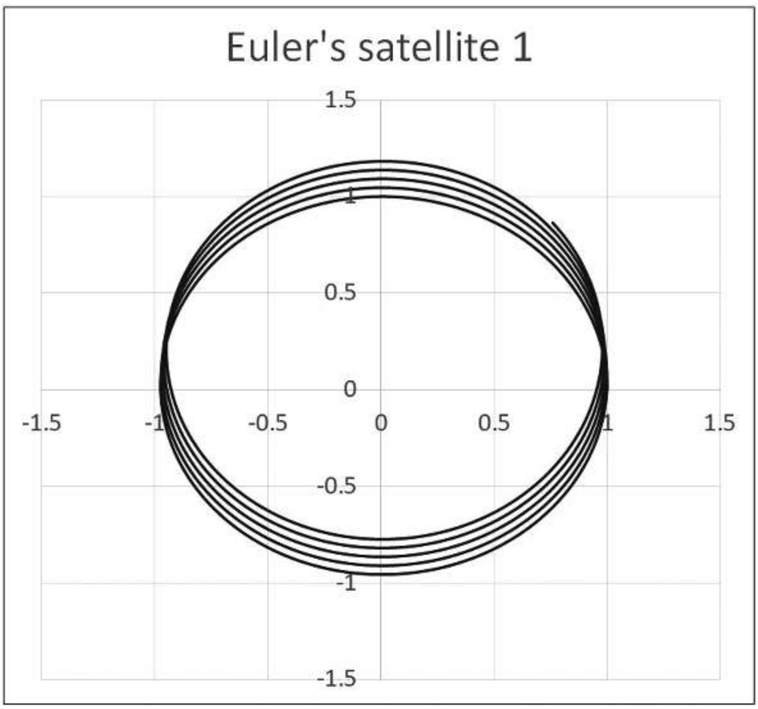


FIGURE 1.11A Orbits of Euler's satellite. Two planets are separated well (d=10): the satellite is orbiting around M_1. The initial position of the satellite is (1, 0) and the initial velocity is (0, 2π). The position of M_2 is not shown in this diagram.

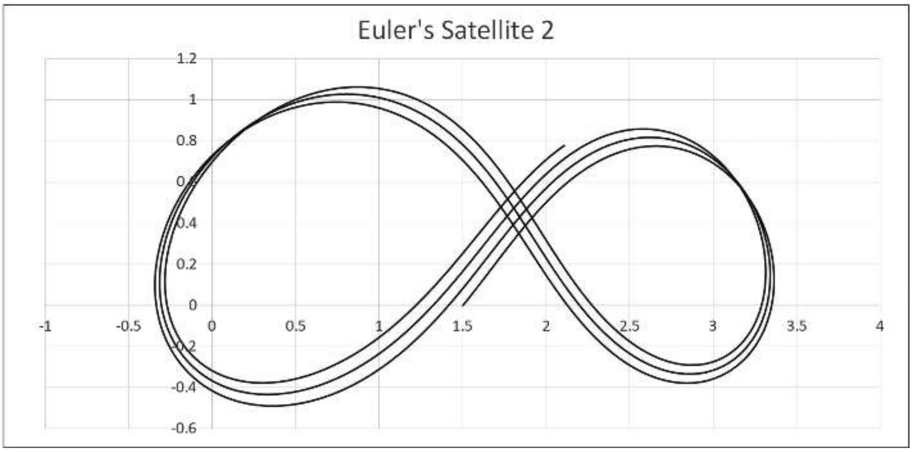


FIGURE 1.11B Orbits of Euler's satellite. Two planets are relatively close (d=3): the satellite is orbiting around M_1 and M_2. The initial position of the satellite is (1.5, 0) and the initial velocity is (3.5, 3.5).

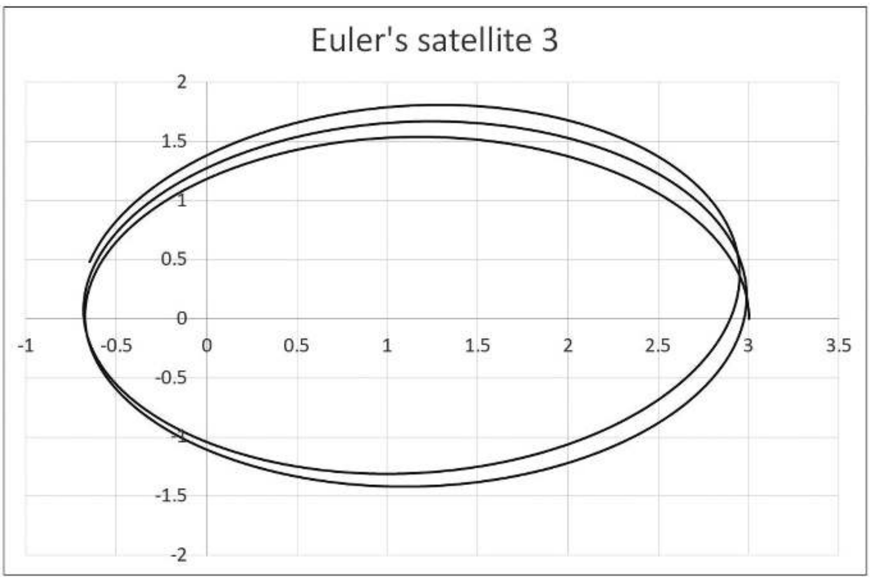


FIGURE 1.11C Orbits of Euler's satellite. Two planets are close (d=0.5): the satellite is orbiting enclosing M_1 and M_2. The initial position of the satellite is (3.0, 0) and the initial velocity is (3.14, 0).

1.3.4 Lagrange Points

There are unique points in the three-body system, called the Lagrange points. The Lagrange points are points of equilibrium for a small-mass object such as the James Webb Space Telescope (JWST) in the gravitational field due to two massive orbiting bodies [3]. Figure 1.12 illustrates the Lagrange points. There are five Lagrange points where the net universal gravitational forces of the Earth and the Sun on a small object m provide balance with the centrifugal force of the orbiting object as observed from the Earth. Equation 1.20

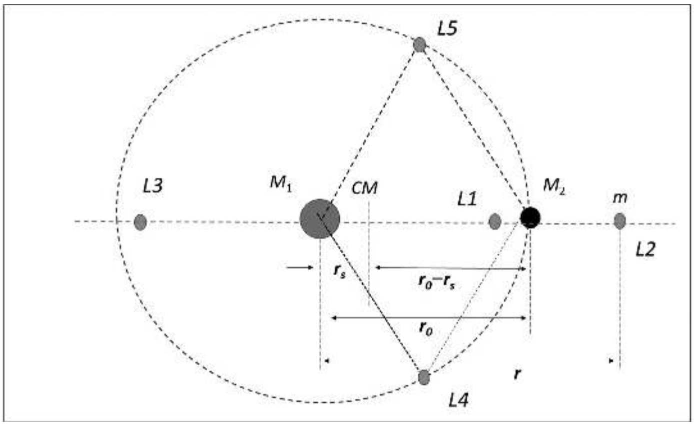


FIGURE 1.12 Lagrange points.

derived below describes this balancing condition. *L*2 is one of the five points in space where JWST has been deployed. *L*2 is behind the Earth from the Sun and enables JWST's sunshield to effectively protect its instruments from the electromagnetic radiation and heat of the Sun, Earth, and Moon.

Let us find where *L*2 is. Let M_1 be the Sun and M_2 be the Earth. These two celestial bodies M_1 and M_2 are huge compared with the third body m. Let the coordinates frame (X, Y) be the frame fixed to the Sun-Earth system. The origin of the XY-frame is the center of mass of the Sun and the Earth (*CM* in Figure 1.12). Notice that the XY-frame is a rotating frame around the center of mass. Referring to Figure 1.12, the distance between the Sun and the origin, r_s, is given by

$$r_s = \frac{M_2}{M_1 + M_2} r_0 = \frac{(M_2 / M_1)}{1 + (M_2 / M_1)} r_0 \tag{1.18}$$

where r_0 is the distance between M_1 and M_2. Between the Sun and the Earth, r_0 =1 AU = 1.496×10^8 km.

Because the XY-frame is a rotating frame with angular velocity ω_0, the relative motion of the third body as observed in the XY-frame is due to the forces exerted on the third body, which are the centrifugal force and the Coriolis force in addition to the universal gravities of m-M_1 and m-M_2. Thus, the equation of motion of m in the XY-frame is given by

$$m\vec{a} = \vec{F}_1 + \vec{F}_2 + m\omega_0^2\vec{r} + 2m(\vec{v} \times \vec{\omega}). \tag{1.19}$$

In the above equation, $|\vec{F}_1| = G\frac{mM_1}{r_1^2}$ and $|\vec{F}_2| = G\frac{mM_2}{r_2^2}$ where r_1 and r_2 are the distances between M_1 and m and M_2 and m, respectively.

If the third object is at a point where the net force acting on the third body vanishes, the *third object must be at rest as observed in the XY-frame*. In other words, from the Earth, the velocity and the acceleration in Equation 1.19 are both zero and Equation 1.19 becomes

$$\vec{F}_1 + \vec{F}_2 + m\omega_0^2\vec{r} = 0. \tag{1.20}$$

As shown in Figure 1.12, Equation 1.20 for the Lagrange point *L2* is one-dimensional and Equation 1.20 reads

$$-G\frac{mM_1}{r^2}-G\frac{mM_2}{(r-r_0)^2}+m\omega_0^2(r-r_s)=0 \tag{1.21}$$

where r_0–r_s is the distance from the center of mass to the Earth, and r–r_s is the distance from the center of mass to the third object. The angular velocity ω_0 of the Sun and the Earth can be calculated from the rotational motion of the Sun around the center of mass,

$$M_1 r_s \omega_0^2 = G\frac{M_1 M_2}{r_0^2}$$

and we obtain

$$\omega_0=\sqrt{G\frac{(M_1+M_2)}{r_0^3}}=\sqrt{GM_1\frac{(1+M_2/M_1)}{r_0^3}}. \tag{1.22}$$

Plug Equation 1.22 into Equation 1.21 to obtain

$$-\frac{1}{r^2}-\frac{M_2/M_1}{(r-r_0)^2}+\frac{1+M_2/M_1}{r_0^3}(r-r_s)=0.$$

Let $\alpha = M_2/M_1$ and $\beta = (1+\alpha)/r_0^3$, then

$$-(r-r_0)^2-\alpha r^2+\beta r^2(r-r_0)^2(r-r_s)=0. \tag{1.23}$$

Therefore, the Lagrange point *L2* is the point that satisfies the following equation,

$$f(r)=\alpha r^2(r-r_0)^2-\beta r^2(r-r_0)^2(r-r_s)=0. \tag{1.24}$$

Figure 1.13 lists the VBA code to find the Lagrange point *L*2, where the net force on the third body vanishes. *L2* is the root of Equation 1.24, which can be found numerically. The algorithm used here to find the root of the function *f*(*r*) is simple [4]. The algorithm starts from a trial value of *r* guaranteed to be less than the root and increases the trial value by small positive steps, backing up and having the step size every time *f*(*r*) changes sign. The values of *r* generated by this procedure converge to the root, and the root-seeking step can be terminated whenever the step size becomes less than the preset tolerance. The boxed part of the code of Figure 1.14 shows this algorithm.

Figure 1.14 shows the calculated net force *f*(*r*) by changing the distance between the third object and the Sun, *r*. The "zero point" of the force function *f*(*r*) is subtle and unstable, indicating that the point *L2* is not a stable equilibrium point. The calculated zero point is 1.01004 AU. Thus, the distance between the Earth and the third object is given by $r - r_0 =$ 0.01004 AU = 1.502×10^6 km [5].

```
Sub Root()
Cells(2, 1) = "Finding L2 (Sun -Earth)"
'Data
   Msun = 1.99E+30
   Mearth = 5.98E+24
'Distance from Sun to Earth is 1 AU= 1.496E8 km.
   Cells(2, 4) = "Mearth/Msun": alpha = Mearth / Msun: Cells(3, 4) = alpha
   Cells(2, 5) = "CM": rs = alpha / (1 + alpha): Cells(3, 5) = rs
   Cells(4, 1) = "r"
   Cells(4, 2) = "Net force"
   beta = 1 + alpha
'Calculate sum of gravity and centripetal force
   For i = 0 To 150
      r  = i / 100
         NetForce = Fr(r, alpha, beta, rs)
            Cells(5 + i, 1) = r
            Cells(5 + i, 2) = NetForce
   Next i
'Find L2
 Tolerance = 1.0E-6                   'to find the zero with this tolerance.
   Cells(5, 5) = "Iteration"
   Cells(5, 6) = "Root"
   'Initial guess from the net force
     r = 1.01    'Starting point
     fold = Fr(r, alpha, beta, rs)      'Net force at the starting point. Fold>0
       dr = 0.0001                      'Increment of distance
         Iter = 0
          While Abs(dr) > Tolerance
           Iter = Iter + 1
           r = r + dr
           Cells(5 + Iter, 5) = Iter: Cells(5 + Iter, 6) = r
             If fold * Fr(r, alpha, beta, rs) > 0 Then GoTo Skip
               r = r - dr
               dr = dr / 2              'Narrowing the increment width
       Skip: Wend
End Sub
_______________________________________________________________
Function Fr(r, alpha, beta, rs)
Fr = (r - 1) ^ 2 + alpha * r ^ 2 - beta * (r - rs) * r ^ 2 * (r - 1) ^ 2
End Function
```

Finding a root of equation (1.24).

FIGURE 1.13 VBA code for finding the second Lagrange point.

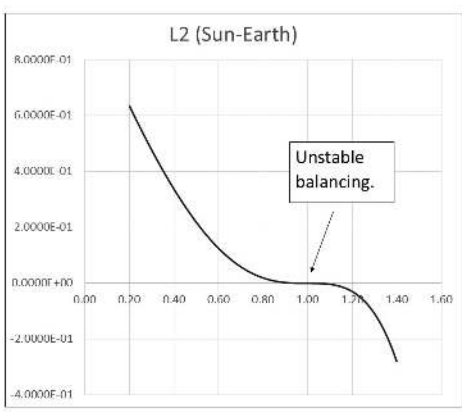


FIGURE 1.14 Net force on the third object.

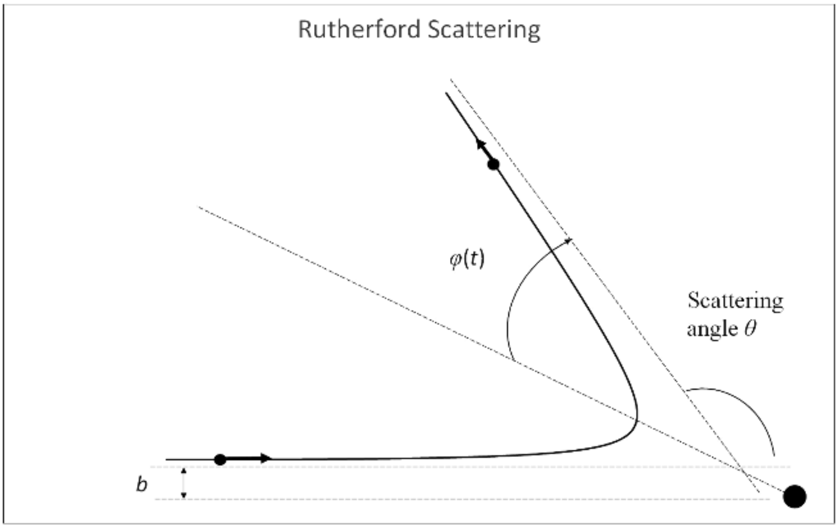


FIGURE 1.15 Scattering of a charged particle by a heavy nucleus.

1.4 RUTHERFORD SCATTERING – SCATTERING IN CENTRAL FORCE FIELD

1.4.1 Theory

Rutherford scattering describes the motion of an incoming charged particle such as an alpha-particle scattered by a heavy target nucleus due to the Coulomb repulsive force [6]. The target nucleus (charge Ze) is assumed to be at rest in space. An incident particle (charge ze and mass m) has an initial velocity v_∞ far away from the nucleus as shown in Figure 1.15. This is the same as the Kepler problem, similar to the discussion in Section 1.3.1, except that the force is repulsive. Using conventional notations, the equation of motion of the incident particle is

$$m\frac{d^2\vec{r}}{dt^2} = \frac{1}{4\pi\varepsilon_0}\frac{ze(Ze)}{r^2}\frac{\vec{r}}{r}. \tag{1.25}$$

In Figure 1.15, the length of a vertical line from the target nucleus to the incident direction of the incoming particle is called the impact parameter b. Recall that the target nucleus is fixed at the origin.

The radial part of the Equation 1.25 of motion of is

$$m\left[\frac{d^2r}{dt^2} - r\left(\frac{d\varphi}{dt}\right)^2\right] = \frac{K}{r^2} \text{ where } K = \frac{1}{4\pi\varepsilon_0}zZe^2. \tag{1.26}$$

Because the Coulomb force has no angular component, the angular part of Equation 1.25 is

$$m\frac{1}{r}\frac{d}{dr}\left(r^2\frac{d\varphi}{dt}\right) = 0, \tag{1.27}$$

and thus, $r^2 \frac{d\varphi}{dt} = \frac{L}{m}$ where L is angular momentum. Combining Equations 1.26 and 1.27, we obtain

$$\frac{d^2r}{dt^2} - \frac{r}{m}\left(\frac{L}{mr^2}\right)^2 = \frac{K}{mr^2}.$$

Using $\frac{d}{dt} = \frac{d\varphi}{dt}\frac{d}{d\varphi}$ and $u = \frac{1}{r}$, we obtain

$$\frac{d^2u}{d\varphi^2} + u = -m\frac{K}{L^2} \equiv -D \text{ where } D = \frac{mK}{L^2}. \tag{1.28}$$

Let us find a solution in the form of $u(\varphi) = A\cos(\varphi - \alpha) - D$ or $r(\varphi) = 1/[A\cos(\varphi - \alpha) - D]$ where A and α are integral constants. This function u indeed satisfies Equation 1.28. Define angle $\varphi = 0$ when the particle is at its turning point, i.e., $dr/d\varphi = 0$ at $r = r_{\text{min}}$:

$$\varphi = 0 \text{ when } \left.\frac{dr}{d\varphi}\right|_{r=r_{\min}} = \left.\frac{d(1/u)}{d\varphi}\right|_{r=r_{\min}} = -\left.\frac{1}{u^2}\frac{du}{d\varphi}\right|_{r=r_{\min}} = 0. \tag{1.29}$$

With this selection of coordinates, the constant α becomes zero. (1.30)

In order to determine the other constant A, we use the total energy of the motion,

$$E = \left[\left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\varphi}{dt}\right)^2\right] + \frac{K}{r} = \frac{L^2}{2m}\left[\left(\frac{du}{d\varphi}\right)^2 + u^2\right] + Ku. \tag{1.31}$$

Let $u_{\text{m}} = 1/r_{\text{min}}$, then u_{m} satisfies

$$E = \frac{L^2}{2m}u_m^2 + Ku_m \tag{1.32}$$

at the turning point where $du/d\varphi = 0$. Equation 1.32 may be solved to obtain the root u_{m}. Because u_{m} must be non-negative, we find

$$u_m = -\frac{mK}{L^2} + \sqrt{\left(\frac{mK}{L^2}\right)^2 + \frac{2mE}{L^2}}. \tag{1.33}$$

Thus, $u_m = A\cos\varphi\big|_{\varphi=0} - D = A - \frac{mK}{L^2}$, and we obtain

$$A = u_m + \frac{mK}{L^2} = \sqrt{\left(\frac{mK}{L^2}\right)^2 + \frac{2mE}{L^2}} = \left(\frac{mK}{L^2}\right)\sqrt{1 + \frac{2EL^2}{mK^2}}. \tag{1.34}$$

Using the obtained α, A, and D, the solution, $u = A\cos(\varphi - \alpha) - D$, of the differential Equation 1.28 becomes a hyperbolic function,

$$u = \frac{1}{r} = A\cos\varphi + \frac{mK}{L^2} = \left(\frac{mK}{L^2}\right)\sqrt{1+\frac{2EL^2}{mK^2}}\cos\varphi - \frac{mK}{L^2} = \left(\frac{mK}{L^2}\right)\left[-1+\sqrt{1+\frac{2EL^2}{mK^2}}\cos\varphi\right],$$

or
$$r = \frac{r_0}{-1+\varepsilon\cos\varphi} \text{ where } r_0 = \frac{L^2}{mK} \text{ and } \varepsilon = \sqrt{1+\frac{2EL^2}{K^2}} = \sqrt{1+\frac{r_0^2}{b^2}}. \tag{1.35}$$

In the above Equation 1.35, $E = (1/2)mv_\infty{}^2$ and $L = mv_\infty b$, where v_∞ is the incident velocity, and b is the impact parameter. By conversely expressing r_0 with ε, we obtain

$$r = \frac{b^2(\varepsilon^2-1)}{-1+\varepsilon\cos\varphi}. \tag{1.36}$$

Therefore, we observe $\cos\varphi_\infty = \pm 1/\varepsilon$ for the incoming α-particle and $\pi \pm 1/\varepsilon$ for the outgoing α-particle where the upper branch (i.e., the upper part of Figure 1.17) takes the positive sign and the lower branch takes the negative sign.

The scattering angle θ shown in Figure 1.15 is expressed by $\theta = \pi - 2\varphi_\infty$, and thus,

$$\tan\left(\frac{\theta}{2}\right) = \cot(\varphi_\infty) = \frac{\cos\varphi_\infty}{\sqrt{1-\cos^2\varphi_\infty}} = \sqrt{1-\varepsilon^2} = \frac{r_0}{b},$$

and

$$\tan(\varphi_\infty) = \frac{b}{r_0}. \tag{1.37}$$

Therefore, tan (φ_∞) is proportional to the impact parameter.

The differential cross-section $\sigma(\theta)$ is defined as the probability of scattering within the unit solid angles $d\Omega = 2\pi\sin\theta d\theta$ along the θ-direction from the incident α-particles passing through the area between b and $b + db$, which is given by $2\pi b$db, and

$$\sigma(\theta) = -\frac{2\pi b db}{2\pi\sin\theta d\theta} = \left(\frac{K}{2mv_\infty^2}\right)\frac{1}{\sin^4(\theta/2)} \text{ where } K = \frac{zZe^2}{4\pi\varepsilon_0}. \tag{1.38}$$

1.4.2 Numerical Analysis

Let the equation of motion for a computational analysis of the two-dimensional case.

$$\begin{cases} m\dfrac{d^2x}{dt^2} = \dfrac{1}{4\pi\varepsilon_0}\dfrac{zZe^2}{(x^2+y^2)^{2/3}}x \\ m\dfrac{d^2y}{dt^2} = \dfrac{1}{4\pi\varepsilon_0}\dfrac{zZe^2}{(x^2+y^2)^{2/3}}y \end{cases} \tag{1.39}$$

The equation of motion of an incoming α-particle is analogous to that of a motion under universal gravity, and the computational analysis can apply the Runge-Kutta method (Appendix A3).

```
Sub Rutherford()
Cells(1, 1) = "Rutherford Scattering"
'Parmeter Alpha is the constant.
     Cells(2, 1) = "Alpha": Alpha = 10#: Cells(2, 2) = Alpha
'Writing labels and initial value in cells:
         Cells(3, 2) = "Initial t": t = 0: Cells(4, 2) = t
         Cells(3, 3) = "Initial x" : x = -40: Cells(4, 3) = x
        'Cells(3, 4) = "Initial y": y = 5: Cells(4, 4) = y
         Cells(3, 5) = "Initial vx": vx = 1: Cells(4, 5) = vx
         Cells(3, 6) = "Initial vy": vy = 0: Cells(4, 6) = vy
         Cells(3, 7) = "delta t": h = 0.05: Cells(4, 7) = h
'Runge-Kutter method:
 n = 2000 ' Iteration #
 Cells(10, 2) = "t"
   For j = 1 To 15
          t = Cells(4, 2)
          x = Cells(4, 3)
          y = j
          vx = Cells(4, 5)
          vy = Cells(4, 6)
          Cells(10, 1) = "t"
          Cells(10, 2 + 3 * (j - 1)) = "x"
          Cells(10, 3 + 3 * (j - 1)) = "y+"
          Cells(10, 4 + 3 * (j - 1)) = "y-"
        For i = 0 To n
           Cells(i + 11, 1) = t
           Cells(i + 11, 2 + 3 * (j - 1)) = x
           Cells(i + 11, 3 + 3 * (j - 1)) = y
           Cells(i + 11, 4 + 3 * (j - 1)) = -y
    LX1 = gx(Alpha, t, x, y)
    Ly1 = gy(Alpha, t, x, y)
    Kx1 = fx(t, x, y, vx, vy)
    Ky1 = fy(t, x, y, vx, vy)
    LX2 = gx(Alpha, t + h / 2, x + h * Kx1 / 2, y + h * Ky1 / 2)
    Ly2 = gy(Alpha, t + h / 2, x + h * Kx1 / 2, y + h * Ky1 / 2)
    Kx2 = fx(t + h / 2, x + h * Kx1 / 2, y + h * Ky1 / 2, vx + h * LX1 / 2,  vy + h * Ly1 / 2)
    Ky2 = fy(t + h / 2, x + h * Kx1 / 2, y + h * Ky1 / 2, vx + h * LX1 / 2, vy + h * Ly1 / 2)
    LX3 = gx(Alpha, t + h / 2, x + h * Kx2 / 2, y + h * Ky2 / 2)
    Ly3 = gy(Alpha, t + h / 2, x + h * Kx2 / 2, y + h  * Ky2 / 2)
    Kx3 = fx(t + h / 2, x + h * Kx2 / 2, y + h * Ky2 / 2, vx + h * LX2 / 2, vy + h * Ly2 / 2)
    Ky3 = fy(t + h / 2, x + h * Kx2 / 2, y + h * Ky2 / 2, vx + h * LX2 / 2, vy + h * Ly2 / 2)
    LX4 = gx(Alpha, t + h, x + h * Kx3, y + h * Ky3)
    Ly4 = gy(Alpha, t + h, x + h * Kx3, y + h * Ky3)
    Kx4 = fx(t + h, x + h * Kx3, y + h * Ky3, vx + h * LX3, vy + h * Ly3)
    Ky4 = fy(t + h, x + h * Kx3, y + h * Ky3, vx + h * LX3, vy + h * Ly3)
        vx = vx + h * (LX1 + 2 * LX2 + 2 * LX3 + LX4) / 6
        vy = vy + h * (Ly1 + 2 * Ly2 + 2 * Ly3 + Ly4) / 6
        x = x + h * (Kx1 + 2 * Kx2 + 2 * Kx3 + Kx4) / 6
        y = y + h * (Ky1 + 2 * Ky2 + 2 * Ky3 + Ky4) / 6
      t = t + h
      Next i
 Next j
End Sub
```

FIGURE 1.16 VBA code to compute the trajectories of Rutherford scattering.

Figure 1.16 lists the VBA code to compute the trajectories by changing the impact parameters 1 to 15. Figure 1.17 shows the calculated trajectories.

From Equation 1.37, $\tan(\varphi_\infty)$ is expected to be proportional to the impact parameter b. Figure 1.18 shows the data of the coordinates (x, y) of the minimum r for given impact parameters. From the coordinates, we calculate $\cot(\varphi_\infty/2) = 1/\tan(\varphi_\infty/2) = r_0/b$.

```
Function gx(Alpha, t, x, y)
'dvx/dt=gx
      gx = Alpha * x / ((x ^ 2 + y ^ 2) ^ 1.5)
End Function
Function gy(Alpha, t, x, y)
'dvy/dt=gy
      gy = Alpha * y / ((x ^ 2 + y ^ 2) ^ 1.5)
End Function
Function fx(t, x, y, vx, vy)
'vx=dx/dt
      fx = vx
End Function
Function fy(t, x, y, vx, vy)
'vy=dy/dt
      fy = vy
End Function
```

FIGURE 1.16 Continued.

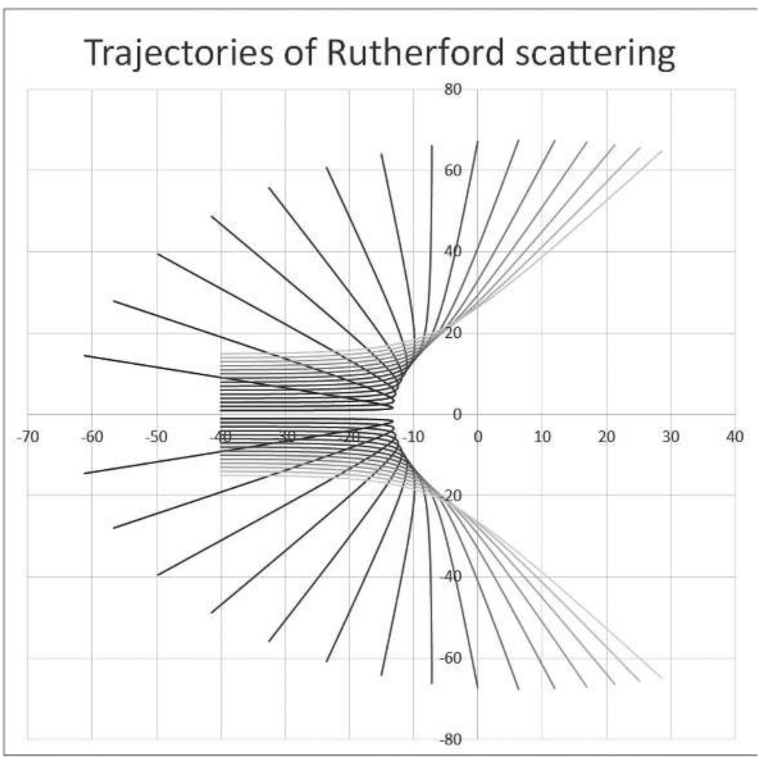
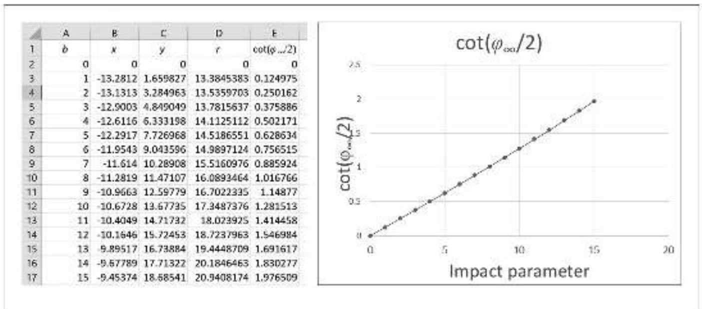


FIGURE 1.17 Trajectories of Rutherford scattering.



	A	B	C	D	E
1	b	x	y	r	cot(φ∞/2)
2	0	0	0	0	0
3	1	-13.2812	1.659827	13.3845383	0.124975
4	2	-13.1313	3.284963	13.5359703	0.250162
5	3	-12.9003	4.849049	13.7815637	0.375886
6	4	-12.6116	6.333198	14.1125112	0.502171
7	5	-12.2917	7.726968	14.5186551	0.628634
8	6	-11.9543	9.043596	14.9897124	0.756515
9	7	-11.614	10.28908	15.5160976	0.885924
10	8	-11.2819	11.47107	16.0893464	1.016766
11	9	-10.9663	12.59779	16.7022335	1.14877
12	10	-10.6728	13.67735	17.3487376	1.281513
13	11	-10.4049	14.71732	18.023925	1.414458
14	12	-10.1646	15.72453	18.7237963	1.546984
15	13	-9.89517	16.73884	19.4448709	1.691617
16	14	-9.67789	17.71322	20.1846463	1.830277
17	15	-9.45374	18.68541	20.9408174	1.976509

FIGURE 1.18 Scattering angle vs impact parameter.

1.5 ROTATIONAL MOTIONS

1.5.1 Rotational Motion with Reducing Radius

An object attached to a pivot point of a friction-free surface by a string is rotating on the surface as shown in Figure 1.19. The string is being shortened by a constant radial force F such that the string length is $r(t) = r_0(1 - \varepsilon t)$ where r_0 is the initial length and ε is the reduction rate. The mass of the object is m and the angular velocity of the object is $\omega(t)$. The basic equations for these rotational motions are:

Equation of motion: $\dfrac{d\vec{L}}{dt} = \vec{\tau}$ where $\vec{L}$ is angular momentum and $\vec{\tau}$ is torque;

Moment of inertia: $I = \sum_i m_i r_i^2$ and $I = mr^2$ in this case;

Angular momentum: $\vec{L} = I\vec{\omega}$; and

Rotational kinetic energy: $K = \dfrac{1}{2} I\omega^2$.

Because the force pulling the string does cause no torque, the angular momentum is conserved and we obtain

$$I(t)\omega(t) = I_0\omega_0, \text{ or } mr^2(t)\omega(t) = mr_0^2\omega_0. \tag{1.40}$$

Thus, the time dependence of the angular velocity is

$$\omega(t) = \left(\frac{r_0}{r(t)}\right)^2 \omega_0 = \left(\frac{1}{1-\varepsilon t}\right)^2 \omega_0. \tag{1.41}$$

The rotational kinetic energy is not conserved. The change in the kinetic energy is given by

$$\Delta K = \frac{1}{2} I\omega^2 - \frac{1}{2} I_0\omega_0^2 = \frac{1}{2} m r_0^2 \omega_0^2 \left(\frac{1}{r^2} - \frac{1}{r_0^2}\right)^2. \tag{1.42}$$

```
Sub AngMomentum()
Cells(1, 1) = "Rotational motion of an object while the string attached to the object is reduced."
Dim Omega(1001)
Dim Theta(1001)
Dim x(1000)
Dim y(1000)
Dim Radius(1001)
Dim TanSpeed(1001)
Dim KE(1001)
Dim F(1001)
Epsilon = 0.5                                   'Reduction rate of radius
Omega0 = 10 * 3.1415: R0 = 1#: m = 2#            'Initial values of angular velocity and radius, and mass
TanSpeed(0) = R0 * Omega0                        'Initial tangential speed
Cells(2, 1) = "R0": Cells(2, 2) = "Omega0": Cells(2, 3) = "Radius reduction rate"
Cells(3, 1) = R0: Cells(3, 2) = Omega0: Cells(3, 3) = Epsilon
Cells(5, 2) = "Time": Cells(5, 3) = "R adius": Cells(5, 4) = "Omega": Cells(5, 5) = "Theta"
Cells(5, 6) = "x": Cells(5, 7) = "y": Cells(5, 8) = "Tan v"
Cells(5, 9) = "KE": Cells(5, 10) = "Fc"
'Initialization:
For i = 0 To 1000
  Omega(i) = 0: Theta(i) = 0: x(i) = 0: y(i) = 0
  Radius(i) = 0: TanSpeed(i) = 0: KE(i) = 0: F(i) = 0
Next i
   For i = 0 To 999
     t = 0.001 * i
     Radius(i) = R0 - Epsilon * t
     Omega(i) = (R0 / Radius(i)) ^ 2 * Omega0
     Theta(i) = Omega(i) * t
     x(i) = Radius(i) * Cos(Theta(i))
     y(i) = Radius(i) * Sin(Theta(i))
     TanSpeed(i) = Radius(i) * Omega(i)
      KE(i) = m * (TanSpeed(i)) ^ 2 / 2
     F(i) = m * Radius(i) * (Omega(i)) ^ 2
        Cells(6 + i, 2) = t
        Cells(6 + i, 3) = Radius(i)
        Cells(6 + i, 4) = Omega(i)
        Cells(6 + i, 5) = Theta(i)
        Cells(6 + i, 6) = x(i)
        Cells(6 + i, 7) = y(i)
        Cells(6 + i, 8) = TanSpeed(i)
        Cells(6 + i, 9) = KE(i)
       Cells(6 + i, 10) = F(i)
   Next i
End Sub
```

FIGURE 1.19 Rotational motion of an object while the radius is reduced.

The change in the kinetic energy is due to the work done by the pulling force which is the centripetal force.

$$W = \int_{r_0}^{r} F_c dr = -\int_{r_0}^{r} m\frac{(r\omega)^2}{r}dr = -\int_{r_0}^{r} m\frac{r_0^4\omega_0^4}{r^3}dr = \frac{1}{2}mr_0^4\omega_0^4\left(\frac{1}{r^2}-\frac{1}{r_0^2}\right). \tag{1.43}$$

Figure 1.19 shows the VBA code where $r_0 = 1$, $\varepsilon = 0.5$, $\omega_0 = 10\pi$, and the time interval is 1 s.

Figure 1.20 shows the trajectory and the angular velocity of the object. The angular velocity ω increases as the radius is reduced.

1.5.2 Euler's Equation for Rotational Motions

Figure 1.21 depicts two coordinate systems: the lab (space)-fixed *xyz*-frame and a rotating *XYZ*-frame. Consider a point *P*, e.g., the center of mass, in a rigid body, and the coordinates

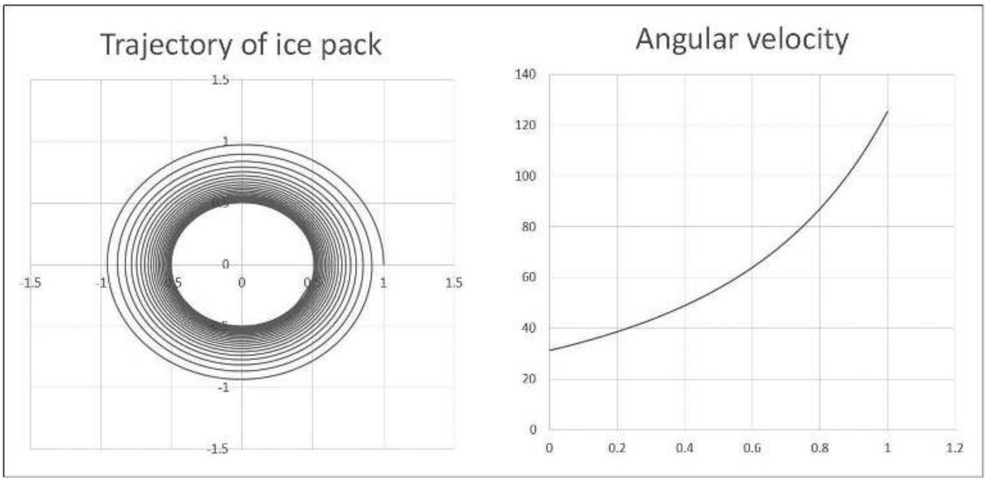


FIGURE 1.20 Trajectory and angular velocity of rotating object.

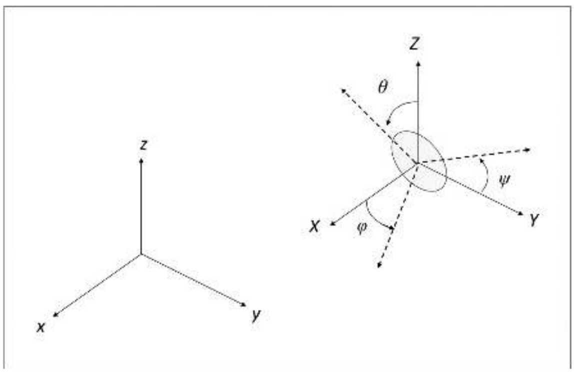


FIGURE 1.21 Lab-fixed frame and body-fixed frame.

of the point P in a lab-fixed xyz-frame. Let the XYZ-frame be attached to the rigid body with the origin at the point P. The position and orientation of the body is completely given in terms of the origin of the body-fixed frame (X, Y, Z) and the orientation of the body-fixed frame (X, Y, Z) with respect to the lab frame (x, y, z). The orientation of the body-fixed frame is expressed using Euler's angles (θ, φ, ψ). For the definition of Euler's angles, refer to Appendix A5.

A rigid body has three mutually orthogonal principal axes, along which principal moment of inertia can be defined as I_i; $i = 1, 2, 3$ [7, 8]. Using the principal axes, kinematic variables such as angular momentum and rotational kinetic energy may be written without cross terms among the principal axes. Assign the body-fixed frame along the principal axes of a rigid body (1, 2, 3).

The rotational equation motion, called Euler equation, in the body-fixed XYZ-frame, which is rotating with respect to the spaced-fixed frame, is given by

$$\frac{dL_i}{dt} + \left(\vec{\omega} \times \vec{L}\right)_i = \tau_i \text{ where } i = 1, 2, 3. \tag{1.44}$$

Here, L, ω, and τ are angular momentum, angular velocity, and torque, respectively. For a rigid body, they are generally different along each of the principal axes. Thus, the explicit forms of equation (1.44) are

$$\begin{cases} I_1\dot{\omega}_1 + \omega_2\omega_3(I_3 - I_2) = \tau_1 \\ I_2\dot{\omega}_2 + \omega_3\omega_1(I_1 - I_3) = \tau_2 \\ I_3\dot{\omega}_3 + \omega_1\omega_2(I_2 - I_1) = \tau_3 \end{cases} \text{ where } \dot{\omega}_i = \frac{d\omega_i}{dt} \text{ and } L_i = I_i\omega_i;\ i = 1, 2, 3. \tag{1.45}$$

In the above Equation 1.45, I_i (i = 1, 2, 3) are the principal moments of inertia. If a rigid body has an axis of symmetry, then rotations about that axis will be dynamically balanced. That is, that axis is a principal axis, and we can use the symmetries of a body to recognize principal axes.

The angular velocities ω's are given by the Euler angles (θ, φ, ψ) and their time derivatives.

$$\begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} \cos\psi & \sin\theta\sin\psi & 0 \\ -\sin\psi & \sin\theta\cos\psi & 0 \\ 0 & \cos\theta & 1 \end{pmatrix} \begin{pmatrix} \dot{\theta} \\ \dot{\varphi} \\ \dot{\psi} \end{pmatrix} = \begin{pmatrix} \dot{\theta}\cos\psi + \dot{\varphi}\sin\theta\sin\psi \\ -\dot{\theta}\sin\psi + \dot{\varphi}\sin\theta\cos\psi \\ \dot{\varphi}\cos\theta \end{pmatrix} \tag{1.46}$$

The Euler angles are called "θ = nutation," "φ = precession," and "ψ = spin" for rigid body dynamics.

In order to describe the motion of a rotating body, we need to solve:

(1) Euler's Equation 1.42 is applied to obtain ω_1, ω_2, and ω_3 and

(2) The directions of the principal axes change with respect to the lab frame.

1.5.3 Free Rotation of a Symmetrical Top

Free rotation means that there is no external torque. The equation of rotational motion in the space-fixed frame is given by

$$\frac{d\vec{L}}{dt} = \vec{\tau} = 0. \tag{1.47}$$

Thus, the angular momentum is constant in its direction and magnitude as observed in the space-fixed frame. Let us take the Z-axis of the body-fixed frame along the angular momentum. In the body-fixed frame, angular momentum is given by $L_i = I_i\omega_i$, i = 1, 2, 3 along the principal axes. For a symmetrical top, take $I_1 = I_2 \neq I_3$ where I_3 is along the spinning axis (Z-axis) of the top. With these conditions, the Euler Equation 1.45 in the body-fixed frame are

$$\begin{cases} I_1\dot{\omega}_1 + \omega_2\omega_3(I_3 - I_1) = \tau_1 = 0 \\ I_2\dot{\omega}_2 + \omega_3\omega_1(I_1 - I_3) = \tau_2 = 0. \\ I_3\dot{\omega}_3 = \tau_3 = 0 \end{cases} \tag{1.48}$$

From the third equation, ω_3 = constant, which means $L_3 = L\cos\theta$ along the Z-axis, and $\omega_3 = L_3/I_3 = (L\cos\theta)/I_3$ where L is the magnitude of the angular momentum. The projection of the angular velocity ω_{xy} on the XY-plane is constant. Define the projection of the angular momentum L_{xy} on the XY-plane, and $\omega_{xy} = L_{xy}/I_1 = L\sin\theta/I_1$.

Let the angular velocity of precession ω_{pr}: $\omega_{pr} = L/I_1$. (1.49)

The angular velocity vector is given by $\vec{\omega} = \omega_3\hat{k} + \omega_{pr}\vec{L}/L$ where $\check{k}$ is the unit vector along the spinning Z-axis. Notice that $\omega_{xy} = L\sin\theta/I_1 = \omega_{pr}\sin\theta$. As shown in Figure 1.22, the motion of a free rotation of a symmetrical top consists of a spin rotation, with a constant rate $\omega_3 = (L\cos\theta)/I_3$ around the body-fixed axis, combined with a precession with a constant angle θ and a rate $\omega_{pr} = L/I_1$ of the body-fixed axis with respect to the space-fixed z-axis.

Figure 1.23 lists the VBA code to compute the free rotation of a symmetrical body by applying the Runge-Kutta method (Appendix A3). Since we expect θ = constant and $d\theta/dt = 0$, from Equation 1.46, we use the following equation to calculate θ, φ, and ψ:

$$\begin{pmatrix}\omega_1\\ \omega_2\\ \omega_3\end{pmatrix} = \begin{pmatrix}\dot{\varphi}\sin\theta\sin\psi\\ \dot{\varphi}\sin\theta\cos\psi\\ \dot{\varphi}\cos\theta\end{pmatrix}, \text{ and we obtain } \begin{cases}\theta = \cos^{-1}(L_3/L).\\ \dot{\varphi} = \sqrt{\omega_1^2+\omega_2^2}/\sin\theta = L/I_1.\\ \dot{\psi} = \omega_3 - \dot{\varphi}\cos\theta = (L_3/I_3) - (L/I_1)\cos\theta.\end{cases} \tag{1.50}$$

Figure 1.24 is a screenshot of the calculated results where `theta1`, `theta2`, `theta3`, `omega1`, `omega2`, `omega3`, `L3`, and `L` are in the body-fixed frame. Principal moments of inertia `I1`, `I2`, and `I3` are also shown on the sheet. Angles `θ(theta)`, `φ(phi)`,

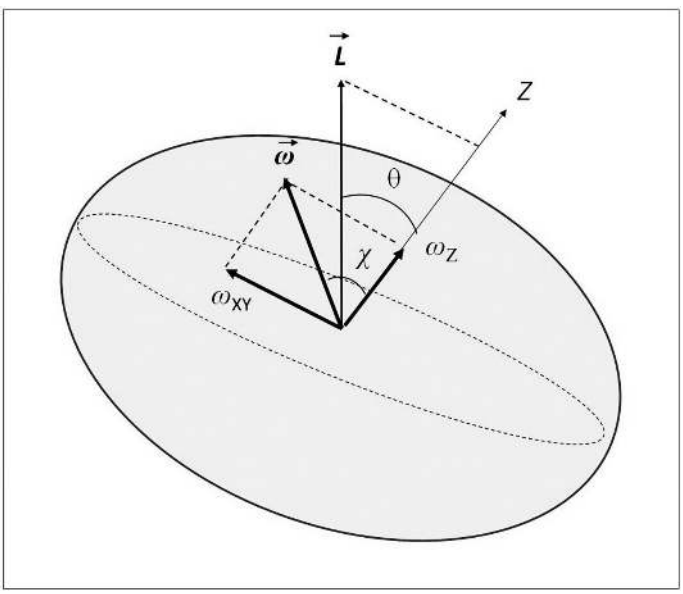


FIGURE 1.22 Free rotation of a symmetrical top.

```
Sub FreeTop()
Cells(1, 1) = "Free rotation of symmetrical top with no external torque"
'Principal moment of inertia of symmetrical top: I 1=I2
   Cells(2, 2) = "I1=": I1 = 1#: Cells(2, 3) = I1
   Cells(2, 5) = "I2=": I2 = I1: Cells(2, 6) = I2
   Cells(2, 8) = "I3=": I3 = 2#: Cells(2, 9) = I3
   Pi = 3.14159265
'Initial conditions to assume the top starts at rest with a give orientation.
   Cells(5, 1) = "time": t = 0: Cells(6, 1) = t
   Cells(5, 2) = "theta1": theta1 = 0: Cells(6, 2) = theta1          'Angle between principal axis 1 and z-axis
   Cells(5, 3) = "theta2": theta2 = 0: Cells(6, 3) = theta2          'Rotation around z-axis
   Cells(5, 4) = "theta3": theta3 = 0: Cells(6, 4) = theta3          'Rotation around new z-axis after theta2-rotation
   Cells(5, 5) = "omega1": omega1 = 1: Cells(6, 5) = omega1
   Cells(5, 6) = "omega2": omega2 = 1: Cells(6, 6) = omega2
   Cells(5, 7) = "omega3": omega3 = Pi: Cells(6, 7) = omega3
   Cells(5, 8) = "L3": L10 = I1 * omega1: L30 = I3 * omega3: Cells(6, 8) = L30          'Initial L1 & L3
   Cells(5, 9) = "L": L0 = ((I1 * omega1) ^ 2 + (I2  * omega2) ^ 2 + (I3 * omega3) ^ 2) ^ 0.5: Cells(6, 9) = L0        'Initial L
   Cells(5, 10) = "theta": theta0 = WorksheetFunction.Acos(L30 / L0): Cells(6, 10) = theta0
   Cells(5, 11) = "phi": Phi = 0: Cells(6, 11) = Phi
   Cells(5, 12) = "psi": psi = 0: Cells(6, 12) = psi
   Cells(5, 13) = "d(phi)/dt": Precession = L / I1: Cells(6, 13) = Precession
   Cells(5, 14) = "d(psi)/dt": Spinning = omega 3 - Precession * (L10 / L0): Cells(6, 14) = Spinning
'RK method:
   Cells(3, 1) = "delta-t": h = 0.005: Cells(3, 2) = h
   n = 1000    'Number of repetitions
      For i = 0 To n
         Cells(6 + i, 1) = t
         Cells(6 + i, 2) = theta1
         Cells(6 + i, 3) = theta2
         Cells(6 + i, 4) = theta3
         Cells(6 + i, 5) = omega1
         Cells(6 + i, 6) = omega2
         Cells(6 + i, 7) = omega3
      K11 = f1(I1, I2, I3, t, omega1, omega2, omega3)
      L11 = g1(I1, I2, I3, t, omega1, omega2, omega3)
      K21 = f2(I1, I2, I3, t, omega1, omega2, omega3)
      L21 = g2(I1, I2, I3, t, omega1, omega2, omega3)
      K31 = f3(I1, I2, I3, t, omega1, omega2, omega3)
      L31 = g3(I1, I2, I3, t, omega1, omega2, omega3)
K12 = f1(I1, I2, I3, t + h / 2, omega1 + h * K11 / 2, omega2 + h * K21 / 2, omega3 + h * K31 / 2)
L12 = g1(I1, I2, I3, t + h / 2, omega1 + h * L11 / 2, omega2 + h * L21 / 2, omega3 + h * L31 / 2)
K22 = f2(I1, I2, I3, t + h / 2, omega1 + h * K11 / 2, omega2 + h * K21 / 2, omega3 + h * K31 / 2)
L22 = g2(I1, I2, I3, t + h / 2, omega1 + h * L11 / 2, omega2 +  h * L21 / 2, omega3 + h * L31 / 2)
K32 = f3(I1, I2, I3, t + h / 2, omega1 + h * K11 / 2, omega2 + h * K21 / 2, omega3 + h * K31 / 2)
L32 = g3(I1, I2, I3, t + h / 2, omega1 + h * L11 / 2, omega2 + h * L21 / 2, omega3 + h * L31 / 2)
K13 = f1(I1, I2, I3, t + h / 2, omega1 + h * K12 / 2, omega2 + h * K22 / 2, omega3 + h * K32 / 2)
L13 = g1(I1, I2, I3, t + h / 2, omega1 + h * L12 / 2, omega2 + h * L22 / 2, omega3 + h * L32 / 2)
K23 = f2(I1, I2, I3, t + h / 2, omega1 + h * K12 / 2, omega2 + h * K22 / 2, omega3 +  h * K32 / 2)
L23 = g2(I1, I2, I3, t + h / 2, omega1 + h * L12 / 2, omega2 + h * L22 / 2, omega3 + h * L32 / 2)
K33 = f3(I1, I2, I3, t + h / 2, omega1 + h * K12 / 2, omega2 + h * K22 / 2, omega3 + h * K32 / 2)
L33 = g3(I1, I2, I3, t + h / 2, omega1 + h * L 12 / 2, omega2 + h * L22 / 2, omega3 + h * L32 / 2)
K14 = f1(I1, I2, I3, t + h, omega1 + h * K13, omega2 + h * K23, omega3 + h * K33)
L14 = g1(I1, I2, I3, t + h, omega1 + h * L13, omega2 + h * L23, omega3 + h * L33)
K24 = f2(I1, I2, I3, t + h, omega1 + h *  K13, omega2 + h * K23, omega3 + h * K33)
L24 = g2(I1, I2, I3, t + h, omega1 + h * L13, omega2 + h * L23, omega3 + h * L33)
K34 = f3(I1, I2, I3, t + h, omega1 + h * K13, omega2 + h * K23, omega3 + h * K33)
L34 = g3(I1, I2, I3, t + h, omega1 + h * L13, omeg a2 + h * L23, omega3 + h * L33)
omega1 = omega1 + h * (L11 + 2 * L12 + 2 * L13 + L14) / 6
omega2 = omega2 + h * (L21 + 2 * L22 + 2 * L23 + L24) / 6
omega3 = omega3 + h * (L31 + 2 * L32 + 2 * L33 + L34) / 6
theta1 = theta1 + h * (K11 + 2 * K12 + 2 * K13 + K14) / 6
theta2 = theta2 + h * (K21 + 2 * K22 + 2 * K23 + K24) / 6
theta3 = theta3 + h * (K31 + 2 * K32 + 2 * K33 + K34) / 6
   L1 = I1 * omega1: L2 = I2 * omega2: L3 = I3  * omega3
   L = (L1 ^ 2 + L2 ^ 2 + L3 ^ 2) ^ 0.5
```

FIGURE 1.23 VBA code for analyzing motion of free rotor.

```
            Precession = L / I1                                          'd(phi)/dt=L/I1
            Spinning = omega3 - Precession * Cstheta                     'd(psi)/dt
              theta = WorksheetFunction.Acos(L3 / L)                     'theta=arccos(L3/L)
              Phi = Precession * t + Phi                                 'phi=phi+d(phi)/dt
              psi = Spinning * t + psi                                   'psi=psi+d(psi)/dt
            Cells(6 + i, 8) = L3
            Cells(6 + i, 9) = L
            Cells(6 + i, 10) = theta
            Cells(6 + i, 11) = Phi
            Cells(6 + i, 12) = psi
            Cells(6 + i, 13) = Precession                                  'd(phi)/dt
            Cells(6 + i, 14) = Spinning                                    'd(psi)/dt
          t = t + h
        Next i
End Sub
_______________________________________________________________________________
Function g1(I1, I2, I3, t, omega1, omega2, omega 3)
'g1=d(omega1)/dt is the second time derivative of theta1.
    g1 = (I2 - I3) / I1 * omega2 * omega3
End Function
_______________________________________________________________________________
Function g2(I1, I2, I3, t, omega1, omega2, omega3)
'g2=d(omega2)/dt is the second time derivative of theta1.
    g2 = (I3 - I1) / I2 * omega3 * omega1
End Function
_______________________________________________________________________________
Function g3(I1, I2, I3, t, omega1, omega2, omega3)
'g3=d(omega3)/dt is the second time derivative of theta1.
    g3 = (I1 - I2) / I3 * omega1 * omega2
End Function
_______________________________________________________________________________
Function f1(I1, I2, I3, t, omega1, omega2, omega3)
'f1=d(theta1)/dt
    f1 = omega1
End Function
_______________________________________________________________________________
Function f2(I1, I2, I3, t, omega1, omega2, omega3)
'f2=d(theta2)/dt
f2 = omega2
End Function
_______________________________________________________________________________
Function f3(I1, I2, I3, t, omega1, omega2, omega3)
'f3=d(theta3)/dt
    f3 = omega3
End Function
```

FIGURE 1.23 Continued.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Free rotation of symmetrical top with no external torque											
2		I1=	1		I2=	1		I3=	2			
3	delta-t	0.002										
4												
5	time	theta1	theta2	theta3	omega1	omega2	omega3	L3	L	theta	phi	psi
6	0	0	0	0	0.01	0.01	0.314159	0.628319	0.628478	0.02250411	0	0
7	0.002	2E-05	2E-05	0.000629	0.009994	0.010006	0.314159	0.628319	0.628478	0.02250411	0.001257	0.000628
8	0.004	4E-05	4.01E-05	0.001258	0.009987	0.010013	0.314159	0.628319	0.628478	0.02250411	0.003771	0.001885
9	0.006	6E-05	6.01E-05	0.001887	0.009981	0.010019	0.314159	0.628319	0.628478	0.02250411	0.007542	0.00377
10	0.008	8E-05	8.02E-05	0.002516	0.009975	0.010025	0.314159	0.628319	0.628478	0.02250411	0.01257	0.006283
11	0.01	1E-04	0.0001	0.003145	0.009969	0.010031	0.314159	0.628319	0.628478	0.02250411	0.018854	0.009425

FIGURE 1.24 Result from the VBA code listed in Figure 1.23.

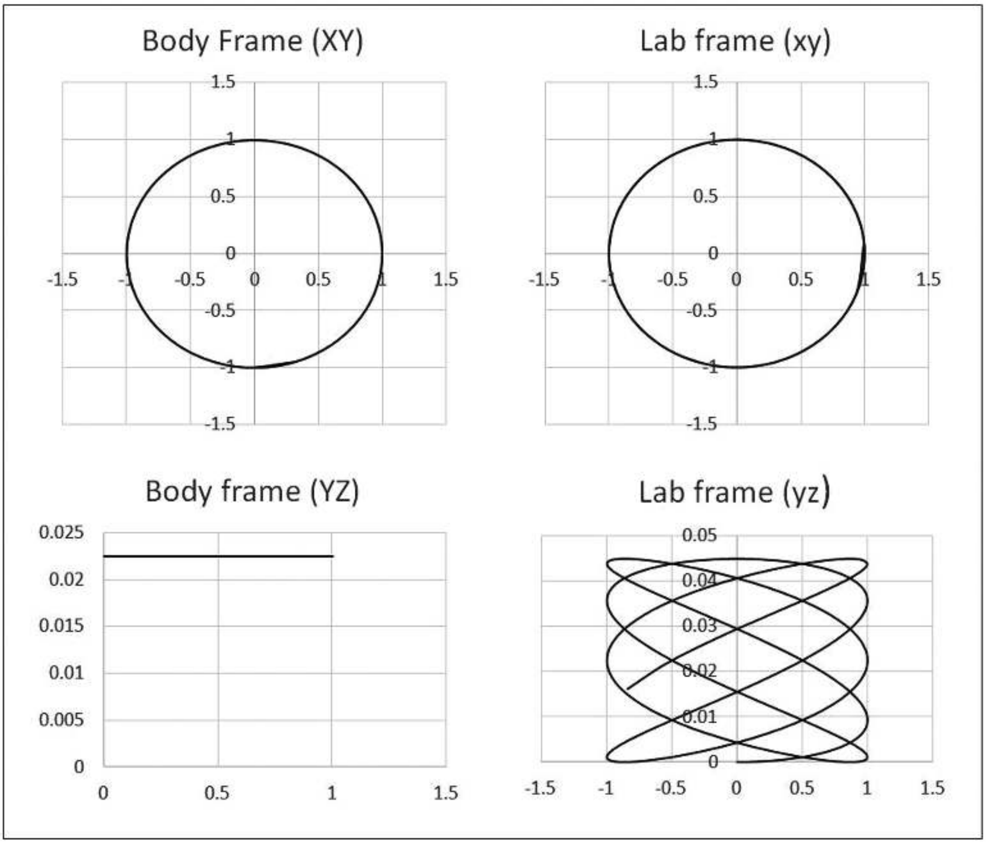


FIGURE 1.25 Trajectories of free rotor.

ψ(psi) are as observed from the lab-fixed frame. As we expect, angular momentum L and its Z-component L_3, angle θ, the precession rate $d\varphi/dt$, and the spinning rate $d\psi/dt$ are constant in time.

Figure 1.25 shows the trajectories in the body (XY) frame and in the lab (xy) frame.

Note: ***Free rotation of the Earth*** [9]. The moments of inertia I_1, I_2, and I_3 of the Earth are $I_1 = I_2 < I_3$ and $(I_3 - I_1)/I_1 = \varepsilon$ is approximately 1/300. The direction of the rotating body (the Earth) which is the fixed axis Z points to the North Pole. The direction of the angular momentum $\vec{L}$ is very close to the North Pole. Referring to Figure 1.22, the angle θ between the Z-axis and $\vec{L}$is $\theta \approx 0.1$" of arc., which is an actual distance 10 m or so on the surface of the Earth between the North Pole and the point where the $\vec{L}$-vector out of the Earth. The direction of $\vec{\omega}$ can be measured by locating the center of diurnal motions of stars. Accurate measurement shows that the direction of $\vec{\omega}$ moves with respect to the Earth, making a circle of radius of about 10 m in 400 days.

We may analyze this motion. In Section 1.5.3, we obtained

$$\Theta = \text{constant},\ \omega_3 = L_3/I_3 = (L\cos\theta)/I_3, \text{ and } \omega_{xy} = L\sin\theta/I_1 = \omega_{pr}\sin\theta.$$

In Figure 1.22, the angle between $\vec{\omega}$ and the Z-axis is χ, and

$$\tan\chi = \frac{\omega_{XY}}{\omega_3} = \frac{I_3}{I_1}\tan\theta. \text{ Thus, } \chi \text{ is slightly larger than } \theta.$$

The period of a circular motion of the tip of $\vec{\omega}$ around the North Pole is given by $\dot{\psi}$. This is the rate with which an observer fixed to the rotating *XYZ*-frame of the Earth sees the *z*-axis. The space-fixed *z*-axis is in the direction of $\vec{L}$ which makes a cone of angle θ around the direction of the Earth-fixed *Z*-axis toward the North Pole. From Equations 1.48 and 1.49,

$$\omega_{pr} = \frac{L}{I_1} = \dot{\varphi} \text{ and } \omega_3 = \dot{\varphi}\cos\theta + \dot{\psi} = \frac{L}{I_3}\cos\theta.$$

Therefore, $\dot{\psi} = L\left(\frac{1}{I_3} - \frac{1}{I_1}\right)\cos\theta = -\frac{L}{I_1}\varepsilon\cos\theta = -\frac{I_1}{I_3}\varepsilon\cos\theta\dot{\varphi}.$

Because $I_1/I_3 \approx 1$, $\cos\theta \approx 1$, and $\dot{\varphi} = 1$ turn per day, we obtain $\dot{\psi} = 1$ turn per 300 days. The observed rate is 1 per 400 days, and the difference may be primarily due to non-rigid properties of the Earth.

1.5.4 A Symmetric Top Rotating about a Fixed Point in the Presence of Gravity

The gravitational force *mg* produces torque, and unlike the free rotation discussed earlier, the angular momentum is not aligned with the lab z-axis but processes about the *z*-axis [8]. The angular momentum in the body-fixed frame is $L_i = I_i\omega_i$, $i = 1, 2, 3$. Equations 1.47 and 1.48 are applicable to this problem. We study the motion of the top in θ and φ while allowing it to spin with angular velocity $\dot{\psi}$ relative to a frame rotating with angular velocity $\vec{\omega}$. We also assume the spinning rate $\dot{\psi}$ is much faster than both $\dot{\theta}$and $\dot{\varphi}$. The angular velocity and the angular momentum of the symmetric top in the body-fixed frame are given by

$$\begin{cases} \omega_1 = \dot{\theta} \\ \omega_2 = \dot{\varphi}\sin\theta \\ \omega_3 = \dot{\varphi}\cos\theta + \dot{\psi} \end{cases} \quad \text{and} \quad \begin{cases} L_1 = I_1\omega_1 = I_1\dot{\theta} \\ L_2 = I_1\omega_2 = I_1\dot{\varphi}\sin\theta \\ L_3 = I_3\omega_3 = I_3(\dot{\varphi}\cos\theta + \dot{\psi}) \equiv p_\psi \end{cases} \tag{1.51}$$

Because the external force is only the gravity *mg*, the Euler equations 1.51 become

$$\begin{cases} I_1\left(\ddot{\theta} - \dot{\varphi}^2\sin\theta\cos\theta\right) + I_3\dot{\varphi}\sin\theta\left(\dot{\varphi}\cos\theta + \dot{\psi}\right) = mgl\sin\theta \\ I_1\left(\ddot{\varphi}\sin\theta + 2\dot{\varphi}\dot{\theta}\cos\theta\right) - I_3\dot{\theta}\left(\dot{\varphi}\cos\theta + \dot{\psi}\right) = 0 \\ I_3\left(\ddot{\psi} + \ddot{\varphi}\cos\theta - \dot{\varphi}\dot{\theta}\sin\theta\right) = 0 \end{cases} \tag{1.52}$$

where *l* is the distance from the fixed point to the center of mass of the top.

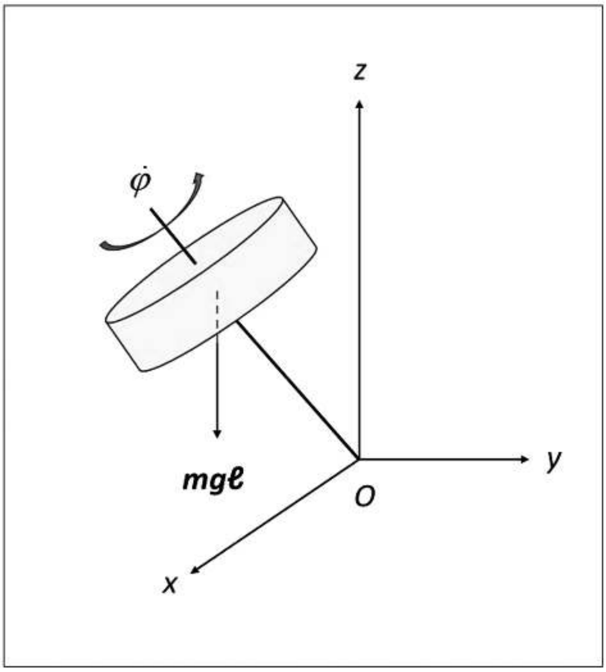


FIGURE 1.26 Steady precession of a top with a fixed point under gravity.

1.5.5 Steady Precession about the Space-Fixed *z*-Axis

The top rotates with spin velocity $\dot{\psi}$ about its principal axis and makes a precession with angular velocity $\dot{\varphi}$ while angle θ is kept constant: $\ddot{\varphi}=0$ and $\dot{\varphi}=\dot{\varphi}_0$; $\ddot{\theta}=0$ and $\dot{\theta}=\dot{\theta}_0$; $\ddot{\psi}=0$ and $\dot{\psi}=\dot{\psi}_0$. Because we assume $\dot{\psi}\gg\dot{\varphi}$, in the first Equation 1.49, $\dot{\varphi}\cos\theta+\dot{\psi}\approx\dot{\psi}$ and $\dot{\varphi}\dot{\psi}-\dot{\varphi}^2\approx\dot{\varphi}\dot{\psi}$. Thus, $I_3\dot{\varphi}\dot{\psi}=mgl$ and the precession angular velocity is given by $\dot{\varphi}=mgl/I_3\dot{\psi}$. Figure 1.26 depicts the steady precession of a top about the space-fixed *z*-axis.

1.5.6 Unsteady Precession

Rearrange Equations 1.52 to express the second-time derivatives of θ, φ, and ψ using their first derivatives,

$$\begin{cases} \ddot{\theta}=\left(1-\dfrac{I_3}{I_1}\right)\dot{\varphi}^2\sin\theta\cos\theta-\dfrac{I_3}{I_1}\dot{\varphi}\dot{\psi}\sin\theta+\dfrac{mgl}{I_1}\sin\theta \\ \ddot{\varphi}=\left(\dfrac{I_3}{I_1}-2\right)\dfrac{\cos\theta}{\sin\theta}\dot{\theta}\dot{\varphi}+\dfrac{I_3}{I_1}\dfrac{1}{\sin\theta}\dot{\theta}\dot{\psi} \\ \ddot{\psi}=-\cos\theta\ddot{\varphi}+\sin\theta\dot{\varphi}\dot{\theta}=-\cos\theta\left[\left(\dfrac{I_3}{I_1}-2\right)\dfrac{\cos\theta}{\sin\theta}\dot{\theta}\dot{\varphi}+\dfrac{I_3}{I_1}\dfrac{1}{\sin\theta}\dot{\theta}\dot{\psi}\right]+\sin\theta\dot{\varphi}\dot{\theta} \\ =\left[\left(2-\dfrac{I_3}{I_1}\right)\dfrac{\cos\theta}{\sin\theta}+\sin\theta\right]\dot{\theta}\dot{\varphi}-\dfrac{I_3}{I_1}\dfrac{1}{\sin\theta}\dot{\theta}\dot{\psi} \end{cases} \tag{1.53}$$

Equations 1.53 are the coupled differential equations that can be numerically solved with the Runge-Kutta method (Appendix A3). As $\theta(t)$ is computed, $\varphi(t)$ and $\psi(t)$ are also computed.

There are three constant quantities during the motion. From the second and the third equations of the set of Equations 1.52,

$$\begin{aligned} &\frac{d}{dt}\left[(I_1\sin^2\theta)\dot{\varphi}+I_3(\dot{\psi}+\dot{\phi}\cos\theta)\cos\theta\right]=\frac{dp_\phi}{dt}=0,\\ &\frac{d}{dt}\left[I_3(\dot{\psi}+\dot{\varphi}\sin\theta)\right]=\frac{dp_\psi}{dt}=0. \end{aligned} \tag{1.54}$$

Thus, the ψ-component of angular momentum

$$p_\psi = I_3\left(\dot{\psi}+\dot{\varphi}\cos\theta\right) \tag{1.55}$$

and the φ-component of angular momentum

$$p_\varphi = I_1\dot{\varphi}\sin^2\theta + I_3\left(\dot{\psi}+\varphi\cos\theta\right)\cos\theta = I_1\dot{\varphi}\sin^2\theta + p_\psi\cos\theta \tag{1.56}$$

are constants in time. The total energy is also a constant in time.

$$\begin{aligned} E &= \frac{1}{2}I_1\left(\dot{\theta}^2+\dot{\varphi}^2\sin^2\theta\right)+\frac{1}{2}I_3\left(\dot{\psi}+\dot{\varphi}\cos\theta\right)^2+mg\ell\cos\theta\\ &=\frac{1}{2}I_1\dot{\theta}^2+\frac{\left(p_\varphi-p_\psi\cos\theta\right)^2}{2I_1\sin^2\theta}+\frac{1}{2I_3}p_\psi^2+mg\ell\cos\theta. \end{aligned} \tag{1.57}$$

Figure 1.27 lists the VBA code to compute the coupled equations 1.55 to 1.57. We calculate the trace of the tip of the top in the XYZ-frame using $X = \sin\theta\cos\varphi$, $Y = \sin\theta\sin\varphi$, and $Z = \cos\theta$. The traces are displayed in the top view (XY-plane) and the side view (YZ-plane). The number of iteration and the time step are adjusted so that motions per about one turn are displayed. The code also calculates p_φ, p_ψ, and E.

We observe three different patterns of nutation. Below is a theoretical description of the patterns and their examples from the computational results. Let $\cos\theta = z$ in the total energy of the top, Equation 1.57 becomes

$$\begin{aligned} &(1-z^2)E=\frac{1}{2}I_1\dot{z}^2+\frac{1}{2I_1}\left(p_\varphi-p_\psi z\right)^2+\left(\frac{1}{2I_3}p_\psi^2+mg\ell\right)\left(1-z^2\right)\text{ or}\\ &\dot{z}^2=(1-z^2)(\alpha-az)-(\beta-bz)^2\equiv f(z) \end{aligned} \tag{1.58}$$

where

$$\alpha=\frac{2E}{I_1}-\frac{p_\psi^2}{I_1I_3},\ \beta=\frac{p_\psi}{I_1},\ a=\frac{2mg\ell}{I_1}>0\text{ , and }b=\frac{p_\psi}{I_1}.$$

```
Sub TopUnderGravity()
Cells(1, 1) = "Top with a fixed point under gravity"
'Principal moment of inertia                    'Symmetrical top means I1=I2
Cells(2, 2) = "I1=": I1 = 1: Cells(2, 3) = I1    'Moment of inertia along body-fixed X-axis.
Cells(2, 5) = "I2=": I2 = I1: Cells(2, 6) = I2   'Along body-fixed Y-axis.
Cells(2, 8) = "I3=": I3 = 2: Cells(2, 9) = I3    'Along body-fixed  Z-axis.
MGL = 20                                          'MGL = m * g * lgt / I3 'The max MGL depends on I 1 and I3.
Pi = 3.141592654
'Initial conditions to assume the top starts at rest with a give orientation.
Cells(5, 1) = "Time": t = 0: Cells(6, 1) = t
Cells(5, 2) = "theta": theta = Pi / 3: Cells(6, 2) = theta     'Nutation=theta = theta: angle between principal axis 1 and z-axis
Cells(5, 3) = "phi": phi = 0: Cells(6, 3) = phi   'Precession=phi = phi: rotation around z-axis
Cells(5, 4) = "psi": psi = Pi / 8: Cells(6, 4) = psi  'Spinning=psi = psi: rotation around new z-axis after phi-rotation
Cells(5, 5) = "dtheta": dtheta = 5: Cells(6, 5) = dtheta 'Nutation rate: dtheta = d(theta) / dt
Cells(5, 6) = "dphi": dphi = 0.5: Cells(6, 6) = dphi      'Precession  rate: dphi = d(phi) / dt
Cells(5, 7) = "dpsi": dpsi = 2.5 * Pi: Cells(6, 7) = dpsi 'Spinn rate: dpsi = d(psi) / dt
Cells(5, 8) = "L3": L3 = I3 * dpsi: Cells(6, 8) = L3
Cells(5, 9) = "L": L = ((I1 * dtheta) ^ 2 + (I2 * dphi) ^ 2 + (I3 * dpsi) ^ 3) ^ 0.5
Cells(6, 9) = L
Cells(5, 10) = "p(psi)": Ppsi = I3 * dpsi: Cells(6, 10) = Ppsi
Cells(5, 11) = "p(phi)": Pphi = I1 * dphi * Sin(theta) ^ 2 + Ppsi * Cos(theta)
Cells(6, 11) = Pphi
  omega1 = dtheta * Cos(psi) + dphi * Sin(theta) * Sin(psi)
  omega2 = dphi * Sin(theta) * Cos(psi) - dtheya * Sin(psi)
  omega3 = dpsi + dphi * Cos(theta)
Cells(5, 12) = "Total E": E = 0.5 * (I1 * mega1 ^ 2 + I2 * omega2 ^ 2 + I3 * omega3 ^ 2)
Cells(6, 12) = E
Cells(5, 14) = "X": X = Sin(theta) * Cos(phi):  Cells(6, 14) = X       'Body-fixed X-component
Cells(5, 15) = "Y": Y = Sin(theta) * Sin(phi): Cells(6, 15) = Y         'Y-component
Cells(5, 16) = "Z": Z = Cos(theta): Cells(6, 16) = Z                    'Z-component
'RK method:
Cells(3, 1) = "del-t": h = 0.003: Cells(3, 2) = h
n = 1000    'Number of repetitions
For i = 0 To n
 Cells(6 + i, 1) = t
 Cells(6 + i, 2) = theta
 Cells(6 + i, 3) = phi
 Cells(6 + i, 4) = psi
 Cells(6 + i, 5) = dtheta
 Cells(6 + i, 6) = dphi
 Cells(6 + i, 7) = dpsi
  omega1 = dtheta * Cos(psi) + dphi * Sin(theta) * Sin(psi)
  omega2 = dphi * Sin(theta) * Cos(psi) - dtheta * Sin(psi)
  omega3 = dpsi + dphi * Cos(theta)
  L3 = I3 * omega3:  Cells(6 + i, 8) = L3
  L = ((I1 * omega1) ^ 2 + (I2 * omega2) ^ 2 + (I3 * omega3) ^ 2) ^ 0.5 :  Cells(6 + i, 9) = L
   Ppsi = I3 * (dpsi + dphi * Cos(theta)): Cells( 6 + i, 10) = Ppsi
   Pphi = I1 * Sin(theta) ^ 2 * phi + Ppsi: Cells( 6 + i, 11) = Pphi
   E = 0.5 * (I1 * omega1 ^ 2 + I2 * omega2 ^ 2 + I3 * omega3 ^ 2): Cells(6 + i, 12) = E
     X = Sin(theta) * Cos(phi):  Cells( 6 + i, 14) = X
     Y = Sin(theta) * Sin(phi): Cells( 6 + i, 15) = Y
     Z = Cos(theta): Cells( 6 + i, 16) = Z
L11 = g1(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
K11 = f1(I1, I3, MGL, t, theta, p hi, psi, dtheta, dphi, dpsi)
L21 = g2(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
K21 = f2(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
L31 = g3(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
K31 = f3(I1, I3, MGL, t, theta, phi, psi,  dtheta, dphi, dpsi)
L12 = g1(I1, I3, MGL, t + h / 2, theta + h * L11 / 2, phi + h * L21 / 2, psi + h * L31 / 2, dtheta + h * L11 / 2, dphi + h * L21 / 2, dpsi + h * L31 / 2)
K12 = f1(I1, I3, MGL, t + h / 2, theta + h * K11 / 2, phi + h * K21 / 2, psi + h  * K31 / 2, dtheta + h * K11 / 2, dphi + h * K21 / 2, dpsi + h * K31 / 2)
L22 = g2(I1, I3, MGL, t + h / 2, theta + h * L11 / 2, phi + h * L21 / 2, psi + h * L31 / 2, dtheta + h * L11 / 2, dphi + h * L21 / 2, dpsi + h * L31 / 2)
K22 = f2(I1, I3, MGL, t + h / 2, theta + h * K11 / 2, phi + h * K21 / 2, psi + h * K31 / 2, dtheta + h * K11 / 2, dphi + h * K21 / 2, dpsi + h * K31 / 2)
L32 = g3(I1, I3, MGL, t + h / 2, theta + h * L11 / 2, phi + h * L21 / 2, psi + h * L31 / 2, dtheta + h * L11 / 2, dphi + h *   L21 / 2, dpsi + h * L31 / 2)
```

FIGURE 1.27 VBA code for unsteady precession.

```
K32 = f3(I1, I3, MGL, t + h / 2, theta + h * K11 / 2, phi + h * K21 / 2, psi + h * K31 / 2, dtheta + h * K11 / 2, dphi + h * K21 / 2, dpsi + h * K31 / 2)
L13 = g1(I1, I3, MGL, t + h / 2, theta + h * L12 / 2, phi + h * L22 / 2, psi +  h * L32 / 2, dtheta + h * L12 / 2, dphi + h * L22 / 2, dpsi + h * L32 / 2)
K13 = f1(I1, I3, MGL, t + h / 2, theta + h * K12 / 2, phi + h * K22 / 2, psi + h * K32 / 2, dtheta + h * K12 / 2, dphi + h * K22 / 2, dpsi + h * K32 / 2)
L23 = g2(I1, I3, MGL, t + h  / 2, theta + h * L12 / 2, phi + h * L22 / 2, psi + h * L32 / 2, dtheta + h * L12 / 2, dphi + h * L22 / 2, dpsi + h * L32 / 2)
K23 = f2(I1, I3, MGL, t + h / 2, theta + h * K12 / 2, phi + h * K22 / 2, psi + h * K32 / 2, dtheta + h * K12 / 2, dphi + h *   K22 / 2, dpsi + h * K32 / 2)
L33 = g3(I1, I3, MGL, t + h / 2, theta + h * L12 / 2, phi + h * L22 / 2, psi + h * L32 / 2, dtheta + h * L12 / 2, dphi + h * L22 / 2, dpsi + h * L32 / 2)
K33 = f3(I1, I3, MGL, t + h / 2, theta + h * K12 / 2, phi + h * K22 / 2, psi  + h * K32 / 2, dtheta + h * K12 / 2, dphi + h * K22 / 2, dpsi + h * K32 / 2)
L14 = g1(I1, I3, MGL, t + h, theta + h * L13, phi + h * L23, psi + h * L33, dtheta + h * L13, dphi + h * L23, dpsi + h * L33)
K14 = f1(I1, I3, MGL, t + h, theta + h * K13, phi + h  * K23, psi + h * K33, dtheta + h * K13, dphi + h * K23, dpsi + h * K33)
L24 = g2(I1, I3, MGL, t + h, theta + h * L13, phi + h * L23, psi + h * L33, dtheta + h * L13, dphi + h * L23, dpsi + h * L33)
K24 = f2(I1, I3, MGL, t + h, theta + h * K13, phi + h * K 23, psi + h * K33, dtheta + h * K13, dphi + h * K23, dpsi + h * K33)
L34 = g3(I1, I3, MGL, t + h, theta + h * L13, phi + h * L23, psi + h * L33, dtheta + h * L13, dphi + h * L23, dpsi + h * L33)
K34 = f3(I1, I3, MGL, t + h, theta + h * K13, phi + h * K23,  psi + h * K33, dtheta + h * K13, dphi + h * K23, dpsi + h * K33)
    dtheta = dtheta + h * (L11 + 2 * L12 + 2 * L13 + L14) / 6
    dphi = dphi + h * (L21 + 2 * L22 + 2 * L23 + L24) / 6
    dpsi = dpsi + h * (L31 + 2 * L32 + 2 * L33 + L34) / 6
    theta = theta + h * (K11 + 2 * K12 + 2 * K13 + K14) / 6
    phi = phi + h * (K21 + 2 * K22 + 2 * K23 + K24) / 6
    psi = psi + h * (K31 + 2 * K32 + 2 * K33 + K34) / 6
      alpha = psi ^ 2 / (I1 * I3) - 2 * E / I1
      beta = I1 * Sin(theta) ^ 2 * dphi + Ppsi
      a = 2 * MGL / I1
      b = Ppsi / I1
        Cells(2, 14) = "alpha / a": Cells(3, 14) = alpha / a
        Cells(2, 15) = "beta / b": Cells(3, 15) = beta / b
  t = t + h
 Next i
End Sub
________________________________________________________________________________
Function g1(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
'g1=d(dtheta)/dt is the second time derivative of theta.
  g1 = (1 - I3 / I1) * Sin(theta) * Cos(theta) * dphi ^ 2 - (I3 / I1) * Sin(theta) * dphi * dpsi + (MGL / I1) * Sin(theta)
 End Function
________________________________________________________________________________
Function g2(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dps i)
'g2=d(dphi)/dt is the second time derivative of theta.
 g2 = ((I3 / I1 - 2) * Cos(theta) * dphi + (I3 / I1) * dpsi) * dtheta / Sin(theta)
End Function
________________________________________________________________________________
Function g3(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
'g3=d(dpsi)/dt is the second time derivative of theta.
 g3 = (((2 - I3 / I1) * Cos(theta) ^ 2 / Sin(theta) + Sin(theta)) * dphi  - (I3 / I1) * Sin(theta) * dpsi) * dtheta
End Function
________________________________________________________________________________
Function f1(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
'f1=d(theta)/dt
   f1 = dtheta
End Function
________________________________________________________________________________
Function f2(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
'f2=d(phi)/dt
   f2 = dphi
End Function
________________________________________________________________________________
Function f3(I1, I3, MGL, t, theta, phi, psi, dtheta, dphi, dpsi)
'f3=d(psi)/dt
   f3 = dpsi
End Function
________________________________________________________________________________
```

FIGURE 1.27 Continued.

```
Function f1(I1, I3, MGL, t, ang1, ang2, ang3, omega1, omega2, omega3)
'f1=d(theta)/dt
f1 = omega1
End Function
Function f2(I1, I3, MGL, t, ang1, ang2, ang3, omega1, omega2, omega3)
'f2=d(ang2)/dt
f2 = omega2
End Function
Function f3(I1, I3, MGL, t, ang1, ang2, ang3, omega1, omega2, omega3)
'f3=d(ang3)/dt
f3 = omega3
End Function
```

FIGURE 1.27 Continued.

Notice that the cubic function (1.58) has the properties,

$$f(\pm 1) = -(\beta \mp 1)^2 < 0 \text{ and } f(z) > 0 \text{ if } z >> 1. \tag{1.59}$$

Figure 1.28 is a schematic graph of $f(z)$. As shown in the figure, $f(z)$ should have three roots that satisfy $f(z_i) = 0$ where $i = 1, 2, 3$ and $-1 < z_1 < z_2 < +1 < z_3$. Since $f(z)$ is square of the time derivative of $z = \cos\theta$, $f(z)$ must be non-negative. Therefore, physically possible roots must be z_1 and z_2. Let $z_1 = \cos\theta_1$ and $z_2 = \cos\theta_2$. For $0 \le \theta \le \pi/2$, since $\cos\theta_1 < \cos\theta_2$, $\theta_1 \le \theta \le \theta_2$. The nutation of θ will be limited between θ_1 and θ_2.

From the angular momentum p_φ, the time derivative of the angle φ is given by

$$\dot{\varphi} = \frac{p_\varphi - p_\psi \cos\theta}{I_1 \sin^2\theta}. \tag{1.60}$$

Define angle θ_3 such that $\dot{\varphi} = 0$, i.e., $\cos\theta_3 = \dfrac{p_\varphi}{p_\psi}$. Then, comparing the smaller angle θ_1 for the nutation with θ_3, we have three different cases that determine the nutation: case 1: $\dot{\varphi} > 0$ if $\theta_1 > \theta_3$, case 2: $\dot{\varphi} < 0$ if $\theta_1 < \theta_3$, and case 3: $\dot{\varphi} = 0$ if $\theta_1 = \theta_3$.

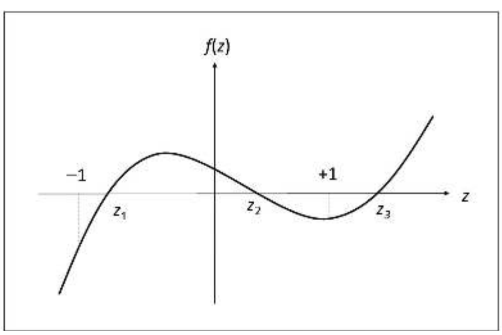


FIGURE 1.28 Function $f(z) = (1 - z^2)(\alpha - az) - (\beta - bz)^2$.

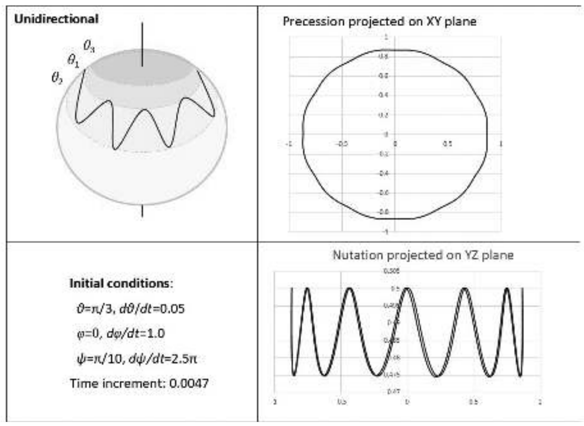


FIGURE 1.29 Unidirectional precession.

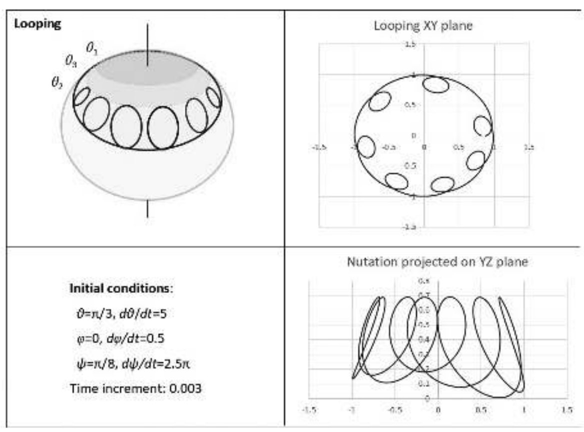


FIGURE 1.30 Looping precession.

Case1: $\boldsymbol{\theta_1 > \theta_3}$. The time derivate of φ is positive throughout the nutation, and the rotational direction of φ does not change. This motion is called unidirectional precession. Figure 1.29 shows the motion of this case and an actual computational result we obtained.

Case2: $\boldsymbol{\theta_1 < \theta_3}$. The time derivate of φ can change its sign, whence the rotational direction of φ becomes backward and the top axis moves backward. This motion is called looping precession. Figure 1.30 shows the motion of this case and an actual computational result.

Case3: $\boldsymbol{\theta_1 = \theta_3}$. The top, spinning about its axis with angular velocity $\omega_3 = \dot{\psi} + \dot{\varphi}\cos\theta$ is held with its axis initially at rest at an angle θ_1, and then released. Initially, we have $\theta = \theta_1$, $\dot{\theta} = 0$, $\dot{\varphi} = 0$, and $\dot{\psi} = \omega_3$. Then, $p_\psi = I_3\omega_3$and$p_\varphi = I_3\omega_3 \cos\theta_1$ at $t = 0$. This motion is called cuspidal precession. The schematic diagram of the motion of this case and a corresponding actual result are shown in Figure 1.31.

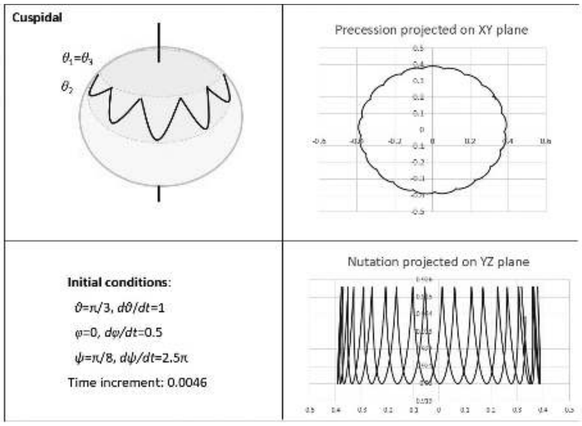


FIGURE 1.31 Cuspidal precession.

SUGGESTED FURTHER STUDY

Perhaps the readers would have seen a photograph of Niels Bohr and Wolfgang Pauli playing with a special top called tippe top. The dynamics of a tippe top is complicated and beyond our scope, but it is worth reading related articles [10]. Another interesting topic is the Dzhanibekov effect or tennis racket theorem. The effect was discovered in a space-station but had been kept secret for decades. Watch a video or read articles to know more about this strange effect [11, 12].

REFERENCES

1. Howell E, NASA's Mighty Saturn V Moon Rocket: 10 Surprising Facts. *Space*. https://www.space.com/38720-nasa-saturn-v-rocket-surprising-facts.html.
2. NASA, Astronomical Unit (AU). Jet Propulsion Laboratory Solar System Dynamics. https://ssd.jpl.nasa.gov/glossary/au.html.
3. NASA. What Is a Lagrange Point? *NASA Science*. https://science.nasa.gov/resource/what-is-a-lagrange-point/.
4. DeVries P L and Hasbun J E, *A First Course in Computational Physics*. James and Bartlett Publishers, 2011.
5. NASA, Where Is Webb? *James Webb Space Telescope: Goddard Space Flight Center*. https://jwst.nasa.gov/content/webbLaunch/whereIsWebb.html.
6. Goldstein H, *Classical Mechanics*, Addison-Wesley, 2011.
7. Symon K, *Mechanics*, Addison-Wesley, 1971.
8. Peraire J and Widnall S, Lecture L28 – 3D Rigid Body Dynamics: Equations of Motion; Euler's Equations. *Dynamics*. https://ocw.mit.edu/courses/16-07-dynamics-fall-2009/resources/mit16_07f09_lec28/.
9. Korringa J, *Lecture note on Classical Mechanics*, The Ohio State University, 1979.
10. Pan S-A, *The Tippe Top*, Stanford University, 2007.
11. YouTube, Dzhanibekov Effect Demonstration in Microgravity, NASA. (Tennis racket theorem). https://www.youtube.com/watch?v=1x5UiwEEvpQ&t=14s.
12. COMSOL, Why Do Tennis Rackets Tumble? The Dzhanibekov Effect Explained. *COMSOL Blog*. https://www.comsol.com/blogs/why-do-tennis-rackets-tumble-the-dzhanibekov-effect-explained.

CHAPTER 2

Oscillations

KNOWLEDGE OF OSCILLATIONS AND waves is on the front line with regard to advancement in physics. We discuss classical harmonic oscillations with driving and/or damping force to describe the phenomena of resonance, weak oscillation, strong damping, and critical damping. Parametric excitations, which can be seen in swing motions and electronic devices, are noteworthy for acquiring knowledge of distinct oscillations and resonance. We also discuss a pair of pendulums with a nonlinear coupling mechanism between them. It is fascinating to view how these two pendulums interact with each other depending on their initial conditions.

2.1 HARMONIC OSCILLATION WITH EXTERNAL FORCES

2.1.1 Periodic Driving Force

The equation of a harmonic oscillator with an external force is given by

$$\frac{d^2x(t)}{dt^2} + \omega_0^2 x(t) = f(t) \tag{2.1}$$

where ω_0 is the angular frequency of the harmonic oscillator without the external force $f(t)$ [1]. Assume that the driving force is periodic of angular frequency ω, i.e., $f(t)=F\sin\omega t$, then Equation 2.1 becomes

$$\frac{d^2x(t)}{dt^2} + \omega_0^2 x(t) = F\sin(\omega t). \tag{2.2}$$

The solution of differential Equation 2.2 can be given by adding a general solution of the homogenous equation, where $F = 0$ and any special solution of Equation 2.2. The general solution may have a form of $y(t) = A\sin(\omega_0 t + c)$, where A and c are constants. Assume a special solution $y(t) = A\sin(\omega t)$. From Equation 2.2, we obtain

$$(\omega_0^2 - \omega^2)A = F, \text{ and thus } x(t) = \frac{F}{(\omega_0^2 - \omega^2)}\sin(\omega t) \text{ is a special solution.} \tag{2.3}$$

DOI: 10.1201/9781003516347-2

Therefore, a general solution of Equation 2.2 is given by

$$x(t) = A\sin(\omega_0 t + c) + \frac{F}{(\omega_0^2 - \omega^2)}\sin(\omega t) \tag{2.4}$$

where c and A are determined by the initial condition. The above solution becomes infinite when $\omega = \omega_0$. In other words, when the frequency of the driving force $f(t)$ is the same as the natural frequency of the harmonic oscillator, resonance occurs. Notice if $\omega < \omega_0$, the second term of Equation 2.4 is out of phase of the external driving force. On the other hand, if $\omega > \omega_0$, the second term becomes out of phase. There is a good demonstration conducted by the MIT Physics Lecture Demonstration Group [2].

Figure 2.1 lists the VBA code to calculate the displacement and velocity of the oscillator in Equation 2.2 using the Runge-Kutta method (Appendix A3). In this code, the trial angular frequency is set to 1 while the external driving frequency is changed.

Figure 2.2 shows the computed results of the VBA code. The broken curve in black is the oscillation without the external driving force, and the large red line is the resonating oscillation with the angular frequency of the periodic driving force being equal to the natural angular frequency of the oscillator. Other oscillation patterns in green and blues are when the driving frequencies are 0.5 and 1.5, which do not excite the oscillation. Recall the phase of the natural oscillation, and the resonating oscillation is out of phase. The diagram of the phase space is an alternative view of the forced oscillation. The amplitude of the oscillation or the energy of the oscillation is rapidly accumulated in the oscillator.

2.1.2 Damping Force

Suppose the damping force is proportional to the velocity dx/dt, we obtain

$$\frac{d^2x}{dt^2} + 2k\frac{dx}{dt} + \omega_0^2 x = 0 \tag{2.5}$$

where the periportal constant of the damping force is $2k$.

Let $y(t) = e^{\gamma t}$, then $\gamma^2 + 2k\gamma + \omega_0^2 = 0$ and the roots are

$$\gamma = \frac{-2k \pm \sqrt{4k^2 - 4\omega_0^2}}{2} = \frac{-k \pm \sqrt{D}}{2} \tag{2.6}$$

where $D = k^2 - \omega_0^2$. There are three distinct oscillation patterns depending on the numerical value of D.

Case 1 (D <0): Weak damping.

Possible roots (2.6) are $\gamma_1 = -k + i\omega$ and $\gamma_2 = -k - i\omega$, where $\omega = \sqrt{\omega_0^2 - k^2}$. Thus, the general solution is given by

$$x(t) = Ae^{\gamma_1 t} + Be^{\gamma_2 t} = e^{-kt}\left[(A+B)\cos\omega t + i(A-B)\sin\omega t\right].$$

```
Sub ForcedOsci1()
Cells(1, 1) = "Harmonic oscillation with damping term and external periodic driving force"
'd(2)x/dt(2)+(omega0)^2x=F*sin(omega*t)   OR dv/dt= -(0mega0)^2x+Fsin(omega*t) and dx/dt=v
'Write labels and initial values in cells:
    Cells(3, 1) = "Initial t": t = 0: Cells(4, 1) = t
    Cells(3, 2) = "Initial x": x = 1: Cells(4, 2) = x
    Cells(3, 3) = "Initial v": v = 0: Cells(4, 3) = v
    Cells(3, 4) = "dt": h = 0.1: Cells(4, 4) = h
omega0 = 1            'Natural oscillation frequency without external factor
                      'Driving term F*sin(omega*t) where F=1 and omega=0.2 to 2.0 by step 0.2.
 jj = 1
For j = 0 To 200 Step 25
   omega = j / 100
   t = 0
   x = 1
   v = 0
   Cells(6, 2 + 2 * (jj - 1)) = "omega"
   Cells(7, 2 + 2 * (jj - 1)) = omega
   Cells(8, 1) = "time"
   Cells(8, 2 + 2 * (jj - 1)) = "x"
   Cells(8, 3 + 2 * (jj - 1)) = "v"
'Runge-Kutta parameters:
   n = 200 ' Iteration # (n*h = range of x; 0 to 5 by step h=0.1)
   For i = 0 To n
      Cells(i + 9, 1) = t
      Cells(i + 9, 2 + 2 * (jj - 1)) = x
      Cells(i + 9, 3 + 2 * (jj - 1)) = v
         K1 = f(t, x, v)
         L1 = g(omega0, omega, t, x, v)
         K2 = f(t + h / 2, x + h * K1 / 2, v + h * L1 / 2)
         L2 = g(omega0, omega, t + h / 2, x + h * K1 / 2, v + h * L1 / 2)
         K3 = f(t + h / 2, x + h * K2 / 2, v + h * L2 / 2)
         L3 = g(omega0, omega, t + h  / 2, x + h * K2 / 2, v + h * L2 / 2)
         K4 = f(t + h, x + h * K3, v + h * L3)
         L4 = g(omega0, omega, t + h, x + h * K3, v + h * L3)
      t = t + h
         x = x + h * (K1 + 2 * K2 + 2 * K3 + K4) / 6
         v = v + h * (L1 + 2 * L2 + 2 * L3 + L4) / 6
   Next i
   jj = jj + 1
Next j
End Sub
________________________________________________________________________________
Function g(omega0, omega, t, x, v)
'g=dv/dt
   g = -omega0 ^ 2 * x + Sin(omega * t)
End Function
________________________________________________________________________________
Function f(t, x, v)
'f=dx/dt
   f = v
End Function
```

Defined by the differential equation.

FIGURE 2.1 VBA code for forced oscillation.

Because $x(t)$ should be real, both $c \equiv A+B$ and $d \equiv i(A-B)$ must be real. Conversely, A and B can be expressed by c and d: $A = (c - id)/2$ and $B = (c + id)/2$. Thus, A and B are complex conjugates. Using c and d, we obtain

$$x(t) = e^{-kt}\left[c\cos\omega t + d\sin\omega t\right] = ae^{-kt}\cos(\omega t + \varphi) \tag{2.7}$$

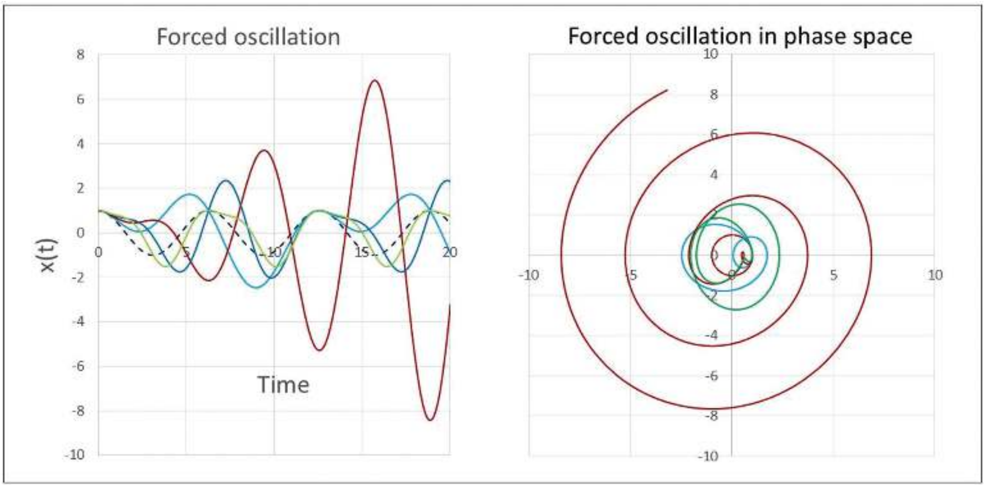


FIGURE 2.2 Forced oscillation.

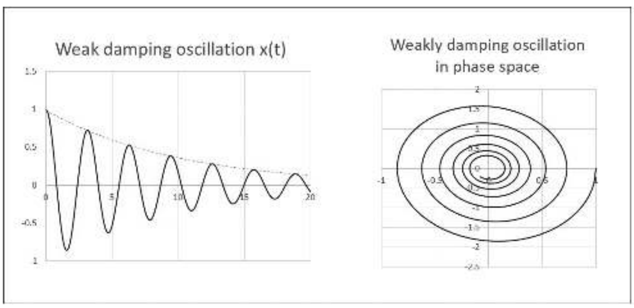


FIGURE 2.3 Time dependence of displacement and trajectory of v(x) of weakly damping oscillation.

where $a = (c^2 + d^2)^{1/2}$ and $\tan\varphi = d/c$. The trajectory of $x(t)$ is an exponentially decreasing periodic function and the one of $v(x)$ in the phase space is a spiral-like curve as shown in Figure 2.3. The period is given by

$$T = 2\pi / \omega = 2\pi / \sqrt{\omega_0^2 - k^2}\,.$$

The VBA code for damping oscillations is similar to the one listed in Figure 2.3 except the statement of `function g` of the Ruge-Kutta algorithm. We used **`g = -a*v-4*x,`** where $a = 2k$ and $\omega_0 = 2$. Make your own code and run to observe the trajectories.

Case 2 (D >0): Strong damping.

Two roots of γ become: $\gamma_1 = -k + \omega'$ and $\gamma_2 = -k - \omega'$, where $\omega' = \sqrt{k^2 - \omega_0^2}$. The general solution is $x(t) = Ae^{\gamma_1 t} + Be^{\gamma_2 t}$, where A and B are both real. Both terms are exponentially decreasing because

$$-k \pm \omega' = -k\left[1 \mp \sqrt{1 - (\omega_0 / k)^2}\,\right] < 0. \tag{2.8}$$

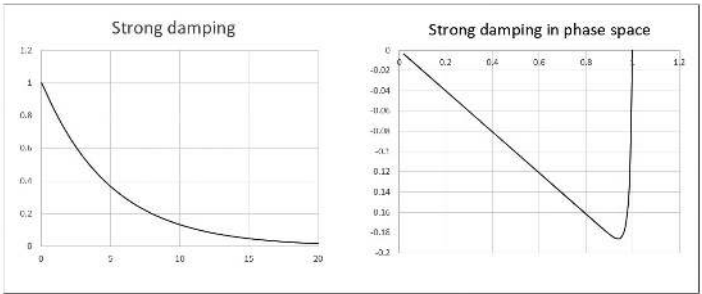


FIGURE 2.4 Time dependence of displacement and trajectory of $v(x)$ of strong damping oscillation.

Figure 2.4 shows the exponentially decreasing trajectory of $x(t)$ and abruptly settling $v(x)$ due to the strong damping.

Case 3 (D = 0): Critical damping.
Two roots of γ are $\gamma_1 = \gamma_2 = -k$. The general solution of Equation 2.5 has one solution. One may find if it can be a form of $x(t) = g(t)e^{-kt}$.

$$\frac{dx}{dt} = 2\left(\frac{dg}{dt} - kg\right)e^{-kt} \text{ and } \frac{d^2x}{dt^2} = \left(\frac{d^2g}{dt^2} - 2k\frac{dg}{dt} + k^2\right)e^{-kt}. \tag{2.9}$$

Thus, Equation 2.5 should satisfy $\dfrac{d^2g}{dt^2} - \left(k^2 - \omega_0^2\right)g = 0.$ (2.10)

Because $D = 0$, i.e., $k = \omega_0$, $g(t) = A + Bt$ and $x(t) = (A + Bt)e^{-kt}$, where A and B are constants.

Figure 2.5 shows the shortest time to cease the oscillation and the gradually settling $v(x)$. The graph in the phase space exhibits a different pattern from that of the strong damping.

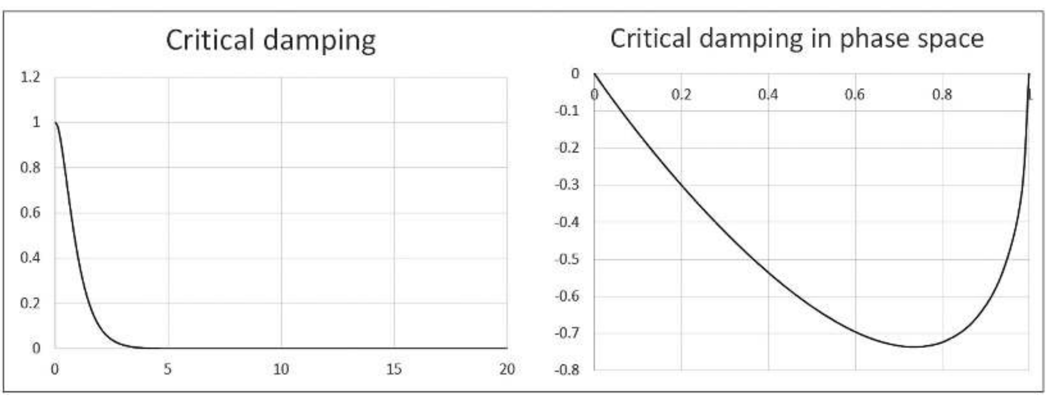


FIGURE 2.5 Time dependence of displacement and trajectory of v(x) of weakly damping oscillation.

2.1.3 Both Driving and Damping Forces

If both driving and damping forces are applied to the harmonic oscillator and Equations 2.2 and 2.3 are combined, we have

$$\frac{d^2x}{dt^2}+2k\frac{dx}{dt}+\omega_0^2 x = F\sin(\omega t). \tag{2.11}$$

The general solution of Equation 2.11 is given by adding the general solution of Equation 2.5, which is calculated, and a special solution of Equation 2.11. Let us find a special solution of a form of $A\sin(\omega t - \delta)$ including a phase delay δ. From Equation 2.11, we obtain

$$-\omega^2 A\sin(\omega t-\delta)+2k\omega A\cos(\omega t-\delta)+\omega_0^2 A\sin(\omega t-\delta) = F\sin(\omega t). \tag{2.12}$$

By applying the addition theorem of trigonometric functions, we obtain

$$\begin{cases}\left[2k\omega_0 A\sin\delta+(\omega_0^2-\omega^2)^2 A\sin\delta\right]\sin\omega t = F\sin\omega t\\ \left[(\omega_0^2-\omega^2)^2 A\sin\delta-2k\omega A\cos\delta\right]=0.\end{cases} \tag{2.13}$$

Solving them for A and $\tan\delta$ gives

$$\begin{cases}A\sin\delta=\dfrac{2k\omega}{(\omega_0^2-\omega^2)^2+4k^2\omega^2}F\\ A s\cos\delta=\dfrac{(\omega_0^2-\omega)^2}{(\omega_0^2-\omega^2)^2+4k^2\omega^2}F\end{cases}, \text{ and } \begin{cases}A=\dfrac{1}{\omega_0^2\sqrt{(1-(\omega/\omega_0)^2)^2+4(k/\omega_0)^2(\omega/\omega_0)^2}}F\\ \tan\delta=\dfrac{2(k/\omega_0)(\omega/\omega_0)}{1-(\omega/\omega_0)^2}\end{cases}. \tag{2.14}$$

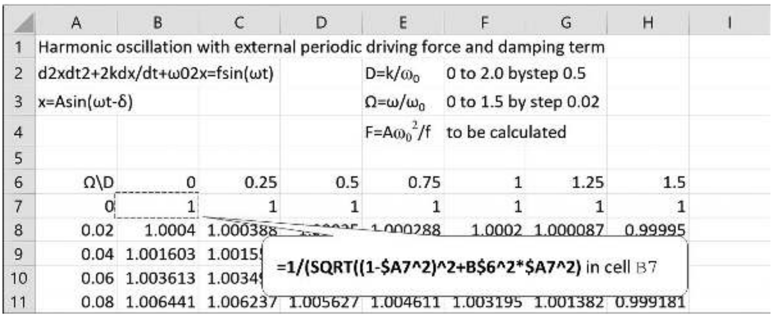
The amplitude A becomes a maximum value when $(\omega_0^2-\omega^2)^2+4k^2\omega^2$ becomes a minimum value, i.e., when $(\omega_0^2-\omega^2)+4k^2\omega^2=0$. The phase δ vanishes as the angular frequency of the external driving force approaches that of the harmonic oscillation. Notice that after a sufficiently long time, only the term of this special solution, which is a forced oscillation, remains.

Let $D = k/\omega_0$ and $\Omega = \omega/\omega_0$. From Equation 2.14, we obtain

$$\frac{A\omega_0^2}{F}=\frac{1}{\sqrt{(1-\Omega^2)^2+4D^2\Omega^2}} \text{ and } \tan\delta=\frac{2D\Omega}{1-\Omega^2}. \tag{2.15}$$

Figure 2.6 shows a screenshot of the angular frequency ($\Omega = \omega/\omega_0$) dependence of the amplitude ($A\omega_0^2/F$) for different values of damping terms ($D = k/\omega_0$). Excel's *AutoFill* feature is applied to this calculation. For *AutoFill*, refer to Appendix A1.1.

Steps for this two-factor calculation using Excel's *AutoFill* feature are given below. Notes in Rows `1` to `4` are ranges of variables **Ω** and **D**. Column `A` is the range of ***Ω*** (0–1.5 by



	A	B	C	D	E	F	G	H	I
1	Harmonic oscillation with external periodic driving force and damping term								
2	d2xdt2+2kdx/dt+ω02x=fsin(ωt)				D=k/ω0	0 to 2.0 bystep 0.5			
3	x=Asin(ωt-δ)				Ω=ω/ω0	0 to 1.5 by step 0.02			
4					F=Aω0^2/f	to be calculated			
5									
6	Ω\D	0	0.25	0.5	0.75	1	1.25	1.5	
7	0	1	1	1	1	1	1	1	
8	0.02	1.0004	1.000388	[illegible]	1.000288	1.0002	1.000087	0.99995	
9	0.04	1.001603	1.0015[illegible]						
10	0.06	1.003613	1.0034[illegible]						
11	0.08	1.006441	1.006237	1.005627	1.004611	1.003195	1.001382	0.999181	

FIGURE 2.6 Calculated frequency dependence of amplitude with different damping terms.

increment 0.02) and Row 6 is the range of **D** (0–2.0 by increment 0.5). "**Ω\D**" in cell A6 is an optional remark.

The letters and numbers in bold are to be entered in a specified cell of a spreadsheet.

Ω-values(*x*-axis):

1) Enter **0** into Cell A7;
2) Enter **= A7−0.02** into Cell A8;
3) *AutoFill* to Cell A107.

D-values (*y*-axis):

4) Enter **0** into Cell B6;
5) Enter **=B5+0.5** into C6;
6) *AutoFill* to cell H6.

Enter function of Equation 2.15:

7) Click on cell B7 and enter

   =1/(SQRT((1-$A7^2)^2+B$6^2*$A7^2))

8) *AutoFill* to cell H7 (to the right);
9) Continue *AutoFill* to H107 (downward).

Create a graph:

10) Highlight Cell A7 to B107;
11) From the drop-down menu, select [Insert] → [Chart] → [Scatter with Smooth Lines];
12) Expand the created chart if necessary;

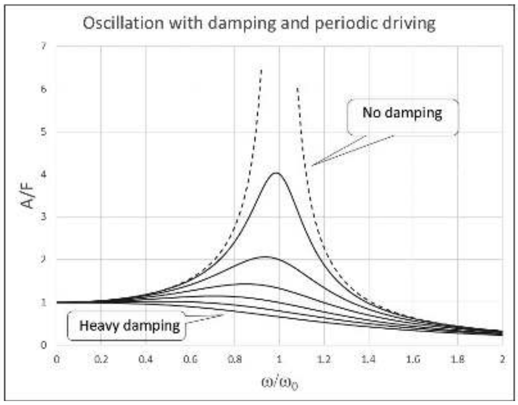


FIGURE 2.7 Resonance curve of forced harmonic oscillation.

	A	B	C	D	E	F	G	H	I
1				D=k/ω0	0 to 2.0 bystep 0.5				
2	tanδ			Ω=ω/ω0	0 to 1.5 by step 0.02				
3				F=Aω0²/f	to be calculated				
4									
5	Ω\D	0	0.25	0.5	0.75	1	1.25	1.5	
6	0	0	0	0	0	0	0	0	
7	0.02	0	0.01[illegible]	0.020008	0.030012	0.040016	0.05002	0.060024	
8	0.04	0	0.0[illegible]	[illegible]	[illegible]	[illegible]8	0.10016	0.120192	
9	0.06	0	0.0[illegible]	[illegible]	[illegible]	[illegible]4	0.150542	0.18065	
10	0.08	0	0.040258	0.080515	0.120773	0.161031	0.201288	0.241546	

=2*B$5*$A6/(1-$A6^2) in cell B6

FIGURE 2.8 Calculated frequency dependence of phase with different damping factors.

13) Right-click on the graph to display a pop-up menu to select [`Select Data`] →[`Add`] for adding the graph from the data from Column `C`, etc.

Figure 2.7 is the final graph of the amplitude from the calculated data.

Figure 2.8 shows a screenshot of calculating the angular frequency (ω/ω_0) dependence of phase (tan δ) for different values of damping factor (k/ω_0). The phase changes across the resonating condition where tan δ diverges. The calculation procedure is very much the same as the amplitude calculation.

Figure 2.9 shows the final graph of tanδ from the calculated data.

2.2 PARAMETRIC OSCILLATION

Figure 2.10 illustrates a parametric pendulum where the string length varies periodically [3, 4].

The equation of motion using angular momentum and torque is given by

$$\frac{d}{dt}\left(mL^2\frac{d\theta}{dt}\right) = -mgL\sin\theta \tag{2.16}$$

where g is the gravitational constant, and the string length ℓ has a slow periodic time dependence $L(t) = L_0\left[1 + h\sin(\omega t + \delta)\right]$ and 0<h<< 1.

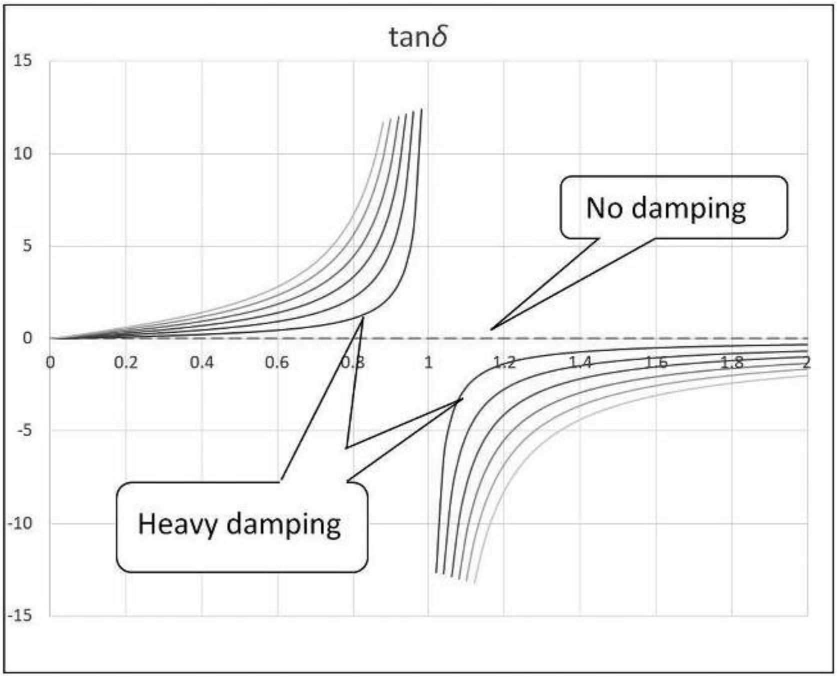


FIGURE 2.9 Phase change of force harmonic oscillation.

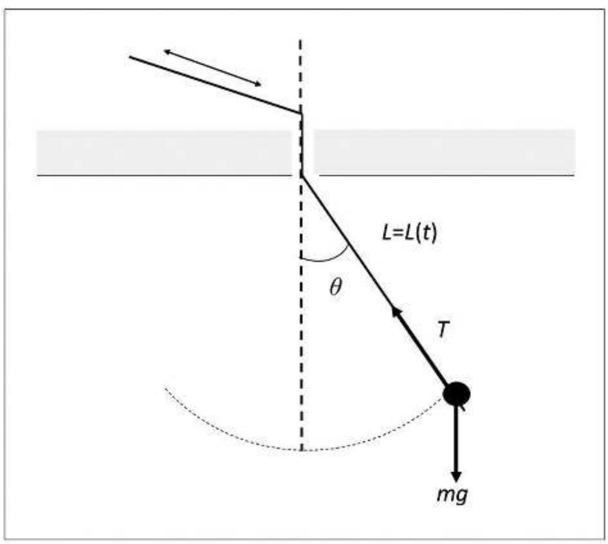


FIGURE 2.10 Pendulum oscillation with parametric excitation

We assume the small angle approximation ($\sin\theta \approx \theta$). Converting the variable from the angle to the arc length $x = L\theta$, Equation 2.16 becomes

$$\frac{d^2x(t)}{dt^2} + \frac{1}{L}\left(g - \frac{d^2L}{dt^2}\right)x(t) = 0 \text{ or } \frac{d^2x(t)}{dt^2} + G(t)x(t) = 0, \text{ and}$$

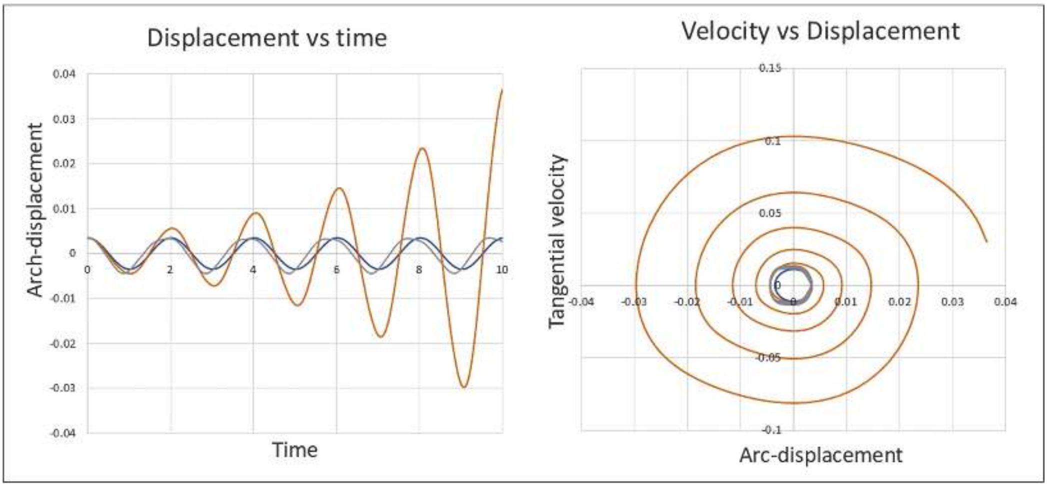


FIGURE 2.11 Arc length and velocity of a pendulum with the parametric excitation.

$$G(t) = \frac{1}{L}\left(g - \frac{d^2L}{dt^2}\right) = \frac{g + L_0\omega^2\delta\sin(\omega t + \delta)}{L_0[1 + \delta\sin(\omega t + \delta)]} = \omega_0^2\frac{1 + n^2\delta\sin(\omega t + \delta)}{1 + \delta\sin(\omega t + \delta)} \tag{2.17}$$

where $\omega_0 = \sqrt{g / L_0}$ when L is fixed to L_0 and $\omega = n\omega_0$.

Note: The VBA code for the parametric oscillation is similar to that shown in Figure 2.1. The only difference is the form of `function g` of the Runge-Kutta algorithm (Appendix A3). For the parametric oscillation,

```
function g = -x * Omega0 ^ 2 * (1 + dl * (kk ^ 2) *
Sin(Omega * t + phi)) / (1 + dl * Sin(Omega * t + phi))
```

from Equation 2.17.

Figure 2.11 shows the arch length vs time and velocity vs time with different multiplication factors n. As we may expect from swings, the arc length exponentially increases when $\omega = 2\omega_0$.

2.3 COUPLED PENDULUMS

Figure 2.12 is a schematic diagram of two identical pendulums of length L connected with a nonlinear spring [5]. Assume the spring force is given by $k_1\Delta x + \varepsilon k_2(\Delta x)^3$, where k_1, k_2, ε = 1/3! are constants and Δx is the length change of the spring.

Equations of motion are:

$$\begin{cases} mL\dfrac{d^2x_1}{dt_2} = -mgx_1 - k_1(x_1 - x_2) - \varepsilon k_2(x_1 - x_2)^3 \\ mL\dfrac{d^2x_2}{dt_2} = -mgx_2 - k_2(x_2 - x_1) - \varepsilon k_2(x_2 - x_1)^3 \end{cases}. \tag{2.18}$$

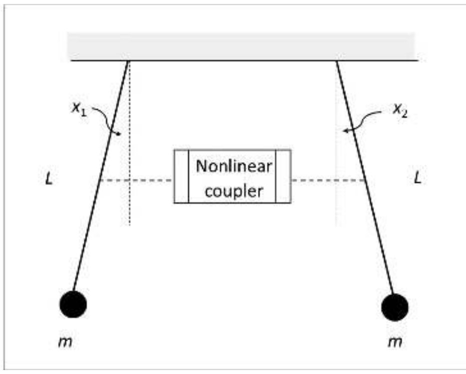


FIGURE 2.12 Two pendulums connected with a spring.

Let $x_1 + x_2 = y_1$ and $x_1 - x_2 = y_2$. Equations 2.18 become

$$\frac{d^2 y_1}{dt^2} + \omega_1^2 y_1 = 0 \text{ and } \frac{d^2 y_2}{dt^2} + \omega_1^2 y_2 = -\varepsilon k y_2^3 \tag{2.19}$$

where $\omega_1^2 = g / L$, $\omega_2^2 = g / L + 2k_1 / mL$, and $k = 2k_2 mL$.

The solution of y_1 is a harmonic oscillation while y_2 yields a nonlinear osculation. The coupling between two pendulums is nonlinear, and their motions may not be simple. Let us compute their motions, and then obtain x_1 and x_2 from calculated y_1 and y_2.

Case 1: Small oscillations

Figure 2.13 shows y_1 and y_2. We set the coupling coefficient $\varepsilon = 1/6$ in the nonlinear term in Equation 2.15. The angular momentum $\omega_1{}^2 = g/L = 9.8$ is set to 3.13 and $k_1 = k_2 = 1$. The initial displacements are $y_1 = 0.5$ and $y_2 = -0.5$. It seems that both y_1 and y_2 yield harmonic oscillations. With these initial settings, the coupling may not be seen except by the pair of pendulums' gradual energy exchange due to the weak coupling.

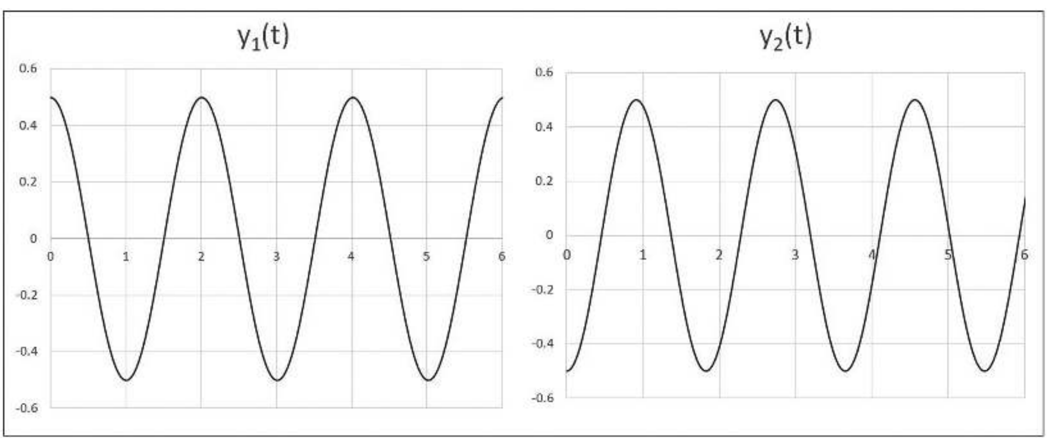


FIGURE 2.13 Coupled pendulums with $y_1 = 0.5$ and $y_2 = -0.5$ at $t = 0$.

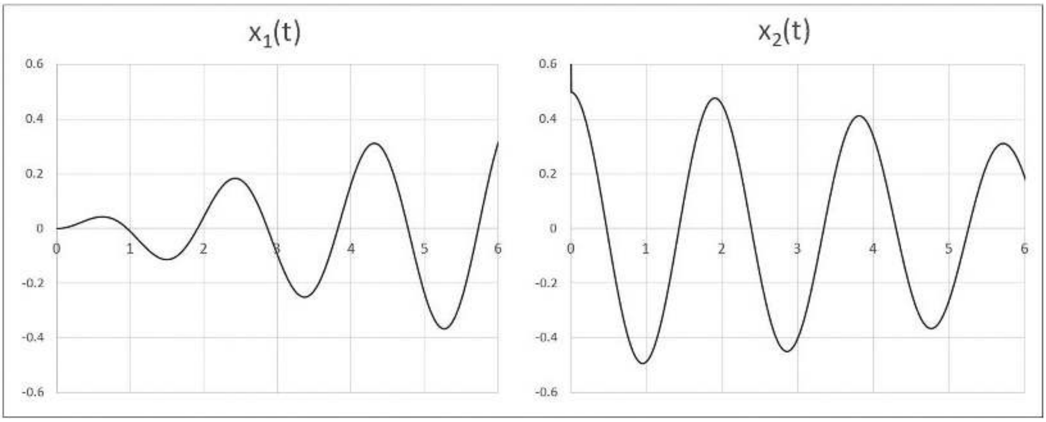


FIGURE 2.14 Observable displacements of coupled pendulums with small nonlinear coupling.

Figure 2.14 shows observable displacements x_1 and x_2 with an initial condition of x_1 = 0 and x_2 = 1 at t = 0. There is energy transfer from pendulum 2 to pendulum 1 due to the coupling.

Case 2: Large oscillations

Taking the third orders of sin(x_1) and sin(x_2): $\sin x_1 \approx x_1 + \varepsilon x_1^3$ and $\sin x_2 \approx x_2 + \varepsilon x_2^3$, where $\varepsilon = 1/3!$,

$$\begin{cases} mL\dfrac{d^2x_1}{dt_2} = -mgx_1 + \varepsilon mgx_1^3 - k_1(x_1 - x_2) - \varepsilon k_2(x_1 - x_2)^3 \\ mL\dfrac{d^2x_2}{dt_2} = -mgx_2 + \varepsilon mgx_2^3 - k_1(x_2 - x_1) - \varepsilon k_2(x_2 - x_1)^3 \end{cases}. \tag{2.20}$$

Using the same definitions of y_1 and y_2, we obtain

$$\frac{d^2y_1}{dt^2} + \omega_1^2 y_1 = \varepsilon f_1(y_1, y_2) \text{ and } \frac{d^2y_2}{dt^2} + \omega_2^2 y_1 = \varepsilon f_2(y_1, y_2) \tag{2.21}$$

where $f_1(y_1, y_2) = (g/4L)y_1(y_1^2 + 3y_2^2)$, $f_2(y_1, y_2) = (g/4L)y_1(y_1^2 + 3y_2^2) - 2(k_2/mL)y_2^3$,

$\omega_1 = g/L$, and $\omega_2^2 = g/L + 2k_1/m$. The coefficient ε is a measure of deviation from linearity.

Figures 2.15 shows the motions of y_1 and y_2 from the nonlinear oscillations. Initially we set $y_1 = 0.5$ and $y_2 = -0.5$. A gradual energy transfer from y_1 to y_2 is observed with the nonlinear coupling. The coupling coefficient $\varepsilon = 1/6$ is the same as in Case 1.

Figure 2.16 shows the observable displacements $x_1 = (y_1+y_2)/2$ and $x_2 = (y_1-y_2)/2$. The initial displacements are $x_1 = 0$ and $x_2 = 1$ at $t = 0$. Changes in their displacements are more noticeable due to the nonlinear cubic terms of x_1 and x_2.

Try and observe what their motions are. It's fun!

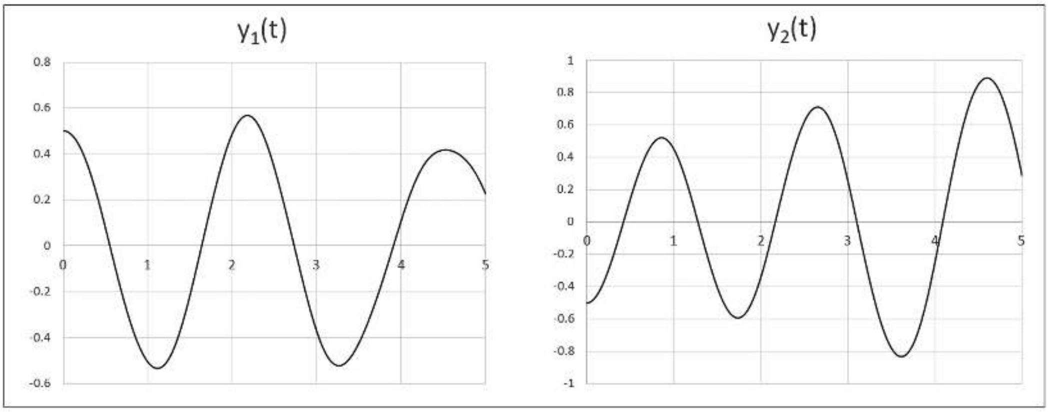


FIGURE 2.15 Nonlinear pendulums with nonlinear coupling. $y_1 = 0.5$ and $y_2 = -0.5$ at $t = 0$.

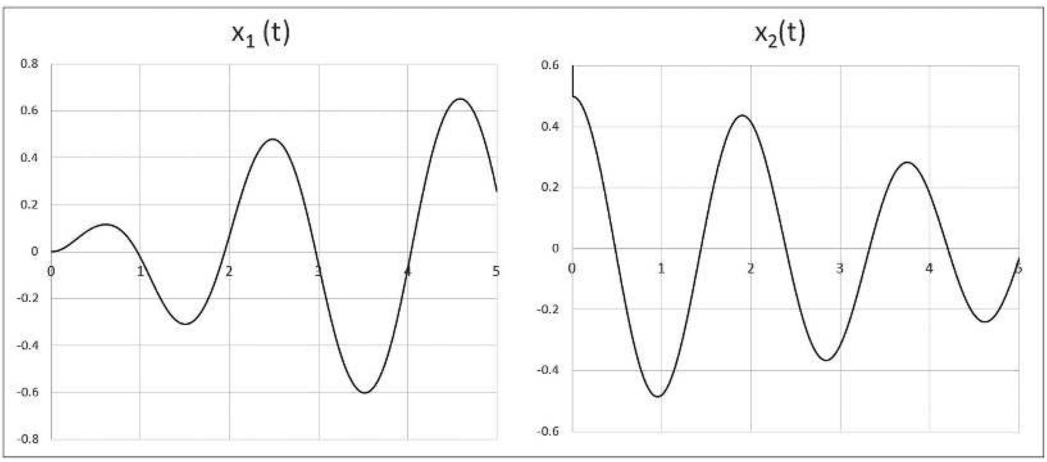


FIGURE 2.16 Observable displacements of nonlinear pendulums with nonlinear coupling.

SUGGESTED FURTHER STUDY

Although this book does not cover nonlinear oscillations, there are many important topics in nonlinear oscillations. For example, electronic devices including diodes and transistors are actually nonlinear components [6]. There is an old-fashioned computer using parametrons conceived by the parametric oscillation [7]. Nonlinear optics is a fascinating technology applied in medicine and science [8]. Chaos is caused by nonlinear dynamics such as large oscillations of a pendulum and double pendulums [9].

REFERENCES

1. OpenStax, *University Physics*, Vol. 1, Rice University, https://openstax.org/details/books/university-physics-volume-1.
2. MIT Physics Lecture Demonstration Group, Driven Mechanical Oscillator. *YouTube*. https://www.youtube.com/watch?v=aZNnwQ8HJHU.
3. MIT Open Course Ware, *Parametric Oscillators: Lecture Notes 6*. https://dspace.mit.edu/bitstream/handle/1721.1/84612/12-006j-fall-2006/contents/lecture-notes/lecnotes6.pdf.

4. Garanin D, *Parametric Resonance*, Lehman College, 2008. https://www.lehman.edu/faculty/dgaranin/Mechanics/Parametric_resonance.pdf
5. University of Toronto, *Coupled Oscillators*. https://www.physics.utoronto.ca/~sandra/PHY238Y/Lectures/Lect4_Coupl_osc.pdf.
6. Horowitz P and Hill W, *The Art of Electronics*, Cambridge University Press, 2015.
7. Goto, E, et al., The Parametron: A Digital Computing Element Which Utilizes Parametric Oscillation. *Proceedings of the IRE* 47, 8, 2007.
8. Brown University, *Introduction to Nonlinear Optics: Lecture 35*. https://www.brown.edu/research/labs/mittleman/sites/brown.edu.research.labs.mittleman/files/uploads/lecture35_0.pdf.
9. Cho S, *Monte Carlo Simulations using Microsoft Excel®*, Springer Nature, 2003.

CHAPTER 3

Waves

Wave phenomena could be understood better by conducting computational analyses of waves. Analyses are done to show diagrams of interference, standing waves, the classical/relativistic Doppler effect, muon detection using the Doppler effect, the law of refraction based on wave and particle models, and diffraction phenomena through a two-dimensional aperture. In relation to standing waves, the Fourier series are introduced to demonstrate that an arbitrary periodic wave can be expressed in terms of trigonometric functions.

3.1 WAVE EQUATION

Let the wave velocity be v. In the Cartesian coordinate system, a three-dimensional wave is given by the following equations [1].

$$\frac{\partial^2 u(\vec{r},t)}{\partial t^2} = v^2\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)u(\vec{r},t) = v^2\nabla^2 u(\vec{r},t) \text{ where } v^2 = v_x^2+v_y^2+v_z^2. \tag{3.1}$$

A plane wave, $u(\vec{r},t) = A\sin(\vec{k}\cdot\vec{r}-\omega t+\delta)$, is a solution of the wave equation, where A is the amplitude, $\vec{k}=(k_x,k_y,k_z)$ is the wave number vector, $\vec{k}\cdot\vec{r}=k_x x+k_y y+k_z z$, ω is the angular frequency, δ is the initial phase, and $v = \omega/k = f\lambda$, where $f = 2\pi/\omega$ is the frequency and $\lambda = 2\pi/k$ is the wavelength. A spherical wave, $u(\vec{r},t)=\frac{A}{r}\sin(kr-\omega t+\delta)$, is also a solution, where $r=\sqrt{x^2+y^2+z^2}$ and $k=\sqrt{k_x^2+k_y^2+k_z^2}$. A spherical wave is isotropic, i.e., $u(\vec{r},t)=u(r,t)$ and satisfies $\nabla^2 u(r,t)=\frac{1}{r}\frac{\partial^2}{\partial r^2}u(r,t)$.

Notice that the wave equation is a linear differential equation. It means that, if u_1 and u_2 satisfy the wave equation, their linear combination, e.g., $u = au_1 + bu_2$, where a and b are constants, is also a solution of the wave equation. This is the foundation of the superposition principle discussed below.

DOI: 10.1201/9781003516347-3

```
Sub SineInterference()
Cells(1, 1) = "Demonstration of interference of two plane waves"
  Dim y1(1001)
  Dim y2(1001)
  Dim x(1001)
  Pi = 3.14159
  alpha = 0.1
    Cells(2, 1) = "Phase difference =": phase = alpha * Pi
    Cells(2, 3) = alpha * Pi: Cells(2, 4) = "rad"
    Cells(3, 2) = "x"
    Cells(3, 3) = "y1"
    Cells(3, 4) = "y2"
    Cells(3, 5) = "y1+y2"
For i = 0 To 1000
  x(i) = i * 0.01
  Cells(4 + i, 2) = x(i)
Next i
  f = 1
  k = 0.5
  a = 1
  For i = 0 To 1000
    y1(i) = a * Sin(2 * Pi * k * x(i) - 2 * Pi * f * j / 50)
    y2(i) = a * Sin(2 * Pi * k * x(i) - 2 * Pi * f * j / 50 + phase)
      Cells(4 + i, 3) = y1(i)
      Cells(4 + i, 4) = y2(i)
      Cells(4 + i, 5) = y1(i) + y2(i)
  Next i
End Sub
```

FIGURE 3.1 VBA code to calculate the interference of two sine waves.

3.2 SUPERPOSITION PRINCIPLE

The superposition principle is the cause of several key wave phenomena. We describe interference, beat, and standing waves in relation to this principle [2].

3.2.1 Interferences

Suppose there are two plane waves in space: $u_1(x,t) = A\sin(kx - \omega t)$ and $u_2(x,t) = A\sin(kx - \omega t + \delta)$, the resultant wave is the algebraic sum of the two waves [3]. They are interfered constructively if $\delta = 0$ and destructively if $\delta = \pi$. Figure 3.1 lists the VBA code to calculate the interference.

Figure 3.2 shows an interference pattern of two sine waves with a small phase difference of 0.1π to demonstrate the superposition of the two waves clearly.

The interference pattern can also be created by superposing two spherical waves at a certain time. Here we consider two-dimensional circular waves. Two circular waves of the same angular frequency generated from two different sources at slightly different locations of $(0, \pm y_s)$ and supposed them.

$$u = \frac{\sin(kr_1 - \omega t)}{r_1} + \frac{\sin(kr_2 - \omega t)}{r_2} \tag{3.2}$$

where $r_1 = \left[x^2 + (y - y_s)^2\right]$ and $r_2 = \left[x^2 + (y + y_s)^2\right]$.

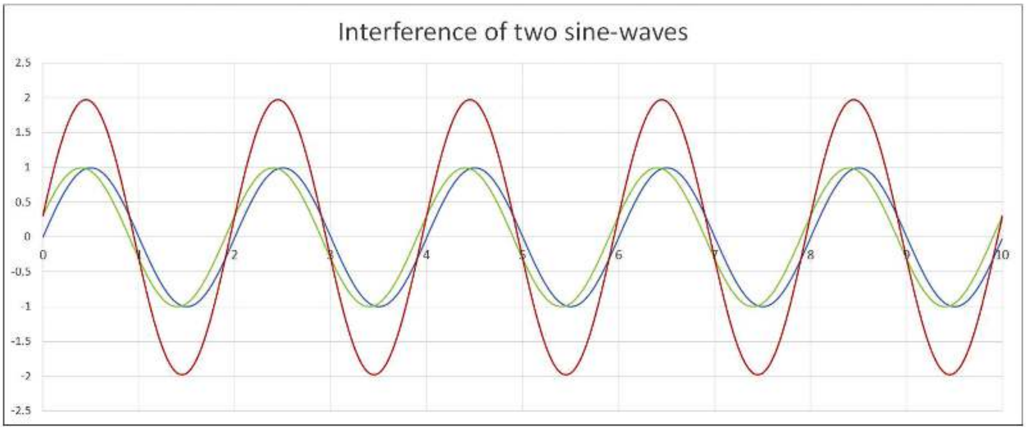


FIGURE 3.2 Interference of two sine waves with path difference of 0.1π.

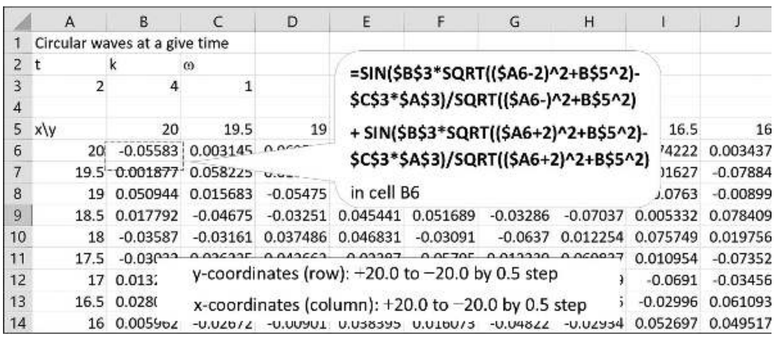


FIGURE 3.3 Calculation of the interference pattern of two circular waves.

Parameter setting

Wave number: $k = 4$; angular frequency: $\omega = 1$; time $t = 2$; and locations of circular wave sources (0, ±2.0).

The area to create the interference pattern is set to x: [–20.0, 20.0], y: [–20.0, 20.0] with an increment of 0.5 in the x and y directions. Figure 3.3 is a screenshot of the calculation using Excel's *AutoFill* feature (Appendix A1.1).

Calculation step:

The letters and numbers in bold are to be entered in a specified cell of a spreadsheet.

1) Enter **`t`** in cell `A2`, **k** in cell `B2`, and **ω** in cell `C2`, and then enter **2** in cell `A3`, **4** in `B3`, and **1** in cell `C3`. Note: These values may be changed after drawing the chart. "**`x\y`**" at cell `A5` is an optional memo.

Determine range and step:

x-axis:

2) Enter **`20`** into Cell `A6`;
3) Enter **`=A6−0.5`** into Cell `A7`;
4) *AutoFill* to Cell `A86`.

y-axis:

5) Enter **20** into Cell B5;
6) Enter **=B5-0.5** into C5;
7) *AutoFill* to cell CD5.

Superpose circular waves:

8) Click on cell B6 and enter
   =SIN($B$3*SQRT(($A6-2)^2+B$5^2)-$C$3*$A$3)/SQRT(($A6-)^2+B$5^2)
   +SIN($B$3*SQRT(($A6+2)^2+B$5^2)-$C$3*$A$3)/SQRT(($A6+2)^2+B$5^2),
   and then, AutoFill to cell CD5 (to the right);
9) Continue *AutoFill* to CD86 (downward).

Create 3D Surface Chart:

10) Highlight Cell B5 to CD86;
11) From the pulldown menu, select [Insert] → [Chart] → [Surface];
12) Expand the created chart if necessary;
13) Right click on the graph to display a pop-up menu and select [3-D Rotation];
14) Rotate your graph to obtain the best view.

Figure 3.4 shows computed 3D charts with the given wave parameters setting and a specific view angle.

Depending on the path difference between two circular waves that arrive at the same point determines the constructive or destructive interference: Constructive if the path difference is $m\lambda$ and destructive if the path difference is $(m + 1/2)\lambda$, where $m = 0, 1, 2, \ldots$

3.2.2 Beat

When two sound frequencies are slightly different by a few Hertz or so, we hear a beat [4]. Musical instruments such as pianos and guitars are tuned by listening to beats. Suppose two sound waves are

$$u_1 = A\cos(k_1 x - \omega_1 t) \text{ and } u_2 = A\cos(k_2 x - \omega_2 t),$$

when an observer at position $x = 0$ hears two sounds at the same time, the resultant sound is their superposition,

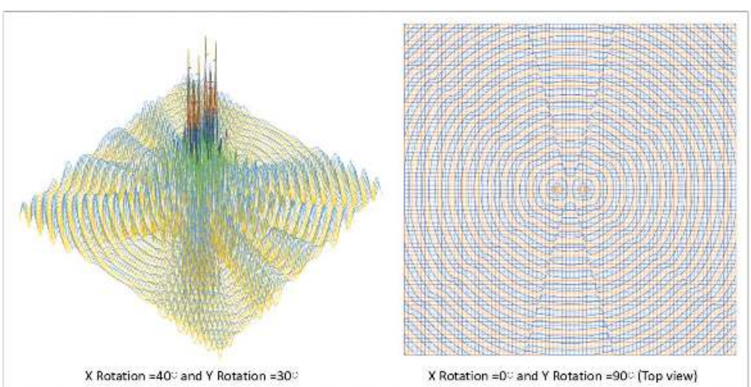


FIGURE 3.4 Interference of circular waves.

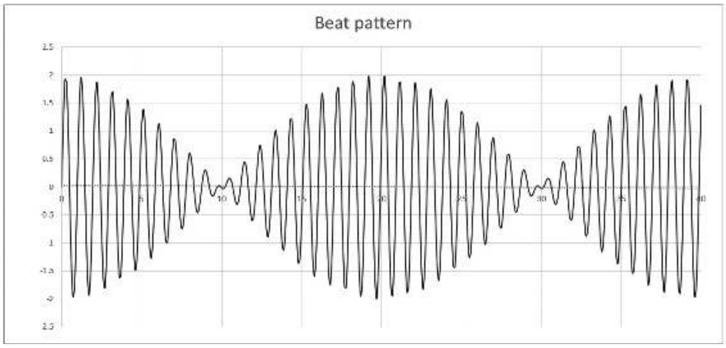


FIGURE 3.5 The beat pattern from two sine waves.

$$u = u_1 + u_2\Big|_{x=0} = 2A\cos\left(\frac{\omega_2 + \omega_1}{2\pi}\right)\cos\left(\frac{\omega_2 - \omega_1}{2}t\right). \tag{3.3}$$

The beat frequency is defined by $f_{beat} = \left|\frac{\omega_2 - \omega_1}{2\pi}\right| = |f_2 - f_1|$.

The VBA code to create the beat is similar to that shown in Figure 3.1. For obtaining the beat, the observer's position is fixed while the time varies. The essential part of the VBA code is

```
For i = 0 To 400 'time increment
    y1(i) = Sin(2 * Pi * f1 * i / 10)
    y2(i) = Sin(2 * Pi * f2 * i / 10)
        Cells(1 + i, 2) = i / 10
        Cells(1 + i, 3) = y1(i) + y2(i)
Next i
```

Figure 3.5 shows the beat pattern, where $f_1 = 1.00$, $f_2 = 1.05$, and $f_1 - f_2 = 0.05$. In this figure, the period of the beat is 20.0, and the beat frequency is also calculated as $f_{\text{beat}} = 1/20 = 0.05$.

3.2.3 Standing Waves

Assume a sine wave traveling to the right on a string, $u_R(x,t) = A\sin(kx - \omega t)$, is reflected at the end on the right side of the fixed string to produce a reflected wave, $u_L(x,t) = A\sin(kx + \omega t)$. The superpose wave is

$$u(x,t) = u_R + u_L = A\sin(kx - \omega t) + A\sin(kx + \omega t) = 2A\sin(kx)\cos(\omega t). \tag{3.4}$$

The resultant wave forms a standing wave, which is not traveling to the right nor left but is a stationary wave pattern with a time-varying amplitude [5]. Figure 3.6 shows a standing wave pattern. The VBA code to obtain the standing wave pattern is similar to that shown in Figure 3.1.

It should be noted that establishing a standing wave requires specific boundary conditions and string length, as well as the tension in the string, which determines the wave speed. For this reason, standing waves are categorized as a boundary value problem. That

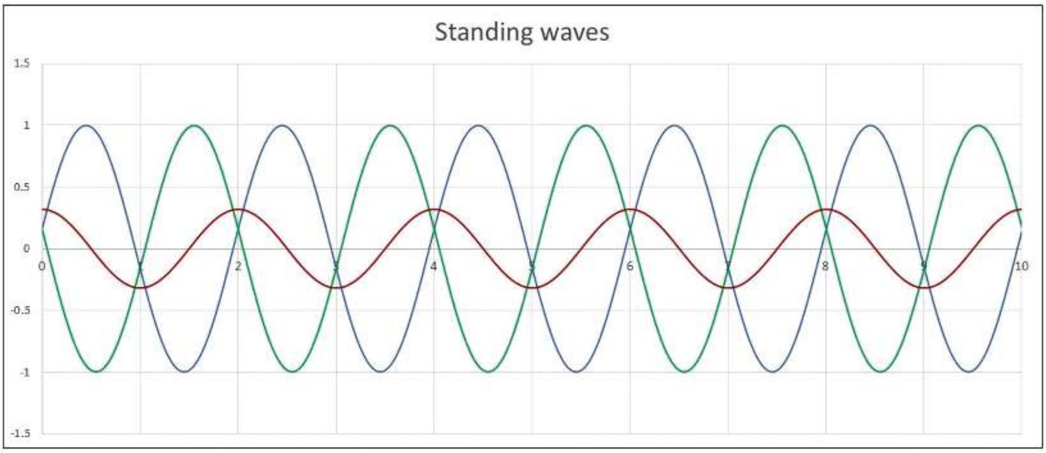


FIGURE 3.6 A standing wave.

is, standing waves on a string of length L having both ends fixed are the solutions of the wave equation,

$$\frac{\partial^2 u(x,t)}{\partial t^2} = v^2 \frac{\partial^2 u(x,t)}{\partial x^2} \tag{3.5}$$

with the boundary condition of fixed ends, $u(0,t) = u(L,t) = 0$, where $u(x, t)$ is the displacement, $v = (F/\mu)^{1/2}$ is the wave speed, F is the tension in the string, and μ is line density of the string.

By separating the variables, $u(x, t) = U(x)\Gamma(t)$, the equation $U(x)$ for the x-coordinate becomes what we call the Helmholtz equation, whereas the equation $\Gamma(t)$ for time is an equation of harmonic oscillation,

$$\frac{d^2U(x)}{dx^2} + \lambda U(x) = 0 \text{ where } U(0) = U(L) = 0, \text{ and } \frac{d^2\Gamma(t)}{dt^2} + \lambda v^2 \Gamma(t) = 0. \tag{3.6}$$

(1) Solutions of $U(x)$ are given using $\sin(n\pi x/L)$, where $\lambda_n = (n\pi/L)^2$ and $n = 1, 2, 3, \ldots$. By the superposition principle, a general solution or an arbitrary wave form with the same boundary condition is given by

$$U(x) = \sum_{m=0}^{\infty} a_m \sin mx. \tag{3.7}$$

(2) The solution of the time part, $\Gamma(t)$, for a given λ_n is

$$\Gamma_n(t) = C_n \sin\left[\left(\frac{n\pi}{L} v\right) t + \delta_n\right].$$

(3) $u(x, t) = U(x)\Gamma(t)$ is given by

$$u(x,t) = \sum_{n=1} a_n C_n \sin(\frac{n\pi v}{L} t + \delta_n) \sin(\frac{n\pi}{L} x) = \sum_{n=1} A_n(t) \sin(\frac{n\pi}{L} x) \tag{3.8}$$

where $A_n(t) = a_n C_n \sin(\frac{n\pi v}{L} t + \delta_n)$ is the time-varying amplitude of the n^{th} standing wave.

3.3 FOURIER THEOREM

Equation 3.7 can also be interpreted in such a way that an arbitrary form of oscillation $u(x, t)$ on a string of fixed ends is the superposition of discrete standing waves or oscillation modes [6, 7]. Assume an observed wave pattern on a string of length $2L$ ($-L \le x \le +L$) at a certain time is given as shown in Figure 3.7, where $L = 1$. This wave contains five modes of standing waves,

$$f(x) = \sin(\pi x) + 0.5\sin(2\pi x) - 0.2\sin(3\pi x) + 0.4\sin(4\pi x) - 0.1\sin(5\pi x).$$

Is it possible to find the frequencies and amplitudes that constitute a given wave pattern? More generally, would it be possible to express an arbitrary function $f(\xi)$, where the variable ξ is a spatial coordinate or time, as a series of sinusoidal functions? This is called the Fourier series of $f(\xi)$. Because the sinusoidal functions are well known and are easy to apply, the Fourier series is valuable for analyzing periodic motions.

The Fourier series can be constructed in the following way. An arbitrary periodic function $f(x)$ in the interval $[-L, +L]$ can be expressed by a series expansion of trigonometric functions.

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_k \cos\left(\frac{n\pi}{L} x\right) + \sum_{n=1}^{\infty} b_k \sin\left(\frac{n\pi}{L} x\right) \tag{3.9}$$

where

$$a_m = \frac{1}{L} \int_{-L}^{L} f(x) \cos\left(\frac{m\pi}{L} x\right) dx \text{ and } b_m = \frac{1}{L} \int_{-L}^{L} f(x) \sin\left(\frac{m\pi}{L} x\right) dx. \tag{3.10}$$

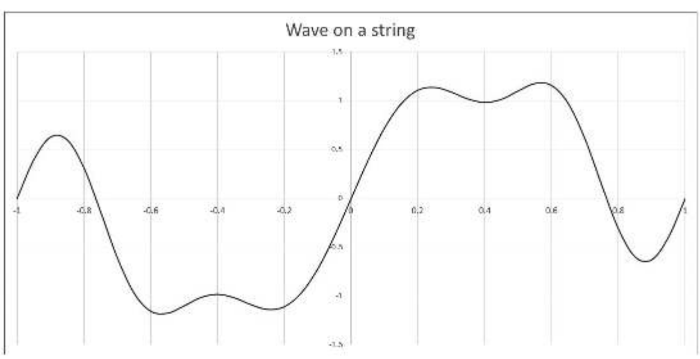


FIGURE 3.7 An observed wave on string.

The Fourier coefficients are calculated using the orthogonal property of sinusoidal functions. Refer to Section 6.1.2 for the orthogonal property.

Using the inner product, ⟨ ... | ... ⟩, defined by Equation 1.17, we obtain

$$\langle \cos(mx) | \cos(nx) \rangle = \int_{-L}^{L} \cos(mx)\cos(nx)dt = 0; \qquad (m \neq n)$$

$$\langle \sin(mx) | \sin(nx) \rangle = \int_{-L}^{L} \sin(mx)\sin(nx)dt = 0; \qquad (m \neq n)$$

and

$$\langle \cos(mx) | \sin(nx) \rangle = \int_{-L}^{L} \cos(mx)\sin(nx)dt = 0. \qquad \text{(including m = n)} \tag{3.11}$$

Depending on the symmetric property of the original periodic function $f(x)$, a Fourier series may have only sine terms or cosine terms. If the function $f(x)$ is an *even* function in the interval $[-L, +L]$, the sine terms must be excluded, and the Fourier series has only cosine terms,

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_k \cos\left(\frac{n\pi}{L} x\right). \tag{3.12}$$

Similarly, if the periodic function $f(x)$ is an *odd* function in the interval $[-L, +L]$, the Fourier series has only sine terms,

$$f(x) = \sum_{n=1}^{\infty} b_k \sin\left(\frac{n\pi}{L} x\right). \tag{3.13}$$

We can also use the periodicity of time. A periodic function $f(t)$ of period T ($-T/2 < t \leq +T/2$) can be expressed by a Fourier series,

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\omega_0 t) + \sum_{n=1}^{\infty} b_n \sin(n\omega_0 t) \tag{3.14}$$

where $\omega_0 = 2\pi/T$ is the angular frequency of the fundamental mode, and the Fourier coefficients a_m and b_m are given by

$$a_m = \frac{2}{T}\int_{--T/2}^{T/2} f(t)\cos(m\omega_0 t)dt \text{ and } b_m = \frac{2}{T}\int_{-T/2}^{+T/2} f(t)\sin(m\omega_0 t)dt. \tag{3.15}$$

Additionally, we can obtain a Fourier series in a complex exponential form. By applying Euler's formula, $e^{i\theta} = \cos\theta + i \sin\theta$, the Fourier series of complex variables are

$$f(t) = \sum_{n=-\infty}^{n=+\infty} c_n e^{in\omega_0 t} \tag{3.16}$$

where the complex Fourier coefficient is given by

$$c_n = \frac{1}{T}\int_{-T/2}^{+T/2} f(\tau)e^{-in\omega_0 t}\,d\tau. \tag{3.17}$$

The complex Fourier coefficient represents the magnitude of the frequency component and the phase.

What if we only know the numerical data of the unknown function $f(x)$? What if the function is non-periodic? Numerical calculations of the integrals to find the coefficients a_n and b_n seem to be very time-consuming computational tasks. To overcome the computational difficulty, we can apply another mathematical theory, which is an extension of the Fourier series, called the Fourier transform. Also, a fast computational algorithm of the Fourier transform called the fast Fourier transform (FFT) has been widely used for numerical computation. For the basic idea of Fourier transform, refer to Section 3.6.1. For detailed discussions on FFT, refer to other books [8].

3.4 DOPPLER EFFECT AND SHOCKWAVE

3.4.1 Doppler Effect

When a sound source is moving to one direction, e.g., to the right, the center of each new wavefront is moved to the right direction. As a result, the wavefronts begin to bunch up on the right side (in front) and spread further apart on the left (behind) of the source. As a result, an observer at rest on the right side will hear a higher pitch sound when the sound source is approaching the observer and a lower pitch sound when the sound source is moving away from the observer. If the observer is also moving at a velocity, the following frequency change will be observed:

$$f_{obs} = f_{souce}\frac{v_{sound} + v_{observer}}{v_{sound} - v_{source}} \tag{3.18}$$

where $v_{\mathrm{observer}} > 0$ if the observer is approaching the sound source and $v_{\mathrm{souce}} > 0$ if the sound source is approaching the observer. For a detailed explanation, refer to a standard education material [9].

Figure 3.8 lists a VBA code to generate wave patterns as the sound source approaches a stationary observer. At a given time, a circle of the wavefront is calculated. The wave speed is 10 m/s and the source speed is 8 m/s (Mac = $v_{\mathrm{source}}/v_{\mathrm{sound}}$ = 0.8)

At $t = 0$, a circle is drawn using the calculated values of `xw` and `yw` in the VBA code. The successive circles at later times are added to the one at $t = 0$. Figure 3.9 shows the schematic diagram of the final result.

3.4.2 Relativistic Doppler Effect

A general physics course may briefly mention the relativistic Doppler effect by pointing out a resemblance to the acoustic Doppler effect. However, its quantitative discussion is seldom found in an introductory physics textbook, and it may be helpful to be aware of the relativistic effect [10, 11].

```
Sub Doppler()
Cells(1, 1) = "Wave pattern of Doppler effect"
Dim x(6)                                    'Position of the source.
Dim rw(6)                                   'Wave propagation from the source.
Dim xw(37)                                  'x-coordinate of the wave front.
Dim yw(37)                                  'y-coordinate of the wave front.
  Cells(2, 2) = "Wave speed v": v = 10: Cells(3, 2) = v
  Cells(2, 4) = "Mac": Mac = 2: Cells(3, 4) = Mac
  Cells(2, 6) = "Source speed u": u = v * Mac: C ells(3, 6) = u
  h = 1                                     'Time increment.
  n = 5                                     'n*h is the total time interval.
'Initialization:
t = 0
  For i = 0 To n
    x(i) = 0: rw(i) = 0
  Next i
    For j = 0 To 36
      xw(j) = 0: yw(j) = 0
    Next j
'Positions of generating circular waves:
  For i = 0 To 5                                ' i*h is time increment.
    x(i) = i * h * u                            'Position of the source at time i*h.
  Next i
Cells(5, 1) = "Time="
Cells(6, 1) = "Source at"
  For i = 0 To 5
  Cells(6, 2 + 2 * i) = "(x"
  Cells(6, 3 + 2 * i) = "y)"
    Cells(7, 2 + 2 * i) = x(i)
    Cells(7, 3 + 2 * i) = 0
    Cells(8, 2 + 2 * i) = 0
    Cells(8, 3 + 2 * i) = 0
  Next i
'Time development of wave patterns:
 For i = 0 To n                                   'time interval i*h
  Cells(5, 2 + 2 * i) = t
  Cells(9, 2 + 2 * i) = "xw": Cells(9, 3 + 2 * i) = "yw"
  For j = 0 To 5
    rw(j) = (n - j) * h * v                       'Wave front circle at a given time.

      For k = 0 To 36                             'Define 36 points on a circle.
        theta = 2 * 3.14 * k / 36                 'Angle at each point on a circle
          xw(j) = x(j) + rw(j) * Cos(theta)       'x value of the circular wave.

          yw(j) = rw(j) * Sin(theta)              'y value of the circular wave.
            Cells(10 + k, 2 + 2 * j) = xw(j)
            Cells(10 + k, 3 + 2 * j) = yw(j)
      Next k
  Next j
 Next i
End Sub
```

FIGURE 3.8 VBA code for visualizing the Doppler effect.

Define a sine plane wave as observed in a frame S,

$$\sin(\vec{k}\cdot\vec{r}-\omega t)=\sin(k_x x+k_y y+k_z z-\omega t) \text{ where } \omega = ck. \tag{3.19}$$

Let $\breve{n}$ be the unit vector of the wave number vector $\vec{k}$ and $\vec{k}=k\breve{n}=(\omega/c)\breve{n}$. Assume there is another frame S' moving at velocity $\vec{v}$ with respect to frame S. The Lorentz transform of the wave number vector has exactly the same form as the position vector. That is,

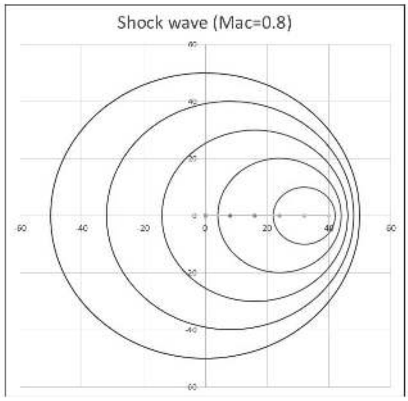


FIGURE 3.9 The Doppler effect.

$$k' = \frac{k - \dfrac{\omega v}{c^2}}{\sqrt{1-\beta^2}} \text{ and thus, } \omega' = ck' = \frac{ck - \dfrac{\omega v}{c}}{\sqrt{1-\beta^2}} = \frac{\omega - kv}{\sqrt{1-\beta^2}} = \omega\frac{1-(\breve{n}\cdot\vec{v}/c)}{\sqrt{1-\beta^2}} \text{ where } \beta = v/c. \tag{3.20}$$

where k is the wave number as observed in frame S, and k' is the wave number emitted from frame S'. Thus, the velocity dependence of the angular frequency is directional.

1) If $\breve{n}$ is parallel to $\vec{v}$, then

$$\omega' = \omega\frac{1-v/c}{\sqrt{1-\beta^2}} = \omega\sqrt{\frac{1-\beta}{1+\beta}} \text{ or } \frac{\omega}{\omega'} = \sqrt{\frac{1+\beta}{1-\beta}} \tag{3.21}$$

where ω is the angular frequency as observed in frame S and ω' is the angular frequency as observed in frame S' which is moving in the direction $\breve{n}$ with respect to frame S. Figure 3.10 shows the longitudinal Doppler effect where frame S' is approaching frame S, and moving away from frame S.

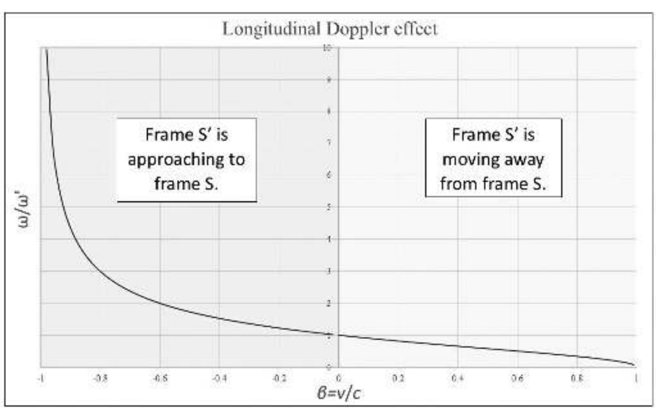


FIGURE 3.10 The Longitudinal Doppler effect.

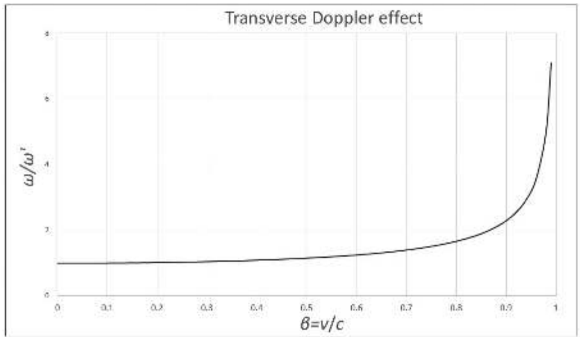


FIGURE 3.11 The Transverse Doppler effect.

2) If $\check{n}$ is perpendicular to $\vec{v}$, then we obtain $\omega = \omega'\sqrt{1-\beta^2}$. Figure 3.11 shows the velocity dependence of the ratio ω'/ω. This velocity dependence is called the transverse Doppler effect. The transverse Doppler effect is unique and not observed in the acoustic Doppler effect. For the transverse Doppler effect, $\omega < \omega'$, i.e., $\lambda > \lambda'$, which is called redshift [12]

3.4.3 Shockwave

When the speed of a wave source exceeds the speed of the generated wave, the wavefronts lag behind the wave source, forming a cone-shaped region with the source at the vertex [13]. The front edge of the cone forms a supersonic wave within which sound energy is confined. In Figure 3.12, $Mac = v_{soruce}/v_{sound} = 20/10 = 2.0$, and the vertex is at $x = 100$.

Note: *Cherenkov radiation and muon detector*. One of the interesting shockwave phenomena is the Cherenkov radiation [14, 15]. The relativistic theory states that the speed of light in a vacuum is constant c, while in media of the index of refraction n, the speed of light is given by $c/n < c$. For example, the propagation speed in water is only $0.75c$. Particles can be accelerated by nuclear reactions or particle accelerators to exceed the propagation speed in the medium (although never exceeding the speed of light c in a vacuum). Cherenkov

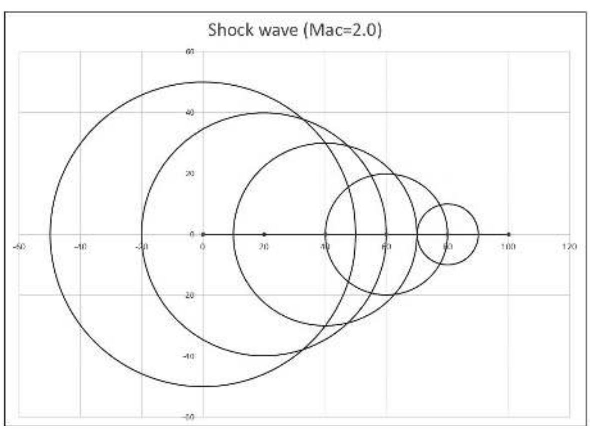


FIGURE 3.12 Wavefronts of shockwave.

radiation is emitted when a charged particle passes through a (non-insulating) dielectric material at a speed faster than the speed of light in that medium.

When a charged particle passes through such a medium, the local electromagnetic field in the material is disturbed. Electrons in the atoms of the medium are moved and polarized by the passing charged particle's field. When the electrons return to equilibrium states after the field disturbance has passed, photons are emitted (in conductors, they return to equilibrium without emitting photons). In a normal case, the photons interfere destructively and no radiation is detected. However, when the field disturbance propagates faster than the speed of light in the material, the photons interfere constructively and the observed radiation is amplified.

Cherenkov radiation is often compared to the shockwave. As shown in Figure 3.12, the sound waves generated by a supersonic object cannot leave the object itself because they do not have enough speed. Thus, the sound waves accumulate, and a shock front is formed. In the same way, a charged particle also generates a shockwave of photons as it passes through a medium.

Figure 3.13 depicts the directions of particle motion and its shockwave. In the diagram, a particle passes through a medium with a velocity v. If n is the refractive index of the material, the propagation speed of the emitted electromagnetic wave is $v_{em} = c/n$. The left vertex of the triangle represents the position of the particle at an initial time ($t = 0$). The right vertex represents the position of the particle at a certain time t. For a certain t, the distance traveled by the particle is $x_p = v_p t$, and the distance traveled by the radiated electromagnetic wave is $x_{em} = (c/n)t$. Therefore, the radiation angle is $\cos\theta = x_{em}/x_{p.}$

It is interesting to know that a neutrino detector catches the Cherenkov radiation [16]. When a charged particle fired by a neutrino travels through water with a speed faster than that of light, the Cherenkov radiation is emitted. The emitted Cherenkov radiation forms a cone shape in the direction of the charged particle's movement as shown in Figure 3.10. Photomultiplier tubes attached to the wall of the water tank capture this Cherenkov radiation. The photomultiplier tubes provide information about the amount of radiation received and the time at which it was received. Based on this, the energy, direction, position, and type of the charged particle are determined. The Super-Kamiokande experiment detects neutrinos using a huge water tank equipped with approximately 13,000 photomultiplier tubes (11,129 in the inner tank and 1,885 in the outer tank) [17].

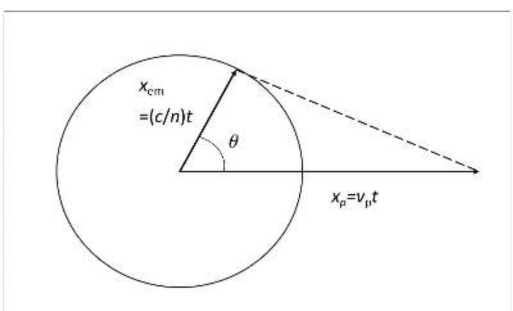


FIGURE 3.13 The direction of a shockwave (Cherenkov radiation).

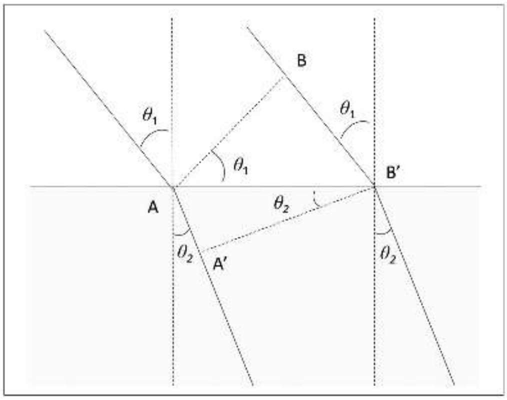


FIGURE 3.14 Refraction of light across two different media.

3.5 REFRACTION

3.5.1 Huygens's Principle

As shown in Figure 3.14, when the incident wavefront just reaches the interface at point A, point B is still well within medium 1. In the time Δt it takes for a wavelet to travel from B to B′ on the interface at speed $v_1 = c/n_1$, a wavelet from A travels into medium 2 at a distance of AA' = $v_2\Delta t$, where $v_2 = c/n_2$ and c is the speed of light in a vacuum and n_1 and n_2 are indices of refraction in the respective medium. Notice

$$\overline{AB'} = \frac{\overline{BB'}}{\sin\theta_1} = \frac{\overline{AA'}}{\sin\theta_2}, \text{ and } \overline{AB'} = \frac{(c/n_2)\Delta t}{\sin\theta_1} = \frac{(c/n_1)\Delta t}{\sin\theta_2}. \tag{3.22}$$

In this way, we obtain Snell's law: $n_1\sin\theta_1 = n_2\sin\theta_2$. To confirm Snell's' law, one may use

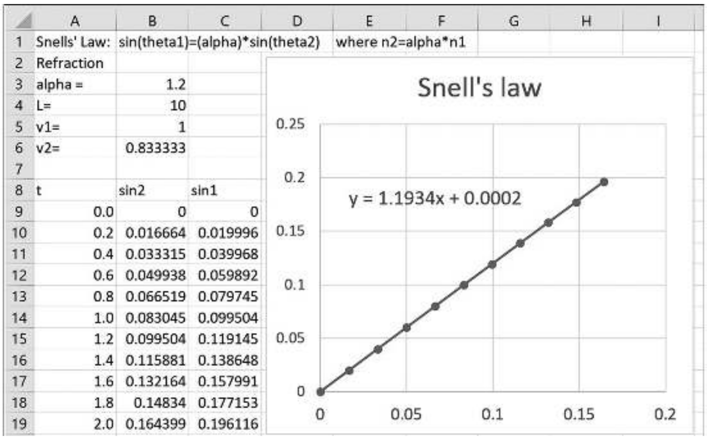
$$\sin\theta_1 = \frac{\overline{BB'}}{\overline{AB'}} = \frac{v_1\Delta t}{\sqrt{L^2+(v_1\Delta t)^2}} \text{ and } \sin\theta_2 = \frac{\overline{AA'}}{\overline{AB'}} = \frac{v_2\Delta t}{\sqrt{L^2+(v_1\Delta t)^2}} = \frac{(v_1/\alpha)\Delta t}{\sqrt{L^2+(v_1\Delta t)^2}} \tag{3.23}$$

where AB = L and $\alpha = n_2/n_1$. Figure 3.15 shows the calculation for sine values at different Δ-values using $v_1 = 1$, $L = 1$, and $\alpha = 1.2$. The slope of the graph is the index of refraction n_2, which is the same as the assumed α-value.

3.5.2 Principle of Least Traveling Time

Figure 3.16 depicts an optical path across the interface between the two different media. The traveling time from point A (0, 0) to point B (l, m) via point M (a, y) on the interface is given by

$$\tau = \frac{\sqrt{a^2+y^2}}{v_1} + \frac{\sqrt{b^2+(l-y)^2}}{v_2}. \tag{3.24}$$



	A	B	C
1	Snells' Law:	sin(theta1)=(alpha)*sin(theta2)	where n2=alpha*n1
2	Refraction		
3	alpha =	1.2	
4	L=	10	
5	v1=	1	
6	v2=	0.833333	
7			
8	t	sin2	sin1
9	0.0	0	0
10	0.2	0.016664	0.019996
11	0.4	0.033315	0.039968
12	0.6	0.049938	0.059892
13	0.8	0.066519	0.079745
14	1.0	0.083045	0.099504
15	1.2	0.099504	0.119145
16	1.4	0.115881	0.138648
17	1.6	0.132164	0.157991
18	1.8	0.14834	0.177153
19	2.0	0.164399	0.196116

FIGURE 3.15 Snell's law.

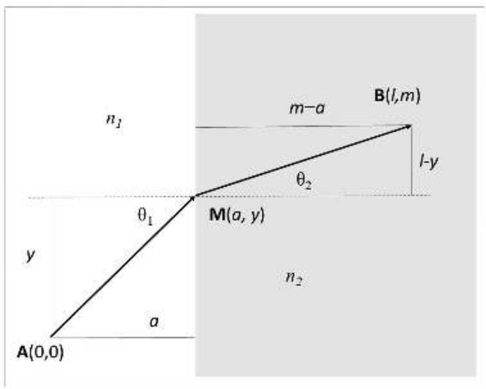


FIGURE 3.16 Optical path while being refracted.

The least traveling time should satisfy

$$\frac{d\tau}{dx} = 0 = \frac{y}{v_1\sqrt{a_2 + y^2}} - \frac{\ell - y}{v_2\sqrt{b^2 + (\ell - y)^2}}. \tag{3.25}$$

Referring to the geometry of Figure 3.14, the incident and the refracted angles satisfy

$$\frac{y}{\sqrt{a^2 + y^2}} = \sin\theta_1 \text{ and } \frac{\ell - y}{v_2\sqrt{b^2 + (\ell - y)^2}} = \sin\theta_2. \tag{3.26}$$

Therefore, the condition of the least traveling time becomes

$$\frac{d\tau}{dx} = \frac{\sin\theta_1}{v_1} - \frac{\sin\theta_2}{v_2} = 0. \tag{3.27}$$

Because $v_1 = c/n_1$ and $v_2 = c/n_2$, Equation 3.24 yields to Snell's law: $n_1 \sin\theta_1 = n_2 \sin\theta_2$. For determining the optical path using Excel's Solver, refer to [18].

3.5.3 Particle Model

With the particle model of light, the law of refraction is a consequence of the conservation laws of momentum and energy. Consider that a particle of mass m goes across the interface. Referring to Figure 3.13, the momentum component along the interface is conserved: $mv_1\sin\theta_1 = mv_2\sin\theta_2$. If the total energy of the particle is only the kinetic energy, $(1/2)mv_1^2 = (1/2)mv_2^2$ by the energy conservation value. Combining both conservation laws, we obtain $n_2\sin\theta_1 = n_1\sin\theta_2$, but this is not Snell's law! In fact, this discrepancy was one of the reasons for the failure of the particle model of light, and Huygens's principle is better equipped to support the wave model of light. We need to carefully reconsider the "velocity of light particle."

Because the particle is a photon, the energy of the particle in each medium is given by $E_i = p_i c = p_i(c/n_i)$, where c is the speed of light in a vacuum, and in E_i and p_i, $i = 1, 2$, are relativistic energy and momentum of the respective medium [19]. The conservation of momentum,

$$p_1\sin\theta_1 = p_2\sin\theta_2 \text{ becomes } (n_1/cE_1)\sin\theta_1 = (n_2/cE_2)\sin\theta_2, \tag{3.28}$$

which gives Snell's law because $E_1 = E_2$. Alternatively, De Broglie wavelength, $\lambda = h/p$, can also be applied, where h is the Planck's constant.

$$p_1 \sin\theta_1 = p_2 \sin\theta_2 \text{ becomes } (h/m\lambda_1)\sin\theta_1 = (h/m\lambda_2)\sin\theta_2. \tag{3.29}$$

Because $\lambda_i = v_i/f_i = c/(n_i f_i)$, $i = 1, 2$, but $f_1=f_2$, the de Broglie wavelength can also derive Snell's law.

3.6 DIFFRACTION

3.6.1 Fourier Transform

We apply the Fourier transform to spectral analysis where we want to decompose a time-varying signal to its frequency components to acquire the spectrum of the signal [20]. The Fourier transform of a function $f(t)$ constitutes a pair of integrals:

$$F(\omega) = \int_{-\infty}^{+\infty} f(t)e^{-i\omega t}dt \text{ and } f(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} F(\omega)e^{i\omega t}d\omega. \tag{3.30}$$

The second integral of the above pair is called the inverse Fourier transform. Equations 3.16 are applied to analyses of signals of mechanics, acoustics, and electromagnetism. Here, let us acquire the energy spectrum of the damped oscillation that we discussed in Section 2.1. We use a simplified version of Equation 2.7 as a displacement of a damping oscillation of angular frequency ω_0.

$$x(t) = e^{-kt}\sin\omega_0 t, \text{ where the damping factor is 2k.} \tag{3.31}$$

The Fourier transform of Equation 3.31 is

$$X(\omega)=\int_{-\infty}^{+\infty}x(t)e^{-i\omega t}dt=\int_{0}^{+\infty}(e^{-kt}\sin\omega_0 t)e^{-i\omega t}dt=\frac{1}{2i}\int_{0}^{+\infty}e^{-kt}(e^{i\omega_0 t}-e^{-i\omega_0 t})e^{-i\omega t}dt$$
$$=\frac{1}{2i}\left[\frac{1}{k-i(\omega-\omega_0)}+\frac{1}{k+i(\omega+\omega_0)}\right]=\frac{1}{2}\left[\frac{1}{(\omega-\omega_0)+ik}-\frac{1}{(\omega+\omega_0)-ik}\right]. \tag{3.32}$$

Assume that the damping is very slow and k/ω_0 <<1. Then

$$X(\omega)\approx\frac{1}{2}\left[\frac{1}{(\omega-\omega_0)+ik}\right]\text{ when }\omega\approx\omega_0,\text{ and }\left|X(\omega)\right|^2\approx\frac{1}{4\left[(\omega-\omega_0)^2+k^2\right]}. \tag{3.33}$$

Figure 3.17 shows the beginning part of Excel's spreadsheet of calculating $|X(f)|^2$ of $x(t)$ = $e^{-t}\sin(20\pi t)$. The total number of data is N = 1024. The sampling time interval is set to 10^{-3} s, and the frequency resolution is 1000/N = 0.9766 Hz. Figure 3.18 shows the calculated $x(t)$ and $|X(f)|^2$.

Remark: Excel has a built-in Fourier transform. To use it, an *Add-in* option, *Analysis ToolPak*, must be installed. Refer to Appendix A1.2 for installing the option.

Mathematically, the Fourier transform connects two different variable spaces that are canonically conjugate. For example, the coordinate $\{q\}$ and the momentum $\{p\}$ (or the wave vector $\{k\}$) are canonically conjugates. The Fourier transform of a function $f(x)$ constitutes a pair of the following integrals.

	A	B	C	D	E	F	G
1	Data no.	Time (s)	Data	FFT	Freq (Hz)	|X|	|X|^2
2	0	0	0	15.2774914968487	0	15.2774915	233.401746
3	1	0.001	0.062728	15.4244109679968-0.611493127633584i	0.9766	15.4365274	238.286378
4	2	0.002	0.125083	15.8823911470968-1.2623027900403i	1.9532	15.9324749	253.843757
5	3	0.003	0.18682	16.7083954792871-2.00058583187578i	2.9298	16.8277397	283.172823
6	4	0.004	0.247697	18.0182955763862-2.89667698773015i	3.9064	18.2496497	333.049713
7	5	0.005	0.307476	20.0333194619014-4.0697881196539i	4.883	20.4425308	417.897064
8	6	0.006	0.365922	23.1948075781147-5.75320562614962i	5.8596	23.8976667	571.098474

FIGURE 3.17 The Fourier transform of damped oscillation.

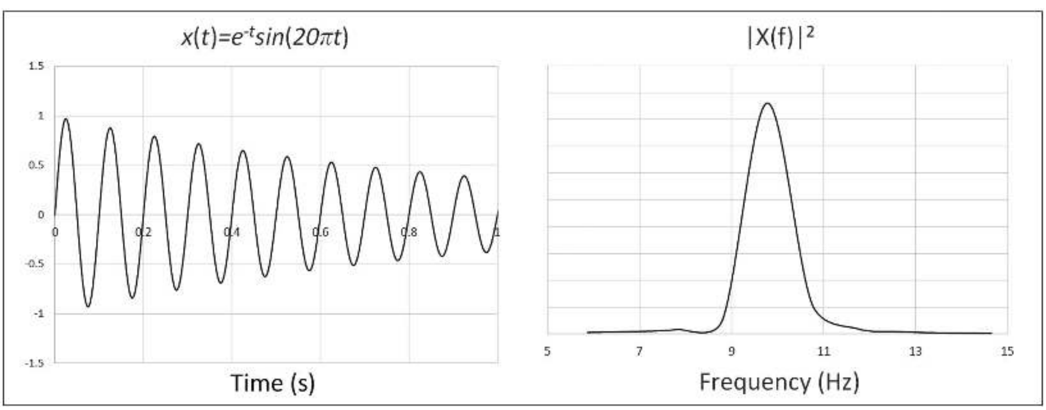


FIGURE 3.18 Damping oscillation and its power spectrum.

$$F(k)=\int_{-\infty}^{+\infty} f(x)e^{-ikx}dx \text{ and its inverse Fourier transform } f(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} F(k)e^{ikx}dk. \quad (3.34)$$

Equation 3.34 is used in wave optics and quantum mechanics.

3.6.2 Diffraction pattern

Diffraction phenomena are the best representation of what a wave is. Any wave exhibits its diffraction. Huygens's principle explains that diffraction through a small aperture is a superposition of the secondary waves from each point on the aperture. Figure 3.19 illustrates a schematic diagram of observing two-dimensional diffraction. In this figure, the amplitude of a diffraction pattern observed at point $P(X, Y)$ on the screen is given by the two-dimensional integral of the spherical wave over the aperture:

$$U_P(X,Y)=\int_{apature}\frac{C\exp(ikr)}{i\lambda r}g(x,y)dxdy \quad (3.35)$$

where C is a constant, r is the distance from a point inside the aperture to the observing point on the screen, $g(x, y)$ is called the aperture function, where $g(x, y) = 1$ if a point (x, y) on the screen is inside the aperture and 0 otherwise. The integral element of $dxdy$ is the area element of the aperture.

The aperture size is comparable to the wavelength for diffraction, and the distance from the light source to the aperture plane is very long, and the distance from the aperture to the observation screen – denoted as R – is also much larger than the aperture size. Under this circumstance, the incident and diffracted spherical waves have negligible curvatures. The angular spread of the diffracted light is small, and we can regard both the incident and diffracted waves as *plane waves*. This is called the Fraunhofer diffraction, and Equation (3.35) becomes

$$U_P(X,Y)=\frac{C}{i\lambda R}\int_{apature} g(x,y)\exp(ikr)dxdy. \quad (3.36)$$

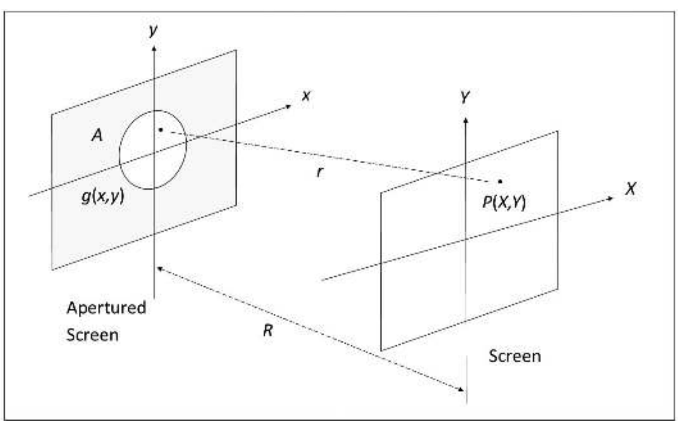


FIGURE 3.19 Schematic diagram of two-dimensional diffraction.

Now, we apply the "Fresnel approximation" to Equation 3.36. Because *R* in Figure 3.17 is considerably large it is denoted as (*x*–*X*) and (*y*–*Y*), and the distance *r* can be approximated to be

$$r=\sqrt{R^2+(x-X)^2+(y-Y)^2}=R\sqrt{1+\frac{(x-X)^2+(y-Y)^2}{R^2}}$$
$$\approx R+\frac{1}{2R}\left[(x-X)^2+(y-Y)^2\right]=R+\frac{1}{2R}\left[(x^2+y^2)+(X^2+Y^2)\right]-\frac{1}{R}(xX+yY). \tag{3.37}$$

Furthermore, because the aperture size is very small, we may drop the term (x^2+y^2) from Equation (3.37) to get

$$r=R+\frac{1}{2R}\left[(X^2+Y^2)\right]-\frac{1}{R}(xX+yY), \tag{3.38}$$

whence the diffraction pattern U_P becomes

$$U_P(X,Y)=\frac{C}{i\lambda R}e^{ikR}e^{i\frac{k}{2R}(X^2+Y^2)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}g(x,y)\exp\left[-\frac{ik}{R}\left(xX+yY\right)\right]dxdy$$
$$=C'\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}g(x,y)\exp\left[-\frac{ik}{R}\left(xX+yY\right)\right]dxdy \tag{3.39}$$

where $C'=\left(C/i\lambda R\right)e^{ikR}e^{i\frac{k}{2R}(X^2+Y^2)}$. Equation 3.39 indicates that the diffraction pattern, U_p, is the two-dimensional Fourier transform of the geometrical shape of the aperture function $g(x, y)$.

Remark: If $g(x, y) = g_x(x)g_y(y)$, then the two-dimensional Fourier transform becomes a product of two independent one-dimensional Fourier transforms. The two-dimensional FFT is separated into each component. Unfortunately, Excel does not have a built-in two-dimensional FFT, but it is not difficult to make a VBA code [8].

3.6.3 Rectangular Aperture

If the aperture is a rectangle of size D_x by D_y, $g(x, y) = 1$ if $-D_x/2 \le x \le D_x/2$ and $-D_y/2 \le y \le D_y/s$; it is otherwise, 0. The integral of the diffraction pattern $U_P(X, Y)$ can be calculated easily to obtain

$$U_P(x_s,y_s)=C'\int_{-D_x/2}^{D_x/2}\int_{-D_y/2}^{Dy/2}\exp\left[-\frac{ik}{R}\left(xX+yY\right)\right]dxdy$$
$$=C'D_xD_y\frac{\sin\left(\frac{kD_x}{2R}X\right)}{\left(\frac{kD_x}{2R}\right)X}\cdot\frac{\sin\left(\frac{kD_y}{2R}Y\right)}{\left(\frac{kD_y}{2R}\right)Y}. \tag{3.40}$$

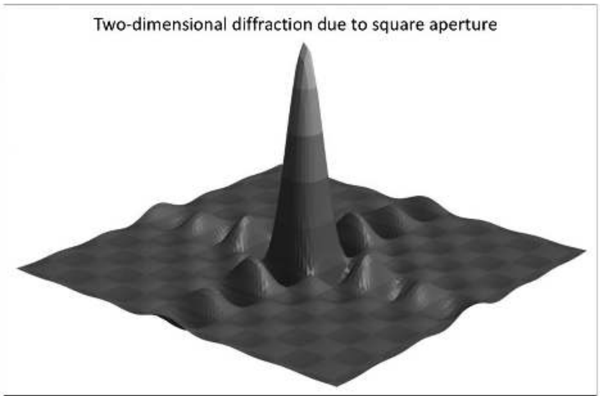


FIGURE 3.20 Diffraction pattern due to a square aperture.

Figure 3.20 shows the intensity of the diffraction pattern through a square aperture, where $C' = 1$, $D_x = D_y = 1$, and $k/2R = 1$. The procedure to create the diffraction pattern is similar to that of Figure 3.3. In order to avoid the singular pit $X = Y = 0$, we select the range of X and Y to be $-20.1 \le X$ (and Y) $\le +19.9$ with increments of 0.5. Excel's *AutoFill* and *3-D Surface* chart options are used.

SUGGESTED FURTHER STUDY

There are excellent articles and books on periodic motions [21, 22]. The author recommends that everyone read these books and a series of OpenCourseWare by MIT. The Fourier transform is a valuable mathematics tool for various physics subjects including spectral analysis and optics [6–8].

REFERENCES

1. *Wave and Wave Equations*: Brown University. https://www.brown.edu/research/labs/mittleman/sites/brown.edu.research.labs.mittleman/files/uploads/lecture02_0.pdf.
2. Nation J, *Superposition Principle*, Georgia Institute of Technology, 2024. https://www.physicsbook.gatech.edu/Superposition_Principle.
3. Moebs W, Ling SJ, and Sanny J, *Wave Interaction: Superposition and Interference*, Open Stax, University Physics Vol 1: Rice University, 2021. https://openstax.org/books/physics/pages/13-3-wave-interaction-superposition-and-interference.
4. Zhabinskaya D, *Beats*. https://phys.libretexts.org/Courses/University_of_California_Davis/UCD%3A_Physics_7C_-_General_Physics/8%3A_Waves/8.6%3A_Beats.
5. Moebs W, Ling SJ, and Sanny J, *Wave Interaction: Superposition and Interference*, Open Stax, University Physics Vol 1: Rice University, 2021. https://openstax.org/books/physics/pages/16-6-standingwaves and resonance.
6. Zhabinskaya D, *Fourier Series and Integrals*, MIT mathematics. https://phys.libretexts.org/Courses/University_of_California_Davis/UCD%3A_Physics_7C_-_General_Physics/8%3A_Waves/8.6%3A_Beats.
7. Morin D, *Fourier Analysis*, Scholars at Harvard, 2009. https://scholar.harvard.edu/files/david-morin/files/waves_fourier.pdf.
8. Cho S, *Fourier Transform and Its Applications Using Microsoft Excel® Second Edition*, IOP Publishing, Inc., 2023.

9. Zhabinskaya D, *Doppler Effect*. https://phys.libretexts.org/Courses/University_of_California_Davis/UCD%3A_Physics_7C_-_General_Physics/8%3A_Waves/8.4%3A_Doppler_Effect.
10. Jackson JD, *Classical Electrodynamics*, John Wiley & Sons, Inc., 1999. https://archive.org/details/john-david-jackson-classical-electrodynamics-wiley-1999.
11. Bettex M, *Explained: The Doppler effect*, MIT News, 2010. https://news.mit.edu/2010/explained-doppler-0803\.
12. Howell B and Dobrijevic D, *Redshift and Blueshift: What Do They Mean?*, SPACE.com, 2023. https://www.space.com/25732-redshift-blueshift.html.
13. Elert G, *Shock Waves*, The Physics Hypertextbook, 2004. https://physics.info/shock/.
14. Alaeian H, *An Introduction to Cherenkov Radiation*, Stanford University, 2014. http://large.stanford.edu/courses/2014/ph241/alaeian2/.
15. Cherenkov Radiation, Explained, *Department of Energy* [Blog]. https://www.energy.gov/ne/articles/cherenkov-radiation-explained.
16. Scholberg K, *Supernova Neutrino Detection in Water Cherenkov Detectors*, Journal of Physics Conference Series 309 (2011), IOP Publishing. https://www.energy.gov/ne/articles/cherenkov-radiation-explained.
17. Suzuki, Y, *The Super-Kamiokande Experiment*, 2019. https://link.springer.com/article/10.1140/epjc/s10052-019-6796-2.
18. Cho S, *Numerical Calculation for Physics Laboratory Projects Using Microsoft Excel®*, IOP Publishing, Inc., 2019.
19. Drosdoff D and Widom A, *Snell's Law from an Elementary Particle Viewpoint*, Northeastern University, 2005. https://arxiv.org/pdf/physics/0502054.
20. FFT Spectrum Analysis (Fast Fourier Transform), *Dewesoft*. https://training.dewesoft.com/online/course/fft-spectral-analysis.
21. Georgi H, *The Physics of Waves*, MIT OpenCourseWare, 1993. https://ocw.mit.edu/courses/8-03sc-physics-iii-vibrations-and-waves-fall-2016/ef731c1b91d77a6db003f6c27e300d25_MIT8_03SCF16_Textbook.pdf.
22. Crawford FS, *Waves* (Berkeley Physics Course, Vol. 3), McGraw-Hill, 1968.

Electromagnetism

After reviewing vector algebra, we start with time-independent Maxwell's equations to discuss the electric potential and the electric field, as well as vector potential and magnetic field. Although computation of EM fields by solving Poisson's equation requires a complicated algorithm, Excel offers an option for "iterative calculation," which allows us to compute EM fields in relatively simple boundary conditions without programming. From time-dependent Maxwell's equations in free space, we derive wave equations of E-field and B-field. Huygens's principle and Snell's law of refraction can be naturally derived from these EM fields. Alternative approaches to the law of refraction are also discussed.

4.1 VECTOR ALGEBRA

Here are the formulas for the addition of two vectors and scalar and vector products. Let $\vec{a} = (a_x, a_y, a_z)$ and $\vec{b} = (b_x, b_y, b_z)$. Vector sum/subtraction is given by

$$\vec{a} \pm \vec{b} = (a_x \pm b_x, a_y \pm b_y, a_z \pm b_z);$$

the scalar product is

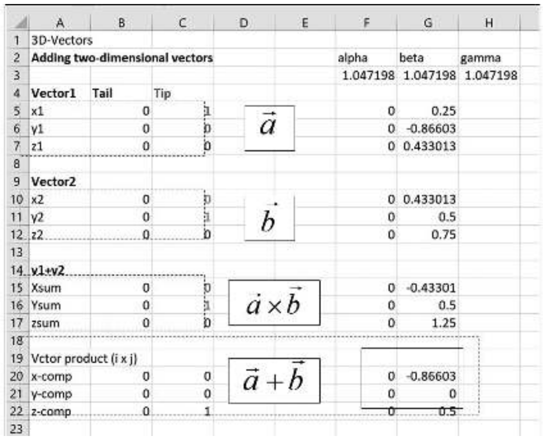
$$\vec{a} \cdot \vec{b} = (a_x b_x + a_y b_y + a_z b_z); \text{ and}$$

the three components of the vector product, $\vec{a} \times \vec{b}$, are

$$\left(\vec{a} \times \vec{b}\right)_x = a_y b_z - a_z b_y, \left(\vec{a} \times \vec{b}\right)_y = a_z b_x - a_x b_z, \text{ and } \left(\vec{a} \times \vec{b}\right)_z = a_x b_y - a_y b_z.$$

These numerical results may be shown with three-dimensional graphs created by applying the Euler angles. For given vectors, a spreadsheet of Excel can be used to calculate these components of vector sums and vector products as shown in Figure 4.1. For the vector addition, $\vec{a} = (1, 0, 4)$ and $\vec{b} = (0, 2, 0)$ are used. For the vector product, unit vectors $\vec{i} = (1,0,0)$ and $\vec{j} = (0,1,0)$ are used.

DOI: 10.1201/9781003516347-4



	A	B	C	D	E	F	G	H
1	3D-Vectors							
2	**Adding two-dimensional vectors**					alpha	beta	gamma
3						1.047198	1.047198	1.047198
4	**Vector1**	**Tail**	Tip					
5	x1	0	1			0	0.25	
6	y1	0	0	$\vec{a}$		0	-0.86603	
7	z1	0	0			0	0.433013	
8								
9	**Vector2**							
10	x2	0	0			0	0.433013	
11	y2	0	1	$\dot{b}$		0	0.5	
12	z2	0	0			0	0.75	
13								
14	v1+v2							
15	Xsum	0	0			0	-0.43301	
16	Ysum	0	1	$\vec{a}\times\vec{b}$		0	0.5	
17	zsum	0	0			0	1.25	
18								
19	Vctor product (i x j)							
20	x-comp	0	0	$\vec{a}+\vec{b}$		0	-0.86603	
21	y-comp	0	0			0	0	
22	z-comp	0	1			0	0.5	
23								

FIGURE 4.1 Calculation of vector addition and vector product.

For creating their three-dimensional representations, a small VBA code is created which reads the calculated values and displays their charts from an arbitrary set of the Euler angles (Appendix A5). The VBA code is shown in Figure 4.2. A vector is defined by the coordinates of its tip and tail and displays the vector on screen using the [`scatter with straight line`] chart.

Figure 4.3 shows the addition of the vectors $\vec{a} = (1,0,4)$ and $\vec{b} = (0,2,0)$, and the unit vector product $\vec{k} = \vec{i} \times \vec{j}$. Both are projected on a YZ plane created by a set of Euler angles (alpha = π/3, beta = π/3, gamma = 0 for the addition, and alpha = π/4, beta = −π/6, gamma = 0 for the vector product).

4.2 LORENTZ FORCE

The Lorenz force on a moving point with charge q and a velocity $\vec{v}$ in an external electric field $\vec{E}$ and a magnetic field $\vec{B}$ is given by $\vec{F} = q\vec{E} + q\vec{v} \times \vec{B}$. Suppose a charged particle with charge q is initially at the origin and is fired in the y-direction with $v_y = v_0$, there is a uniform E-field and a uniform B-field along the z-direction, and the force components are

$$\begin{cases} F_x = qE_x + q(v_y B_z - v_z B_y) = qv_y B_z \\ F_y = qE_y + q(v_z B_x - v_x B_z) = -qv_x B_z \, . \\ F_z = qE_z + q(v_x B_y - v_y B_x) = qE_z \end{cases} \tag{4.1}$$

Figure 4.4 shows the VBA code to calculate the position (x, y, z) of the changed particle when $\vec{E} = (0,0,1)$, $\vec{B} = (0,0,-1)$, $\vec{v}(t=0) = (0,1,0)$, and the charge-to-mass ratio $q/m = 2$.

Figure 4.5 shows the trajectory projected on the xy-plane of the lab coordinates and on the YZ-plane of the tilted plane by the Euler angles. The trajectory is a spiral with an acceleration in the axial direction because there is a vertical acceleration due to the electric field along the z-axis. For better visibility, two dots at the starting and ending points are added.

```
Sub Vector3D()
Cells(1, 1) = "3D-Vectors"
Pi = 3.14159265358979
'Rotational angles of coordinates
  Cells(2, 6) = "alpha": alpha = Pi / 3: Cells(3, 7) = alpha
  Cells(2, 7) = "beta": beta = Pi / 3: Cells(3, 8) = beta
  Cells(2, 8) = "gamma": Gamma = 0: Cells(3, 9) = Gamma
  x1 = Cells(5, 3)
  y1 = Cells(6, 3)
  z1 = Cells(7, 3)
  x2 = Cells(10, 3)
  y2 = Cells(11, 3)
  z2 = Cells(12, 3)
  xsum = Cells(15, 3)
  ysum = Cells(16, 3)
  zsum = Cells(16, 3)
  xp = Cells(20, 3)
  yp = Cells(21, 3)
  zp = Cells(22, 3)
    fx1 = x1 * (Cos(beta) * Cos(alpha) * Cos(Gamma)  - Sin(alpha) * Sin(Gamma)) + y1  * (Cos(beta) * Sin(alpha) * Cos(Gamma) +
        Cos(alpha) * Sin(Gamma))  - z1 * Sin(beta) * Cos(Gamma)
    fy1 = -x1 * (Cos(beta) * Cos(alpha) * Sin(Gamma) + Sin(alpha) * Cos(Gamma))  - y1 * (Cos(beta) * Sin(alpha) * Sin(Gamma)  -
        Cos(alpha) * Cos(Gamma)) + z 1 * Sin(beta) * Sin(Gamma)
    fz1 = x1 * Sin(beta) * Cos(alpha) + y1 * Sin(beta) * Sin(alpha) + z1 * Cos(beta)
          Cells(5, 6) = 0: Cells(5, 7) = fx1
          Cells(6, 6) = 0: Cells(6, 7) = fy1
          Cells(7, 6) = 0: Cells(7, 7) = fz1
    fx2 = x2 * (Cos(beta) * Cos(alpha) * Cos(Gamma)  - Sin(alpha) * Sin(Gamma)) + y2 * (Cos(beta) * Sin(alpha) * Cos(Gamma) +
        Cos(alpha) * Sin(Gamma))  - z2 * Sin(beta) * Cos(Gamma)
    fy2 = -x2 * (Cos(beta) * Cos(alpha)  * Sin(Gamma) + Sin(alpha) * Cos(Gamma))  - y2 * (Cos(beta) * Sin(alpha) * Sin(Gamma)  -
        Cos(alpha) * Cos(Gamma)) + z2 * Sin(beta) * Sin(Gamma)
    fz2 = x2 * Sin(beta) * Cos(alpha) + y2 * Sin(beta) * Sin(alpha) + z2 * Cos(beta)
          Cells(10, 6) = 0: Cells(10, 7) = fx2
          Cells(11, 6) = 0: Cells(11, 7) = fy2
          Cells(12, 6) = 0: Cells(12, 7) = fz2
  fxsum = xsum * (Cos(beta) * Cos(alpha) * Cos(Gamma)  - Sin(alpha) * Sin(Gamma)) + ysum  * (Cos(beta) * Sin(alpha) * Cos(Gamma) +
        Cos(alpha) * Sin(Gamma))  - zsum * Sin(beta) * Cos(Gamma)
  fysum = -xsum * (Cos(beta) * Cos(alpha) * Sin(Gamma) + Sin(alpha) * Cos(Gamma))  - ysum * (Cos(beta) * Sin(alpha) * Sin(Gamma)  -
        Cos(alpha) * Cos(Gamma))  + zsum * Sin(beta) * Sin(Gamma)
  fzsum = xsum * Sin(beta) * Cos(alpha) + ysum * Sin(beta) * Sin(alpha) + zsum * Cos(beta)
          Cells(15, 6) = 0: Cells(15, 7) = fxsum
          Cells(16, 6) = 0: Cells(16, 7) = fysum
          Cells(17, 6) = 0: Cells(17, 7) = fzsum
  fxp = xp * (Cos(beta) * Cos(alpha) * Cos(Gamma)  - Sin(alpha) * Sin(Gamma)) + yp * (Cos(beta) * Sin(alpha) * Cos(Gamma) + Cos(alpha) *
        Sin(Gamma)) - zp * Sin(beta) * Cos(Gamma)
  fyp = -xp * (Cos(beta) * Cos(alpha) * Sin(Gamma) + Sin(alpha) * Cos(Gamma))  - yp * (Cos(beta) * Sin(alpha) * Sin(Gamma)  - Cos(alpha) *
        Cos(Gamma)) + zp * Sin(beta) * Sin(Gamma)
  fzp = xp * Sin(beta) * Cos(alpha) + yp * Sin(beta) * Sin(alpha) + zp * Cos(beta)
          Cells(30, 6) = 0: Cells(30, 7) = fxp
          Cells(31, 6) = 0: Cells(31, 7) = fyp
          Cells(32, 6) = 0: Cells(32, 7) = fzp

End Sub
```

FIGURE 4.2 Vector sum $\vec{c} = \vec{a} \times \vec{b}$ and vector product of unit vectors $\vec{i} \times \vec{j} = \vec{k}$.

4.3 MAXWELL'S EQUATIONS FOR STATIC ELECTROMAGNETIC FIELDS

4.3.1 Static Electric Field

From the Coulomb force, the static electric field and the electric potential can be given by a charge distribution $\rho(\vec{r})$ and the permittivity of free space ε_0:

$$\vec{E}(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \int_V \frac{\rho(\vec{r}\,')}{\left|\vec{r} - \vec{r}\,'\right|} \left(\vec{r} - \vec{r}\,'\right) d^3\vec{r}\,', \text{ and}$$

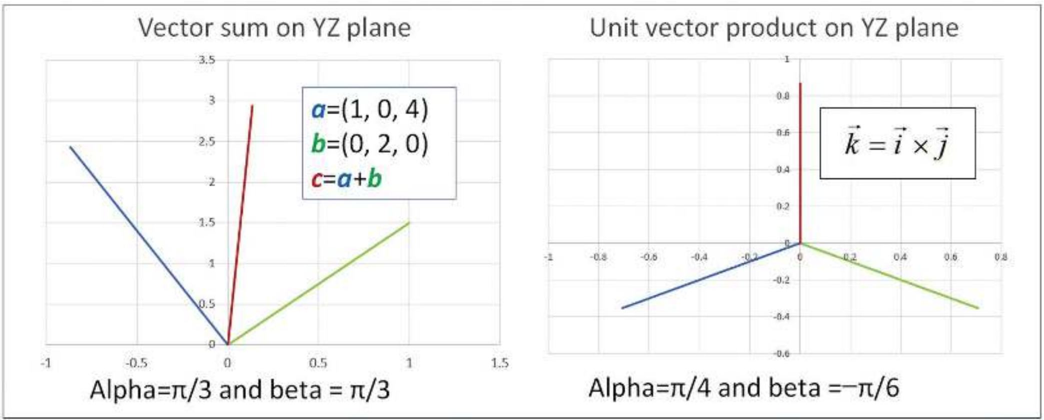


FIGURE 4.3 VBA code for three-dimensional display of a vector sum and a unit vector product.

$$\phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_V \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} d^3\vec{r}\,'. \tag{4.2}$$

Let us find the differential equations for the electric field [1]. Gauss' law, which is a consequence of Coulomb's law of $1/r^2$ dependence of the electrostatic force, states that the closed surface integral is the total charge within the volume enclosed by the closed surface divided by ε_0:

$$\int_S \vec{E}(\vec{r})\cdot d\vec{A} = \frac{1}{\varepsilon_0}\int_V \rho(\vec{r})dV. \tag{4.3}$$

By applying the Gauss theorem of vector calculus, the closed surface integral of Equation 4.3 can be changed to a volume integral: $\int_S \vec{V}(\vec{r})\cdot d\vec{A} = \int_V (\nabla\cdot\vec{V}(\vec{r}))dV$ for any vector function $\vec{V}$.

Thus, $\int_S \vec{E}(\vec{r})\cdot d\vec{A} = \int_V \nabla\cdot\vec{E}(\vec{r})dV = \frac{1}{\varepsilon_0}\int_V \rho(\vec{r})dV.$

Therefore, we obtain the differential form of Maxwell's equation, $\nabla\cdot\vec{E}(\vec{r}) = \frac{\rho(\vec{r})}{\varepsilon_0}$. (4.4)

Using the electric potential defined by $\vec{E} = -\nabla\phi$, Equation 2.3 can be expressed by another differential equation for the electric potential called Poisson's equation: $\nabla^2\phi(\vec{r}) = -\frac{\rho(\vec{r})}{\varepsilon_0}$.
(4.5)

Note that $\nabla\times\vec{E} = -\nabla\times(\nabla\phi) = 0$ for any scalar function ϕ. In summary, the static electric field can be described with the following two Maxwell's equations:

$$\nabla\cdot\vec{E}(\vec{r}) = \frac{\rho(\vec{r})}{\varepsilon_0} \text{ and } \nabla\times\vec{E} = 0 \tag{4.6}$$

where $\vec{E} = -\nabla\phi$ and the electric potential satisfies Poisson's Equation 4.5.

```
Sub ChargedParticle()
 Cells(1, 1) = "Charged particle in Static EM-field."
 Cells(2, 1) = "Both E-field and B-field are in the z-direction."
 Cells(3, 1) = "A charged particle is fired to the yz-direction from the origin on the xy-plane of the lab frame."
'Parmeter Charge/Mass is the electrical charge of the particle.
   QM = 2
'Writing labels and initial value in cells:
     Cells(3, 2) = "Initial t": t = 0: Cells(4, 2) = t
     Cells(3, 3) = "Initial x": x = 0: Cells(4, 3) = x
     Cells(3, 4) = "Initial y": y = 0: Cells(4, 4) = y
     Cells(3, 5) = "Initial z": z = 0: Cells(4, 5) = z
     Cells(3, 6) = "Initial vx": vx = 0: Cells(4, 6) = vx
     Cells(3, 7) = "Initial vy": vy = 10: Cells(4, 7) = vy
     Cells(3, 8) = "Initial vz": vz = 0.5: Cells(4, 8) = vz
     Cells(3, 9) = "delt": h = 0.005: Cells(4, 9) = h
'Parmeter names:
          Cells(10, 2) = "t"
          Cells(10, 3) = "x"
          Cells(10, 4) = "y"
          Cells(10, 5) = "z"
          Cells(10, 6) = "vx"
          Cells(10, 7) = "vy"
          Cells(10, 8) = "vz"
          Cells(9, 10) = "Euler angled coordinates"
          Cells(10, 10) = "X"
          Cells(10, 11) = "Y"
          Cells(10, 12) = "Z"
'Runge-Kutta method:
    Pi = 3.14159265358979
'Rotational angles of coordinates
   Cells(5, 1) = "Euler angles for 3D display "
   Cells(6, 1) = "alpha": alpha = Pi / 6: Cells(7, 1) = alpha
   Cells(6, 3) = "beta": beta = -Pi / 3: Cells(7, 3) = beta
   Cells(6, 5) = "gamma": Gamma = 0: Cells(7, 5) = Gamma
n = 5000  'Iteration #
  For i = 0 To n
     Lx1 = gx(QM, t, x, y, z, vx, vy, vz)
            Ly1 = gy(QM, t, x, y, z, vx, vy, vz)
          Lz1 = gz(QM, t, x, y, z, vx, vy, vz)
          Kx1 = fx(x, y, z, vx, vy, vz)
          Ky1 = fy(x, y, z, vx, vy, vz)
          Kz1 = fz(x, y, z, vx, vy, vz)
 Lx2 = gx(QM, t, x + h * Kx1 / 2, y + h * Ky1 / 2, z + h * Kz1 / 2, vx + h * Lx1 / 2, vy + h * Ly1 / 2, vz + h * Lz1 / 2)
 Ly2 = gy(QM, t, x + h * Kx1 / 2, y + h * Ky1 / 2, z + h * Kz1 / 2, vx + h * Lx1 / 2, vy + h * Ly1 / 2, vz + h * Lz1 / 2)
 Lz2 = gz(QM, t, x + h * Kx1 / 2, y + h * Ky1 / 2, z + h * Kz1 / 2, vx + h * Lx1 / 2, vy + h * Ly1 / 2, vz + h * Lz1 / 2)
     Kx2 = fx(x + h * Kx1 / 2, y + h * Ky1 / 2, z + h * Kz1 / 2, vx + h * Lx1 / 2, vy + h * Ly1 / 2, vz + h * Lz1 / 2)
     Ky2 = fy(x + h * Kx1 / 2, y + h * Ky1 / 2, z + h * Kz1 / 2, vx + h * Lx1 / 2, vy + h * Ly1 / 2, vz + h * Lz1 / 2)
     Kz2 = fz(x + h * Kx1 / 2, y + h * Ky1 / 2, z + h * Kz1 / 2, vx + h * Lx1 / 2, vy + h * Ly1 / 2, vz + h * Lz1 / 2)
 Lx3 = gx(QM, t, x + h * Kx2 / 2, y + h * Ky2 / 2, z + h * Kz2 / 2, vx + h * Lx2 / 2, vy + h * Ly2 / 2, vz + h * Lz2 / 2)
 Ly3 = gy(QM, t, x + h * Kx2 / 2, y + h * Ky2 / 2, z + h * Kz2 / 2, vx + h * Lx2 / 2, vy + h * Ly2 / 2, vz + h * Lz2 / 2)
 Lz3 = gz(QM, t, x + h * Kx2 / 2, y + h * Ky2 / 2, z + h * Kz2 / 2, vx + h * Lx2 / 2, vy + h * Ly2 / 2, vz + h * Lz2 / 2)
     Kx3 = fx(x + h * Kx2 / 2, y + h * Ky2 / 2, z + h * Kz2 / 2, vx + h * Lx2 / 2, vy + h * Ly2 / 2, vz + h * Lz2 / 2)
     Ky3 = fy(x + h * Kx2 / 2, y + h * Ky2 / 2, z + h * Kz2 / 2, vx + h * Lx2 / 2, vy + h * Ly2 / 2, vz + h * Lz2 / 2)
     Kz3 = fz(x + h * Kx2 / 2, y + h * Ky2 / 2, z + h * Kz2 / 2, vx + h * Lx2 / 2, vy + h * Ly2 / 2, vz + h * Lz2 / 2)
 Lx4 = gx(QM, t, x + h * Kx3, y + h * Ky3, z + h * Kz3, vx + h * Lx3, vy + h * Ly3, vz + h * Lz3)
 Ly4 = gy(QM, t, x + h * Kx3, y + h * Ky3, z + h * Kz3, vx + h * Lx3, vy + h * Ly3, vz + h * Lz3)
 Lz4 = gz(QM, t, x + h * Kx3, y + h * Ky3, z + h * Kz3, vx + h * Lx3, vy + h * Ly3, vz + h * Lz3)
     Kx4 = fx(x + h * Kx3, y + h * Ky3, z + h * Kz3, vx + h * Lx3, vy + h * Ly3, vz + h * Lz3)
     Ky4 = fy(x + h * Kx3, y + h * Ky3, z + h * Kz3, vx + h * Lx3, vy + h * Ly3, vz + h * Lz3)
     Kz4 = fz(x + h * Kx3, y + h * Ky3, z + h * Kz3, vx + h * Lx3, vy + h * Ly3, vz + h * Lz3)
```

FIGURE 4.4 VBA code for calculating Lorentz force.

```
        vx = vx + h * (Lx1 + 2 * Lx2 + 2 * Lx3 + Lx4) / 6
        vy = vy + h * (Ly1 + 2 * Ly2 + 2 * Ly3 + Ly4) / 6
        vz = vz + h * (Lz1 + 2 * Lz2 + 2 * Lz3 + Lz4) / 6
        x = x + h * (Kx1 + 2 * Kx2 + 2 * Kx3 + Kx4) / 6
        y = y + h * (Ky1 + 2 * Ky2 + 2 * Ky3 + Ky4) / 6
        z = z + h * (Kz1 + 2 * Kz2 + 2 * Kz3 + Kz4) / 6
            Cells(i + 11, 2) = t
             Cells(i + 11, 3) = x
                  Cells(i + 11, 4) = y
                  Cells(i + 11, 5) = z
                  Cells(i + 11, 6) = vx
                  Cells(i + 11, 7) = vy
                  Cells(i + 11, 8) = vz
          t = t + h
'Euler's angles
      EulerX = x * (Cos(beta) * Cos(alpha) * Cos(Gamma) - Sin(alpha) * Sin(Gamma)) + y * (Cos(beta) * Sin(alpha) * Cos(Gamma) + Cos(alpha)
* Sin(Gamma)) - z * Sin(beta) * Cos(Gamma)
      EulerY = -x * (Cos(beta) * Cos(alpha) * Sin(Gamma) + Sin(alpha) * Cos(Gamma)) - y * (Cos(beta) * Sin(alpha) * Sin(Gamma) - Cos(alpha)
* Cos(Gamma)) + z * Sin(beta) * Sin(Gamma)
      EulerZ = x * Sin(beta) * Cos(alpha) + y * Sin(beta) * Sin(alpha) + z * Cos(beta)
            Cells(i + 11, 10) = EulerX
            Cells(i + 11, 11) = EulerY
            Cells(i + 11, 12) = EulerZ
   Next i
End Sub
_________________________________________________________________
Function gx(QM, t, x, y, z, vx, vy, vz)
'dvx/dt=gx
      gx = QM * (Ex(x, y, z) + vy * Bz(x, y, z) - vz * By(x, y, z))
End Function
_________________________________________________________________
Function gy(QM, t, x, y, z, vx, vy, vz)
'dvy/dt=gy
      gy = QM * (Ey(x, y, z) + vz * Bx(x, y, z) - vx * Bz(x, y, z))
End Function
_________________________________________________________________
Function gz(QM, t, x, y, z, vx, vy, vz)
'dvz/dt=gz
      gz = QM * (Ez(x, y, z) + vx * By(x, y, z) - vy * Bx(x, y, z))
End Function
_________________________________________________________________
Function fx(x, y, z, vx, vy, vz)
'vx=dx/dt
      fx = vx
End Function
_________________________________________________________________
Function fy(x, y, z, vx, vy, vz)
'vy=dy/dt
      fy = vy
End Function
```

FIGURE 4.4 Continued.

4.3.2 Difference Equations for the Electric Potential and the Field

Let us focus on two-dimensional spaces to find the electric potential and the electric field from a given charge distribution:

$$\frac{\partial^2\phi(x,y)}{\partial x^2}+\frac{\partial^2\phi(x,y)}{\partial y^2}=-\frac{\rho(x,y)}{\varepsilon_0}, \text{ and } \begin{cases} E_x(x,y)=-\dfrac{\partial\phi(x,y)}{\partial x} \\ E_y(x,y)=-\dfrac{\partial\phi(x,y)}{\partial y} \end{cases}. \tag{4.7}$$

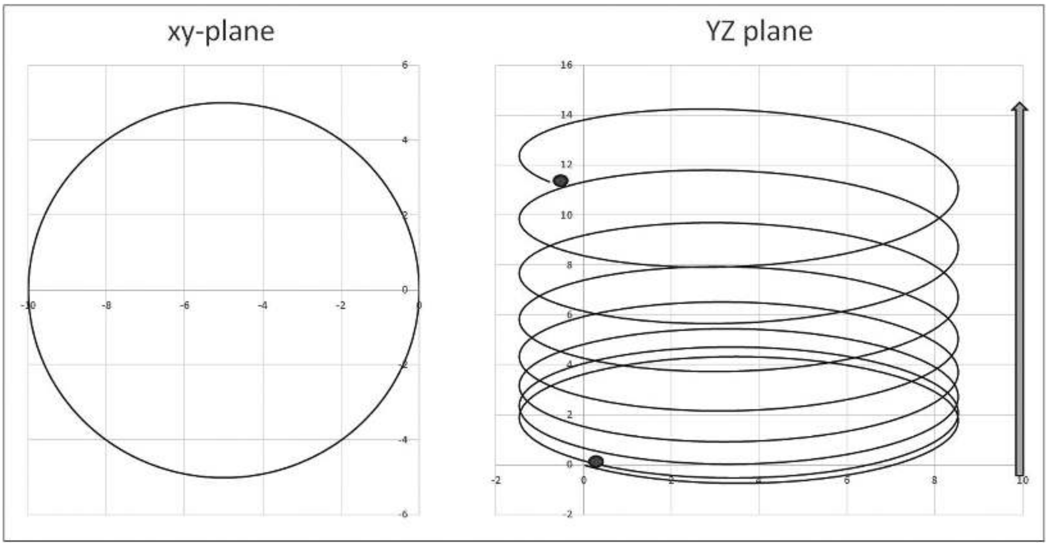


FIGURE 4.5 Trajectories on the xy-plane of the lab frame and on the XY-plane of the tilted plane.

We discretize the independent variables x and y: $x = i\Delta x$ and $y = j\Delta y$, where i and j are integers, and the electric potential function, $\phi(x, y)$, is defined as $\phi(i, j)$. Partial derivatives for a continuous and smooth function are calculated as

$$\begin{cases} \dfrac{\partial\phi(x,y)}{\partial x} \approx \dfrac{\phi(i+1,j)-\phi(i,j)}{\Delta x} \\ \dfrac{\partial\phi(x,y)}{\partial y} \approx \dfrac{\phi(i,j+1)-\phi(i,j)}{\Delta x} \end{cases} \text{or} \begin{cases} \dfrac{\partial\phi(x,y)}{\partial x} \approx \dfrac{\phi(i,j)-\phi(i-1,j)}{\Delta x} \\ \dfrac{\partial\phi(x,y)}{\partial y} \approx \dfrac{\phi(i,j)-\phi(i,j-1)}{\Delta x} \end{cases}. \tag{4.8}$$

Using the forward and backward derivatives, the second derivatives are given by

$$\begin{cases} \dfrac{\partial^2\phi(x,y)}{\partial x^2} \approx \dfrac{1}{\Delta x}\left[\left(\dfrac{\phi(i+1,j)-\phi(i,j)}{\Delta x}\right)-\left(\dfrac{\phi(i,j)-\phi(i-1,j)}{\Delta x}\right)\right] \\ \dfrac{\partial^2\phi(x,y)}{\partial y^2} \approx \dfrac{1}{\Delta y}\left[\left(\dfrac{\phi(i,j+1)-\phi(i,j)}{\Delta y}\right)-\left(\dfrac{\phi(i,j)-\phi(i,j-1)}{\Delta y}\right)\right], \end{cases} \tag{4.9}$$

and the Poisson equation discretized for numerical calculation becomes:

$$\begin{aligned} &\frac{1}{h}\left[\left(\frac{\phi(i+1,j)-\phi(i,j)}{h}\right)-\left(\frac{\phi(i,j)-\phi(i-1,j)}{h}\right)\right] \\ &+\frac{1}{h}\left[\left(\frac{\phi(i,j+1)-\phi(i,j)}{h}\right)-\left(\frac{\phi(i,j)-\phi(i,j-1)}{h}\right)\right] = -\frac{\rho(i,j)}{\varepsilon_0}. \end{aligned} \tag{4.10}$$

From Equation 4.9, the electric potential at the point (i, j) is

$$\phi(i,j) = \frac{\phi(i+1,j)+\phi(i-1,j)+\phi(i,j+1)+\phi(i,j-1)}{4} + \frac{h^2\rho(i,j)}{4\varepsilon_0}. \tag{4.11}$$

4.3.3 Electric Dipole Potential

With Equation 7.6, the two-dimensional electric potential can be calculated from a given charge distribution, $\rho(i, j)$. Let us calculate the dipole field from which we obtain the 3D equipotential surface of Figure 4.7. Excel has an option called *Iterative Calculation*, which is "the repeated recalculation of a worksheet until a specific numeric condition is met." [2]. Refer to Appendix A.1.5 for enabling this option.

Here is the iteration routine for the electric potential:

1) Use A*utoFill* to write x-coordinate values from **−10** to **+10** in Row `1` (the x-coordinates) and Column `A` (the y-coordinates).
2) Enter the boundary condition: $\phi(+10, y) = \phi(-10, y) = \phi(x, +10) = \phi(x, -10) = 0$ for $-10 \le x \le +10$ and $-10 \le y \le +10$. Enter **0** in Cells `B2:B42` of Column `B`, Cells `AP2:AP42` of Column `AP`, Cells `B2:AP2` of Row `2`, and Cells `B42:AP42` of Row `42`.
3) Enter the charges: **±1** ($=h^2\rho/4\varepsilon_0$) in Cells `R23` and `AB23`, respectively.
4) Enter **`=(B2+C1+D3+C4)/4`** in Cell `C3`. Figure 4.6 shows the difference equation and its equation for Excel.

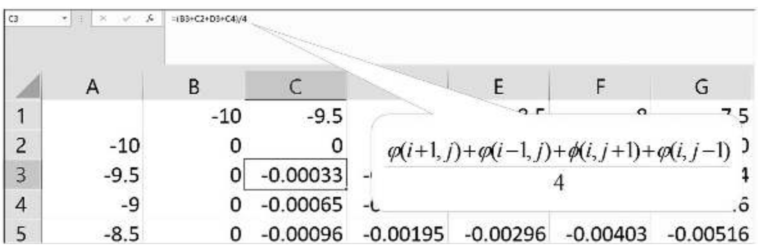


FIGURE 4.6 Preparing the integrative calculation.

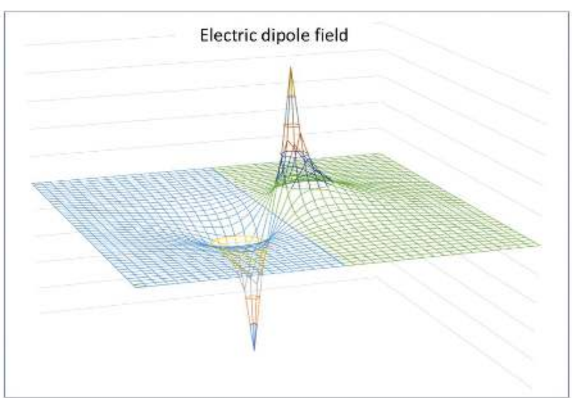


FIGURE 4.7 Two-dimensional electric dipole potential surface.

5) *AutoFill* `C3` to `C42` and then *AutoFill* `C3` to `AQ3`. Continue *AutoFill* along rows and columns. Do not worry even if the cell values are all zero until reaching Column `O`. Once Column `P` is *AutoFilled*, the cell values change by the *Iteration Calculation* option. For Column `Q`, *AutoFill* `Q3:Q21` and `Q23:Q42` to avoid Cells `Q22`.

6) Highlight `A1:AP42` and insert a `[Wire frame 3-D surface]` graph.

4.3.4 Two-Dimensional Electric Field from Electric Potential

The electric field can be calculated from the electric potential: $\vec{E}(x,y,z) = -\nabla\phi(x,y,z)$. Because the electric field is a vector, it needs two separate tables for $E_x(x, y)$ and $E_y(x, y)$. For the two-dimensional potential, the following approximation of position derivatives can be used.

$$E_x(x,y) = -\frac{\partial\phi(x,y)}{\partial x} \approx -\frac{1}{2}\left[\frac{\phi(i+1,j)-\phi(i,j)}{h} + \frac{\phi(i,j)-\phi(i-1,j)}{h}\right] = -\frac{\phi(i+1,j)-\phi(i-1,j)}{2h}, \tag{4.12}$$

and

$$E_y(x,y) = -\frac{\partial\phi(x,y)}{\partial y} \approx -\frac{1}{2}\left[\frac{\phi(i,j+1)-\phi(i,j)}{h} + \frac{\phi(i,j)-\phi(i,j-1)}{h}\right] = -\frac{\phi(i,j+1)-\phi(i,j-1)}{2h}. \tag{4.13}$$

From the spreadsheet of the electric dipole potential obtained through steps (17) to (22), the electric field, $E_x(x, y)$ and $E_y(x, y)$, can be calculated. Here, rows change the x-coordinates: Cells `B2:AP2` correspond to the coordinate (–10, –10) to (+10, –10) by increments of 0.5, and columns change the y-coordinates: Cells `A2:A42` correspond to the coordinates (–10, –10) to (–10, +10).

Calculation of $E_x(x, y)$

7) Use *AutoFill* and enter the x-coordinates from **–10** to **+10** in Cells `B45:AP45` of Row `46` by step 0.7. Similarly, enter the y-coordinates from **–10** to **+10** in Cells `A45:A85` of Column `A`.

8) Enter the boundary value 0 in Cells `B45:AP45`, `B45:B84`, `AP45:AP84`, and `B85:AP87`.

9) Enter **`=-(C3-B3)`** in Cell `B46` and *AutoFill* to `AP46`.

10) Highlight Cells `B46:AP46` and *AutoFill* to Cells `B84:AP84`.

Figure 4.8 shows the initial part of E_x.

	A	B	C	D	E	F	G	H	I	J	K	L	M
44	Ex												
45		-10	-9.5	-9	-8.5	-8	-7.5	-7	-6.5	-6	-5.5	-5	-4.5
46	-10	0	0	0	0	0	0	0	0	0	0	0	0
47	-9.5	0	0.000678	0.000657	0.000624	0.000579	0.000521	0.00045	0.000365	0.000267	0.000156	3.46E-05	-9.6E-05
48	-9	0	0.001368	0.001325	0.00126	0.00117	0.001055	0.000913	0.000744	0.000547	0.000324	7.78E-05	-0.00019
49	-8.5	0	0.002079	0.002016	0.001919	0.001787	0.001616	0.001404	0.00115	0.000853	0.000514	0.000139	-0.00027

FIGURE 4.8 Initial part of E_x.

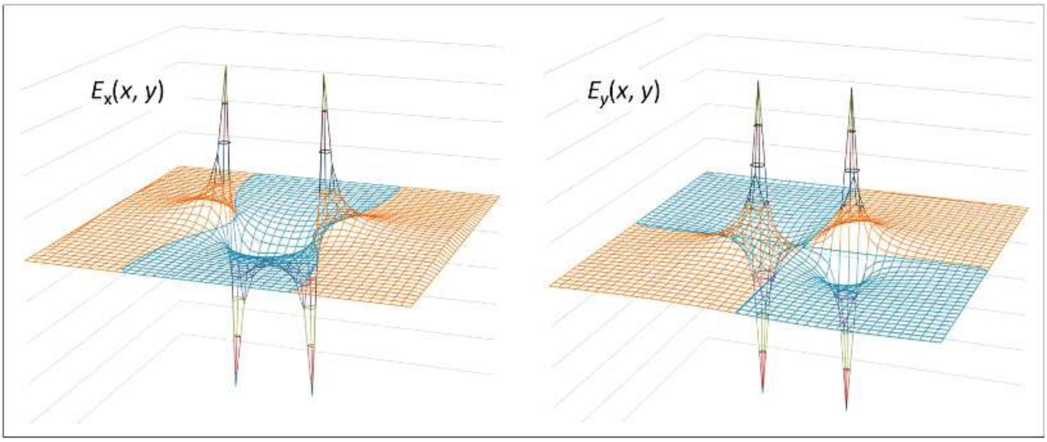


FIGURE 4.9 Electric field patters E_x and E_y.

Calculation of $E_y(x, y)$

11) Use *AutoFill* and enter the x-coordinates from –10 to +10 in Cells B89:AP89 of Row 89 by step 0.7. Enter the y-coordinates from –10 to +10 in Cells A90:A130 of Column A.
12) Enter the boundary value **0** in Cells B90:AP90, B90:B130, AP90:AP130 and B130:AP130.
13) Enter **=-(C4-C3)** in Cell B91. *AutoFill* to AP91.
14) Highlight Cells B91:AP91 and *AutoFill* to Cells B129:AP129.

4.3.5 A Charged Square Conductor in a Uniform Electric Field

Apply potential difference V across a pair of large parallel plates to produce a uniform E-field. Place a square conductor that initially carries no charge in the field. How can we compute equipotential lines?

Figure 4.10 shows a part of the initial setting of a spreadsheet. There are 40 × 40 points to calculate the potential distribution. The ranges of x and y coordinates are set to be [–10, +10] with 0.5 increments. Column B (cells B4:B44) represents a plate of zero potential and Column AP (Cell AP4:AP44) represents the plate of potential of a constant positive voltage V. They are highlighted in yellow. The cells highlighted in green (Cells U19:X19) represent the square conductor. Assume that the region between the plates is large and potential values on both sides of the region should be linear from 0 to V volts.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1	Two-dimensional dipole potential																								
2																									
3		-10	-9.5	-9	-8.5	-8	-7.5	-7	-6.5	-6	-5.5	-5	-4.5	-4	-3.5	-3	-2.5	-2	-1.5	-1	-0.5	0	0.5	1	1.5
4	-10	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
5	-9.5	0	0	1.582616	2.737578	3.765298	4.750549	5.719673	6.681813	7.640567	8.597603	9.553883	10.51013	11.46701	12.42524	13.3856	14.34894	15.31618	16.28823	17.26599	18.25023	19.24157	20.24038	21.24678	22.26059
6	-9	0	0.582856	1.592861	2.602966	3.573027	4.517179	5.446287	6.366966	7.282809	8.195923	9.107767	10.01959	10.93265	11.84834	12.76821	13.69399	14.62753	15.57076	16.5255	17.49338	18.47568	19.47519	20.48615	21.5142
7	-8.5	0	0.738538	1.603566	2.505944	3.407204	4.298784	5.181261	6.056884	6.927714	7.795451	8.661619	9.52777	10.39564	11.26723	12.14488	13.00125	13.92921	14.84178	15.77187	16.72212	17.69459	18.69057	19.71046	20.75366
8	-8	0	0.767696	1.576868	2.41057	3.250979	4.089403	4.922999	5.751503	6.575626	7.396471	8.21542	9.034175	9.854845	10.68002	11.51283	12.3569	13.21628	14.09527	14.99811	15.92866	16.89	17.88407	18.91147	19.97131
9	-7.5	0	0.755339	1.525576	2.308407	3.096645	3.884746	4.66972	5.450401	6.226716	6.999297	7.769336	8.5386	9.309493	10.08515	10.86948	11.66722	12.48374	13.32491	14.19665	15.10444	16.0527	17.04429	18.08009	19.15879
10	-7	0	0.72804	1.461624	2.200747	2.942344	3.683102	4.420621	5.153551	5.881434	6.604565	7.323944	8.041324	8.759323	9.481548	10.21272	10.95873	11.72655	12.524	13.35918	14.23976	15.1721	16.16036	17.20583	18.30667
11	-6.5	0	0.695153	1.39206	2.090523	2.788775	3.484583	4.175992	4.861629	5.540795	6.213486	6.880462	7.543359	8.204869	8.868959	9.541094	10.22841	10.93974	11.68536	12.47631	13.32336	14.23562	15.21924	16.27626	17.404
12	-6	0	0.660465	1.320872	1.980418	2.637543	3.29035	3.937016	4.576065	5.206521	5.828025	6.440974	7.04671	7.647782	8.248287	8.854262	9.474072	10.11866	10.8014	11.53737	12.34177	13.22783	14.20478	15.27602	16.45772
13	-5.5	0	0.625792	1.250478	1.872649	2.490531	3.102149	3.705547	4.298987	4.881098	5.451028	6.008621	6.55466	7.091212	7.62211	8.153574	8.694952	9.259411	9.864226	10.53004	11.27857	12.12917	13.09609	14.18537	15.39175
14	-5	0	0.592185	1.182538	1.769091	2.349693	2.922068	3.483937	4.033139	4.567764	5.086287	5.587754	6.07204	6.540254	6.995338	7.442957	7.892746	8.359819	8.866071	9.440016	10.11332	10.91426	11.86507	12.97767	14.24574
15	-4.5	0	0.560377	1.118342	1.671415	2.217001	2.752408	3.274904	3.781784	4.270453	4.738533	5.184007	5.605445	6.002393	6.376007	6.73016	7.073257	7.421058	7.800241	8.250662	8.820466	9.549499	10.47232	11.61457	12.97326
16	-4	0	0.530952	1.058994	1.581167	2.094419	2.595587	3.081415	3.548568	3.993667	4.41333	4.804247	5.163306	5.487839	5.776124	6.028412	6.24907	6.450925	6.663191	6.94195	7.368418	7.990991	8.860183	10.03506	11.53965
17	-3.5	0	0.504413	1.005477	1.499794	1.983865	2.45405	2.906543	3.337352	3.742265	4.116829	4.456312	4.755666	5.009517	5.212231	5.358294	5.443692	5.470395	5.459667	5.48555	5.720293	6.185895	6.942399	8.125888	9.902604
18	-3	0	0.481204	0.958678	1.428631	1.887155	2.330159	2.753314	3.15199	3.521177	3.855382	4.148483	4.393516	4.582324	4.704988	4.748848	4.697019	4.52731	4.219546	3.820307	3.84133	4.089921	4.59766	5.623523	8.035755
19	-2.5	0	0.461714	0.919377	1.368873	1.805938	2.226088	2.624536	2.996093	3.335051	3.635023	3.888714	4.087586	4.221278	4.276555	4.2351	4.068237	3.722292	3.070914	1.734814	1.734814	1.734814	1.734814	1.734814	6.090016
20	-2	0	0.446264	0.888232	1.32153	1.741619	2.143703	2.522633	2.872783	3.187904	3.46094	3.683767	3.846841	3.938655	3.944868	3.846774	3.618551	3.222721	2.607015	1.734814	1.734814	1.734814	1.734814	1.734814	5.324016
21	-1.5	0	0.435106	0.865751	1.287391	1.695297	2.084468	2.449508	2.784501	3.082848	3.337075	3.538586	3.677372	3.741653	3.717506	3.588598	3.336488	2.943042	2.399621	1.734814	1.734814	1.734814	1.734814	1.734814	4.990203
22	-1	0	0.428407	0.852278	1.266984	1.667715	2.049369	2.406439	2.732877	3.021928	3.265944	3.456153	3.582431	3.633102	3.59493	3.453646	3.195784	2.813353	2.313627	1.734814	1.734814	1.734814	1.734814	1.734814	4.85563
23	-0.5	0	0.426247	0.847972	1.260562	1.659221	2.038867	2.39402	2.718659	3.006069	3.248646	3.43768	3.563127	3.613425	3.575496	3.435298	3.179671	2.800978	2.30673	1.734814	1.734815	1.734815	1.734815	1.734815	4.848519
24	0	0	0.428615	0.852812	1.268084	1.669755	2.052881	2.412139	2.7417	3.055076	3.284925	3.482829	3.61901	3.68201	3.658367	3.532411	3.286651	2.904179	2.377513	1.734815	1.734815	1.734815	1.734815	1.734815	4.967431
25	0.5	0	0.43541	0.866588	1.289225	1.698858	2.090789	2.459985	2.800962	3.107646	3.373191	3.589745	3.748115	3.837281	3.843589	3.749365	3.53037	3.151597	2.564342	1.734815	1.734815	1.734815	1.734815	1.734815	5.280144
26	1	0	0.446446	0.888921	1.323389	1.745689	2.151464	2.536086	2.894557	3.221398	3.510493	3.754889	3.946473	4.075454	4.129387	4.091129	3.933902	3.607524	2.993457	1.734815	1.734815	1.734815	1.734815	1.734815	6.010613
27	1.5	0	0.461463	0.919278	1.369744	1.809072	2.233328	2.638378	3.019827	3.37294	3.692545	3.972897	4.207485	4.388723	4.507422	4.551904	4.506622	4.351169	4.067169	3.699262	3.730469	3.981268	4.485997	5.500717	7.880104
28	2	0	0.480141	0.957	1.427263	1.88756	2.334433	2.764311	3.173478	3.558041	3.913901	4.23672	4.521901	4.764583	4.959726	5.102489	5.189558	5.223397	5.224821	5.264622	5.506557	5.973818	6.727218	7.901986	9.663096
29	2.5	0	0.502112	1.001337	1.494774	1.979502	2.452571	2.910999	3.351781	3.771896	4.168349	4.538237	4.878872	5.188036	5.464461	5.70882	5.925772	6.128083	6.344137	6.627887	7.057357	7.680266	8.547111	9.716955	11.2145

FIGURE 4.10 Electric potential around a square conductor (shown in green) in uniform *E*-field.

The computational step of the electric potential is similar to that in Section 4.3.3.

Boundary conditions:

1) Enter **`0`** in cells `B4` to `B44`.
2) Enter **`=B4+1`** in cell `C4` and AutoFill to cell `AP4`.
3) Enter **`=B4+1`** in cell `C44` and AutoFill to cell `AP44`.
4) The conductor forms an equipotential region but the potential value is unknown. We set the numerical value in cells of the square conductor to calculate the average value of the surrounding cell. Enter

   `=(T18+T19+T20+T21+T22+T23+T24+T25+T26+T27+U27+V27+W27+X27+X26+X25+X24+X23+X22+X21+X19+X18+W18+V18+U18)/40`

   in Cell `U19`, and then copy and paste it to other cells of the square conductor. Each cell of `U19:X19` has the same calculation formula.
5) Enter **`=(B5+C4+D5+C6)/4`** in Cell `C5`.
6) Apply Excel's *Iterative Calculation* feature. *AutoFill* `C5` to `C44` and then *AutoFill* `C5` to `AP44`, ***avoiding the cells of the square conductor***.

Figure 4.11 shows the final result of the electric potential distribution around the square conductor.

4.3.6 Static Magnetic Field

Since there is no magnetic monopole, the Gauss' law for the magnetic field is

$$\int_A \vec{B}\cdot d\vec{A} = 0, \text{ which leads to } \nabla\cdot\vec{B} = 0. \tag{4.14}$$

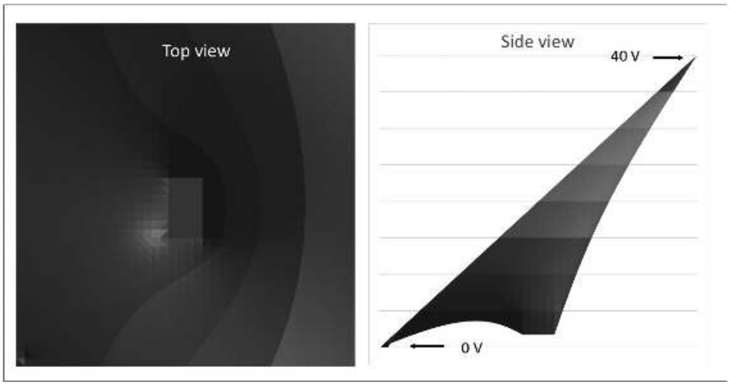


FIGURE 4.11 Electric potential distribution around a square conductor.

Using the current density, $\vec{j}(\vec{r})$, Ampere's law can be expressed to be $\oint_\ell \vec{B} \cdot d\vec{s} = \mu_0 \int_A \vec{j} \cdot d\vec{A}$.

Now, Stokes' theorem forms vector calculus, and the line integral of the above equation can be changed to a surface integral $\oint_\ell \vec{B} \cdot d\vec{s} = \int_A (\nabla \times \vec{B}) \cdot d\vec{A}$, and thus, $\int_A (\nabla \times \vec{B}) \cdot d\vec{A} = \mu_0 \int_A \vec{j} \cdot d\vec{A}$. (4.15)

Therefore, we obtain the differential form of Maxwell's equation for B-field, $\nabla \times \vec{B} = \mu_o \vec{j}$.

The magnetic field can be expressed in the form of $\vec{B} = \nabla \times \vec{A}$, where $\vec{A}$ is the vector potential of the magnetic field. Since $\nabla \cdot (\nabla \times \vec{A}) = 0$ for any vector, Equation (4.14) is automatically satisfied with the vector potential defined in this way [3].

Use Equation (4.15) with $\vec{B} = \nabla \times \vec{A}$ to obtain $\nabla \times \vec{B} = \nabla \times (\nabla \times \vec{A}) = \nabla(\nabla \cdot \vec{A}) - \nabla^2 \vec{A} = \mu_0 \vec{j}$. (4.16)

Now, because any scalar function χ satisfies $\nabla \times (\nabla \chi) = 0$, another vector potential $\vec{A} = \vec{A}' + \nabla \chi$ also satisfies $\vec{B} = \nabla \times \vec{A} = \nabla \times \vec{A}' + \nabla \times (\nabla \chi) = \nabla \times \vec{A}'$. This means that both the vector potentials $\vec{A}$ and $\vec{A}'$yield the same magnetic field. Back to Equation (4.16), we may choose the vector potential such that $\nabla \cdot \vec{A} = 0$. With this condition on the vector potential, we obtain $-\nabla^2 \vec{A} = \mu_0 \vec{j}$. (4.17)

In summary, the static magnetic field can be described with the following two Maxwell's equations:

$$\nabla \cdot \vec{B} = 0 \text{ and } \nabla \times \vec{B} = \mu_o \vec{j} \tag{4.18}$$

where $\vec{B} = \nabla \times \vec{A}$ and the vector potential satisfies $-\nabla^2 \vec{A} = \mu_0 \vec{j}$.

Similar to the electric potential, the vector potential and the magnetic field in two-dimensional space can be computed by the following difference equations.

4.3.7 Iteration Method to Compute Vector Potential and Magnetic Field

Magnetic fields can be calculated using vector potential. For a two-dimensional field,

$$B_x(x,y) = \frac{\partial A_z(x,y)}{\partial y} \text{ and } B_y(x,y) = -\frac{\partial A_z(x,y)}{\partial x} \tag{4.19}$$

where the vector potential satisfies

$$\frac{\partial^2 A_z(x,y)}{\partial x^2} + \frac{\partial^2 A_z(x,y)}{\partial y^2} = -\mu_0 J_x(x,y). \tag{4.20}$$

Similar to the numerical solution of the Poisson equation (4.7) for an electric field, the vector potential can be numerically given by

$$A_z(i,j) = \frac{A_z(i+1,j)+A_z(i-1,j)+A_z(i,j+1)+A_z(i,j-1)}{4} + \mu_0 \frac{h^2 J_z(i,j)}{4}. \tag{4.21}$$

The magnetic field given by Equation 4.19 can be calculated as the average of the forward and backward derivatives:

$$\begin{aligned} B_y(x,y) &= -\frac{\partial A_z}{\partial x} \approx -\frac{1}{2}\left[\frac{A_z(x+\Delta x,y)-A_z(x,y)}{\Delta x} + \frac{A_z(x,y)-A_z(x-\Delta x,y)}{\Delta x}\right] \\ &= -\frac{A_z(x+\Delta x,y)-A_z(x-\Delta x,y)}{2\Delta x} \Rightarrow B_y(i,j) = -\frac{A_z(i+1,j)-A_z(i-1,j)}{2h}, \end{aligned} \tag{4.22}$$

and

$$\begin{aligned} B_x(x,y) &= \frac{\partial A_z}{\partial y} \approx \frac{1}{2}\left[\frac{A_z(x,y+\Delta y)-A_z(x,y)}{\Delta y} + \frac{A_z(x,y)-A_z(x,y-\Delta y)}{\Delta y}\right] \\ &= \frac{A_z(x,y+\Delta y)-A_z(x,y-\Delta y)}{2\Delta y} \Rightarrow B_x(i,j) = \frac{A_z(i,j+1)-A_z(i,j-1)}{2h}. \end{aligned} \tag{4.23}$$

4.3.8 Vector Potential and Magnetic Field due to a Pair of Current Wires

Here is how to calculate the magnetic field using a pair of straight current wires with opposite current directions along the z-axis. The positive current, +1, is at x = +1.25 and the negative current −1, is at x = −1.25 in the two-dimensional space, $-10 \le x \le +10$, $-10 \le y \le +10$.

First of all, make sure that the [`Iterative Calculation`] option is enabled. Refer to A.1.5 for enabling this option.

Calculation of the vector potential $A_z(i, j)$

1) Create a spreadsheet with a boundary condition.

   x-axis

   i) Enter **−10** into Cell `B1`

   ii) Enter **`=C2+0.5`** into Cell `2`

   iii) *Autofill* to Cell AP1

   y-axis

   iv) Enter **−10** into Cell `A2`

   v) Enter **`=B3+0.5`** into Cell `A3`

   vi) *Autofill* to Cell A42

2) Enter **0** along the boundaries `B2:AP2`, `B2:B42`, `AP2:AP42`, and `B42:AP42`.

3) Enter current value **−1** in Cell `AA23` ($x = -2.5, y = 0$) and **+2** in Cell `Q23` ($x = +2.5, y = 0$).

4) Enter **`=(A2+B1+C2+B3)/4`** in Cell `B2`.

5) Complete the sheet by applying *AutoFill.*

Figures 4.12 shows the initial part of the spreadsheet and Figure 4.13 shows the 3D surface graph of the completed vector potential due to two current wires: $I_1 = -1$ at (−2.5,0) and $I_2 = +2$ at (+2.5, 0)

Calculation of the magnetic fields $B_x(i, j)$

6) Create coordinate positions (i, j) and boundary conditions

   x-axis:

   i) Enter **−10** into Cell `B44`

   ii) Enter **`=C2+0.5`** into Cell `C44`

   iii) *AutoFill* to Cell `AP44`

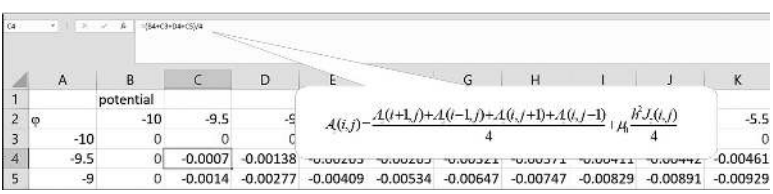


FIGURE 4.12 Beginning part of the spreadsheet for the vector potential.

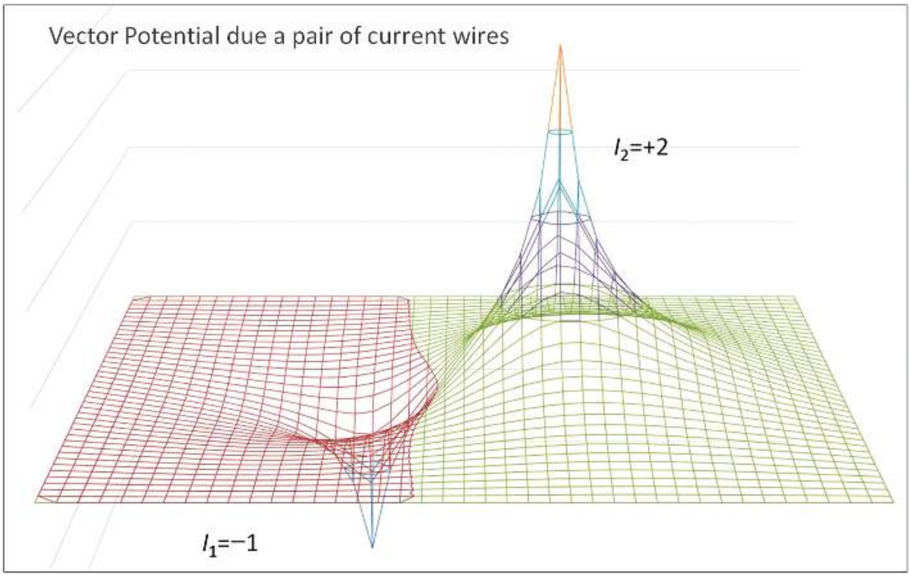


FIGURE 4.13 Vector potential of a pair of opposite-current wires.

y-axis:

iv) Enter **−10** into Cell `AP45`

v) Enter **=B3+0.5** into Cell `A46`

vi) *AutoFill* to Cell `A85`

7) Enter **0** along the boundaries `B45:AP45`, `B45:B85`, `AP45:AP85`, and `B485:AP85`.

8) Enter **=B3−C3** in Cell `C46`.

9) Complete the B_x components (`B45:AP85`) by performing *AutoFill*.

Calculation of the magnetic fields $B_y(i, j)$

10) Create coordinate positions (i, j) and boundary condition

x-axis:

i) Enter **−10** into Cell `B89`

ii) Enter **=C2+0.5** into Cell `C89`

iii) *AutoFill* to Cell `AP89`

y-axis:

iv) Enter **−10** into Cell `A90`

v) Enter =**B3+0.5** into Cell `A91`

vi) *AutoFill* to Cell `A130`

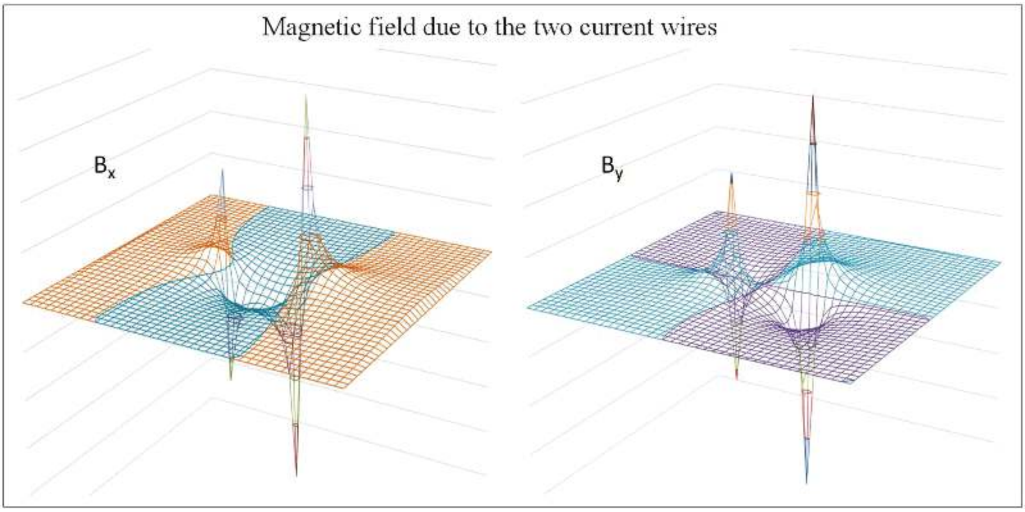


FIGURE 4.14 Magnetic foil produced by two current wires ($I_1 = -1$ and $I_2 = +2$).

11) Enter **0** along the boundaries `B45:AP45`, `B45:B85`, `AP45:AP85`, and `B485:AP85`.

12) Enter **= B2–B4** in Cell `C91`.

13) Complete the B_y components (`B91:AP130`) by performing *AutoFill*.

The pattern of the magnetic field due to the two current wires is similar to the electric dipole field as shown in Figure 4.14.

Note: *Biot-Savart's law from Ampere's law*

Each component of Equation 4.17 is essentially a Poisson's equation. For example, its x-component is $-\nabla^2 A_x = \mu_0 j_x$.

Recall that $\phi(\vec{r}) = \dfrac{1}{4\pi\varepsilon_0}\displaystyle\int_V \dfrac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'$, and we may write $A_x(\vec{r}) = \dfrac{\mu_0}{4\pi}\displaystyle\int_V \dfrac{j_x(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'$. (4.24)

Thus, $\vec{A}(\vec{r}) = \dfrac{\mu_0}{4\pi}\displaystyle\int_V \dfrac{\vec{j}(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'$ can be used to calculate the magnetic field [4, 5].

$$\vec{B}(\vec{r}) = \nabla\times\vec{A}(\vec{r}) = \frac{\mu_0}{4\pi}\nabla\times\left[\int_V \frac{\vec{j}(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'\right], \tag{4.25}$$

which is Biot-Savart's law.

Taking the x-component, we have $B_x(\vec{r}) = \dfrac{\mu_0}{4\pi}\nabla\times\left[\displaystyle\int_V \dfrac{\vec{j}(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'\right]_x$, (4.26) we can calculate B_x.

$$B_x(\vec{r}) = \frac{\mu_0}{4\pi}\left[\frac{\partial}{\partial y}\left\{\int_V \frac{j_z(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'\right\} - \frac{\partial}{\partial z}\left\{\int_V \frac{j_y(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}'\right\}\right]$$
$$= \frac{\mu_0}{4\pi}\left[\int_V j_z(\vec{r}')\frac{\partial}{\partial y}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)d^3\vec{r}' - \int_V j_y(\vec{r}')\frac{\partial}{\partial z}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)d^3\vec{r}'\right]$$
$$= \frac{\mu_0}{4\pi}\left[-\int_V j_z(\vec{r}')\frac{y-y'}{|\vec{r}-\vec{r}'|^3}d^3\vec{r}' + \int_V j_y(\vec{r}')\frac{z-z'}{|\vec{r}-\vec{r}'|}d^3\vec{r}'\right]$$
$$= \frac{\mu_0}{4\pi}\left[\int_V \frac{\left[\vec{j}(\vec{r}')\times(\vec{r}-\vec{r}')\right]_x}{|\vec{r}-\vec{r}'|^3}d^3\vec{r}'\right].$$

Combining all three components, we obtain Biot-Savart's law.

$$\vec{B}(\vec{r}) = \frac{\mu_0}{4\pi}\left[\int_V \frac{\left[\vec{j}(\vec{r}')\times(\vec{r}-\vec{r}')\right]}{|\vec{r}-\vec{r}'|^3}d^3\vec{r}'\right]. \tag{4.27}$$

4.4 TIME-VARYING MAXWELL'S EQUATIONS

4.4.1 Faraday's Law of Magnetic Induction

The induced voltage (*emf*) is proportional to the changing rate of magnetic flux.

$$emf = -\frac{\partial \Phi_B}{\partial t} = -\oint_A \frac{\partial \vec{B}}{\partial t}\cdot d\vec{A}. \tag{4.28}$$

What induces *emf*? An electric field or a magnetic field must be induced, and charges (electrons) are driven by the induced field to produce electrical current and voltage. Note that the magnetic field does not work because the magnetic force is always perpendicular to the displacement of the charges. Therefore, the induced field must be electric. The charge along the closed path by the induced electric field is equal to the electric potential energy due to *emf*.

$$W = \oint_C \vec{F}\cdot d\vec{s} = q\oint_C \vec{E}\cdot d\vec{s} = q(emf), \text{ thus } q\oint_C \vec{E}\cdot d\vec{s} = -\oint_A \frac{\partial \vec{B}}{\partial t}\cdot d\vec{A}. \tag{4.29}$$

By applying Stokes' theorem, $\oint_C \vec{E}\cdot d\vec{s} = -\oint_A \left(\nabla\times\vec{E}\right)\cdot d\vec{A} = -\oint_A \frac{\partial \vec{B}}{\partial t}\cdot d\vec{A}.$ (4.30)

Therefore, Faraday's law states $\nabla\times\vec{E} = -\frac{\partial \vec{B}}{\partial t}.$ (4.31)

4.4.2 Displacement Current

You may notice a similar equation for B-field, i.e., Ampere's law: $\nabla\times\vec{B}=\mu_o\vec{j}$. For a time-varying magnetic field, this equation cannot be used. Here is why. Because $\nabla\cdot(\nabla\times\vec{B})=0$, Ampere's law indicates $\nabla\cdot\vec{j}=0$. This is acceptable for a steady current but not for a time-varying current. For a time-varying current, the conservation of charge, $\partial\rho(\vec{r},t)/\partial t+\nabla\cdot\vec{j}=0$ must be applied.

Recall $\nabla\cdot\vec{E}(\vec{r})=\dfrac{\rho(\vec{r})}{\varepsilon_0}$. The time derivative of this equation,

$$\frac{\partial}{\partial t}\left[\nabla\cdot\vec{E}\right]=\frac{1}{\varepsilon_0}\frac{\partial\rho}{\partial t}=-\frac{1}{\varepsilon_0}\left(\nabla\cdot\vec{j}\right).$$

Thus, $$\nabla\cdot\vec{j}+\varepsilon_0\frac{\partial}{\partial t}\left[\nabla\cdot\vec{E}\right]=\nabla\cdot\left[\vec{j}+\varepsilon_0\frac{\partial\vec{E}}{\partial t}\right]=0. \tag{4.32}$$

The additional term is called the displacement current. Ampere's law is modified to $\nabla\times\vec{B}=\mu_0\left(\vec{j}+\varepsilon_0\dfrac{\partial\vec{E}}{\partial t}\right)$. Maxwell's equations for time-varying fields are now given:

$$\nabla\cdot\vec{E}(\vec{r},t)=\frac{\rho(\vec{r},t)}{\varepsilon_0},\ \nabla\times\vec{E}(\vec{r},t)=-\frac{\partial\vec{B}(\vec{r},t)}{\partial t},$$

$$\nabla\cdot\vec{B}(\vec{r},t)=0,\ \nabla\times\vec{B}(\vec{r},t)=\mu_0\vec{j}(\vec{r},t)+\mu_0\varepsilon_0\frac{\partial\vec{E}(\vec{r},t)}{\partial t}. \tag{4.33}$$

4.4.3 Electromagnetic Wave in Free Space

The most important aspect of Maxwell's equations is that they predict the existence of electromagnetic waves [5]. Faraday's speculation that "visible light is an electromagnetic wave" was proved.

There is neither charge nor current. In this case, Maxwell's Equations 4.33 become

$$\nabla\cdot\vec{E}(\vec{r},t)=0;\ \nabla\times\vec{E}(\vec{r},t)+\frac{\partial\vec{B}(\vec{r},t)}{\partial t}=0;$$

$$\nabla\cdot\vec{B}(\vec{r},t)=0;\text{ and }\nabla\times\vec{B}(\vec{r},t)-\mu_0\varepsilon_0\frac{\partial\vec{E}(\vec{r},t)}{\partial t}=0. \tag{4.34}$$

Calculate

$$\nabla\times\left[\nabla\times\vec{E}(\vec{r},t)+\frac{\partial\vec{B}(\vec{r},t)}{\partial t}\right]=\nabla\cdot(\nabla\cdot\vec{E})-\nabla^2\vec{E}+\frac{\partial(\nabla\times\vec{B}(\vec{r},t))}{\partial t}=0,$$

and thus, $$\nabla^2\vec{E}=-\mu_0\varepsilon_0\frac{\partial^2\vec{E}}{\partial t^2}. \tag{4.35}$$

This is a wave equation and the speed of the electromagnetic wave is $c = 1\big/\sqrt{\mu_0\varepsilon_0} = 2.99\times10^8$ m/s.

Similarly, $\nabla\times(\nabla\times\vec{B}) = \frac{1}{c^2}\nabla\times\left(\frac{\partial\vec{E}}{\partial t}\right)$, which becomes another wave equation, $\nabla^2\vec{B} = \frac{1}{c^2}\frac{\partial^2\vec{B}}{\partial t^2}$.

(4.36)

4.5 HUYGENS'S PRINCIPLE AND GREEN'S FUNCTION

Huygens's principle explains how and where waves propagate. It states that every point on a wavefront itself is the source of spherical wavelets [6]. The sum of these spherical wavelets forms a new wavefront. Here, we describe the principle in non-rigorous mathematics in an analogy of electric potential in the next chapter (Section 4.3).

Suppose there is a distribution of charge density$\rho(\vec{r})$, the electric potential is given by

$$\phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_V \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}' \tag{4.37}$$

where ε_0 is the permittivity of free space and the integral is for volume. As we explain in Section 4.3.1, the potential satisfies the Poisson equation

$$\nabla^2\phi(\vec{r}) = -\frac{\rho(\vec{r})}{\varepsilon_0}. \tag{4.38}$$

Suppose we have a differential equation

$$\nabla^2\phi(\vec{r}) = F(\vec{r}), \tag{4.39}$$

a special solution of this differential equation should be given by

$$\phi(\vec{r}) = -\frac{1}{4\pi}\int_V \frac{F(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3\vec{r}' \text{ by replacing } -\frac{\rho(\vec{r})}{\varepsilon_0} \text{ with } F(\vec{r}). \tag{4.40}$$

If $F(\vec{r})$ is the Dirac's delta function $\delta(\vec{r})$, the solution 3.22 becomes

$$\phi(\vec{r}) = -\frac{1}{4\pi}\int_V \frac{1}{|\vec{r}-\vec{r}'|}d^3\vec{r}'. \tag{4.41}$$

The integrant of Equation 3.23, $G(\vec{r},\vec{r}') = -1/4\pi(|\vec{r}-\vec{r}'|)$, is called Green's function of $\nabla^2\phi(\vec{r}) = \delta(\vec{r})$, and it is a fundamental solution of the Laplace equation $\nabla^2\phi(\vec{r}) = 0$.

The special solution 3.23 of the differential equation 3.21 and the fundamental solution of the Laplace equation constitute a general solution of the differential equation 3.21.

$$G(\vec{r},\vec{r}') = -\frac{1}{4\pi(|\vec{r}-\vec{r}'|)} - \frac{1}{4\pi}\int_V \frac{F(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3\vec{r}'. \tag{4.42}$$

By an analogous argument, we can construct a general solution of the differential equation

$$\nabla^2\phi(\vec{r}) + k^2\phi(\vec{r}) = F(\vec{r}). \tag{4.43}$$

Green's function for the differential equation, a special solution of differential equation 4.43 is given by

$$-\frac{1}{4\pi}\int_V \frac{e^{i\vec{k}|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} F(\vec{r}')d^3\vec{r}', \tag{4.44}$$

and the fundamental solution of the Helmholtz differential equation

$$\nabla^2\phi(\vec{r}) + k^2\phi(\vec{r}) = 0 \tag{4.45}$$

is given by a linear combination of plane waves,$e^{\pm i\vec{k}\cdot\vec{r}}$, and a general solution of Equation 4.45 is given by

$$\phi(\vec{r}) = ae^{i\vec{k}\cdot\vec{r}} + be^{-i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int_V \frac{e^{i\vec{k}|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} F(\vec{r}')d^3\vec{r}'. \tag{4.46}$$

The special solution 4.44 is a spherical wave generated at each point $\vec{r}'$ and that is what Huygens's principle states. For a more rigorous description of Huygens's principle, refer to the advanced book of electrodynamics and optics [7].

SUGGESTED FURTHER STUDY

Wave optics including Huygens's principle and Snell's law discussed in Chapter 3 can be established with Maxwell's equation. Refer to advanced textbooks on electrodynamics for these subjects [8].

REFERENCES

1. Lorrain P and Corson D, *Electromagnetic Fields and Waves*, W.H. Freeman and Company, 1907. https://iopscience.iop.org/article/10.1088/0143-0807/30/6/018/pdf#:~:text=The%20permissible%20use%20of%20different%20combinations%20gives%20rise,signals%20are%20propagated%20with%20an%20arbitrary%20gauge%20velocity.
2. *Numerical Methods – Using Excel to Solve by Iteration*, Elmhurst University. https://crawford.elmhurst.edu/classes/m342/2010S/sec7.1_Excel_instructions.pdf.
3. Wong CW, *Maxwell Equations and the Redundant Gauge Degree of Freedom*, European Journal of Physics, 2009. https://iopscience.iop.org/article/10.1088/0143-0807/30/6/018/pdf#:~:text=The%20permissible%20use%20of%20different%20combinations%20gives%20rise,signals%20are%20propagated%20with%20an%20arbitrary%20gauge%20velocity.

4. Likharev KK, *Vector Potential and Ampère Law: Physics LibreTexts*, Stony Brook University. https://phys.libretexts.org/Bookshelves/Electricity_and_Magnetism/Essential_Graduate_Physics_-_Classical_Electrodynamics_(Likharev)/05%3A_Magnetism/5.02%3A_Vector_Potential_and_the_Ampere_Law.
5. *Maxwell's Equations and Electromagnetic Waves*, MIT OpenCourseWare. https://ocw.mit.edu/courses/8-02-physics-ii-electricity-and-magnetism-spring-2007/2d2f227e6fd26ee25f366759e02f03dc_chapte13em_waves.pdf.
6. Ling SJ, Sanny J, and Moebs W, *Huygens's Principle*, University Physics Vol. 3: OpenStax, Rice University, 2021. https://pressbooks.online.ucf.edu/osuniversityphysics3/chapter/huygenss-principle/.
7. Fowler GR, *Introduction to Modern Optics*, Dover Publications, 2012. Zoboko.com: https://zoboko.com/book/jmovree3/introduction-to-modern-optics.
8. Jackson JD, *Classical Electrodynamics*, John Wiley & Sons, Inc., 1999. https://archive.org/details/john-david-jackson-classical-electrodynamics-wiley-1999.

Entropy

Entropy is one of the important concepts in physics and other fields. Yet, we do not have enough time to contemplate it with examples. Here, we consider the entropy of ideal gas, regular solution, spin system, and quantum harmonic oscillators. There are phenomena where changes in entropy cause interesting consequences. For example, adiabatic demagnetization on reaching a temperature below 1 mK is a fascinating application of entropy and can be modeled with a set of N-independent spins. Although the numerical calculation of change in entropy of two substances of known specific heat capacities and initial temperatures is a typical introductory physics problem, its "general proof" is not discussed. This book shows a diagram of the thermodynamic entropy change only with ratios of specific heat capacity and masses and given initial temperatures.

Although entropy of information may not be introduced in physics courses, it is a vital concept even in the economy of these days. We introduce popular concepts such as the probability distribution of maximum entropy and one-factor entropy. H-function and entropy in Markov processes are also described to validate the increasing entropy. Negative entropy proposed by Erwin Schrödinger is also explained in relation to information science.

5.1 THERMODYNAMIC VARIABLES

This section summarizes the basic properties of thermodynamics of ideal gas of N molecules, having pressure P, temperature T, and volume V [1]. The equation of ideal gas, $PV = Nk_BT$, connects these state variables to express its thermal state.

The first law of thermodynamics states the change in internal energy of a system while absorbing heat and receiving work done on the system: $\Delta E = \Delta Q + \Delta W$, where ΔQ is the heat absorbed by the system and ΔW is the work done on the system. For the ideal gas, $\Delta W = -\int PdV$. The beauty of the first law is that work and heat are not state variables, i.e., they depend on the thermodynamic process but the internal energy is a state variable, and the change in the internal energy does not depend on the thermodynamic processes. In particular, the internal energy of ideal gas depends only on the temperature of the system.

DOI: 10.1201/9781003516347-5

The second law of thermodynamics has various statements. Since we focus on entropy, we use entropy change to state the second law. By the definition of Clausius, the second law states that the change in entropy is $dS = dQ/T$, where dQ is the heat absorbed by the system and T is the absolute temperature of the system during an infinitesimally small reversible process, and $dS \geq 0$ i.e., the entropy of an isolated system never decreases. For an irreversible process, we use the entropy change of a reversible process with the same initial and final states.

The probability that a thermodynamic system at temperature T has internal energy E is given by the canonical ensemble,

$$p(E) = \frac{\Omega(E)\exp(-\beta E)}{Z(T,N)} \text{ where } \beta = \frac{1}{k_B T}. \tag{5.1}$$

In Equation 5.1, $\Omega(E)$ is the number of microscopic states for a given internal energy E, k_B is the Boltzmann constant, and N is the number of particles. The denominator $Z(T, N)$ of Equation 5.1 is called the distribution function,

$$Z(E) = \int \Omega(E)\exp(-\beta E)dE = \int \exp\left[-\left(\beta E - \ln\Omega(E)\right)\right]dE. \tag{5.2}$$

Using the distribution function, thermodynamic functions can be calculated. For example, the average internal energy is

$$\langle E\rangle = \int Ep(E)dE = -\frac{\partial}{\partial\beta}\ln Z(T,N). \tag{5.3}$$

Suppose the distribution function is at its maximum value when $E = E^*$ then the distribution function can be approximated with

$$Z(T,N) \approx \exp\left[-(\beta E^* - \ln\Omega(E^*))\right], \text{ and thus } \ln Z(T,N) = -[\beta E^* - \ln\Omega(E)].$$

Therefore, the Helmholtz free energy may be expressed as

$$F(T,N) = -\frac{1}{\beta}\ln Z(T,N) = E^* - \frac{1}{\beta}\ln\Omega(E) = E^* - TS, \tag{5.4}$$

where entropy S is defined by $S = k_B T \ln\Omega(E)$. Recall that the change in the entropy is thermodynamically defined by $dS = dQ/T$. We bridge these two definitions of entropy in Section 5.2. Once the Helmholtz free energy is calculated,

$$P = -\left(\frac{\partial F}{\partial V}\right)_T \text{ and } S = -\left(\frac{\partial F}{\partial T}\right)_V \tag{5.5}$$

from the change in the free energy, $dF = dE - SdT - PdV$.

5.2 ENTROPY OF AN IDEAL GAS

5.2.1 Change in Entropy during Free Expansion

For obtaining a change in entropy while an ideal gas undergoes free expansion where its volume expands from V_i to V_f, and pressure changes from P_i to P_f, we calculate the equivalent entropy change of isothermal expansion of the same initial and the final states. Note that there is no change in the internal energy because the internal energy of an ideal gas depends only on T. Thus, according to Clausius's definition,

$\Delta S = \int_i^f \frac{dQ}{T} = \frac{1}{T}\Delta Q$ and $\Delta Q = \Delta W = \int_i^f PdV$ because $\Delta E = 0$ for the isothermal process.

Using the ideal gas equation, $\Delta W = \int_i^f \frac{Nk_B T}{V} dV = Nk_B T \ln\left(\frac{V_f}{V_i}\right)$, and the entropy change during an isothermal expansion is given by

$$\Delta S = \frac{\Delta Q}{T} = Nk_B \ln\left(\frac{V_f}{V_i}\right). \tag{5.6}$$

Following Boltzmann, we may consider the entropy change from the "microscopic state" of an ideal gas during the free expansion. Below is a simplified version of his argument. Assume that each particle occupies a microscopic cell of volume V_m. The number of possible allocations of a single particle in a bulk volume V is given by V/V_m. Because $V >> V_m$, $V - V_m \approx V$, and even $V - N \bullet V_m \approx V$. Then, the number of allocating N particles in the bulk volume V is given by $\Omega = (V/V_m)^N$. Therefore, when the volume of the gas expands from V_i to V_f, the number of microscopic states changes from $\Omega_i = (V_i/V_m)^N$ to $\Omega_f = (V_f/V_m)^N$, and we obtain

$$\frac{\Omega_f}{\Omega_i} = \frac{\left(V_f / V_m\right)^N}{(V_i / V_m)^N} = \left(\frac{V_f}{V_i}\right)^N. \tag{5.7}$$

One may formulate entropy based on the number of microscopic states by comparing Equation 5.6 with Equation 5.7 to obtain

$$\Delta S = Nk_B \ln\left(\frac{V_f}{V_i}\right) = k_B \ln\left(\frac{V_f}{V_i}\right)^N = k_B \ln\left(\frac{\Omega_f}{\Omega_i}\right).$$

Thus, the entropy of the ideal gas may be expressed as

$$S = k_B \ln \Omega = Nk_B \ln V. \tag{5.8}$$

The derivations of the number of microscopic states of an ideal gas are shown in standard textbooks [2]. From the classical mechanics,

$$\Omega(E) = \frac{3N}{2} C_{3N} (2m)^{3N/2} V^N E^{(3N/2)-1} \tag{5.9}$$

where $C_{3N} = \dfrac{\pi^{3N/2}}{\Gamma\left(\dfrac{3N}{2}+1\right)}$ is the volume of a $3N$-dimensional unit sphere and $\Gamma(x)$ is a Gamma function described in Section 6.5.5. From the Schrödinger equation,

$$\Omega(E) = \frac{3N}{2} C_{3N} \left(\frac{2m}{h^2}\right)^{3N/2} V^N E^{(3N/2)-1}. \tag{5.10}$$

The essential part of the entropy of an ideal gas is given by $S = Nk_B \ln V$ from both classical and quantum systems.

5.2.2 Mixing Entropy

Assume two ideal gas systems of *the same pressure and temperature* but different numbers of particles and volume: $PV_1 = N_1k_BT$ and $PV_2 = N_2k_BT$. Each of them is placed in two separate compartments of volume V_1 and V_2 of a box with the total volume $V = V_1 + V_2$.

Imagine there is a partition between the compartments. By removing the partition, we can mix the gases. The equation of the mixed gas is given by $PV = Nk_BT$. Because $V = V_1 + V_2$ and $N = N_1 + N_2$, $V_1 = N_1V/N$ and $V_2 = N_2V/N$, and the entropies are given by

$$S_1 = N_1 k_B \ln V_1 = N_1 k_B \ln\left(N_1 V / N\right), \text{ and } S_2 = N_2 k_B \ln V_2 = N_2 k_B \ln(N_2 V / N). \tag{5.11}$$

Before mixing, the total entropy is the sum of S_1 and S_2, that is,

$$S_1 + S_2 = N_1 k_B \ln\left(N_1 V / N\right) + N_2 k_B \ln\left(N_2 V / N\right) = N \ln V + k_B\left[N_1 \ln(N_1/N) + N_2 \ln(N_2/N)\right].$$

After mixing, the entropy of the mixed gas is $S = Nk_B \ln V$, and thus, the change in entropy by mixing is

$$\begin{aligned} \Delta S = S_{mix} - (S_1 + S_2) &= -k_B\left[N_1 \ln(N_1/N) + N_2 \ln(N_2/N)\right] \\ &= k_B\left[N_1 \ln(N/N_1) + N_2 \ln(N/N_2)\right] > 0. \end{aligned} \tag{5.12}$$

Figure 5.1 is a screenshot of the calculation of the mixing entropy given by Equation 5.10. The total number of gas particles is kept to $N = 100$ while changing N_1 and N_2 from 1 to 99.

Figure 5.2 shows the dependence of the mixing entropy on the mixing ratio N_1/N_2. The mixing entropy becomes maximum when $N_1 = N_2$.

5.2.3 Gibbs Paradox

Imagine that a box has two parts of equal volume V separated with a partition. Place two *different* ideal gases (e.g., two different kinds of inert gases) of *the same* V, T, and N into the box. Each of the gas systems is placed into each of the two separate parts of the box. Using the calculation in Section 5.2.2, the total entropy before mixing is $S_{tot} = S_1 + S_2 = 2Nk_B \ln V$, where $N_1 = N_2 = N$. Next, remove the partition to mix the gases. Each gas expands to the

	A	B	C	D	E	F
1	Mixing two gasses			N1+N2	100	
2						
3	N1	N2	ΔS			
4	1	99	5.600153			
5	2	98	9.803911			
6	3	97	13.47422			
7	4	96	16.79441			
8	5	95	19.85152			
9	6	94	22.69675			
10	7	93	25.36389			
11	8	92	27.87694			

Enter `=($E$1/A4)*Ln($E$1/A4) + (1-$E$1/A4)* Ln(1-$E$1/A4)` and apply *AutoFill*.

FIGURE 5.1 Calculation table of mixing entropy.

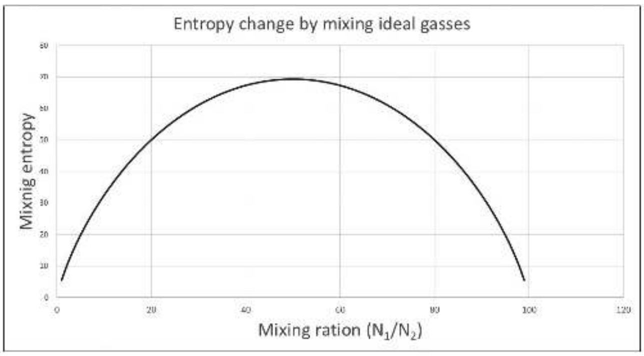


FIGURE 5.2 Mixing entropy of ideal gases.

volume of 2*V*, and the entropy after mixing should be $S'_{tot} = 2Nk_B\ln(2V)$, and the entropy change by mixing should be given by $S'_{tot} - S_{tot} = 2k_B\ln 2 > 0$.

Now, consider the same mixing procedure using two sets of gases of the *same* kind. Because the gases are identical, the "mixing" has no meaning, and entropy should exhibit no change. Since N, T, P, and V do not reflect the particle types, the above result of entropy change by mixing should be applicable even for the two sets of the same kind of ideal gas. This could be a paradox [3].

Is this really a paradox? The calculations of the number of microscopic states described in Section 5.2.1 did not consider the indistinguishability of the identical particles, which affects the number of allocating N particles. Back to Equation 5.8, we should have used

$$S = k_B \ln\left(\frac{V^N}{N!}\right) = Nk_B \ln V - k_B \ln N! \approx Nk_B \ln V - k_B\left(N\ln N - N\right) \tag{5.13}$$

where we used the Stirling formula, $\ln N! \approx N\ln N - N$ for $N >> 1$.

Using the Stirling formula again, the total entropy of the two ideal gases of the same type should be

$$S_{tot} = 2\left(Nk_B \ln V - k_B \ln N!\right) \approx 2Nk_B \ln V - 2k_B N\ln N + 2k_B N \text{ before mixing,}$$

and

$S'_{tot} = 2Nk_B \ln(2V) - k_B \ln[(2N)!] = 2Nk_B \ln(2V) - 2k_B N \ln(2N) + 2k_B N$ after mixing. Thus, the mixing entropy is $S_{mix} = S'_{tot} - S_{tot} = 0$ as we expect.

How about mixing two sets of ideal gases of *different numbers of particles* (N_1 and N_2) *and different volumes* (V_1 and V_2) *and pressures* (P_1 and P_2) to reach the final state of $N = N_1 + N_2$, $V = V_1 + V_2$, and T? Using Equation 5.11,

$$S_1 = N_1 k_B \ln\left(\frac{N_1 V}{N}\right) - k_B \ln N_1! \text{ and } S_2 = N_2 k_B \ln\left(\frac{N_2 V}{N}\right) - k_B \ln N_2!.$$

$$S'_{tot} = k_B \ln\left(\frac{V^N}{N_1! N_2!}\right) = Nk_B \ln V - k_B \ln(N_1!) - k_B \ln(N_2!).$$

Therefore, the change of entropy by mixing is calculated below, which results in the same as Equation 5.12.

$$\begin{aligned} S_{mix} &= S'_{tot} - (S_1 + S_2) = Nk_B \ln V - N_1 k_B \ln\left(\frac{N_1 V}{N}\right) - N_2 k_B \ln\left(\frac{N_2 V}{N}\right) \\ &= Nk_B \ln V - (N_1 + N_2) k_B \ln V - k_B \left[N_1 \ln\left(\frac{N_1}{N}\right) + N_2 \ln\left(\frac{N_2}{N}\right) \right] \\ &= k_B \left[N_1 \ln\left(\frac{N}{N_1}\right) + N_2 \ln\left(\frac{N}{N_2}\right) \right] = Nk_B \left[\left(\frac{N_1}{N}\right) \ln\left(\frac{N}{N_1}\right) + \left(\frac{N_2}{N}\right) \ln\left(\frac{N}{N_2}\right) \right]. \end{aligned} \tag{5.14}$$

It is remarkable that the indistinguishable property of identical particles that appeared in quantum mechanics must be considered when mixing the entropy of an ideal gas!

5.2.4 Mixing Entropy of Ideal Solutions

An ideal solution or an ideal mixture is a solution that exhibits thermodynamic properties analogous to those of a mixture of ideal gases [4, 5]. Consider mixing two components of molecules N_1 and N_2 in a solution with volume. We use the lattice model of the solution. Suppose there are N lattices in volume V. Let b^3 be the volume of a lattice cell, then $V = b^3 N$, and there will be no vacancy, i.e., $N = N_1 + N_2$. Mathematically, this model is very much similar to mixing two ideal gases as discussed earlier, and the total number of N_1 molecules and N_2 molecules in the volume is

$$\begin{aligned} S &= k_B \ln\left(\frac{N_t!}{N_1! N_2!}\right) = k_B \left[N \ln N + N_t - \left(N_1 \ln N_1 + N_1 - N_2 \ln N_2 + N_2 \right) \right] \\ &= k_B \left[(N_1 + N_2) \ln N_t - N_1 \ln N_1 - N_2 \ln N_2 \right] \\ &= k_B \left[N_1 \ln\left(\frac{N_t}{N_1}\right) + N_2 \ln\left(\frac{N_t}{N_2}\right) \right] = Nk_B \left[\frac{N_1}{N_t} \ln\left(\frac{N_t}{N_1}\right) + \frac{N_2}{N_t} \ln\left(\frac{N_t}{N_2}\right) \right]. \end{aligned} \tag{5.15}$$

The mixing entropy has the same dependence on N_1 and N_2 as shown in Figure 5.1.

5.3 THERMODYNAMICS OF TWO-LEVEL SYSTEMS

5.3.1 Spin 1/2 Particles in a Uniform Magnetic Field

Suppose there are N independent spins in a magnetic field B. Each spin can take either the spin up state of energy $-\mu_B B = -\varepsilon_0$ or the spin down state of energy $+\mu_B B = +\varepsilon_0,$ where μ_B is the magnetic moment [6]. The total magnetic energy is $E = (N_d - N_u)\,\varepsilon_0 = M\varepsilon_0,$ where N_d is the number of down spins and N_u is the number of up spins, $N = N_d + N_u$, and $M = N_d - N_u.$

The number of possible spin configurations is given by

$$\Omega_N = \frac{N!}{\left[(1/2)(N-M)!\right]\left[(1/2)(N+M)!\right]}, \tag{5.16}$$

and the entropy of this spin system is given by

$$S = -k_B\left[N_u \ln\left(\frac{N_u}{N}\right) + N_d \ln\left(\frac{N_d}{N}\right)\right] = Nk_B\left[p\ln(1/p) + (1-p)\ln(1/1-p)\right] \tag{5.17}$$

where $p = N_d/N$ and $N_u/N = 1 - p$. Similar to the ideal gas as shown in Figure 5.2, entropy is at its maximum when $p = 0.5$. The temperature of the system is given by

$$\frac{1}{T} = \frac{1}{\varepsilon_0}\frac{\partial S}{\partial M} = \frac{1}{2}\frac{k_B}{\varepsilon_0}\ln\left(\frac{N-M}{N+M}\right). \tag{5.18}$$

Note that if $M > 0$ (or $E > 0$), then the temperature will be negative, $T < 0$. That is, the system is not normal because of the negative temperature. On the other hand, if $M < 0$ (or $E < 0$), then $T > 0$. This is acceptable and we consider $M < 0$.

Figure 5.3 shows a screenshot of these calculations using the *AutoFill* feature.

Figure 5.4 shows entropy (S/Nk_B) vs energy ($E/N\varepsilon_0$), where the positive and negative temperature regions appear.

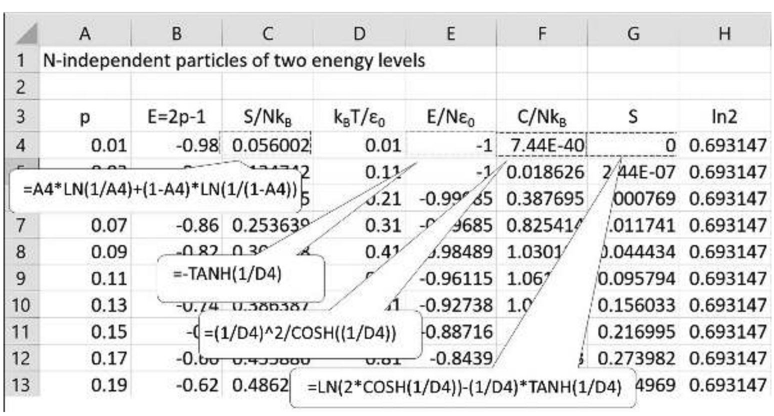


FIGURE 5.3 Calculation of two-level system.

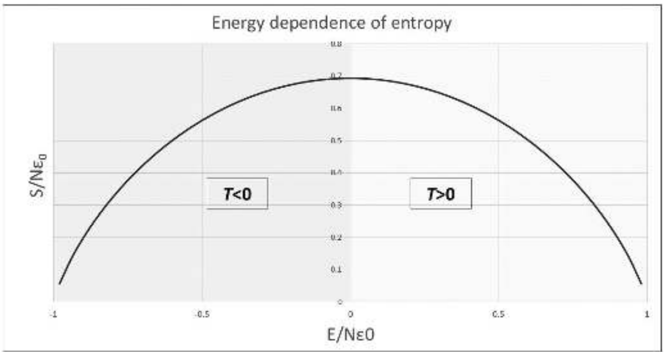


FIGURE 5.4 Entropy vs energy.

For $T > 0$,

$$\frac{N-M}{N+M} = \frac{N_d}{N_u} = \exp\left(\frac{2\varepsilon_0}{k_B T}\right) \text{ from equation (5.18).}$$

Thus, we obtain

$$\frac{N_d}{N} = \frac{\exp(\varepsilon_0 / k_B T)}{\exp(\varepsilon_0 / k_B T) + \exp(-\varepsilon_0 / k_B T)} \text{ and } \frac{N_u}{N} = \frac{\exp(-\varepsilon_0 / k_B T)}{\exp(\varepsilon_0 / k_B T) + \exp(-\varepsilon_0 / k_B T)}. \quad (5.19)$$

Hence, using Equation 5.19, $E = -(N_d - N_u)\varepsilon_0 = -N\varepsilon_0 \tanh\left(\varepsilon_0 / k_B T\right)$. Figure 5.5 shows energy ($E/N\varepsilon_0$) vs temperature ($k_B T/\varepsilon_0$).

The specific heat capacity, $C = dE/dT$, is also calculated below.

$$C = Nk_B \frac{\left(\varepsilon_0 / k_B T\right)^2}{\cosh^2\left(\varepsilon_0 / k_B T\right)} = Nk_B \left(\frac{\varepsilon_0}{k_B T}\right)^2 \frac{\exp(2\varepsilon_0 / k_B T)}{[1 + \exp(2\varepsilon_0 / k_B T)]^2}. \quad (5.20)$$

Figure 5.6 shows the temperature dependence of specific heat capacity (C/Nk_B). This type of specific heat capacity is called the Schottky type [7].

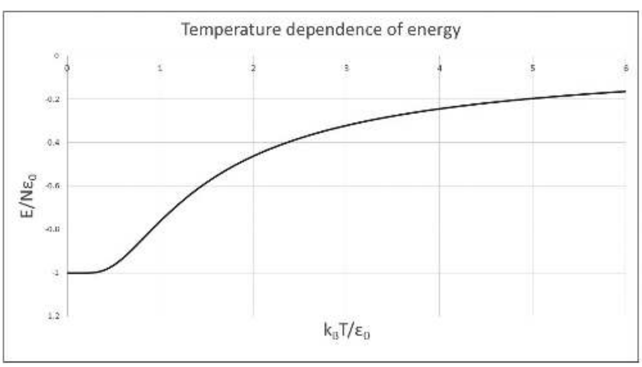


FIGURE 5.5 Temperature dependence of energy.

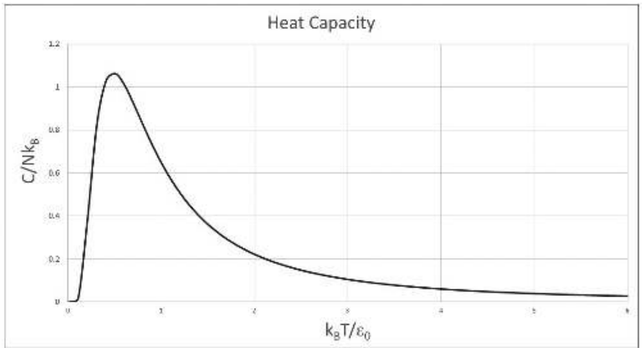


FIGURE 5.6 Schottky type heat capacity of the N-spin system.

5.3.2 Adiabatic Demagnetization

Using the independent spin system described earlier, we may explain the basic idea of adiabatic demagnetization to achieve micro-Kelvin temperature [8]. We apply the canonical distribution or the partition function Z_N to express entropy as a function of temperature. For an N-independent spin system at temperature $\beta = 1/k_B T$,

$$Z_N = \sum_{s_1=\pm 1}\sum_{s_2=\pm 1}\cdots\sum_{s_N=\pm 1}\exp\left(\beta\mu_B B\sum_{i=1}^{N} s_i\right) = Z_1^N \tag{5.21}$$

where $Z_1 = \sum_{s=\pm 1}\exp\left(-\beta\mu_B Bs\right) = 2\cosh(\beta\mu_B B)$. The entropy can be calculated using Equation 5.5.

$$S = -\left(\frac{\partial F}{\partial T}\right) = k_B\beta\left(\frac{\partial F}{\partial \beta}\right) = -Nk_B\beta\left(\frac{\partial}{\partial \beta}(2\cosh(\beta\mu_B B)\right). \tag{5.22}$$

$$\frac{S}{Nk_B} = \frac{1}{\beta}\ln\left(2\cosh(\beta\mu_B B)\right) - \mu_B B\tanh(\beta\mu_B B). \tag{5.23}$$

The cooling steps are as follows:

1) Ramp up the magnetic field from B_1 to B_2 isothermally at temperature T_1. Spins are aligned more and the entropy decreases at an initial temperature T_1; and
2) Ramp down the magnetic field from B_2 to B_1 adiabatically. Since the entropy does not change in this adiabatic process, the argument $\beta\mu_B B$ remains the same, i.e., $\beta_1\mu_B B_2 = \beta_2\mu_B B_1$ *and* $B_2 > B_1$. Thus, $\beta_2 > \beta_1$ or $T_2 < T_1$. The system temperature decreases to T_2.

Figure 5.7 shows a graph of the calculated entropy expression 5.23 with $\mu_B B_1 = 0.1$ and $\mu_B B_2 = 0.2$.

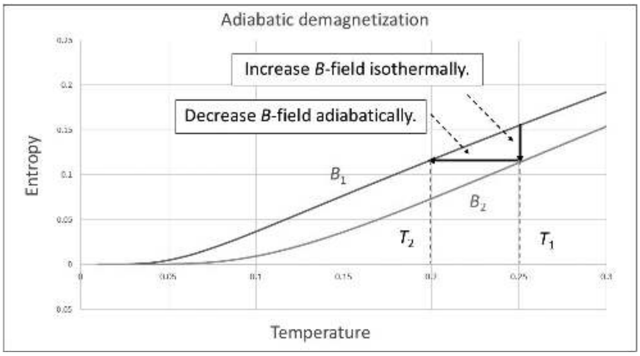


FIGURE 5.7 Model of adiabatic demagnetization.

Note: ***Negative thermodynamic temperature***. If the temperature is negative, the factor $\exp(-E/k_BT)$ in the canonical distribution 5.1 could be infinite, which is unacceptable from a thermodynamics viewpoint as thermal equilibrium states do not have a negative temperature [9]. However, it is possible to create a transient state with a negative temperature. For example, imagine a spin system where spins are lined up in an external magnetic field in the positive z-direction. The spin distribution will have a population inversion where the number of up spins is more than that of the down spins. If the magnetic field is reversed quickly, the spin distribution momentarily creates a negative temperature because the spins of higher energy states are more than those of lower energy states. A new thermal equilibrium state will be established soon with a positive temperature and energy exchange in an interaction other than the spin interaction. Note that if we use a temperature scale $ß = 1/k_BT$, the negative temperature is higher than the positive temperature!

5.3.3 N-Independent Quantum Oscillators

For the energy level of a quantum harmonic oscillator, the total energy of N-independent oscillators is $E = N(n + 1/2)\hbar\omega = N(M/N + 1/2)$, where $M = N\bullet n$, and $n = 0, 1, 2, 3, \ldots$ Denote the quantum number of the i-th oscillator as n_i. The total energy is

$$E = \left(\frac{1}{2}N + M\right)\hbar\omega \tag{5.24}$$

where

$$\sum_{i=1}^{N} n_1 = M. \tag{5.25}$$

The number of possible configurations is equal to the number of possible allocations of M balls into N boxes. Because $n_i = 0$ is allowed, an empty box is also allowed. Thus, the number of possible configurations is equal to the number of possible ways to line up M white balls (corresponding to oscillators) and (N–1) black balls (corresponding to empty boxes). Note that the white balls are indistinguishable and so are the black balls. Therefore,

$$\Omega(E) = \frac{(M+N-1)!}{M!(N-1)!}. \tag{5.26}$$

Entropy is given by $S = k_B \ln \Omega(E) \approx k_B \left[(M+N)\ln(N+M) - M\ln M - N\ln N \right]$. (5.27)

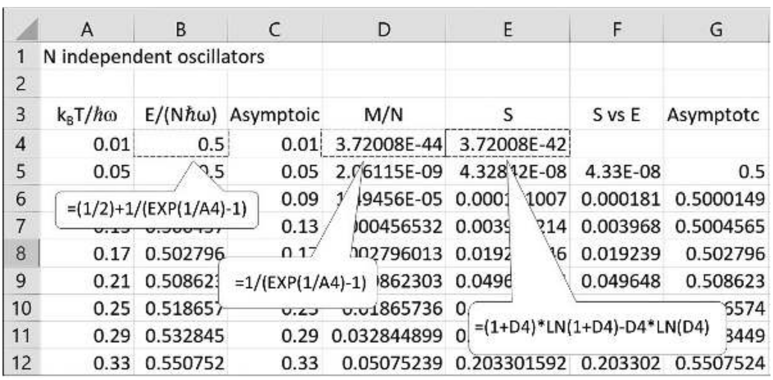
Temperature is $\dfrac{1}{T} = \dfrac{\partial S}{\partial E} = \dfrac{\partial S}{\partial M}\dfrac{\partial M}{\partial E} = \dfrac{k_B}{\hbar\omega}\ln\left[\dfrac{(E/N)+(1/2)\hbar\omega}{(E/N)-(1/2)\hbar\omega}\right]$,

and conversely

$$\frac{(E/N)+(1/2)\hbar\omega}{(E/N)-(1/2)\hbar\omega} = \exp\left(\frac{\hbar\omega}{k_B T}\right) \text{ and } E = N\hbar\omega\left[\frac{1}{2} + \frac{1}{\exp(\hbar\omega/k_B T)-1}\right]. \tag{5.28}$$

Figure 5.8 shows a screenshot of the calculation of energy and entropy of N-independent quantum oscillators.

Figure 5.9 shows the temperature ($k_B T/\hbar\omega$) dependence of energy ($E/N\hbar\omega$). As the temperature increases, energy approaches the classical system. For calculations of M/N and entropy, use Equations 5.27 and 5.28.



	A	B	C	D	E	F	G
1	N independent oscillators						
2							
3	kBT/ħω	E/(Nħω)	Asymptoic	M/N	S	S vs E	Asymptotc
4	0.01	0.5	0.01	3.72008E-44	3.72008E-42		
5	0.05	[illegible]	0.05	[illegible]	[illegible]	4.33E-08	0.5
6	[illegible]	[illegible]	0.09	[illegible]	[illegible]	0.000181	0.5000149
7	[illegible]	[illegible]	0.13	[illegible]	[illegible]	0.003968	0.5004565
8	0.17	0.502796	[illegible]	[illegible]	[illegible]	0.019239	0.502796
9	0.21	[illegible]	[illegible]	[illegible]	[illegible]	0.049648	0.508623
10	0.25	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
11	0.29	0.532845	0.29	0.032844899	[illegible]	[illegible]	[illegible]
12	0.33	0.550752	0.33	0.05075239	0.203301592	0.203302	0.5507524

FIGURE 5.8 Calculation of N quantum oscillators.

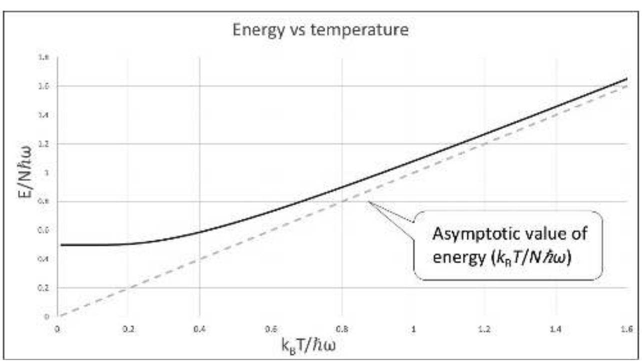


FIGURE 5.9 Temperature dependence of energy of N quantum oscillators.

Using the Stirling formula, the entropy Equation 5.27 can be modified to

$$\frac{S}{Nk_B} = \left(1+\frac{M}{N}\right)\ln\left(1+\frac{M}{N}\right) - \left(\frac{M}{N}\right)\ln\left(1+\frac{M}{N}\right). \tag{5.29}$$

From Equations 5.28, $\frac{M}{N} = \frac{E}{N\hbar\omega} - \frac{1}{2} = x - \frac{1}{2}$ where $x = \frac{E}{N\hbar\omega}$. (5.30)

With Equation 5.30, entropy 5.29 becomes

$$\frac{S}{Nk_B} = \left(x+\frac{1}{2}\right)\ln\left(x+\frac{1}{2}\right) - \left(x-\frac{1}{2}\right)\ln\left(x+\frac{1}{2}\right). \tag{5.31}$$

Figure 5.10 shows the energy ($x = E/N\hbar\omega$) dependence of entropy (S/Nk_B).

5.3.4 Change in Entropy of Two Substances after Making Thermal Contact

Refer to a popular exercise problem relating to entropy in general physics to calculate the entropy change of two substances of known masses and specific heat capacities after reaching thermal equilibrium by thermal contact [10]. The entropy change is given by

$$\Delta S = \int_{T_1}^{T}\frac{dQ_1}{T} + \int_{T_2}^{T}\frac{dQ_2}{T} = m_1c_1\int_{T_1}^{T}\frac{dT}{T} + m_2c_2\int_{T}^{T}\frac{dT}{T} = m_1c_1\ln\left(\frac{T}{T_1}\right) + m_2c_2\ln\left(\frac{T}{T_2}\right) \tag{5.32}$$

and the condition of thermal equilibrium is

$$m_1c_1(T-T_1) + m_2c_2(T-T_2) = 0 \tag{5.33}$$

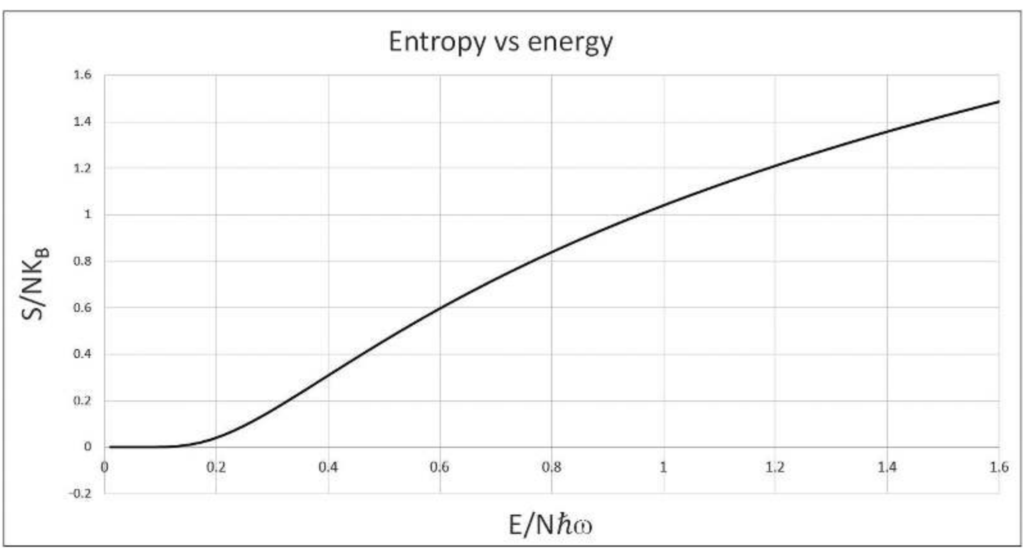


FIGURE 5.10 Energy dependence of entropy.

where T is the equilibrium temperature. While this problem demonstrates that the entropy increases with a given date of masses and specific heat capacities, it is challenging to prove it without numerical data.

Here, we seek a general tendency of the entropy. First, we assume $T_1 > T_2$. Let $T_1 = \alpha T_2$ and $m_1 c_1 = \beta m_2 c_2$, where $\alpha > 1$ with the temperature condition and $\beta > 0$. Using these ratios, Equation 5.32 becomes

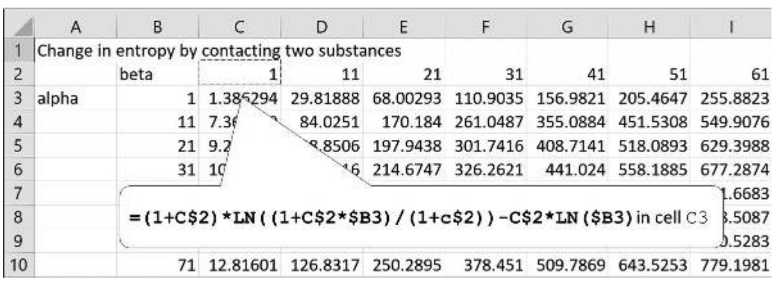
$$\beta(T - \alpha T_2) + (T - T_2) = 0 \text{ or } T = (1 + \alpha\beta)T_2 / (1 + \beta). \tag{5.34}$$

From Equations 5.32 and 5.33, we define "reduced" entropy

$$\Delta\tilde{S} \equiv \frac{\Delta S}{m_2 c_2} = \beta \ln\left[\frac{1+\alpha\beta}{\alpha(1+\beta)}\right] + \ln\left[\frac{1+\alpha\beta}{1+\beta}\right] = (1+\beta)\ln\left(\frac{1+\alpha\beta}{1+\beta}\right) - \beta\ln\alpha. \tag{5.35}$$

Figure 5.11 is a screenshot of the commutation of Equation 5.35. On this spreadsheet, $1 \leq \alpha \leq 1851$ by step 10 and $1 \leq \beta \leq 331$ by step 10.

Figure 5.12 shows the 3D surface chart from the numerical calculation of Equation 5.35, where the ranges of α and β are limited to $1 \leq \alpha \leq 20$ and $0.1 \leq \beta \leq 10.1$. It appears that the entropy is a monotonic increasing function of α and β and never be negative. Although



	A	B	C	D	E	F	G	H	I
1	Change in entropy by contacting two substances								
2		beta	1	11	21	31	41	51	61
3	alpha	1	1.386294	29.81888	68.00293	110.9035	156.9821	205.4647	255.8823
4		11	7.3	84.0251	170.184	261.0487	355.0884	451.5308	549.9076
5		21	9.2	.8506	197.9438	301.7416	408.7141	518.0893	629.3988
6		31	10	6	214.6747	326.2621	441.024	558.1885	677.2874
7		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.6683
8		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.5087
9		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	.5283
10		71	12.81601	126.8317	250.2895	378.451	509.7869	643.5253	779.1981

`=(1+C$2)*LN((1+C$2*$B3)/(1+c$2))-C$2*LN($B3)` in cell C3

FIGURE 5.11 Change in entropy by establishing thermal contact of two substances.

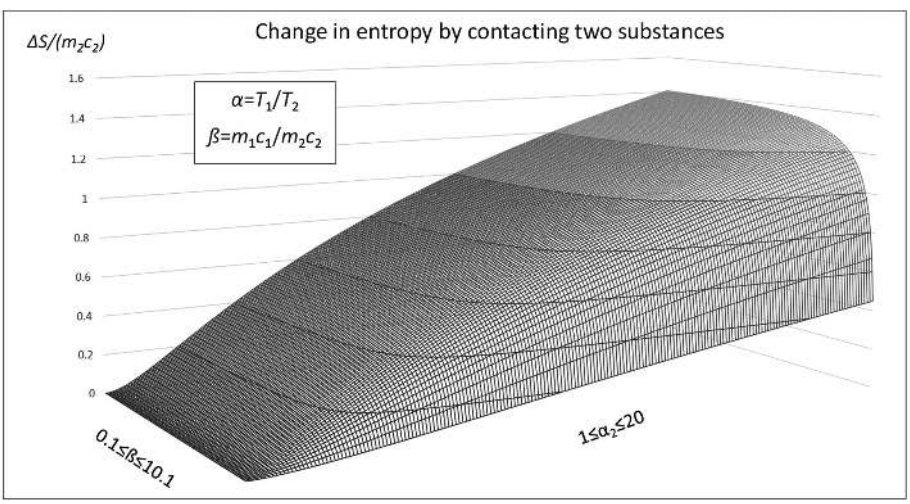


FIGURE 5.12 Change in entropy after making two substances in thermal equilibrium.

we show limited ranges of α and β, expanding their ranges does not change the monotonic increasing tendency.

5.3.5 H-Function and Entropy in Markov Processes

Assume a system is changing its state, following a Markov process that can take finite numbers of state variables x, which may represent a set of several variables, $x_1, x_2, \ldots, x_W$ [11, 12]. Let p_{ji} be the probability of transit from state x_i to state x_j. The conditions on p_{ji} are:

1) In a thermal system, microscopic reversibility means $p_{ji} = p_{ij}$; and

The transition probability p_{ji} satisfies the sum of all possible transitions that must be unity, i.e., $\sum_{j=1}^{W} p_{ji} = 1$.

If the probability that the system is found in the state x_i is $P_i(n)$ after the n^{th} transition, then the probability that the system is found in the state x_j, $P_j(n+1)$ after the $(n+1)^{th}$ transitions is given by

$$P_j(n+1) = \sum_{i=1}^{W} p_{ji} P_i(n). \tag{5.36}$$

Now, consider a convex downward function $f(x)$ where we assume that the variable x follows a probability distribution of a Markov process. Its tangential line is always below $f(x)$ as shown in Figure 5.13. In other words, $f(x) \geq f(<x>) + (\text{constant})(x - <x>)$. Taking an average of $f(x)$, we obtain the following inequality,

$$<f(x)> \geq <f(<x>)> + <(\text{constant})(x - <x>)>.$$

Furthermore, because $<(\text{constant})(x - <x>)> = (\text{constant})<(x - <x>) = 0$,

$$<f(x)> \geq <f(<x>)>. \tag{5.37}$$

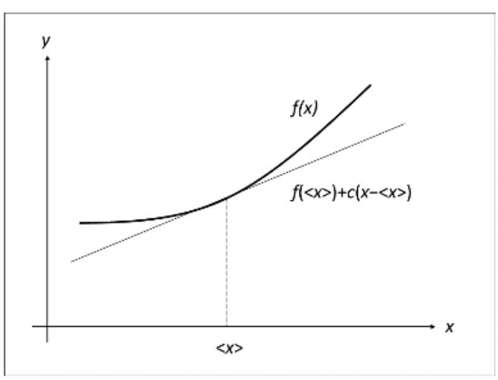


FIGURE 5.13 A convex downward function $f(x)$.

Using Equation 5.36, Equation 5.37 can be interpreted as

$$\sum_{i=1}^{W} p_{ji} f\left(P_i(n)\right) \geq f\left(\sum_{i=1}^{W} p_{ji} P_i(n)\right) = f\left(P_j(n+1)\right). \tag{5.38}$$

Taking the sum of $\sum_{j=1}^{W}$, $\sum_{j=1}^{W}\sum_{i=1}^{W} p_{ji} f\left(P_i(n)\right) = \sum_{i=1}^{W}\left(\sum_{j=1}^{W} p_{ji}\right) f\left(P_i(n)\right) \geq \sum_{j=1}^{W} f\left(P_j(n+1)\right).$ (5.39)

Hence,

$$\sum_{i=1}^{W} f\left(P_i(n)\right) \geq \sum_{j=1}^{W} f\left(P_j(n+1)\right). \tag{5.40}$$

Define H-function as $H(n) \equiv \sum_{j=1}^{W} f\left(P_j(n)\right)$, then $\Delta H = H(n+1) - H(n) \leq 0$ by Equation 5.40.

Therefore, the H-function never increases in a Markov process. Furthermore, if we define entropy,

$$S(n) = -k_B H(n),$$

then we have

$$\Delta S = S(n+1) - S(n) \geq 0, \text{ i.e., the entropy never decreases.}$$

Let $f(x) = x\ln x$. The inequality 5.37 holds, and the above discussion is still valid. Thus,

$$S(n) = -k_B H(n) = -k_B \sum_{i=1}^{W} P_i(n) \ln P_i(n).$$

This is the same entropy form of information we discuss in the next Section 5.4.1. As we will find in the next section, the entropy becomes maximum when $p_i = 1/\Omega$; $i = 1, 2, \ldots, W$, and $S_{max} = k_B \ln\Omega$.

5.4 ENTROPY OF INFORMATION

5.4.1 Quantification of Information and Entropy of Information

When you define the probability of an event occurring as p, $p\sim1$ means the event surely occurs, whereas $p\sim0$ means the event seldom occurs. Using the reciprocal value of probability, called odds, we define self-information,

$$I(p) = K\ln(1/p) = -K\ln(p). \tag{5.41}$$

where the coefficient K is included to compare the entropy of information with that of thermodynamics [13].

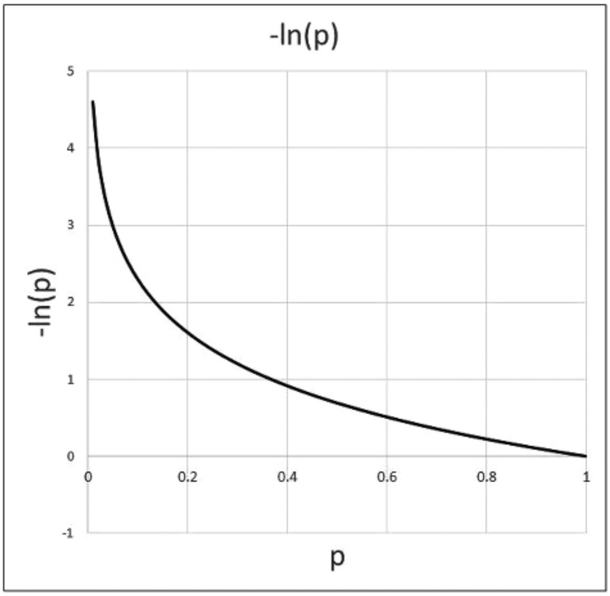


FIGURE 5.14 Self-information.

As shown in Figure 5.14, the self-information is $I(p = 1) = 0$ and becomes a steep function near $p \geq 0$. If something occurs for sure, we do not gain useful information, but if something that would not be expected to occur, the event provides us with much useful information.

We define entropy of information as the expectation value of the self-information:

$$S = -K\sum_i p_i \ln p_i \text{ where } \sum_i p_i = 1. \tag{5.42}$$

What is the probability distribution that leads to maximum entropy? Consider that when the entropy becomes maximum, it is a maximum value for any p_i. Let us apply the Lagrange multiplier to find such a probability distribution. The restriction is that the total probability must be 1. Define

$$L = S(p_1, p_2, \ldots, p_N) + \lambda\left\{\sum_{i=1}^{N} p_i - 1\right\} = 0. \tag{5.43}$$

The function L should satisfy $\dfrac{\partial L}{\partial p_i} = 0;\ i = 1, 2, \ldots, N;$ and $\dfrac{\partial L}{\partial \lambda} = 0.$ (5.44)

1) $\partial L/\partial\lambda = 0$ yields to $\sum p_i = 1.$ (5.45)

2) $$\frac{\partial L}{\partial p_i} = -\frac{\partial}{\partial p_i}\left[K\sum_{j=1}^{N} p_j \ln p_j\right] + \lambda\frac{\partial}{\partial p_i}\left[\sum_{j=1}^{N} p_j\right] = 0, \text{ i.e.,} -K\ln p_i - 1 + \lambda = 0, \tag{5.46}$$

and we obtain $p_i = \exp\left[\left(\lambda - 1\right)/K\right]$.

3) $$\sum_{i=1}^{N} p_i = 1 = \sum_{i=1}^{N} \exp[(\lambda-1)/K] = \exp[(\lambda-1)/K]\sum_{i=1}^{N} 1 = N\cdot\exp[(\lambda-1)/K]. \quad (5.47)$$

Thus, $\exp[(\lambda-1)/K] = \dfrac{1}{N}$ and $p_i = \dfrac{1}{N}$ for $\mathrm{i} = 1, 2, \ldots, N$. (5.48)

In other words, the entropy becomes maximum when the probabilities are all equal to $1/N$. The maximum entropy value is

$$S_{\max} = -K\sum_{i=1}^{n} p_i \ln p_i = -K\sum_{i=1}^{N}\left(\frac{1}{N}\ln\left(\frac{1}{N}\right)\right) = K\ln N. \quad (5.49)$$

5.4.2 Probability Distribution for Maximum Entropy

Assume an event takes positive values of ε_i, $i = 1, 2, \ldots, N$ with the probability of the event being p_i. The average value of information is $E = \sum\varepsilon_\mathrm{i}p_\mathrm{i}$. What is the probability distribution that gives the maximum entropy? In this case, entropy $S = \sum p_\mathrm{i}\ln p_\mathrm{i}$ becomes maximum with the conditions of $\sum p_\mathrm{i} = 1$ and $E = \sum\varepsilon_\mathrm{i}p_\mathrm{i}$. We can also apply the Lagrange multiplier to find such probability distribution with two restrictions, $\sum p_\mathrm{i} = 1$ and $E = \sum\varepsilon_\mathrm{i}p_\mathrm{i}$.

Define

$$L = S(p_1, p_2, \ldots, p_N) + \lambda\left\{\sum_{i=1}^{N} p_i - 1\right\} + \alpha\left\{\sum_{i=1}^{N} \varepsilon_i p_i - E\right\} \quad (5.50)$$

and minimize L.

1) $\partial \mathrm{L}/\partial p_\mathrm{i} = 0$

$$\frac{\partial L}{\partial p_i} = \frac{\partial}{\partial p_i} S(p_1, p_2, \ldots, p_N) + \lambda + \alpha\varepsilon_i = -K\ln p_i + \lambda + \alpha\varepsilon_i = 0, \text{ and thus,}$$

$$p_i = \exp[(\alpha\varepsilon_i - 1 + \lambda)/K].$$

2) $\partial \mathrm{L}/\partial\lambda = 0$

$$\sum_{i=1}^{N} p_i = 1 = \sum_{i=1}^{N} \exp[(\alpha\varepsilon_i - 1 + \lambda)/K] = \exp[(-1+\lambda)/K]), \text{ and thus}$$

$$\exp[(-1+\lambda)/K] = \frac{1}{\sum_{i=1=1}^{N} \exp(\alpha\varepsilon_i/K)}, \text{ and thus}$$

$$p_i = \frac{\exp(\alpha\varepsilon_i / K)}{\sum_{i=1=1}^{N} \exp(\alpha\varepsilon_i / K)} = \frac{\exp(\beta\alpha\varepsilon_i)}{\sum_{i=1=1}^{N} \exp(\beta\alpha\varepsilon_i)}, \text{ where } 1/K = \beta.$$

3) $\partial L/\partial\alpha = 0$

$$\sum_{i=1}^{N} \varepsilon_i p_i - E = 0, \text{ and thus } E = \frac{\sum_{i=1=1}^{N} \varepsilon_i \exp(\beta\alpha\varepsilon_i)}{\sum_{i=1=1}^{N} \exp(\beta\alpha\varepsilon_i)}.$$

5.4.3 Maximum Entropy and Minimum Energy

Assume an event takes positive values of ε_i, $i = 1, 2, \ldots, N$ with the probability of the event being p_i. The average value of information is $E(p_1, p_2, \ldots, p_N)=\sum\varepsilon_i p_i$. What is the probability distribution that gives both maximum entropy $S(p_1, p_2, \ldots, p_N)$ and minimum energy of $E = \sum\varepsilon_i p_i$? We may also apply the Lagrange multiplier to find such probability distribution with the restriction $\sum p_i = 1$. Note that entropy S will never be negative and $E > 0$ with the assumption of $\varepsilon_i > 0$. This time, one finds the probability distribution for maximizing $S(p_1, p_2, \ldots, p_N)/E(p_1, p_2, \ldots, p_N)$ with the restriction of $\sum p_i = 1$.

Define , and minimize M. $M = \dfrac{S(p_1, p_2, \ldots, p_N)}{E(p_1, p_2, \ldots, p_N)} + \lambda\left\{\sum_{i=1}^{N} p_i - 1\right\}$ (5.51)

1) $\partial M/\partial p_i = 0$

$$\frac{\partial M}{\partial p_i} = \frac{\partial}{\partial p_i}\left(\frac{S}{E}\right) + \lambda = \frac{1}{E}\left(\frac{\partial S}{\partial p_i}\right) - \frac{1}{E^2}\left(\frac{\partial E}{\partial p_i}\right)S + \lambda = \frac{1}{E}\left(-\ln p_i - 1\right) - \frac{S}{E^2}\varepsilon_i + \lambda = 0. \quad (5.52)$$

$$\text{Thus, } \ln p_i = -\frac{S}{E}\varepsilon_i + \lambda E - 1; \text{ i} = 1, 2, \ldots, \text{N}. \quad (5.53)$$

By multiplying p_i to the above equation, we obtain

$$p_i \ln p_i = -\frac{S}{E} p_i\varepsilon_i + \lambda E p_i - p_i.$$

Thus,

$$\sum_{i=1}^{N} p_i \ln p_i = -\frac{S}{E}\sum_{i=1}^{N} p_i\varepsilon_i + \lambda E\sum_{i=1}^{N} p_i - \sum_{i=1}^{N} p_i .$$

Because $\sum_{i=1}^{N} p_i = 1$, the above equation becomes $S = -S + \lambda E - 1$, and thus $\lambda = 1/E$.

Back to Equation 5.37, we obtain

$$p_i = \exp\left(-\frac{S}{E}\varepsilon_i\right) = \exp(-\tau\varepsilon_i) \text{ where } \tau = S/E \text{ and } \sum_{i=1}^{N} \exp(-\tau\varepsilon_i) = 1. \tag{5.54}$$

2) $\partial L/\partial \lambda = 0$

$$\sum_{i=1}^{N} p_i = \sum_{i=1}^{N} \exp(\alpha\varepsilon_i - 1 + \lambda) = \exp(-1+\lambda)\sum_{i=1=1}^{N} \exp(\alpha\varepsilon_i) = 1.$$

$$\exp(-1+\lambda) = \frac{1}{\sum_{i=1=1}^{N} \exp(\alpha\varepsilon_i)}, \text{ and thus } p_i = \frac{\exp(\alpha\varepsilon_i)}{\sum_{i=1=1}^{N} \exp(\alpha\varepsilon_i)}. \tag{5.55}$$

Here is an example of how to use Equation 5.55. Let $N = 2$, and $\varepsilon_1 = \varepsilon_0$ and $\varepsilon_2 = 2\varepsilon_0$, where ε_0 is a constant. Imagine a two-energy level system where the higher energy level is twice the lower level. With this condition, $e^{-\varepsilon_0\tau} + e^{-2\varepsilon_0\tau} = 1$ or $x + x^2 = 1$, where $x = e^{-\varepsilon_0\tau}$. Solving the quadrature equation, we obtain $x = \frac{-1 \pm \sqrt{5}}{2} \sim 0.618$ for $x > 0$. Therefore, $p_1 = x = 0.618$ and $p_2 = x^2 = 0.382$. The probability of reaching the higher energy level is proportional to the square of the lower probability.

5.4.4 Negative Entropy

Assume that the number of all possible events is N_0 and each of which has an equal probability, and we knew there were only N_1-events, where $N_1 < N_0$, occurred. As we defined in Section 5.4.1, the information we get from N_1-events is given by

$$I_0 = -K\ln(p_0) = K\ln N_0 \text{ because } p_0 = 1/N_0 \text{ and } I_1 = -K\ln(1/N_1) = K\ln N_1 \text{ because } p_1 = 1/N_1,$$

assuming each event in a group of possible events takes the equal probability. Thus, we lose information when the number of occurring events changes from N_1 to N_0 when $N_1 < N_0$.

The maximum entropy from the N_1-events and N_0-events are given by $S_1 = K\ln N_1$ and $S_0 = K\ln N_0$. Change in entropy from the N_1-events to N_0-events is $\Delta S = S_0 - S_1 = K\ln(N_0/N_1) > 0$ when $N_1 < N_0$. The entropy of a system increases and reaches the maximum in its thermal equilibrium state as the second law of thermodynamics states.

As the entropy of the system increases, information on the system decreases, $\Delta I = I_0 - I_1 = K\ln(N_1/N_0)$. In order to increase or even maintain the amount of information, we must decrease entropy. For a thermodynamic system, it means that from a thermal non-equilibrium state to the equilibrium state, the entropy of the system increases while we lose information on the microscope state of the system. Once the system reaches its thermal equilibrium state, all the microscopic states will have an equal probability.

The concept of negentropy was introduced by Irwin Schrödinger in his book titled *What Is Life?* [14]. According to him, a living organism is not in a thermal equilibrium state while alive and its entropy reaches its maximum upon death. In order for the living tissues to be alive, they must maintain information about reproduction, and we need to feed negentropy!

SUGGESTED FURTHER STUDY

Knowing the history of entropy would open your eyes to thermodynamics [15, 16]. That history was indeed the reason for me to study statistical physics.

In digital data/image processing, the maxim entropy method (MEM) is widely applied. MEM is based on the entropy of information and the power spectrum of a signal to estimate its spectrum by maximizing the entropy. MEM is equivalent to computational processes of determining the coefficients of a linear prediction (LP) filter [17–19]. Furthermore, cepstra constructed by the LP method and Fourier transform (FT) are equivalent. Cepstra are the results of computing the inverse Fourier transform (IFT) of the logarithm of the estimated signal spectrum. MEM may also acquire signal spectra although a two-dimensional MEM has not been established. If readers are interested in these digital technologies, refer to these references. One of our readers would accomplish a new discovery!

For the general description of information theory applied in physics, refer to a collection of research articles [20].

REFERENCES

1. Schwartz M, *Entropy* Scholars at Harvard, 2019. https://scholar.harvard.edu/files/schwartz/files/6-entropy.pdf.
2. Gould H and Tobochnik J, *Statistical and Thermal Physics*, Princeton University Press, 2010.
3. Tatum J, *Entropy of Mixing, and Gibbs Paradox*, LibreTexts. https://phys.libretexts.org/Bookshelves/Thermodynamics_and_Statistical_Mechanics/Heat_and_Thermodynamics_(Tatum)/17%3A_Chemical_Thermodynamics/17.08%3A_Entropy_of_Mixing_and_Gibbs'_Paradox.
4. *Ideal Solution*, LibreTexts Chemistry. https://byjus.com/chemistry/ideal-solution/.
5. *Properties of Ideal Solutions*, LibreTexts Chemistry. https://byjus.com/chemistry/ideal-solution/.
6. Reif F, *Fundamentals of Statistical and Thermal Physics*, McGrwo-Hill, Inc., 1965. https://archive.org/details/fundamentalsofst00fred/page/n7/mode/2up.
7. *Can Somebody Explain the Low Temperature Schottky Anomaly for Two Level Systems*?, Chemistry Stack Exchange, 2019. https://archive.org/details/fundamentalsofst00fred/page/n7/mode/2up.
8. White GK, *Experimental Techniques in Low-Temperature Physics*, Oxford Press, 1979.
9. Schneider U and Bloch I, *A Temperature Below Absolute Zero*, Max-Planck-Gesellschaft, 2013. https://www.mpg.de/research/negative-absolute-temperature.
10. Ling S, Sanny J, and Moeba W, *Second Law of Thermodynamics: Entropy*, University Physics Vol. 2, Open Stax, Rice University, 2021. https://openstax.org/books/physics/pages/12-3-second-law-of-thermodynamics-entropy.
11. Smart B, Roughan M, and Mitchell L, *The Entropy Rate of Linear Additive Markov Processes*, arXiv.org, 2022. https://arxiv.org/abs/2211.05350.
12. Höst Stefan, *Information Theory Lecture 5 Entropy Rate and Markov Sources*, LUND University. https://www.eit.lth.se/fileadmin/eit/courses/eitn45/Lectures/2018/L5-HO.pdf#:~:text=Definition.%20The%20entropy%20rate%20of%20a%20random.
13. Pierce J R, *An Introduction to Information Theory*, Dover Publishings, Inc., 1980.
14. Schoedinger E, *What Is Life*? *The Physical Aspect of the Living Cell & Mind and Matter*, 1944. https://archive.org/details/WhatIsLife-EdwardSchrodinger.

15. *Entropy: Physics Origin*, University of California, Berkeley. https://www.bing.com/ck/a?!&&p=243f9a0e67093249JmltdHM9MTcyODM0NTYwMCZpZ3VpZD0yNjU0ZmNlZi00M2MyLTZjNTItMDFjZi1lOWU3NDI1YjZkZjAmaW5zaWQ9NTE5Nw&ptn=3&ver=2&hsh=3&fclid=2654fcef-43c2-6c52-01cf-e9e7425b6df0&psq=Entropy%3a+physics+origin%3a+University+of+California%2c+Berkley++&u=a1aHR0cHM6Ly93d3cuc3RhdC5iZXJrZWxleS5lZHUvfmJpbnl1LzIxMkEvcGFwZXJzL3NsaWRlcy5wZGY&ntb=1.
16. Müller I, *A History of Thermodynamics the Doctrine of Energy and Entropy*, Springer, 2017. https://www.perplex.ethz.ch/thermo_course/various_thermodynamics_texts/Muller%202007%20A%20history%20of%20thermodynamics.pdf.
17. *Principle of Maximum Entropy*, MIT. https://mtlsites.mit.edu/Courses/6.050/2003/notes/chapter10.pdf.
18. Cho S, *Fourier Transform and Its Applications Using Microsoft Excel® Second Edition*, IOP Publishing, Inc., 2003.
19. Jain AK, *Fundamentals of Digital Image Processing*, Prentice Hall, 1989.
20. Grandy WT, ed., *Information Theory in Physics*, AMERICAN Association of Physics Teachers, 2000.

CHAPTER 6

Boundary Value Problems

HELMHOLTZ DIFFERENTIAL EQUATION, $\nabla^2 U(\vec{r}) + kU(\vec{r}) = 0$, appears in many science subjects. Solving the Helmholtz equation for a specific boundary condition needs a special mathematical function that satisfies the boundary condition. The boundary value problems may be called the eigenvalue problems where these special functions are called "orthonormal bases." Because the boundary conditions are expressed using suitable coordinate systems, we may sort out special functions according to their coordinate systems. While there is a wide variety of mathematical properties that appear in the boundary value problems, this book focuses on their orthonormal properties without mathematical proofs. For their comprehensive descriptions, refer to advanced mathematics books [1–5].

6.1 EIGENFUNCTIONS AS ORTHONORMAL BASES

6.1.1 Separation of Variables of the Helmholtz Equation

One of the methods to solve partial differential equations of the second-order time derivative, $\frac{\partial^2 u(\vec{r},t)}{\partial t^2} = v^2 \nabla^2 u(\vec{r},t)$, is the separation of variables. Assume $u(\vec{r},t) = T(t)U(\vec{r})$ and $T(t) = \exp(\pm i\omega t)$. The differential equations become $\frac{d^2T/dt^2}{T} = -\omega^2 = \frac{v^2\nabla^2 U}{U}$, and the space part becomes the Helmholtz equation $\nabla^2 U + k^2 U = 0$, where $k = \omega/v$. We can also apply the variable separation for partial differential equations with the first order time derivative, $\frac{\partial u(\vec{r},t)}{\partial t} = \lambda \nabla^2 u(\vec{r},t)$ such as heat conduction equation, diffusion equation, and Schrödinger equation. In this case, $\frac{d^2T/dt^2}{T} = \lambda \frac{\nabla^2 U}{U} = -\alpha$, where α is a constant. The space part also becomes the Helmholtz equation, $\nabla^2 U + kU = 0$, where $k = \alpha/\lambda$.

Depending on the coordinate system used to solve the Helmholtz equation, appropriate special functions are applied to describe the solutions. Solutions of the Helmholtz equation satisfying a specific boundary condition are called eigenfunctions, and the k-values for the solutions are called eigenvalues. Recall that with a set of unit vectors an arbitrary vector can be expressed. Likewise, a set of eigenfunctions forms an orthogonal basis with which

DOI: 10.1201/9781003516347-6

an arbitrary function satisfying the boundary condition may be expressed. The general orthonormal properties are described below.

6.1.2 Orthonormal Property of Eigenfunctions

Recall a three-dimensional vector space of the Cartesian coordinate frame. Let a set of unit vectors $\{\vec{e}_i; i = 1,2,3\}$ be in the coordinate frame. We learn that the unit vectors are orthogonal to each other, i.e., their inner products satisfy $(\vec{e}_i \cdot \vec{e}_j) = \delta_{ij}$, where δ_{ij} is the Kronecker delta. With the orthonormal property of the unit vectors, we can express a vector $\vec{V}$ in the coordinate such that

$$\vec{V} = V_1\vec{e}_1 + V_2\vec{e}_2 + V_3\vec{e}_3 \text{ where } V_i = (\vec{V} \cdot \vec{e}_i); \quad i = 1,2,3. \tag{6.1}$$

A similar argument may be made for the solutions of Helmholtz equations with a specific boundary condition. Assume that we have a one-dimensional boundary value problem described by

$$\frac{d^2X}{dx^2} + \lambda X = 0 \text{ where } 0 \le x \le 1. \tag{6.2}$$

The boundary conditions are, for example, $X(0) = X(1) = 1$. Assume we obtain eigenfunctions X_m and X_n for different eigenvalues λ_m and λ_n:

$$\frac{d^2X_m}{dx^2} + \lambda_m X_m = 0 \text{ and } \frac{d^2X_n}{dx^2} + \lambda_n X_n = 0, \tag{6.3}$$

and X_m and X_n satisfy the same boundary condition of $X(0) = X(1) = 0$, $dX(0)/dx = dX(1)dx = 0$, or $X(0) = dX(1)/dx = 0$. From these eigenfunctions, we obtain

$$X_n\frac{d^2X_m}{dx^2} - X_m\frac{d^2X_n}{dx^2} = \frac{d}{dx}\left(X_n\frac{dX_m}{dx} - X_m\frac{dX_n}{dx}\right). \tag{6.4}$$

Thus, $\left(\lambda_m - \lambda_n\right)\int_0^1 X_nX_m dx = \left[X_n\frac{dX_m}{dx} - X_n\frac{dX_m}{dx}\right]_0^1 = 0$ for the boundary conditions.

Because $\lambda_m \ne \lambda_n$, $\int_0^1 X_nX_m dx = 0$. This relationship may be interpreted as the "inner product" of the functions X_n and X_m, and when the inner product becomes zero, we interpreted eigenfunctions X_n and X_m to be orthogonal if $\lambda_m \ne \lambda_n$. Even if $\|X\|^2 \equiv \int_0^1 X_m^2 dx \ne 1$ for a set of orthogonal functions, we may normalize the orthogonal functions to make a set of orthonormal functions,

$$Y_m(x) = \frac{X_m(x)}{\sqrt{\|X(x)\|^2}}. \tag{6.5}$$

Note: The ***Sturm-Liouville differential equation***

The Sturm-Liouville differential equation has the following form [1].

$$\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)-q(x)y+\lambda r(x)y=0$$

or

$$\check{L}y=\lambda ry \text{ where } \check{L}=\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)-q(x). \tag{6.6}$$

Note that the Helmholtz differential equation is a special form with $p(x) = 1$, $q(x) = 0$, and $r(x) = 1$. The solutions of the Sturm-Liouville equation are orthogonal as described below.

Let eigenfunctions of the Sturm-Liouville differential equation for different eigenvalues λ_m and λ_n be X_m and X_n with a given boundary condition for $a \le x \le b$:

$$\check{L}X_m=\lambda_m rX_m \text{ and } \check{L}X_n=\lambda_n rX_n. \tag{6.7}$$

With arbitrary functions, $u(x)$ and $v(x)$, we have

$$u\check{L}v-v\check{L}u=v\frac{d}{dx}\left(p\frac{du}{dx}\right)-u\frac{d}{dx}\left(p\frac{dv}{dx}\right)=\frac{d}{dx}\left[p\left(v\frac{du}{dx}-\frac{dv}{dx}u\right)\right]. \tag{6.8}$$

Let $u = X_n$ and $v = X_m$. Equation 6.8 becomes

$$\left(\lambda_m-\lambda_n\right)X_mX_n=\frac{d}{dx}\left[p\left(X_m\frac{dX_n}{dx}-\frac{dX_m}{dx}X_n\right)\right]. \tag{6.9}$$

Then, the eigenfunctions are orthogonal with a weight function $r(x)$:

$$\left(\lambda_m-\lambda_n\right)\int_a^b rX_mX_ndx=\left[p\left(X_m\frac{dX_n}{dx}-\frac{dX_m}{dx}X_n\right)\right]_a^b=0 \text{ if } \lambda_m\neq\lambda_n. \tag{6.10}$$

6.2 RECTANGULAR COORDINATES

6.2.1 Standing Wave on a Rectangular Membrane

Consider a standing wave on a two-dimensional rectangular membrane. The wave equation is

$$\frac{\partial^2 u(x,y,t)}{\partial t^2}=v^2\left[\frac{\partial^2 u(x,y,t)}{\partial x^2}+\frac{\partial^2 u(x,y,t)}{\partial y^2}\right]. \tag{6.11}$$

The solution of the equation can be obtained by the variable separation. Let $u(x, y, t) = X(x)Y(y)\Gamma(t)$, then Equation 6.1 becomes

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} = \frac{1}{v^2}\frac{\Gamma''(t)}{\Gamma(t)}, \tag{6.12}$$

and $X(x)$ and $Y(y)$ are also separated,

$$\frac{X''(x)}{X(x)} = -k_x^2 \text{ and } \frac{Y''(y)}{Y(y)} = -k_y^2. \tag{6.13}$$

Assume the following initial and boundary conditions for a rectangular membrane:

(i) The initial conditions: $u(x, y, 0) = f_1(x, y)$ and $(\partial u/\partial t)_{t=0} = f_2(x, y)$; and

(ii) The boundary conditions: $u(0, y, t) = u(a, y, t) = 0$ and $u(x, 0, t) = u(x, b, t) = 0$.

The solutions of Equation 6.2 including the boundary condition are

$$X_n(x) = A_n \sin\left(\frac{m\pi}{a}x\right) \text{ where } k_x = \frac{m\pi}{a} \text{ and } m = 1, 2, 3, \ldots; \tag{6.14}$$

$$Y_n(y) = B_n \sin\left(\frac{n\pi}{b}y\right) \text{ where } k_x = \frac{n\pi}{a} \text{ and } n = 1, 2, 3, \ldots; \tag{6.15}$$

and the time part of Equation 6.1 is a harmonic oscillation,

$$\frac{d^2\Gamma(t)}{dt^2} + \omega^2\Gamma(t) = 0 \text{ where } \omega^2 = v^2\left(k_x{}^2 + k_y{}^2\right). \tag{6.16}$$

Because possible values of k_x and k_y are discrete, the angular frequency ω is also discrete:

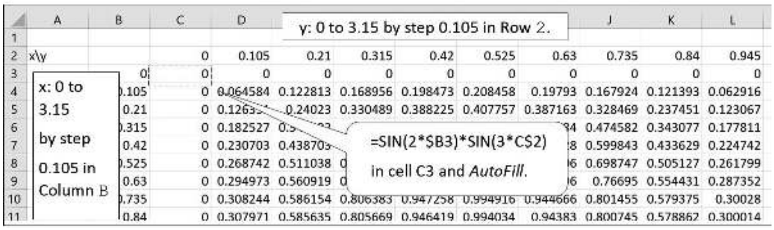
$$\omega_{m,n}^2 = v^2\pi^2\left[\left(\frac{m}{a}\right)^2 + \left(\frac{n}{b}\right)^2\right], \text{ and thus } \Gamma_{m,n}(t) = C_{m,n}\sin\left(\omega_{m,n}t + \varepsilon_{m,n}\right). \tag{6.17}$$

Therefore, the general solution is

$$\begin{aligned} u_{m,n}(x, y, t) &= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} X_m(x)Y_n(y)\Gamma_{m,n}(t) \\ &= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} D_{mn,} \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{b}y\right)\sin\left(\omega_{m,n}t + \varepsilon_{m,n}\right) \end{aligned} \tag{6.18}$$

where $\{D_{m,n}\} = \{A_m B_n C_{m,n};\ m = 1,2,3, \ldots, \text{ and } n = 1, 2, 3, \ldots\}$ and $\{\varepsilon_{m,n}\}$ are determined by the initial condition.

The spatial part is a two-dimensional Fourier series discussed in Section 6.2.2. Figure 6.1 shows a screenshot of the calculated spatial part of $u_{2,3}$ with $a = b = 3.14$ using Equation 6.17. The x-range is specified from 0 to 3.15 with increments of 3.15/30 = 0.105



	A	B	C	D	E	F	G	H	I	J	K	L
1												
2	x\y		0	0.105	0.21	0.315	0.42	0.525	0.63	0.735	0.84	0.945
3		0	0	0	0	0	0	0	0	0	0	0
4		.105	0	0.064584	0.122813	0.168956	0.198473	0.208458	0.19793	0.167924	0.121393	0.062916
5		0.21	0	[illegible]	0.24023	0.330489	0.388225	0.407757	0.387163	0.328469	0.237451	0.123067
6		.315	0	0.182527	[illegible]				[illegible]	0.474582	0.343077	0.177811
7		0.42	0	0.230703	0.43870[illegible]				[illegible]	0.599843	0.433629	0.224742
8		.525	0	0.268742	0.511038				[illegible]	0.698747	0.505127	0.261799
9		0.63	0	0.294973	0.560919				[illegible]	0.76695	0.554431	0.287352
10		.735	0	0.308244	0.586154	0.806383	0.947258	0.994916	0.944666	0.801455	0.579375	0.30028
11		0.84	0	0.307971	0.585635	0.805669	0.946419	0.994034	0.94383	0.800745	0.578862	0.300014

FIGURE 6.1 Two-dimensional standing wave $u_{2,3}$.

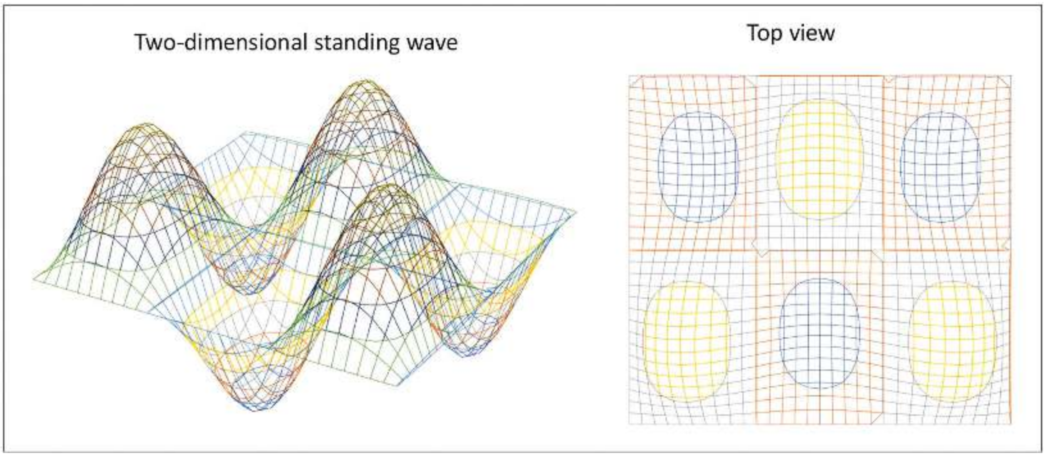


FIGURE 6.2 Two-dimensional standing wave on a square membrane.

in Column B and the y-range is specified from 0 to 3.15 with increments of 3.15/30 = 0.105 in Row 2. Enter **=SIN(2*$B3)*SIN(3*C$2)** and apply *AutoFill*.

Figure 6.2 shows a 3D surface chart from the calculated data.

6.2.2 Trigonometric Functions as an Orthonormal Basis – Fourier Series

Trigonometric functions form a set of orthonormal functions, and a function $f(x)$ can be expressed as a series of trigonometric functions. As we described in Section 3.3., if the function $f(x)$ is a periodic function, a series expansion in terms of trigonometric functions should be suitable.

An arbitrary periodic function $f(x)$ in the interval $[-L, +L]$ can be expressed by a series expansion of trigonometric functions,

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_k \cos\left(\frac{n\pi}{L} x\right) + \sum_{n=1}^{\infty} b_k \sin\left(\frac{n\pi}{L} x\right) \tag{6.19}$$

where the coefficients $\{a_m\}$ and $\{b_m\}$ are given by

$$a_m = \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{m\pi}{L} x\right)dx \text{ and } b_m = \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{m\pi}{L} x\right)dx. \tag{6.20}$$

```
Sub Fourier1D()
Cells(1, 1) = "Fourier series of f(x)=x for |x|<=1"
Pi = 3.141592654
Cells(2, 2) = "x"
Cells(2, 3) = "FT"
Cells(2, 4) = "Exact"
N = 200                          '# of terms to be calculated.
  For j = 1 To 101               '100 segments from x=0 to x=1
    jj = (j - 1) / 100
      temp = 0
        For k = 1 To N
          temp = temp + ((-1) ^ (k + 1)) * Sin(k * Pi * jj) / k
        Next k
    Cells(j + 2, 2) = jj
    Cells(j + 2, 3) = temp * 2 / Pi
    Cells(j + 2, 4) = jj
  Next j
End Sub
```

FIGURE 6.3 VBA code for calculating the Fourier series of $f(x) = x$.

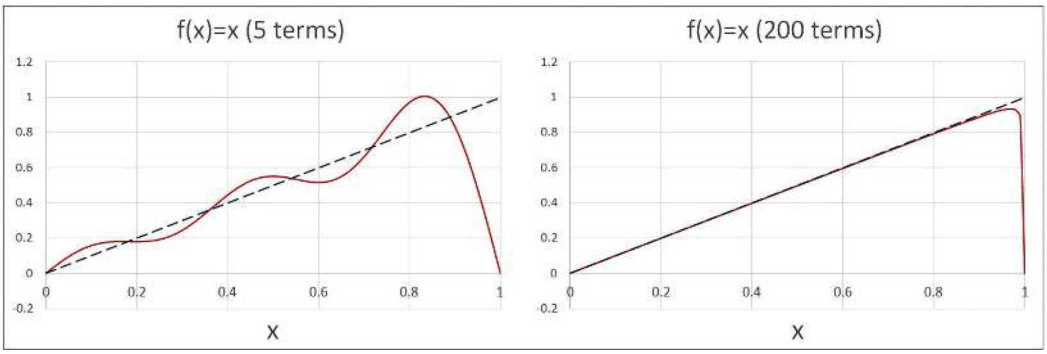


FIGURE 6.4 The Fourier series of $f(x) = x$ for $0 < x < 1$ (5 terms and 200 terms).

Example: a sawtooth wave. The sawtooth wave is a repetition of the function $f(t) = x$ for $-1< x < +1$, and the period is 2. The Fourier series of the above sawtooth wave is

$$f(t) = \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\sin(n\pi x) = \frac{2}{\pi}\left[\sin(\pi x) - \frac{1}{2}\sin(2\pi x) + \frac{1}{3}\sin(3\pi x) - \frac{1}{4}\sin(4\pi x) + \frac{1}{5}\sin(5\pi x) - + \cdots\right]. \tag{6.21}$$

Figure 6.3 lists the VBA code for the iterative summation of the Fourier series of $f(x) = x$ using Equation 6.21.

Figure 6.4 shows the actual Fourier series of up to 5 terms and 200 terms for $0<x<1$. The Fourier series of the first 5 terms is shown for comparison with series expansions of other orthonormal functions in Sections 6.3 and 6.4.

6.2.3 Hermite Polynomials

The Hermite differential equation is given by

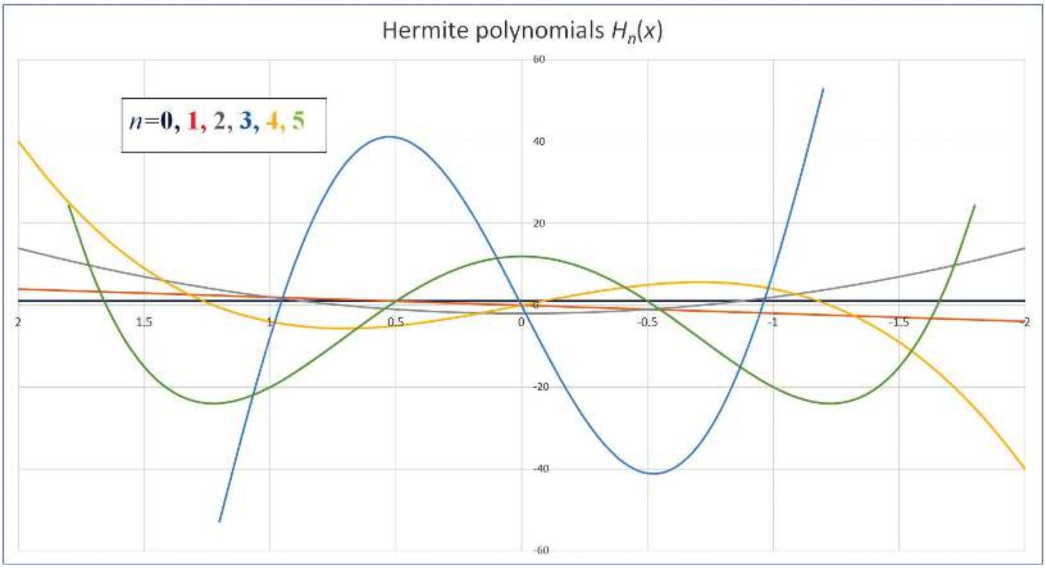


FIGURE 6.5 Hermite polynomials.

$$\frac{d^2F(x)}{dx^2} - 2x\frac{dF(x)}{dx} + 2nF(x) = 0 \text{ where } n = 0, 1, 2, \ldots \tag{6.22}$$

Solutions of the Hermite equation are called Hermite polynomials. The quantum harmonic oscillator can be described by the Hermite equation as we will discuss in Section 7.2.2.

Example of Hermite polynomials (n = 0 to 5):

$H_0(x) = 1$,
$H_1(x) = 2x$,
$H_2(x) = 4x^2 - 2$,
$H_3(x) = 8x^3 - 12x$,
$H_4(x) = 16x^4 - 48x^2 + 12$,
$H_5(x) = 32x^5 - 160x^3 - 120x$. (6.23)

Graphs: Figure 6.5 shows $H_0(x)$ to $H_5(x)$ using Excel's *AutoFill*.
The Hermite polynomials can be generated with the following formula.

Generating function: $H_n(x) = (-1)^n e^{x^2} \dfrac{d^n}{dx^n} e^{-x^2}$ and $e^{2xt-t^2} = \displaystyle\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n$. (6.24)

Recursion formula: $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$. (6.25)

Important properties of the Hermite polynomials are:

Parity: $H_n(-x) = (-1)^n H_n(x)$ (6.26)

Orthonormality: $\int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x) dx = (\sqrt{\pi} 2^n n!) \delta_{nm}$, where δ_{nm} is the Kronecker delta. (6.27)

The orthonormality expressed by Equation 6.27 means that the Hermite polynomials form an orthonormal basis given by

$$h_n(x) = \frac{H_n(x) e^{-x^2/2}}{\left[\sqrt{\pi} 2^n n!\right]^{1/2}}, \; n = 0, 1, 2, 3, \ldots \tag{6.28}$$

Series expansion using the Hermite polynomials is given by

$$f(x) = \sum_{n=0} c_n h_n(x) \tag{6.29}$$

$$\text{where } c_n = \int_{-\infty}^{\infty} f(x) h_n(x) dx = \frac{1}{\left[\sqrt{\pi} 2^n n!\right]^{1/2}} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2/2} dx. \tag{6.30}$$

A few terms of $h_n(x)$ do not represent a good approximation. Figure 6.6 shows two examples: $f(x) = x$ and $f(x) = \sin x$ with up to $n = 5$ terms of the orthonormal bases (6.29). The calculation of the coefficients (6.30) is shown in Appendix A6.1. We apply Simpson's method for the numerical evaluation of the integrals in Equation 6.30. Refer to Appendix A.4 for Simpson's method.

6.2.4 Laguerre polynomials

The Laguerre polynomials, $L_n(\rho)$, are solutions of the Laguerre differential equation:

$$x \frac{d^2 y(x)}{dx^2} + (1 - x) \frac{dy(x)}{dx} + ny(x) = 0 \text{ where } n \text{ is integer.} \tag{6.31}$$

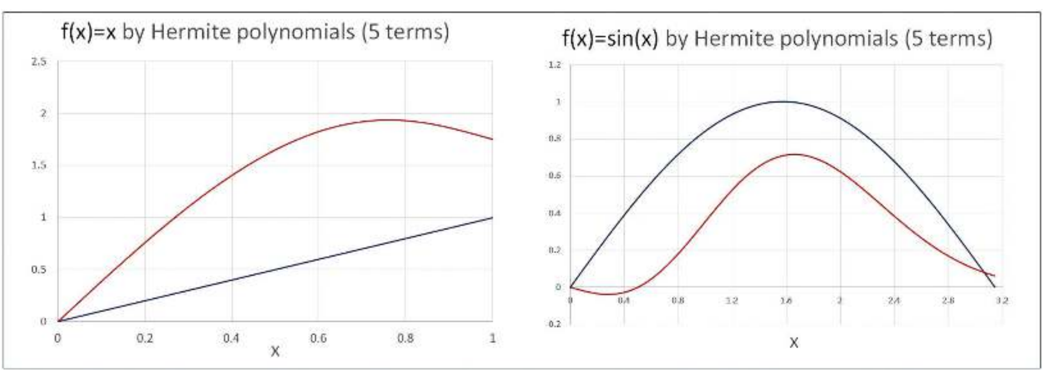


FIGURE 6.6 Series expansions using Hermite polynomials.

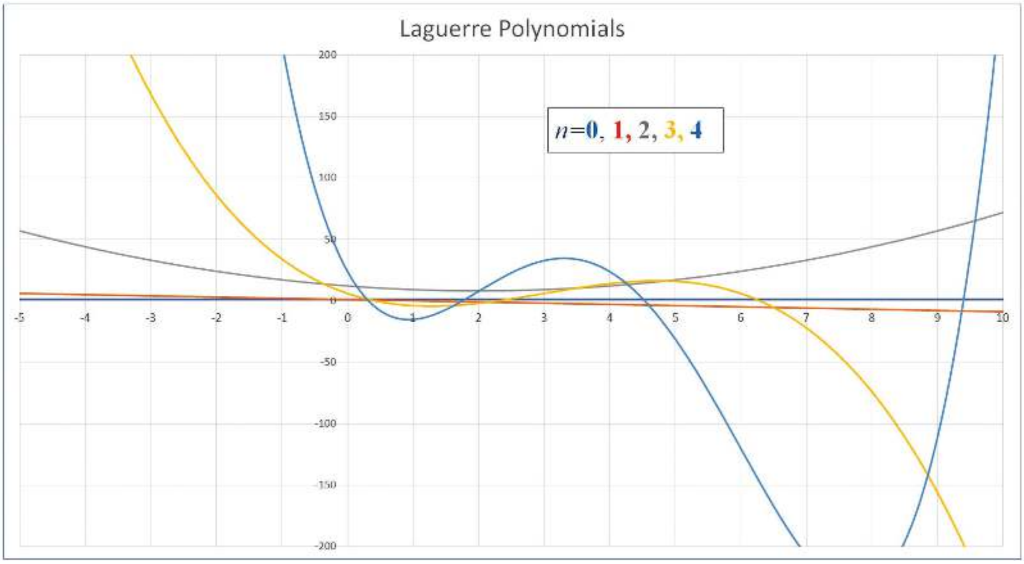


FIGURE 6.7 Laguerre polynomials (n = 1–4).

Examples of Laguerre polynomials ($n = 0 - 4$):

$$
\begin{aligned}
&L_0(x) = 1,\\
&L_1(x) = -x + 1,\\
&L_2(x) = x^2 - 4x + 12,\\
&L_3(x) = -x^3 + 9x^2 - 18x + 6,\\
&L_4(x) = x^4 - 16x^3 + 72x^2 - 96x + 24.
\end{aligned}
\tag{6.32}
$$

Figure 6.7 shows the Laguerre polynomials of n = 0–4 using Excel's *AutoFill*.

Definition: $L_n(x) = e^x \dfrac{d^n}{dx^n}(x^n e^{-x}).$ (6.33)

Generating function: $U(x,t) = \dfrac{1}{1-t}\exp\left(-\dfrac{xt}{1-t}\right) = \displaystyle\sum_{n=0}^{\infty} \dfrac{L_n(x)}{n!} t^n.$ (6.34)

Recursion formula: $L_{n+1}(x) - (2n+1-x)L_n(x) + n^2 L_{n-1}(x) = 0,\ n \geq 1.$

$$L_n{}'(x) - nL_{n-1}{}'(x) + nL_{n-1}(x) = 0.$$

$$xL_n{}''(x) + (1-x)L_n{}'(x) + nL_n(x) = 0 \tag{6.35}$$

where primes denote the differential with respect to x.

Orthonormality: $\displaystyle\int_0^{\infty} e^{-x} L_m(x) L_n(x)\,dx = (n!)^2 \delta_{nm}.$ (6.36)

Laguerre polynomials are also a complete set of functions. An arbitrary function $f(x)$ on the interval $0 \leq x \leq \infty$ may be expanded with the following orthonormal functions:

$$f(x) = \sum_{n=0}^{\infty} c_n \varphi_n(x) \text{ where } \varphi_n(x) = \frac{1}{n!} L_n(x) e^{-x/2} \; \left(n = 0, 1, 2, \ldots\right). \tag{6.37}$$

6.2.5 Associated Laguerre Polynomials

Associated Laguerre differential equation is defined as

$$x \frac{d^2 y(x)}{dx^2} + (\alpha + 1 - x) \frac{dy(x)}{dx} + n y(x) = 0 \text{ where } n = \text{integer and } \alpha \neq 0. \tag{6.38}$$

Solutions of the associated Laguerre differential equation are called associated Laguerre polynomials, $L_n^\alpha(x)$. The associated Laguerre polynomials can be defined as $L_n^\alpha(x) = \frac{d^\alpha}{dx^\alpha} L_n(x)$.

Generating function: The generating function of the Laguerre polynomials (6.34) α-times with respect to *x* gives the generating function for the associated Laguerre polynomials.

$$U_\alpha(x,t) = \frac{(-t)^\alpha e^{-xt/(1-t)}}{(1-t)^{\alpha+1}} = \sum_{n=0}^{\infty} \frac{L_n^\alpha(x)}{n!} t^n. \tag{6.39}$$

Examples of Associated Laguerre Polynomials (n = 0–3):

$$\begin{aligned}
&L_0^\alpha(x) = 1, \\
&L_1^\alpha(x) = -x + \alpha + 1, \\
&L_2^\alpha(x) = (1/2)\left[x^2 - 2(\alpha+2)x + (\alpha+1)(\alpha+2)\right], \\
&L_3^\alpha(x) = (1/6)\left[-x^3 + 3(\alpha+3)x^2 - 3(\alpha+2)(\alpha+3)x + (\alpha+1)(\alpha+2)(\alpha+3)\right].
\end{aligned} \tag{6.40}$$

The radial wave function of the hydrogen atom is reduced to the associated Laguerre differential equation as we will discuss in Section 7.3.3. For more description of the associated Laguerre polynomials, refer to the advanced books listed in Chapter 7.

6.3 CYLINDRICAL COORDINATES

Using the cylindrical coordinates (r, θ, z), the Helmholtz equation becomes

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2} + k^2 u = 0 \text{ where } u = u(r,\theta,z). \tag{6.41}$$

Because the z-component is the same as the rectangular coordinates, let us focus on two-dimensional cases (z = 0). Let $u(r, \theta) = R(r)(\theta)$ for separating variables.

$$r^2 \frac{R''}{R} + r\frac{R'}{R} + k^2 r = -\frac{\Theta''}{\Theta} \tag{6.42}$$

where $R' = \frac{dR(r)}{dr}$, $R'' = \frac{d^2R(r)}{dr^2}$, and $\Theta'' = \frac{d^2\Theta(\theta)}{d\theta^2}$.

Assume $\Theta''/\Theta = -m^2$ and $\Theta(\theta) = A\exp(im\theta)$, where A and m are constants. If the angular part has a periodic boundary condition, $\Theta(\theta) = \Theta(\theta+2\pi)$, then m must be integers, $m = 0$, 1, 2, 3, …

Let $kr = x$ and $R(r) = y(x)$. From Equation 6.42, the radial part $R(r)$ satisfies Bessel differential equation,

$$x^2 y'' + xy' + (x_2 - m^2)y = 0. \tag{6.43}$$

6.3.1 Bessel Functions

A general solution of the Bessel Equation 6.43 is given by

$$\sum_{m=0} \left[a_m J_m(x) + b_m Y_m(x) \right] \text{ where } J_m(x) = \sum_{s=0} \frac{(-1)^s}{s!(s+m)!} \left(\frac{x}{2} \right)^{m+2S}, \tag{6.44}$$

which is called the m^{th}-order Bessel function. It remains finite for all x values. The other solution $Y_m(x)$ is called the m^{th}-order Neuman function. The Neuman function diverges at $x = 0$.

$$Y_m(x) = \lim_{\nu \to m} \frac{\cos(\nu\pi) J_\nu(x) - J_{-\nu}(x)}{\sin(\nu\pi)}. \tag{6.45}$$

Note: Excel has built-in Bessel functions: `BESSELJ` as $J_m(x)$, `BESSELY` as $Y_m(x)$, `BESSELI` as a modified Bessel function, and `BESSELK` as a modified Neuman function.

Graphs: Figure 6.8 plots $J_n(x)$ and $Y_n(x)$, where $n = 0, 1, 2, 3, 4, 5$ using Excel's `BESSELJ(x,M)` as $J_n(x)$ and `BESSELY(x, M)` as $Y_n(x)$ which are found by taking the following steps of menus, `[Formulas]`→`[More Functions]`→`[Engineering]`.

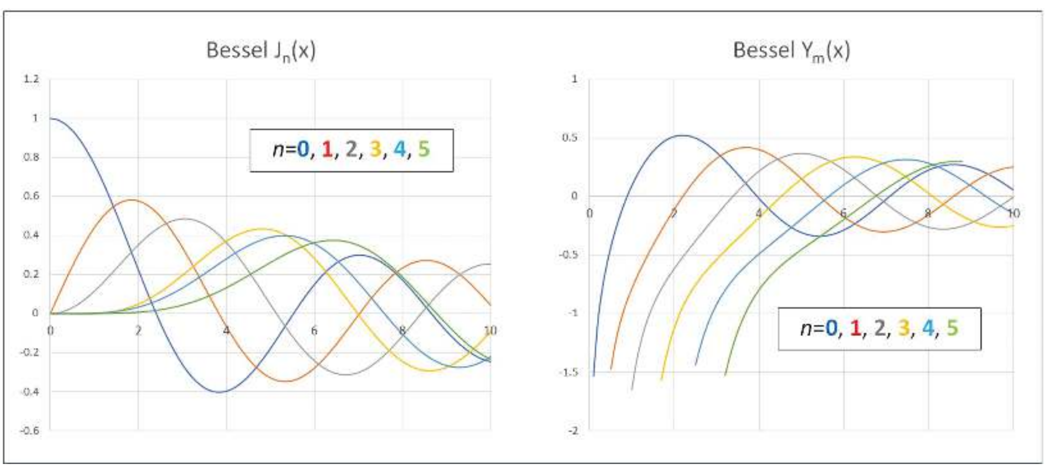


FIGURE 6.8 Bessel function $J_n(x)$ and Neumann Function $Y_n(x)$.

Generating function: $\exp\left[\frac{x}{2}\left(t-\frac{1}{t}\right)\right]=\sum_{m=-\infty}^{+\infty} J_m(x)t^m.$ (6.46)

Note: Let $t = e^{i\theta}$, then $t-(1/t) = 2i\sin\theta$ and the generation function becomes

$$\exp(ix\sin\theta)=\sum_{m=-\infty}^{+\infty} J_m(x)e^{im\theta}\mathbb{F}. \tag{6.47}$$

The real and the imaginary parts are

$$\begin{aligned}\cos(x\sin\theta) &= \sum_{m=-\infty}^{+\infty} J_m(x)\cos(m\theta)=J_0(x)+2\sum_{m=1}^{+\infty} J_{2m}(x)\cos(2m\theta),\\ \sin(x\sin\theta) &= \sum_{m=-\infty}^{+\infty} J_m(x)\sin(m\theta)=J_0(x)+2\sum_{m=1}^{+\infty} J_{2m-1}(x)\sin[(2m-1)\theta].\end{aligned} \tag{6.48}$$

Orthonormality: If $J_m(kx)$ and $J_m(lx)$ vanish at a and b, or if $J_m'(kx)$ and $J_m'(lx)$ vanish at a and b, we obtain

$$\int_a^b J_m(kx)J_m(lx)dx=0 \text{ if } k\neq l; \text{ and} \tag{6.49}$$

$$\int_a^b \left[J_m(kx)\right]^2 dx=\frac{b^2}{2}\left[J_{m+1}(kb)\right]^2-\frac{a^2}{2}\left[J_{m+1}(ka)\right]^2 \text{ if } k=l. \tag{6.50}$$

With the orthogonal property, a function $f(x)$ on the interval $0 < x < 1$ may be expanded in terms of Bessel functions.

$$f(x)=\sum_{n=0}^{\infty} c_n J_n(k_n x) \text{ where the } k_n \text{ are chose so that } J_n\left(k_n a\right)=0, \text{ and} \tag{6.51}$$

the coefficients are given by

$$c_n=\frac{\int_0^a f(x)J_m(k_n x)x dx}{(a^2/2)\left[J_{m+1}(k_n a)\right]^2} \text{ using } \int_0^a J_m(k_p x)J_m(k_q x)x dx=\delta_{pq}(a^2/2)\left[J_m(k_p a)\right]^2. \tag{6.52}$$

Figure 6.9 shows the series expansion of $f(x) = x$ using Equations 6.51 and 6.52. For a detailed calculation, refer to Appendix A6.2. Because Bessel functions $J_n(x)$ of integers n have functional forms similar to trigonometric functions, the series expansion of Bessel functions is similar to that of Fourier transform as shown in Figure 6.6.

6.3.2 Application of Bessel Functions

There are many applications of Bessel functions [6]. An example is standing waves on a circular membrane of radius 1. The wave equation is

$$\frac{\partial^2\psi(x,y,t)}{\partial x^2}+\frac{\partial^2\psi(x,y,t)}{\partial x^2}=\frac{1}{v^2}\frac{\partial^2\psi(x,y,t)}{\partial t^2} \tag{6.53}$$

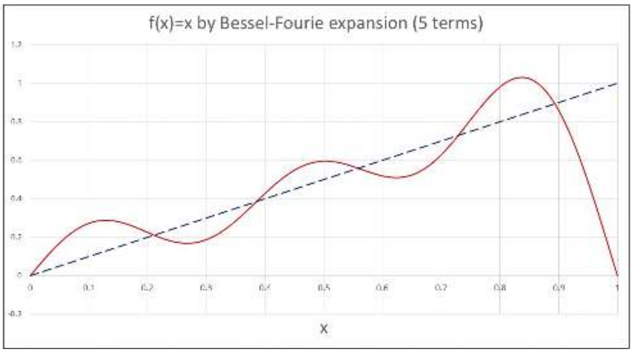


FIGURE 6.9 $f(x) = x$ using Bessel functions of $n = 0–4$.

where we assume the wave speed is $v = 1$.

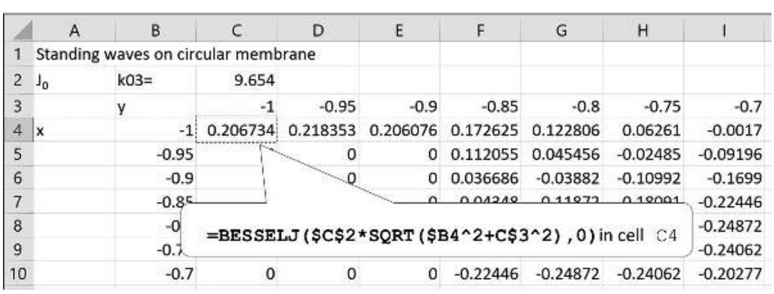
Let $\psi(x, y, t) = u(r, \theta)\sin(kt) = R(r)\Theta(\theta)\sin(kt)$, where $k > 0$, then $u(r, \theta)$ satisfies the Helmholtz Equation 6.2. If the rim of the membrane is fixed, the boundary condition is $R(1) = 0$ in addition to the periodicity of $\Theta(\theta)$. The Neuman function $Y_n(r)$ diverges at $r = 0$, and it is excluded in the solution. Thus, $R(r) = AJ_m(kr)$ and $\Theta(\theta) = Ce^{im\theta}$, where A_m and C are constants. For the fixed boundary condition at $r = 1$, $J_m(k) = 0$. Let the n^{th}-zero-point of the m^{th}-order Bessel function λ_m: $J_m(k_{m,n}) = 0$, where $n = 1, 2, 3, \ldots.$ for a given m. In this book, we define $J_{mn} = J_m(k_{m,n}r)$. The solution is given by

$$\psi(r,t) = \sum_{m=0}\sum_{n=1} D_m J_m(k_{m,n}r)\cos(m\theta)\ r) \text{ where } D_m = A_m C. \tag{6.54}$$

Figure 6.10 is a screenshot for calculating $J_{03} = J_0(k_{03}r)$, where $m = 0$ and $n = 3$. The x-range is entered from −1 to +1 with increments of 0.05 in Column `B` and the y-range is from −1 to +1 with increments of 0.05 in Row `3`. The third zero point of J_0 in Equation 6.54 is $k_{03} = 9.654$, which is entered in Cell `C2`. Then, enter

```
=BESSELJ($C$2*SQRT($B4^2+C$3^2),0)
```

in cell `C4` and apply *AutoFill*.



	A	B	C	D	E	F	G	H	I
1	Standing waves on circular membrane								
2	J_0	k03=	9.654						
3		y	-1	-0.95	-0.9	-0.85	-0.8	-0.75	-0.7
4	x	-1	0.206734	0.218353	0.206076	0.172625	0.122806	0.06261	-0.0017
5		-0.95		0	0	0.112055	0.045456	-0.02485	-0.09196
6		-0.9		0	0	0.036686	-0.03882	-0.10992	-0.1699
7		-0.8[illegible]			0	[illegible]	[illegible]	[illegible]	-0.22446
8		-0[illegible]							-0.24872
9		-0.[illegible]							-0.24062
10		-0.7	0	0	0	-0.22446	-0.24872	-0.24062	-0.20277

FIGURE 6.10 Calculating $J_{03} = J_0(k_{03}r)$.

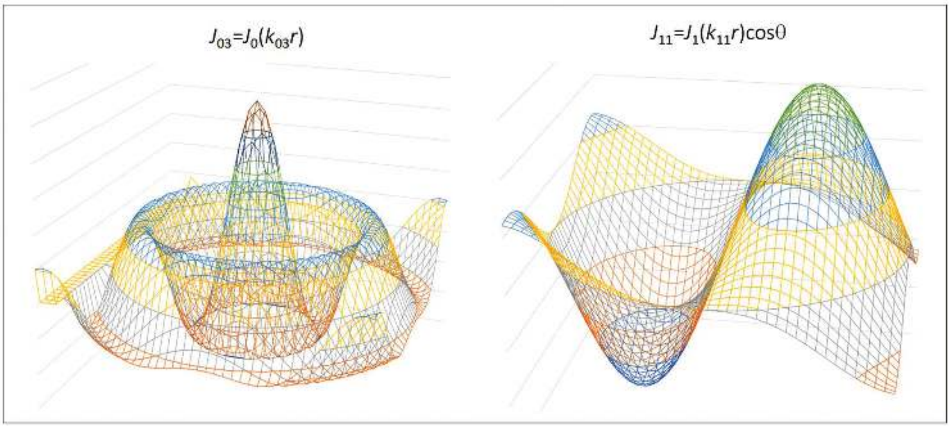


FIGURE 6.11 Standing waves on a circular membrane.

Figure 6.11 shows the standing waves on a circular membrane using Bessel functions. D_m = 1, radius = 1, and the angular part is adjusted to be $\cos(m\theta)$. Here, J_{03} is the third mode of J_0 and $n = 3$ and $J_{11} = J_1(k_{11}r)\cos\theta$.

Figure 6.12 lists the VBA code to compute J_{11} to obtain $n = 1$ and $m = 1$. Here, we used the built-in Bessel function of Excel in the VBA code,

```
Application.WorksheetFunction.BesselJ(k * r, m).
```

```
Sub CircularSheet()
Cells(1, 1) = "Standing wave on a circular sheet of radius 1"
'J1(k11x)*cos(theta)
  Cells(2, 1) = "m=": m = 1: Cells(2, 2) = m
  Cells(2, 4) = "k=": k = 3.832: Cells(2, 5) = k
r = 1 'Radius of circular sheet
h = 0.05
  For Row = 0 To 40
      Cells(Row + 4, 2) = -1 + h * Row
    Next Row
      For Col = 0 To 40
        Cells(3, Col + 3) = -1 + h * Col
      Next Col
  For i = -20 To 20
    x = i / 20
      For j = -20 To 20
        y = j / 20
        r = (x ^ 2 + y ^ 2) ^ 0.5
  ii = i + 24
  jj = j + 23
    If r > 1 Then Cells(ii, jj) = 0: GoTo Skip
    If r <= 1 Then BJ = Application.WorksheetFunction.BesselJ(k * r, m)
      'Angular part
      If r = 0 Then trig = 1
      If r <> 0 Then trig = (x / r)
        Cells(ii, jj) = BJ * trig       'J1(k11x)*cos(theta)
Skip:     Next j
  Next i
End Sub
```

Calling the Excel function BESSELJ

FIGURE 6.12 VBA code to calculate $J_{11}\cos\theta$.

6.4 SPHERICAL COORDINATES

The Schrödinger equation in a central potential energy is essentially

$$\nabla^2\psi(\vec{r})+\left[E-V(r)\right]\psi(\vec{r})=0. \tag{6.55}$$

Using the spherical coordinates (r, θ, φ), Equation 6.54 becomes

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}+E-V(r)\right]\psi(r,\theta,\varphi)=0. \tag{6.56}$$

For separating variables, let $\psi(r,\theta,\varphi)=R(r)\Theta(\theta)\Phi(\varphi)$ to obtain

$$\frac{1}{R(r)}\frac{d}{dr}r^2\frac{d}{dr}R(r)+r^2[E-V(r)]=-\left[\frac{1}{\Theta(\theta)}\frac{1}{\sin\theta}\frac{d}{d\theta}\Theta(\theta)+\frac{1}{\Phi(\phi)}\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}\Phi(\varphi)\right]. \tag{6.57}$$

The angular part is

$$\left[\frac{1}{\Theta(\theta)}\frac{1}{\sin\theta}\frac{d}{d\theta}\Theta(\theta)+\frac{1}{\Phi(\varphi)}\frac{1}{\sin^2\theta}\frac{d^2}{d\varphi^2}\Phi(\varphi)\right]=-\lambda \text{ where } \lambda \text{ is } a \text{ constant.} \tag{6.58}$$

For separating two angular variables,

$$\frac{\sin\theta}{\Theta(\theta)}\frac{1}{\sin\theta}\frac{d}{d\theta}\Theta(\theta)+\lambda\sin^2\theta=-\frac{1}{\Phi(\varphi)}\frac{d^2}{d\varphi^2}\Phi(\varphi)=-a \text{ where } a \text{ is } a \text{ constant.} \tag{6.59}$$

From $\frac{1}{\Phi(\varphi)}\frac{d^2}{d\varphi^2}\Phi(\varphi)=a$, and thus $\Phi(\varphi)=e^{\pm\sqrt{a}\varphi}$.

With the periodic boundary condition, $\Phi(\varphi) = \Phi(\varphi + 2\pi)$, $a = -m^2$, where m is integer and thus

$$\Phi(\varphi)=e^{im\varphi}. \tag{6.60}$$

The θ-part becomes

$$\frac{\sin\theta}{\Theta(\theta)}\frac{1}{\sin\theta}\frac{d}{d\theta}\Theta(\theta)+\lambda\sin^2\theta=m^2. \tag{6.61}$$

6.4.1 Associated Legendre Function

Let $x = \cos\theta$ and $\Theta(\theta) = P(x)$, then from Equation 6.61 becomes

$$\frac{d}{dx}(1-x^2)\frac{d}{dx}P(x)+[\lambda-\frac{m^2}{1-x^2}]P(x)=0. \tag{6.62}$$

For Equation 6.62 to have finite value of solutions for $|x| \leq 1$, it is shown that $\lambda = \ell(\ell + 1)$, where $-\ell \leq m \leq +\ell$ [7]. Therefore,

$$\frac{d}{dx}(1-x^2)\frac{d}{dx}P(x)+[\ell(\ell+1)-\frac{m^2}{1-x^2}]P(x)=0. \tag{6.63}$$

Equation 6.63 is called the associated Legendre differential equation, and their solutions are called the associated Legendre functions $P_\ell^m(x)$.

Examples of associated Legendre polynomials (ℓ = 0 to 2):

$$\begin{aligned}
&\ell=0: P_0^0(x)=1.\\
&\ell=1:, P_1^1(x)=\sqrt{1-x^2},\ P_1^{-1}(x)=-\frac{1}{2}\sqrt{1-x^2}.\\
&\ell=2: P_2^2(x)=3(1-x^2),\ P_2^1(x)=3x\sqrt{1-x^2},\ P_2^0(x)=\frac{1}{2}(3x^2-1).\\
&P_2^{-1}(x)=-\frac{1}{2}x\sqrt{1-x^2},\ P_2^{-2}(x)=\frac{1}{8}(1-x^2).
\end{aligned} \tag{6.64}$$

Let $x = \cos\theta$ to express the polynomials in trigonometric functions:

$$\begin{aligned}
&P_0^0(x)=\cos\theta.\\
&P_1^1(x)=\sin\theta,\ P_1^0(x)=\cos\theta,\ P_1^{-1}(x)=-\frac{1}{2}\sin\theta.\\
&P_2^2(x)=3\sin^2\theta=\frac{3}{2}(1-\cos2\theta),\ P_2^1(x)=3\cos\theta\sin\theta=\frac{3}{2}\sin2\theta,\\
&P_2^0(x)=\frac{1}{2}(3\cos^2\theta-1),\ P_2^{-1}(x)=-\frac{1}{2}\cos\theta\sin\theta,\ P_2^{-2}(x)=\frac{1}{8}\sin^2\theta.
\end{aligned} \tag{6.65}$$

Figure 6.13 shows these functions calculated using Excel's *AutoFill* feature.

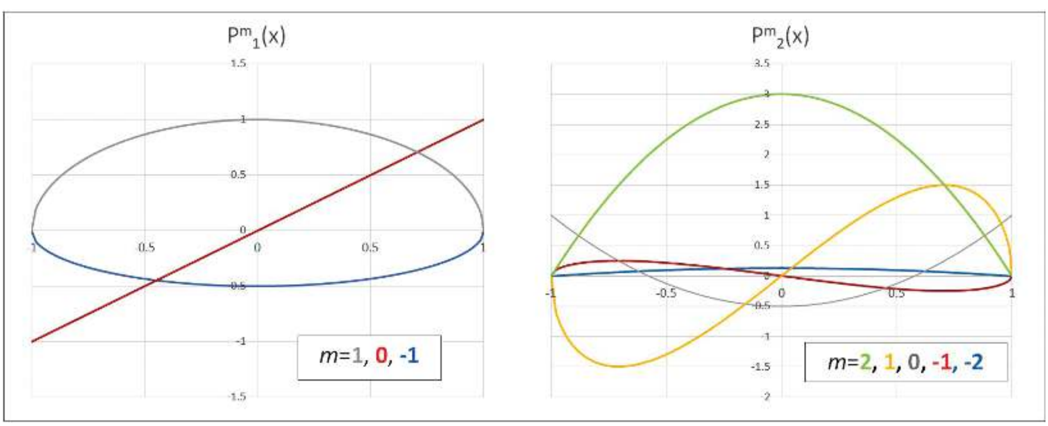


FIGURE 6.13 Associated Legendre functions (ℓ = 1 and 2).

List of important properties of Legendre polynomials.

Rodrigues formula: $P_\ell^m(x) = \frac{1}{2^\ell \ell!}(1-x^2)^{\frac{m}{2}} \frac{d^{\ell+m}}{dx^{\ell+m}}(x^2-1)^\ell$, where $-\ell \leq m \leq +\ell$. (6.66)

Generating function:

$$(\cos\theta + i\sin\theta\cos\phi)^\ell = P_\ell(\cos\theta) + 2\sum_{m=1}^{\ell} i^m \frac{\ell!}{(\ell+m)!}\cos(m\phi)P_\ell^m(\cos\theta) \tag{6.67}$$

where $P_\ell(\cos\theta)$ is the Legendre polynomials discussed in the next section.

Recursion relations:

$$2mxP_\ell^m(x) = \sqrt{1-x^2}\left[P_\ell^{m+1}(x) + (\ell+m)(\ell-m+1)P_\ell^{m-1}(x)\right]. \tag{6.68}$$

$$(\ell-m+1)P_{\ell+1}^m(x) - (2\ell+1)xP_\ell^m(x) + (\ell+m)P_{\ell-1}^m(x) = 0. \tag{6.69}$$

$$\begin{aligned}(1-x^2)\frac{dP_\ell^m(x)}{dx} &= (\ell+1)xP_\ell^m(x) - (\ell-m+1)P_{\ell+1}^m(x)\\ &= (\ell+m)P_{\ell-1}^m(x) - \ell xP_\ell^m(x) = \sqrt{1-x^2}\,P_\ell^{m+1}(x) - mxP_\ell^m(x)\\ &= mxP_\ell^m(x) - (\ell+m)(\ell-m+1)\sqrt{1-x^2}\,P_\ell^{m-1}(x).\end{aligned} \tag{6.70}$$

Parity: $P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!}P_\ell^m(x)$ and $P_\ell^m(-x) = (-1)^n P_\ell^m(x)$. (6.71)

Orthonormality: $\int_{-1}^{+1} P_\ell^m(x)P_n^m(x)dx = \frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}\delta_{\ell n}$. (6.72)

Associated Legendre functions, with a fixed m, also form a set of orthonormal basis, and an arbitrary function $f(x)$ on the interval $-1 \leq x \leq +1$ may be expanded in a series of the form,

$$f(x) = \sum_{\ell=m}^{\infty} c_\ell P_\ell^m(x) \text{ where } c_\ell = \frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}\int_{-1}^{1} f(x)P_\ell^m(x)dx. \tag{6.73}$$

Remark: Although there is another solution of the associated Legendre equation called the associated Legendre functions of the second kind, they are seldom applied to physics problems.

6.4.2 Legendre Polynomials

The associated Legendre differential equation with $m = 0$ is called the Legendre differential equation.

$$\frac{d}{dx}(1-x^2)\frac{d}{dx}P(x) + \ell(\ell+1)P(x) = 0. \tag{6.74}$$

The solutions of Equation 6.74 are called Legendre polynomials and can be given by

$$P_\ell(x)=\sum_{r=0}^{[\ell/2]}\frac{(-1)^\ell(2\ell-2r)!}{2^\ell r!(\ell-r)!(\ell-2r)!}x^{\ell-2r}\text{ ; and }\left|P_\ell\left(x\right)\right|\le 1\text{ for }|x|\le 1. \tag{6.75}$$

Legendre polynomials of lower orders (ℓ = 0–4):

$P_0(x) = 1,$
$P_1(x) = x,$
$P_2(x) = (1/2)(3x^2 - 1),$
$P_3(x) = (1/2)(5x^3 - 3x),$
$P_4(x) = (1/8)(35x^4-30x^2+3), \ldots$

Assume $x = \cos\theta$ to express the polynomials in terms of trigonometric functions:

$P_0(x) = 1,$
$P_1(x) = \cos\theta,$
$P_2(x) = (1/4)(3\cos 2\theta + 1),$
$P_3(x) = (1/8)(5\cos 3\theta + 3\cos\theta),$
$P_4(x) = (35/64)\cos 4\theta + (30/91)\cos 2\theta + 9/64, \ldots$ (6.76)

Figure 6.14 shows Legendre polynomials (ℓ = 0–4). The calculations can be made using Excel's *AutoFill*.

Rodrigues formula: $P_n(x)=n\frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n.$ (6.77)

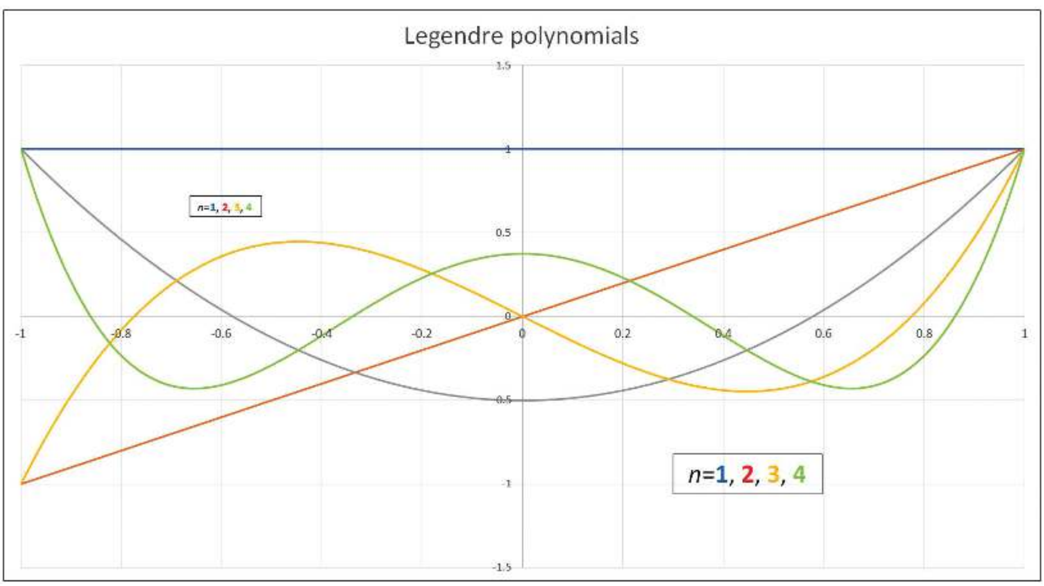


FIGURE 6.14 Legendre polynomials.

Generating function: $$\frac{1}{\sqrt{1-2tx+t^2}}=\sum_{n=0}^{\infty}P_n(x)t^n. \tag{6.78}$$

Recursion formula: $$P_{n+1}(x)=\frac{2n+1}{n+1}xP_n(x)-\frac{n}{n+1}P_{n-1}(x), \text{ using} \tag{6.79}$$

$$\left[(1-x^2)\frac{d}{dx}-(n+1)x\right]P_n(x)=-(n+1)P_{n+1}(x) \text{ and } \left[(1-x^2)\frac{d}{dx}-nx\right]P_n(x)=nP_{n-1}(x).$$

List of important properties of Legendre polynomials.

Parity: $$P_n(-x)=(-1)^nP_n(x). \tag{6.80}$$

Note: $$P_\ell^0(x)=P_\ell(x) \text{ and } P_\ell^m(x)=(1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}P_\ell(x). \tag{6.81}$$

Orthonormality: $$\int_{-1}^{+1}P_m(x)P_n(x)dx=\frac{2}{2n+1}\delta_{nm}. \tag{6.82}$$

Legendre functions also form a set of orthonormal bases. A function $f(x)$ on the interval $-1 \le x \le +1$ may be expanded in a series of the form

$$f(x)=\sum_{\ell=1}^{\infty}c_\ell P_\ell(x) \text{ where } c_\ell=\frac{2\ell+1}{2}\int_{-1}^{1}f(x)P_\ell(x)dx. \tag{6.83}$$

Figure 6.15 shows $f(x) = \sin x$ using 5 terms of $P_n(x)$. Refer to Appendix A6.3 for its detailed calculation. Because Legendre functions originated from the spherical coordinates, which are based on trigonometric functions, the fitting is good for 5 terms.

6.4.3 Spherical Harmonic Functions

In the Schrödinger Equation 6.55, the angular part of the Hamiltonian,

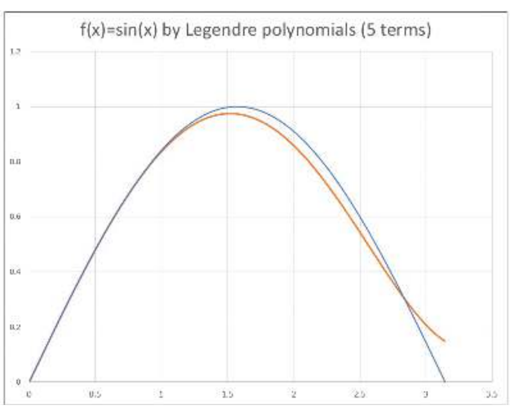


FIGURE 6.15 Series expansion of $\sin x$ using Legendre polynomials (5 terms).

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}, \tag{6.84}$$

expresses the angular momentum operators,

$$\breve{L}^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \text{ and } \breve{L}_z=-i\hbar\frac{\partial}{\partial\varphi}. \tag{6.85}$$

The solution of the angular momentum operators is the spherical harmonic function defined as

$$Y_{\ell m}(\theta,\varphi)=(-1)^m\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\varphi} \tag{6.86}$$

where

$$\begin{cases}\breve{L}^2Y_{\ell m}(\theta,\varphi)=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y_{\ell m}(\theta,\varphi)=\hbar^2\ell(\ell+1)Y_{\ell m}(\theta,\varphi),\\ \breve{L}_zY_{\ell m}(\theta,\varphi)=-i\hbar\frac{\partial}{\partial\phi}Y_{\ell m}(\theta,\varphi)=m\hbar Y_{\ell m}(\theta,\varphi).\end{cases} \tag{6.87}$$

Here are the explicit forms of the spherical harmonic functions.

$\underline{\ell=0}$: $Y_{00}(\theta,\varphi)=\frac{1}{\sqrt{4\pi}}$.

$\underline{\ell=1}$: $Y_{11}(\theta,\varphi)=-\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi}$, $Y_{10}(\theta,\varphi)=\sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_{1-1}(\theta,\varphi)=\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi}$.

$$\underline{\ell=2}: Y_{22}(\theta,\gamma)=\sqrt{\frac{5}{96\pi}}3\sin^2\theta e^{2i\varphi},\ Y_{21}(\theta,\varphi)=-\sqrt{\frac{5}{24\pi}}3\sin\theta\cos\theta e^{i\varphi},\ Y_{20}(\theta,\varphi)=-\sqrt{\frac{5}{4\pi}}\frac{1}{2}(3\sin^2\theta-1),$$

$$Y_{2-1}(\theta,\varphi)=\sqrt{\frac{5}{24\pi}}3\sin\theta\cos\theta e^{-i\varphi},\ Y_{2-2}(\theta,\varphi)=\sqrt{\frac{5}{96\pi}}3\sin^2\theta e^{-2i\varphi}. \tag{6.88}$$

$$\underline{\ell=3}: Y_{30}(\theta,\varphi)=\sqrt{\frac{7}{4\pi}}\left(\frac{5}{2}\cos^3\theta-\frac{3}{2}\cos\theta\right),\ Y_{31}(\theta,\varphi)=-\sqrt{\frac{7}{4\pi}}\frac{1}{4}\sin\theta\left(5\cos^5\theta-1\right)e^{i\varphi},$$

$$Y_{32}(\theta,\varphi)=\sqrt{\frac{105}{2\pi}}\frac{1}{4}\sin^2\theta\cos\theta e^{2i\varphi},\ Y_{33}(\theta,\varphi)=-\sqrt{\frac{35}{4\pi}}\frac{1}{4}\sin^3\theta e^{3i\varphi},\text{ etc.}$$

For displaying spherical harmonic functions using Euler's angles, there are several steps:

1) Convert θ and φ values to x, y, z values: using

   $x = r\cos\theta\cos\varphi$, $y = r\cos\theta\sin\varphi$, and $z = r\sin\theta$ ($r = 1$);

2) Rotate the calculated *xyz*-coordinates to *XYZ*-coordinates using specified Euler's angles; and

3) Select the *XY*, the *YZ*, or the *ZX* plane to display data using the *Scatter chart*.

As is well known, angular parts of wave functions are quite different from the semi-classical theory, and it is fun to produce them on your own computer. Figure 6.16 lists the VBA code to take the above steps to create $|Y_{00}|$.

Figures 6.17 to 6.19 show these spherical harmonic functions ($\ell = 0$–3). Euler's angles: $\alpha = \pi/6$ rad, $\beta = \pi/3$ rad, and $\gamma = \pi/8$ rad.

Orthonormality: $\{Y_{\ell m}(\theta, \varphi)\}$ forms an orthonormal basis on a spherical surface. A function $f(\theta, \varphi)$ on a sphere may be expressed with $\{Y_{\ell m}(\theta, \varphi)\}$.

```
Sub SphericalHarmonics()
Cells(1, 1) = "3D displays of Spherical Harmonics"
   Pi = 3.14159265358979
'Rotational angles of coordinates
   Cells(2, 1) = "alpha": alpha = Pi / 6: Cells(3, 1) = alpha
   Cells(2, 3) = "beta": beta = Pi / 3: Cells(3, 3) = beta
   Cells(2, 5) = "gamma": Gamma = Pi / 8: Cells(3, 5) = Gamma
'Variable labels
   Cells(4, 1) = "phi"
   Cells(4, 2) = "theta"
   Cells(4, 3) = "Y00"
   Cells(4, 5) = "fx"
   Cells(4, 6) = "fy"
   Cells(4, 7) = "fz"
   Cells(4, 9) = "Fx"
   Cells(4, 10) = "Fy"
   Cells(4, 11) = "Fz"
'Calculating spherical harmonics
'For a given theta, change phi from 0 to 2*PI and calculate the given spherical harmonics.
   For i = 0 To 32
      Phi = i * (2 * Pi / 32)
      Cells(5 + 33 * i, 1) = Phi
         For j = 0 To 32
            theta = j * (Pi / 32)
            Y = 1
            Cells(5 + 33 * i + j, 2) = theta
            Cells(5 + 33 * i + j, 3) = Y
               fx = Y * Sin(theta) * Cos(Phi)
               fy = Y * Sin(theta) * Sin(Phi)
               fz = Y * Cos(theta)
                  Cells(5 + 33 * i + j, 5) = fx
                  Cells(5 + 33 * i + j, 6) = fy
                  Cells(5 + 33 * i + j, 7) = fz
'Rotate fx, fy, fz to ffx, ffy, ffz by Euler's angles (alpha, beta, gamma).
      ffx = fx * (Cos(beta) * Cos(alpha) * Cos(Gamma)  - Sin(alpha) * Sin(Gamma)) + fy * (Cos(beta) * Sin(alpha) * Cos(Gamma) + Cos(alpha) *
Sin(Gamma)) - fz * Sin(beta) * Cos(Gamma)
      ffy = -fx * (Cos(beta) * Cos(alpha) * Sin(Gamma) + Sin(alpha) * Cos(Gamma))  - fy * (Cos(beta) * Sin(alpha) * Sin(Gamma)  - Cos(alpha) *
Cos(Gamma)) + fz * Sin(beta) * Sin(Gamma)
      ffz = fx * Sin(beta) * Cos(alpha) + fy * Sin(beta) * Sin(alpha) + fz * Cos(beta)
               Cells(5 + 33 * i + j, 9) = ffx
               Cells(5 + 33 * i + j, 10) = ffy
               Cells(5 + 33 * i + j, 11) = ffz
         Next j
   Next i
End Sub
```

FIGURE 6.16 VBA code to prepare a 3D display of Y.

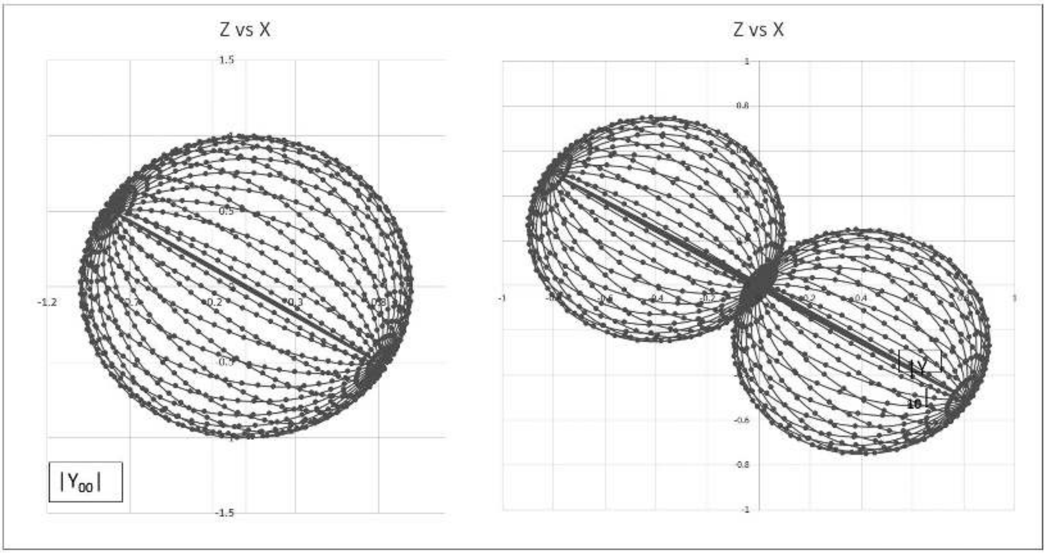


FIGURE 6.17 $|Y_{00}|$ and $|Y_{10}|$.

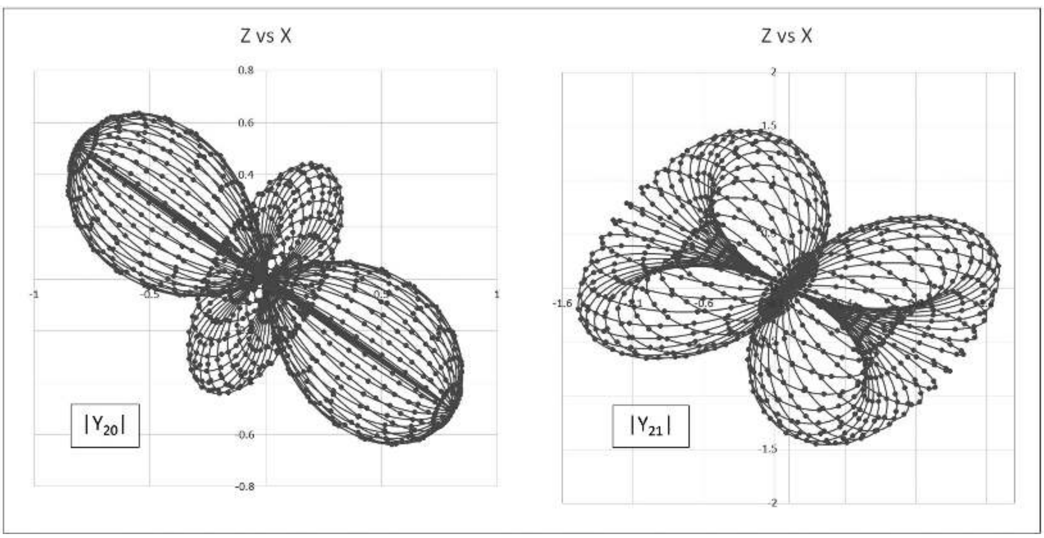


FIGURE 6.18 $|Y_{20}|$ and $|Y_{21}|$.

$$\begin{aligned}
\left(Y_{\ell m}, Y_{\ell' m'}\right) &\equiv \int_0^{2\pi} d\varphi \int_0^{\pi} \overline{Y_{\ell m}(\theta,\varphi)} Y_{\ell' m'}(\theta,\varphi) \sin\theta d\theta = \delta_{\ell\ell'}\delta_{mm'} \\
\left(Y^*_{\ell m}, Y^*_{\ell' m'}\right) &\equiv \int_0^{2\pi} d\varphi \int_0^{\pi} Y^*_{\ell m}(\theta,\varphi) Y^*_{\ell' m'}(\theta,\varphi) \sin\theta d\theta = \delta_{\ell\ell'}\delta_{mm'}.
\end{aligned} \tag{6.89}$$

$$f(\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} f_{\ell m} Y_{\ell m}(\theta,\varphi) \text{ where } f_{\ell m} = \left(Y_{\ell m}, f\right) \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} \overline{Y_{\ell m}(\theta,\varphi)} f(\theta,\varphi) \sin\theta d\theta. \tag{6.90}$$

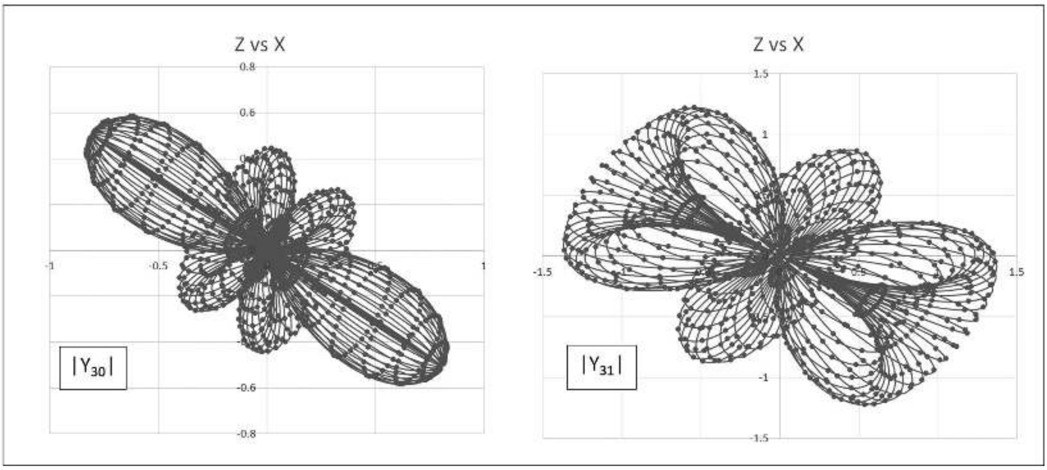


FIGURE 6.19 $|Y_{30}|$ and $|Y_{31}|$.

Note: *Ladder operators of angular momentum.* Ladder operators or raising or lowering operators are mathematical operators that increase or decrease the eigenvalue of another operator. The angular momentum,

$$\begin{aligned} \breve{L}_x &= y\breve{p}_z - z\breve{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \breve{L}_y &= z\breve{p}_x - x\breve{p}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \breve{L}_z &= x\breve{p}_y - y\breve{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned} \tag{6.91}$$

can be expressed in spherical polar coordinates to give

$$\begin{aligned} \breve{L}_x &= i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ \breve{L}_y &= i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right). \\ L_z &= -i\hbar\frac{\partial}{\partial\varphi} \end{aligned} \tag{6.92}$$

Define new

$$\begin{aligned} \breve{L}_+ &\equiv L_x + i\breve{L}_y = e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \\ \breve{L}_- &\equiv L_x - i\breve{L}_y = e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right). \end{aligned} \tag{6.93}$$

Using Equation 6.86, $Y_{\ell m}(\theta,\varphi) = (-1)^m \sqrt{\dfrac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}} P_\ell^m(\cos\theta)e^{im\varphi} \equiv N_{\ell m} P_\ell^m(\cos\theta)e^{im\varphi}$,

$$\begin{aligned} \breve{L}_+ Y_{\ell m}(\theta,\varphi) &= e^{i\varphi} N_{\ell m}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) P_\ell^m(\cos\theta)e^{im\varphi} \\ &= e^{i(m+1)\varphi} N_{\ell m}\left(\frac{dP_\ell^m}{d\theta} - m\frac{\cos\theta}{\sin\theta}P_\ell^m\right). \end{aligned} \tag{6.94}$$

Let $x = \cos\theta$, then $d/d\theta = (dx/d\theta)\bullet d/dx$, and

$$\begin{aligned} \frac{dP_\ell^m}{d\theta} &= -\sqrt{1-x^2}\,\frac{dP_\ell^m}{dx} = -P_\ell^{m+1} + \frac{mx}{\sqrt{1-x^2}}P_\ell^m \\ &= (\ell+m)(\ell-m+1)P_\ell^{m-1} + \frac{mx}{\sqrt{1-x^2}}P_\ell^m - (\ell+m)(\ell-m+1)P_\ell^{m-1} + \cot\theta P_\ell^m. \end{aligned} \tag{6.95}$$

where we used the recursion relations (6.70). Thus, moving the second term from the right side to the left side,

$$\begin{aligned} -\frac{dP_\ell^m}{d\theta} + m\cot\theta P_\ell^m &= P_\ell^{m+1}, \\ \frac{dP_\ell^m}{d\theta} + m\cot\theta P_\ell^m &= (\ell+m)(\ell-m+1)P_\ell^{m+1}, \end{aligned} \tag{6.96}$$

and Equation 6.95 gives

$$\begin{aligned} \breve{L}_+ Y_{\ell m}(\theta,\varphi) &= e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) Y_{\ell m}(\theta,\varphi) \\ &= -e^{i(m+1)\varphi} N_{\ell m} P_\ell^{m+1}(\cos\theta) = -\sqrt{(\ell-m)(\ell+m+1)}\,Y_{\ell m+1}(\theta,\varphi). \end{aligned} \tag{6.97}$$

Similarly, we obtain

$$\begin{aligned} \breve{L}_- Y_{\ell m}(\theta,\varphi) &= e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) Y_{\ell m}(\theta,\varphi) \\ &= -\sqrt{(\ell+m)(\ell-m+1)}\,Y_{\ell m-1}(\theta,\varphi). \end{aligned} \tag{6.98}$$

6.5 TABULATED INTEGRALS

6.5.1 Gamma Functions

Gamma function $\Gamma(x)$ is the generalization of factorial ($n!$). The definition of gamma function is

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt. \tag{6.99}$$

From the definition, $\Gamma(x + 1) = x\,\Gamma(x)$, and $\Gamma(n + 1) = n!$, where n is a positive integer.

$$\text{Notice } \Gamma\left(1/2\right)=\sqrt{\pi} \text{ and } \Gamma(n+1/2)=\frac{(2n-1)!!}{2^n}\sqrt{\pi}, \tag{6.100}$$

where $n!! = n\bullet(n-2)\bullet(n-4)\ldots3\bullet1$ if n is an odd integer and $n!! = n\bullet(n-2)\bullet(n-4)\ldots4\bullet2$ if n is an even integer.

$$\text{If } x<0, \text{ we use } \Gamma(x)\Gamma(1-x)=\frac{\pi}{\sin(\pi x)} \text{ to calculate } \Gamma\left(x\right). \tag{6.101}$$

Excel does not provide the gamma function. However, the gamma function can be created by using the probability distribution function of the gamma distribution, which is the built-in function `GAMMADIST`. Using this built-in function, we can calculate

```
Γ(x)=1/GAMMADIST(1, x, 1, 0)/EXP(1)
```

for $x > 0$. For $x < 0$, use Equation 6.101. Figure 6.20 shows the gamma function using GAMMADIST.

6.5.2 Beta Functions

$$\text{Beta function is defined as } B(x,y)=\int_0^1 t^{x-1}(1-t)^{y-1}dt \text{ where } x>0 \text{ and } y>0. \tag{6.102}$$

Beta function is closely related to gamma function in the following way.

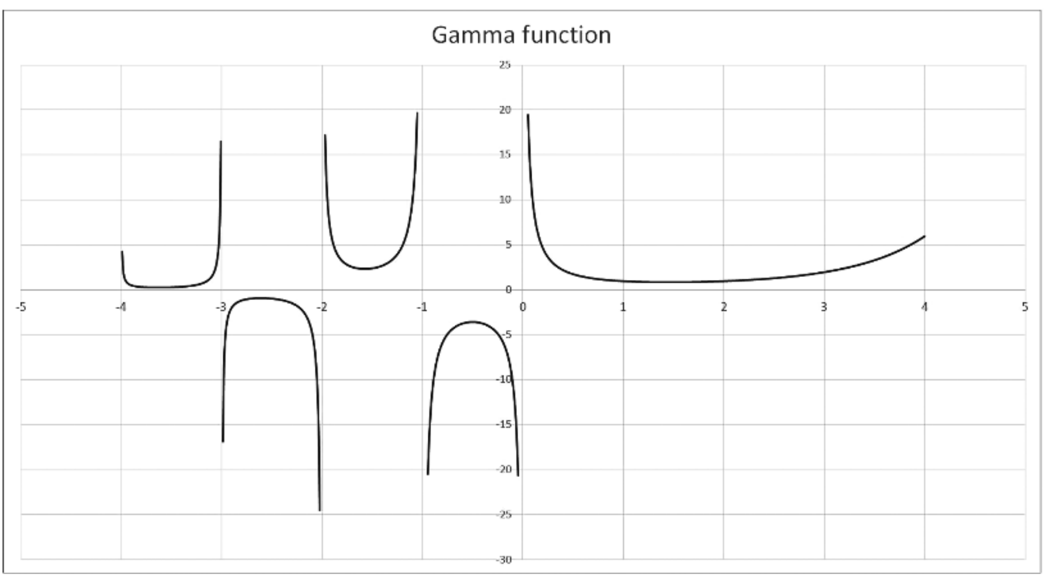


FIGURE 6.20 Gamma function using GAMMADIST.

$$\Gamma(r)\Gamma(s)=\int_0^\infty x^{r-1}e^{-x}dx\int_0^\infty y^{s-1}e^{-y}dx=\int_0^\infty du\int_0^u dxx^{r-1}(u-x)^{s-1}e^{-u} \text{ where } u=x+y. \quad (6.103)$$

Assume $x = ut$, then

$$\Gamma(r)\Gamma(s)=\int_0^\infty due^{-u}u^{r+s-1}\int_0^1 dtt^{r-1}(1-t)^{s-1}=\Gamma(r+s)B(r,s). \quad (6.104)$$

From the above relationship, we can calculate $B(x, y)$ by using `GAMMADIST` in the following way:

B(*x*, *y*)=GAMMADIST(1, *x*+*y*, 1, 0)/GAMMADIST(1, *x*, 1, 0)/GAMMADIST(1, *y*, 1, 0)/EXP(1).

Figure 6.21 is a screenshot for calculating the numerical values of the beta function.

1) The x-axis ranges from 0.05 to 3.0.5 with increments of 0.1 in Column `B` and the y-axis ranges from 0.05 to 3.05 with increments of 0.1 in Row `2`.
2) Enter

   =GAMMADIST(1,$B3+C$2,1,0)/GAMMADIST(1,$B3,1,0)/GAMMADIST(1, C$2,1,0)/EXP(1)

   in cell `C3` and apply *AutoFill*.
3) Highlight the data set (`C3` to `BJ33`) and select [`Wire-frame 3D surface chart`].
4) Expand the graph and select [`Monochrome color`].
5) Right-click on the graph to select [`3-D Rotation`]. Try to rotate your graph to obtain a good view.

Figure 6.22 shows the beta function profile.

6.5.3 Elliptic Functions

The equation of motion of a pendulum of length L under gravity is given by

	A	B	C	D	E	F	G	H	I
1	Beta function B(x,y)								
2	x\y		0.05	0.15	0.2	0.25	0.3	0.35	0.4
3		0.05	39.84695	26.38061	24.65354	23.59663	22.87617	22.34902	21.94348
4		0.15	[illegible]	12.93361	11.2155	10.16711	9.45482	8.935482	8.537436
5		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
6		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
7		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

=GAMMADIST(1,$B3+C$2,1,0)/GAMMADIST(1,$B3,1,0)/GAMMADIST(1,C$2,1,0)/EXP(1)

FIGURE 6.21 Calculating beta function B(x, y).

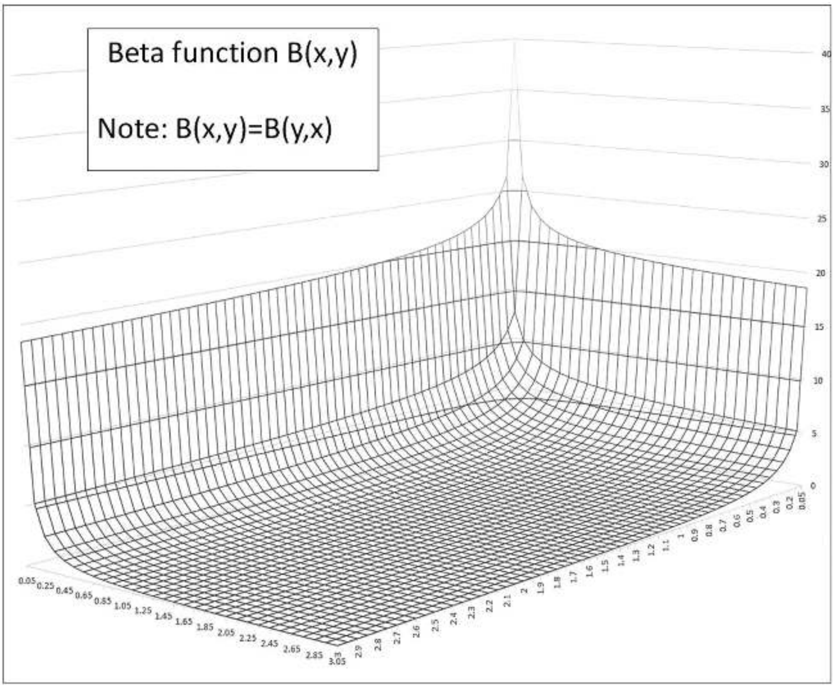


FIGURE 6.22 Beta function.

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta \text{ where } \theta \text{ is the angular displacement to the vertical direction.} \tag{6.105}$$

Multiplying $d\theta/dt$ to the above equation to perform the energy integral.

$$\int_0^t \left(\frac{d\theta}{dt}\right)\left(\frac{d^2\theta}{dt^2}\right)dt = -\frac{g}{L}\int_0^t \sin\theta\left(\frac{d\theta}{dt}\right). \tag{6.106}$$

$$\frac{1}{2}\left[\left(\frac{d\theta}{dt}\right)^2 - \omega_0^2\right] = \frac{g}{L}\int_0^\theta \frac{d(\cos\theta)}{dt} = \frac{g}{L}\left(\cos\theta - 1\right). \tag{6.107}$$

Where we used the initial conditions as $d\theta/dt|_{t=0} = \omega_0$ and $\theta|_{t=0} = 0$.

Considering the case when the angular velocity is positive, we obtain

$$\frac{d\theta}{dt} = \sqrt{\omega_0^2 - \frac{2g}{L}(1-\cos\theta)} = \sqrt{\omega_0^2 - \frac{4g}{L}\sin^2\left(\frac{\theta}{2}\right)}. \tag{6.108}$$

$$\frac{d\theta}{dt} = 2\sqrt{\frac{g}{l}}\sqrt{k^2 - \sin^2\left(\frac{\theta}{2}\right)} \text{ where } k^2 = \frac{L}{4g}\omega_0^2. \tag{6.109}$$

$$\text{Thus, } dt = \frac{1}{2}\sqrt{\frac{L}{g}}\frac{d\theta}{\sqrt{k^2-\sin^2(\theta/2)}}, \text{ and } t = \frac{1}{2}\sqrt{\frac{L}{g}}\int_0^{\theta}\frac{d\theta}{\sqrt{k^2-\sin^2(\theta/2)}}. \tag{6.110}$$

Let $\sin(\theta/2) = kz$, then

$$t = \sqrt{\frac{L}{g}}\int_0^{(1/k)\sin(\theta/2)}\frac{dz}{\sqrt{(1-z^2)(1-k^2z^2)}}. \tag{6.111}$$

The following integral is called elliptic integral:

$$x = \int_0^y \frac{dy}{\sqrt{(1-y^2)(1-k^2y^2)}}. \tag{6.112}$$

Note that Equation 6.112 becomes $x = \sin^{-1}y$ when $k = 0$. In other words, if we define

$$x = \sin^{-1} y = \int_0^y \frac{dy}{\sqrt{1-y^2}},$$

then $y = \sin x$ can be defined as the inverse function of $x = \sin^{-1}y$. Analogues to this idea, elliptic functions are defined as the inverse functions to elliptic integrals. When $k\neq 0$, we denote the inverse function of Equation 6.112 as $y = \mathrm{sn}(x, k)$.

We also define

$$\begin{aligned} cn(x,k) &= \sqrt{1-sn^2(x,k)}, \\ tn(x,k) &= sn(x,k)/cn(x,k), \\ dn(x,k) &= \sqrt{1-k^2sn^2(x,k)}. \end{aligned} \tag{6.113}$$

In particular, these functions with $k = 0$ and $k = 1$ become ordinary trigonometric functions:

$\mathrm{sn}(x,0) = \sin x$, $\mathrm{cn}(x,0) = \cos x$, $\mathrm{tn}(x,0) = \tan x$, and $\mathrm{dn}(x,0) = 1$.
$\mathrm{sn}(x,1) = \tanh x$, $\mathrm{cn}(x,1) = \mathrm{sech} x$, $\mathrm{tn}\,(x,1) = \sinh x$, and $\mathrm{dn}(x,1) = \mathrm{sech} x$.

Figure 6.23 shows these elliptic functions.

SUGGESTED FURTHER STUDY

Hypergeometric functions,

$${}_2F_1(a,b;c;x) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{n=0}^{\infty}\frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)}\frac{x_n}{n!},$$

are a solution of the differential equation called the hypergeometric equation,

$$x(1-x)\frac{d^2y}{dx^2} + \left[c-(a+b+1)x\right]\frac{dy}{dx} - aby = 0.$$

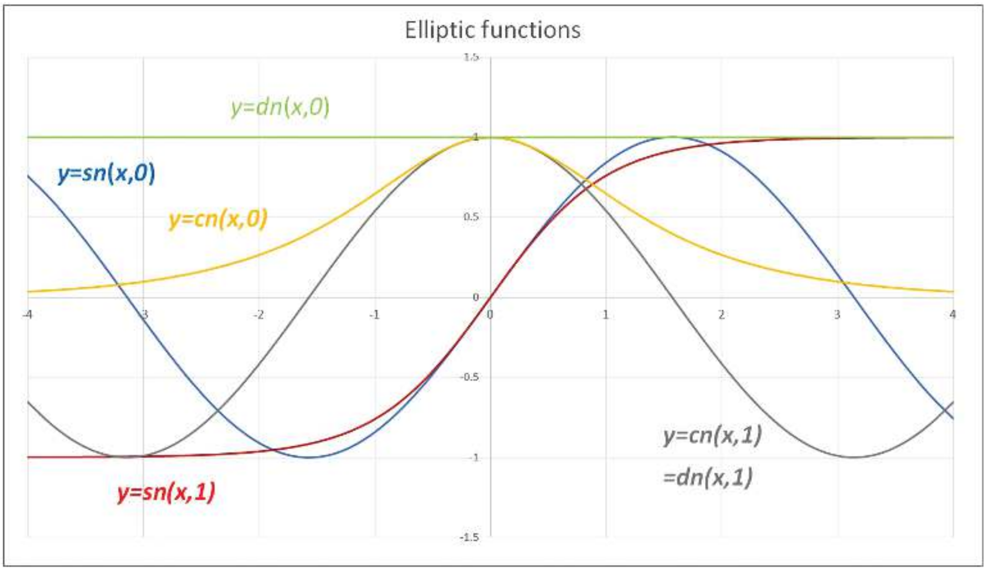


FIGURE 6.23 Elliptic functions.

Mathematical functions we encounter in physics are mostly special cases of ${}_2F_1(a, b, c, x)$ including the Legendre functions, Jacobi polynomials, Bessel functions, Laguerre polynomials, Hermite polynomials, and Fresnel integrals of classical optics. Refer to [1, 8, 9] for hypergeometric functions and equations.

Elliptic functions play an important role in cryptography. "Elliptic integral" was named so by Legendre because it relates to the elliptic arclength. Jacobi called the inverse function of the elliptic integral as an "elliptic function." Riemann considered the relationship between the elliptic function and the algebraic curves. For example, the third-order polynomial curve was expressed using a parametric expression of the elliptic function. Refer to [10] for the historical background. For elliptic cryptography, refer to interesting articles on the Internet [11, 12].

REFERENCES

1. Mathews J, and Walker RL, *Mathematical Methods of Physics*, Internet Archive, 1973. https://archive.org/details/mathematicalmeth0000math.
2. Arfken GB, Weber HJ, and Harris FE, *Mathematical Methods for Physicists*, Internet Archive. 2013. https://archive.org/details/Mathematical_Methods_for_Physicists.
3. Riley KF, Hobson MP, and Bence SJ, *Mathematical Methods for Physics and Engineering*, Cambridge University Press, 2002.
4. Schneider BI, Miller BR, and Saunders BV, *Digital Library of Mathematical Functions*, NIST. https://dlmf.nist.gov/.
5. Abramowitz M, and Stegun IA, *A Handbook of Mathematical Functions with Formula, Graphs, and Mathematical Tables*, National Bureau of Standards, 1972. https://personal.math.ubc.ca/~cbm/aands/frameindex.htm.
6. Zakharov V, *Bessel Functions and their Applications to Solutions of Partial Differential Equations*, University of Arizona, 2009. https://math.arizona.edu/~zakharov/BesselFunctions.pdf.

7. This statement can be also obtained from the Laplace equation. See [3].
8. Mathews WN, Esrick MA, Teoh ZY, and Freericks JK, *A Physicist's Guide to the Solution of Kummer's Equation and Confluent Hypergeometric Functions*, arXiv, Cornell University, 2012. https://arxiv.org/abs/2111.04852.
9. Boyce WE and DiPrima RC, *Elementary Differential Equations*, John Wiley & Sons, Inc., 2003.
10. Ravenel D, *Elliptic Curves: What They Are, Why They Are Called Elliptic, and Why Topologists Like Them*, *I*, Wayne State University Mathematics Colloquium, 2007. https://people.math.rochester.edu/faculty/doug/mypapers/wayne3.pdf#:~:text=Elliptic%20curves%20Recall%20that%20an%20elliptic.
11. Froehlich A Elliptic Curve Cryptography (ECC): TechTarget. https://www.techtarget.com/searchsecurity/definition/elliptical-curve-cryptography.
12. *Elliptic Curve Cryptography*, Avi Networks. https://www.vmware.com/topics/elliptic-curve-cryptography.

CHAPTER 7

Wave Packets and Wave Functions

A WAVE PACKET IS A model to implement the dual nature of a wave-particle in quantum mechanics. From the kinematics of wave packets, we understand:

(1) The difference between the velocities of particle and wave; and

(2) The propagation of a wave packet in a given potential energy.

As we pointed out in Section 3.5.3, when the particle model is applied to the law of refraction, the classical theory does not correctly predict the law. The reason for this discrepancy may be attributed to the difference between the velocities of classical particles and the electromagnetic wave. A computational algorithm proposed by Visscher et al. predicts the kinematics of wave packets correctly. We demonstrate the algorithm for two cases: in a free space and in a potential step.

The algorithm of Euler and Cromer is known as a shooting method for finding the eigenvalues of a bound state Schrödinger equation and other boundary value problems. The shooting method may be extended more generally by applying the Runge-Kutta method with correct boundary conditions to a harmonic oscillator and a hydrogen atom.

7.1 KINEMATICS OF WAVE PACKET

Although a single plane wave cannot be localized, an arbitrary localized wave propagating in the x direction can be created by a wave packet which is superposed plane waves $F(k)e^{i(kx-\omega t)}$ of amplitude $F(k)$:

$$\psi(x,t) = \int_{-\infty}^{+\infty} F(k)e^{i(kx-\omega t)}dk. \tag{7.1}$$

DOI: 10.1201/9781003516347-7

This is equivalent to the Fourier transform, and the "amplitude" $F(k)$ should be the inverse Fourier transform [1].

$$F(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \psi(x,t)e^{-ikx}\,dk. \tag{7.2}$$

If a particle can be a wave packet, what is the speed of a wave packet?

7.1.1 Group Velocity and Phase Velocity

Does the phase velocity, $v_p = \lambda \cdot f = \omega/k$, where ω is the angular frequency and k is the wave number, represent the speed of a particle as a wave [2]? If the particle has the frequency, f, its energy is given by $E = hf = \hbar\omega$. From the de Broglie wavelength of a particle, the momentum of the particle is given by $p = h/\lambda = \hbar k$. The phase velocity is given by

$$v_{phase} = f \cdot \lambda = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{E}{p} = \frac{mc^2}{mv_{particle}} = \frac{c^2}{v_{particle}}. \tag{7.3}$$

The relativistic expressions of energy and momentum are $E = mc^2$ and $p = mv$ where m is the relativistic mass,

$$v_{phase} = \frac{E}{p} = \frac{mc^2}{mv_{particle}} = \frac{c^2}{v_{particle}} = \left(\frac{c}{v_{particle}}\right) \cdot c > c \text{ because } c > v_{particle}. \tag{7.4}$$

The consequence of Equation 7.4 is unacceptable. The phase velocity cannot be the speed of the wave nature of a particle. Instead, the group velocity defined by $v_g = d\omega/dk$ may be used to express the speed of a wave packet [3]. In terms of the particle's parameter, the group velocity can be expressed as

$$v_g = \frac{d\omega}{dk} = \frac{d(E/\hbar)}{d(p/\hbar)} = \frac{dE}{dp}. \tag{7.5}$$

For a particle, the kinetic energy is $E = p^2/2m$, and thus, $v_g = dE/dp = p/m = v$. Energy and momentum of a free particle can be given by $E = \hbar\omega$ and $p = \hbar k$. Because the energy of a free particle is given by $E = p^2/2m$, $\omega = E/\hbar = \hbar k^2/2m$ from which the group velocity is correctly given by $v_g = d\omega/dk = \hbar k/m = p/m$.

How can we incorporate the group velocity in the wave packet [4]? If the distribution $F(k)$ of Equation 7.2 is localized at around k_0, then the angular frequency $\omega(k)$ can be expanded around k_0:

$$\omega(k) = \omega_0 + \left.\frac{d\omega}{dk}\right|_0 (k - k_0) + \ldots \tag{7.6}$$

Plugging Equation 7.6 into Equation 7.1, we obtain

$$\psi(x,t) = \int_{-\infty}^{+\infty} F(k)e^{i\left[kx - (\omega_0 t + \left.\frac{d\omega}{dk}\right|_0 (k-k_0)t + \ldots)\right]}dk = e^{i\omega_0 t + \left.\frac{d\omega}{dk}\right|_0 k_0 t} + \int_{-\infty}^{+\infty} F(k)e^{i\left[kx - \left.\frac{d\omega}{dk}\right|_0 kt\right]}dk. \tag{7.7}$$

Recall the definition of a Fourier transform,

$$\psi(x,0) = \int_{-\infty}^{+\infty} F(k)e^{ikx}dk, \tag{7.8}$$

and we obtain

$$\int_{-\infty}^{+\infty} F(k)e^{i\left[k\left(x-\left.\frac{d\omega}{dk}\right|_0 t\right)\right]}dk = \psi(x',0) \tag{7.9}$$

where $x' = x - \left.\dfrac{d\omega}{dk}\right|_0 t.$

Because $d\omega/dk$ is the group velocity v_g, the position of the wave packet at a later time t is given by $x' = x - v_g t$. This is equivalent to the position of a particle moving at a velocity v_g.

7.1.2 Motion of a Wave Packet in Free Space

We start with Equation 7.1 to describe the motion of a wave packet in free space. In addition, we assume the probability of existence at $t = 0$ is given by a Gaussian distribution function at the origin,

$$|\psi(x,0)|^2 = \frac{1}{\left(2\pi\sigma^2\right)^{1/2}}\exp\left[-\frac{x^2}{2\sigma^2}\right] \tag{7.10}$$

with the standard deviation σ, which represents the uncertainty in the position Δx at $t = 0$. The wave packet at $t = 0$ is given by

$$\psi(x,0) = \frac{1}{\left(2\pi\sigma^2\right)^{1/4}}\exp\left[-\frac{x^2}{4\sigma^2}\right]\exp\left[ik_0x\right]. \tag{7.11}$$

From Equation 7.2, the amplitude $F(k)$ for the Gaussian wave packet is

$$F(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\psi(x,0)e^{-ikx}dx = \left(\frac{2\sigma^2}{\pi}\right)^{1/4}\exp\left[-\sigma^2(k-k_0)^2\right]. \tag{7.12}$$

From equation (7.1), the wave packet $\psi(x, t)$ at time t is given by

$$\begin{aligned}\psi(x,t) &= \left(\frac{2\sigma^2}{\pi}\right)^{1/4}\int_{-\infty}^{+\infty}\exp\left[-\sigma^2(k-k_0)^2 + i(kx-\omega t)\right]dk \\ &= \frac{1}{\sigma^{1/2}}\frac{1}{(1+i\alpha t)^{1/2}}\exp\left[-\left(\frac{(x-i2\sigma^2k_0)^2}{4\sigma^2(1+i\alpha t)} + \sigma^2k_0^2\right)\right].\end{aligned} \tag{7.13}$$

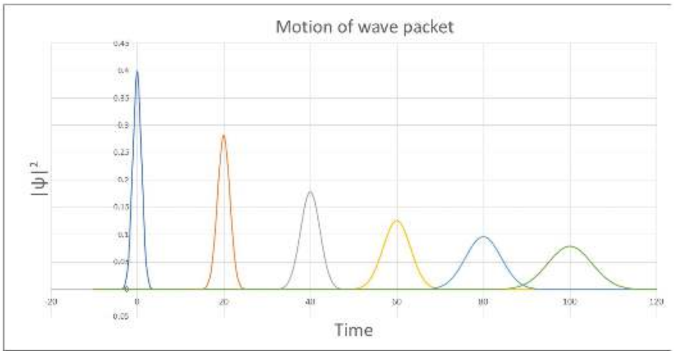


FIGURE 7.1 A time-dependent wave packet.

Where $\alpha = \hbar/2m\sigma^2$. The calculation of the above wave packet is detailed in Appendix A7. The probability distribution function is

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi\sigma^2(1+\alpha^2t^2)}}\exp\left[-\frac{(x-v_0t)^2}{2\sigma^2(1+\alpha^2t^2)}\right] \tag{7.14}$$

where $v_0 = \hbar k_0/m$. This is a "spreading-Gaussian" function with the standard deviation given by $\sigma^2(1+\alpha^2t^2)$. Figure 7.1 is the schematic diagram of the time-dependent wave packet with $v_0 = 1$, $\sigma = 0.2$, and $\alpha = 1$. The Gaussian wave packet is spreading out as time elapses while the peak position is moving at the group velocity v_0.

Figure 7.2 lists the VBA code used to calculate the motion of the Gaussian wave packet.

7.1.3 Wave Packet in a Harmonic Potential

The potential energy of a harmonic oscillator asymptotically becomes infinite and a particle will be trapped inside the potential. How does its wave packet, or more precisely, the probability distribution function of the wave function change dynamically? For analyzing

```
Sub WavePacket()
Cells(1, 1) = "Time dependence of wave packet in free space"
Cells(2, 2) = "sigma": sigma = 1: Cells(3, 2) = sigma
Cells(2, 3) = "alpha": alpha = 0.1: Cells(3, 3) = alpha
Cells(2, 4) = "v0": v0 = 2: Cells(3, 4) = v0
Cells(5, 2) = "x"
Cells(4, 3) = "Time"
Pi = 3.141592654
 For k = 0 To 5
  t = 10 * k
  Cells(5, 3 + k) = t
  j = 0
   For x = -10 To 120
     Cells(6 + j, 2) = x
Probability = (1 / ((2 * Pi * sigma ^ 2) * (1 + (alpha * t) ^ 2)) ^ 0.5) * Exp( -(x - v0 * t) ^ 2 / (2 * (1 + (alpha * t) ^ 2)) * sigma ^ 2)
     Cells(6 + j, 3 + k) = Probability
     j = j + 1
   Next x
 Next k
End Sub
```

FIGURE 7.2 VBA code of the time-dependent wave packet.

the motion, we need to use the Schrödinger equation for the harmonic oscillator [5]. Let us start with the time-dependent wave function,

$$\psi(x,t) = \sum_{n=0} c_n \varphi_n(x) \exp\left[-\frac{i}{\hbar} E_n t\right] \tag{7.15}$$

where the time-independent wave function satisfies the time-independent Schrödinger equation.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2\right]\varphi_n(x) = E_n \varphi_n(x). \tag{7.16}$$

The solution of Equation 7.16 is given by the Hermite polynomials discussed in Section 6.2.3:

$\varphi_n(x) = N_n H_n(\alpha x)\exp(-\alpha^2 x^2)$, where $N_n = \left(\frac{\alpha}{\pi^{1/2} 2^n n!}\right)$, $\alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$,
where

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0,\ n{=}0,\ 1,\ 2,\ \ldots$$

Combining Equations 7.14 and 7.15, we obtain

$$\psi(x,t) = \exp\left[-\frac{i}{2}\omega_0 t\right] \sum_{n=0} c_n \varphi_n(x) \exp\left[-i\omega_0 n t\right]. \tag{7.17}$$

We may predict that the probability distribution function $|\psi(x,t)|^2$ is periodic with a period of $T = 2\pi/\omega_0$.

$$\left|\psi(x, t+uT)\right|^2 = \left|\sum_{n=0} c_n \varphi_n(x) \exp\left[-i(\omega_0 n t + 2\pi n u)\right]\right|^2 \tag{7.18}$$

where u is an integer. Because nu is also an integer, $\exp(-2\pi i n u) = 1$. Therefore,

$$\left|\psi(x, t+uT)\right|^2 = \left|\sum_{n=0} c_n \varphi_n(x) \exp\left[-i\omega_0 n t\right]\right|^2 = \left|\psi(x,t)\right|^2. \tag{7.19}$$

This indicates that the probability distribution function retains the same shape over time.

As the initial condition, take the wave function of the ground state except that the center of gravity is displaced in the positive x direction by an amount x_0:

$$\psi(x,0) = \sum_{n=0}^{\infty} c_n \varphi_n(x) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \exp\left[-\frac{\alpha^2}{2}(x - x_0)^2\right] \text{ where } \alpha = \left(\frac{m\omega_0}{\hbar}\right)^{1/2}. \tag{7.20}$$

The coefficients $\{c_n\}$ are given by $c_n = \frac{(ax_0)^n}{\sqrt{2^n n!}} \exp\left[-\frac{(ax_0)^2}{4}\right]$. Refer to Appendix A9 for the calculation of the coefficients.

The time-dependent wave function of the ground state is given by

$$\psi(x,t)=\left(\frac{\alpha^2}{\pi}\right)^{1/4}\exp\left[-\frac{1}{2}(\alpha x)^2-\frac{1}{4}(\alpha x_0)^2-\frac{1}{2}i\omega_0 t\right]\sum_{n=0}^{\infty}\frac{H_n(\alpha x)}{n!}\left(\frac{1}{2}\alpha x_0 e^{-i\omega_0 t}\right)^n$$

$$=\left(\frac{\alpha^2}{\pi}\right)^{1/4}\exp\left[-\frac{1}{2}\alpha^2x^2-\frac{1}{4}\alpha^2x_0^2-\frac{1}{2}i\omega_0 t-\frac{1}{4}\alpha^2x_0^2e^{-2i\omega_0 t}+\alpha^2xx_0e^{-i\omega_0 t}\right]$$

$$=\left(\frac{\alpha^2}{\pi}\right)^{1/4}\exp\left[-\frac{\alpha^2}{2}(x-x_0\cos(\omega_0 t)^2\right]\times\exp\left[-i\left(\frac{\omega_0 t}{2}+\alpha^2xx_0\sin(\omega_0 t)\right)-\frac{(\alpha x_0)^2}{4}\sin(2\omega_0 t)\right].$$

Thus,

$$|\psi(x,t)|^2=\sqrt{\frac{\alpha^2}{\pi}}\exp\left[-\alpha^2\left(x-x_0\cos(\omega_0 t)\right)^2\right]. \tag{7.21}$$

This shows that ψ represents a wave packet that oscillates without change of shape about $x = 0$, with amplitude x_0 and the classical angular frequency ω_0. In other words, the time dependence of the peak position of the wave packet is the harmonic oscillation with $\cos(\omega_0 t)$, equivalent to the classical harmonic oscillation. Figure 7.5 shows the wave packet in a harmonic potential, where $x_0 = -3$, $m = 1$, $\alpha = 1$, and $\omega_0 = 0.2$. The peak position of the wave packet exhibits a classical harmonic oscillation in $-3 \le x \le +3$.

Figure 7.4 lists the VBA code for calculating the wave packet positions at different times.

7.2 WAVE PACKET APPROACHING THE POTENTIAL STEP

7.2.1 Method of Visscher et al.

When the kinematics of a wave packet is difficult to compute, we may apply a method to obtain the numerical solution of the time-dependent Schrödinger equation developed by Visscher and others [6]. One-dimensional time-dependent Schrödinger equation in a potential of a real function $V(x)$ is given by

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x)\psi(x,t)=\breve{H}\psi(x,t)$$

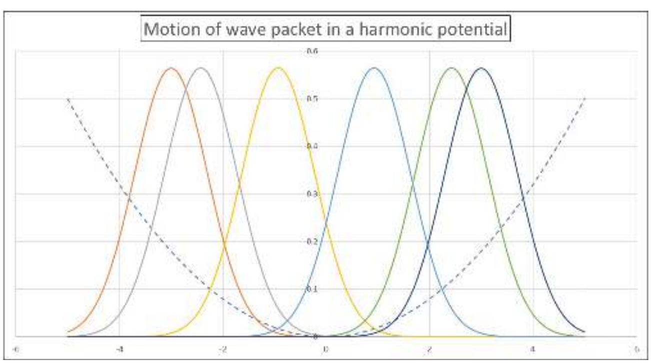


FIGURE 7.3 A wave packet in a harmonic potential.

```
Sub WPacketHO()
Cells(1, 1) = "Motion of wave packet of harmonics oscillator"
Pi = 3.141592654
Cells(2, 1) = "m": m = 1: Cells(3, 1) = m
Cells(2, 2) = "a": a = 1: Cells(3, 2) = a
Cells(2, 3) = "Omega0": omega0 = 0.2: Cells(3, 3) = omega0
Cells(2, 4) = "Initial x0": x0 = -3: Cells(3, 4) = x0
Cells(2, 5) = "Period": Period = 2 * Pi / omega0: Cells(3, 5) = Period
Cells(4, 3) = "Wave packet at a given time. Time step is pi:"
Cells(5, 1) = "x"
Cells(5, 2) = "U(x)"
  For i = 0 To 10
Cells(5, 3 + i) = i   'Time step i*pi
   j = 0.1 * i
   Cells(6, i + 3) = j * Pi
    'Phi(j)= |Wave packet|^2 where j is the x coordinate at a given time.
Next i
  n = 10                                'Number of repetitions
  dt = Pi                               'Time step
  dx = 0.1                              'Coordinate step
'Calculate U(x) and phi(x) at a given time t, starting t=0.
t = 0                                   'Initial time
   For i = 0 To n
      For j = 0 To 100                  'Change the x-coordinate
         x = -5 + j * dx
            Cells(6 + j, 1) = x         'x-coordinate
         U = m * (omega0 * x) ^ 2 / 2   'Potential energy
            Cells(6 + j, 2) = U
         Phi = (a / Pi ^ 0.5) * Exp( -(a * (x - x0 * Cos(omega0 * t)) ^ 2))
            Cells(6 + j, 3 + i) = Phi
        Next j
      t = t + dt
   Next i
End Sub
```

FIGURE 7.4 VBA code for the motion of a wave packet in a harmonic potential.

where

$$\breve{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{7.22}$$

The method by Visscher et al. treats the real and the imaginary parts of the wave function separately and applies a form of the half-step time method to establish difference equations for numerical calculations. Let

$$\psi(x,t) = R(x,t) + iI(x,t)$$

where $R(x, t)$ and $I(x, t)$ satisfy

$$\begin{cases} \dfrac{\partial R(x,t)}{\partial t} = \dfrac{1}{i\hbar}\breve{H}R(x,t) \equiv \breve{H}_v R(x,t) \\ \dfrac{\partial I(x,t)}{\partial t} = -\dfrac{i}{\hbar}\breve{H}I(x,t) \equiv -\breve{H}_v I(x,t) \end{cases}. \tag{7.23}$$

By applying the half-step method, the difference equations we use are given by

```
Sub PotentialStep()
Cells(1, 1) = "Kinematics of wave packet approaching to potential step."
Cells(2, 1) = "Calculate wave packet and probability distribution function at each given time."
Dim RE(1000)                                'Real par of wave packet
Dim IM(1000)                                'Imaginary part of wave packet
Dim IMold(1000)                             'Temporal imaginary part of wave packet
  Pi = 3.1415926
  x0 = -15                                  'Initial position of Gaussian wave packet
  wd = 1: wd2 = wd ^ 2                      'Standard deviation of initial wave packet
  k0 = 2                                    'Initial wave number
  xmax = 60: xmin = -xmax                   'Range of x-coordinate.
  V0 = 2                                    'Height of potential step
  a = 0                                     'Position of rising edge of potential step
  dx = 0.4: dx2 = dx ^ 2                    'dx=division of x-coordinate to calculate wave packet.
  n = 1 + (xmax - xmin) / dx                'n=101 is number of divisions of the x coordinates.
  dt = 0.1                                  'Time increment. To be repeated by RepeatNumber
  RepeatNumber = 210                        'Time change is 0 to RepeatNumber*dt, e.g.,  10*0.1=1.
'Parameter labels
  Cells(3, 2) = "Time"
  Cells(3, 3) = "Psum"                      'Total probability should be 1.
  Cells(5, 1) = "x"                         'x-coordinate
  Cells(5, 2) = "RE(X)"                     'Real part of wave packet
  Cells(5, 3) = "IM(x)"                     'Imaginary part of wave packet
  Cells(5, 4) = "P(x)"                      'Probability distribution function
'Construct initial Gaussian wave packet (t=0)
  t = 0: Cells(4, 2) = t
  Amp = 1 / ((2 * Pi * wd2) ^ 0.25)
  b = k0 * dt / 2
      For i = 1 To n
        x = xmin + (i - 1) * dx
        efact = Exp(-((x - x0) ^ 2 / wd2 / 4))
        RE(i) = Amp * Cos(k0 * (x - x0)) * efact          'Value at t=0
  IM(i) = Amp * Sin(k0 * (x - x0 - b / 2)) * efact        'Value at t=dt/2
          Cells(5, 1) = "x": Cells(5 + i, 1) = x
          Cells(5, 2) = "RE(x)": Cells(5 + i, 2) = RE(i)
          Cells(5, 3) = "IM(x)": Cells(5 + i, 3) = IM(i)
      Next i
      Psum = 0
      Cells(5, 4) = "P(x)"
        For i = 1 To n
          P = RE(i) * RE(i) + IM(i) * IM(i)
          Cells(5 + i, 4) = P
          Psum = Psum + P * dx
        Next i
          Cells(4, 3) = Psum                              'Psum should be 1.
'Time evolution of wave packet
  For j = 1 To RepeatNumber
  jj = 3 * j
    Cells(3, 2 + jj) = "Time": t = t + dt: Cells(4, 2 + jj) = t   'Current time
    Cells(3, 3 + jj) = "Psum"
    Cells(5, 2 + jj) = "RE(X)"                            'Real part of wave packet
    Cells(5, 3 + jj) = "IM(x)"                            'Imaginary part of wave packet
    Cells(5, 4 + jj) = "P(x)"                             'Probability distribution fu nction
      For i = 1 To n
        x = xmin + (i - 1) * dx
       HIM = V(x, V0, a) * IM(i) - 0.5 * (IM(i + 1) - 2 * IM(i) + IM(i - 1)) / dx2
       RE(i) = RE(i) + HIM * dt                           'Real part defined at multiples of dt
          Cells(5 + i, 2 + jj) = RE(i)
      Next i
        For i = 1 To n
          x = xmin + (i - 1) * dx
          IMold(i) = IM(i)                                'dt/2-earlier than real part
       HRE = V(x, V0, a) * RE(i) - 0.5 * (RE(i + 1) - 2 * RE(i) + RE(i - 1)) / dx2
       M(i) = IM(i) - HRE * dt          'dt/2-later than real part
            Cells(5 + i, 3 + jj) = IM(i)
```

FIGURE 7.5 VBA code for a wave packet in free space.

```
            Next i
        Psum = 0
          For i = 1 To n
            P = RE(i) * RE(i) + IM(i) * IMold(i)
            Psum = Psum + P * dx
              Cells(5 + i, 4 + jj) = P
          Next i
            Cells(4, 3 + jj) = Psum                    'Psum should be 1.
      Next j
   End Sub
   ________________________________________________________________
   Function V(x, V0, a)
     V=0
  End Function
```

FIGURE 7.5 Continued.

$$\begin{cases} R(x,t+\Delta t) = R(x,t) + \breve{H}_v I(x,t+\frac{1}{2}\Delta t)\Delta t \\ I(x,t+\frac{3}{2}\Delta t) = I(x,t+\frac{1}{2}\Delta t) - \breve{H}_v R(x,t)\Delta t. \end{cases} \tag{7.24}$$

The initial values are given by $R(x, 0)$ and $I(x, (1/2)(\Delta t)$. Note that they are not defined at the same time. The probability density is assumed to be given by

$$\begin{cases} P(x,t) = R(x,t)^2 + I(x,t+\frac{1}{2}\Delta t)I(x,t-\frac{1}{2}\Delta t) \\ P(x,t+\frac{1}{2}\Delta t) = R(t+\Delta t)R(x,t) + I(x,t+\frac{1}{2}\Delta t)^2 \end{cases}, \text{ and} \tag{7.25}$$

they conserve the total probability. Visscher has shown this algorithm is stable if the potential satisfies the following condition:

$$\frac{-2\hbar}{\Delta t} \le V \le \frac{2\hbar}{\Delta t} - \frac{2\hbar^2}{(m\Delta x)^2}. \tag{7.26}$$

A Gaussian wave packet is selected as the initial wave packet:

$$\psi(x,0) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{ik_0(x-x_0)} \exp\left(-\frac{(x-x_0)^2}{4\sigma^2}\right). \tag{7.27}$$

We need the values of $I(x, (1/2)\Delta t)$ and $R(x, 0)$ to start the half-step algorithm. For calculating $I(x, \Delta t/2)$, note that a plane wave at time t evolving in a zero potential region is related to its value at $t = 0$ by a factor of $e^{-i\omega t}$, where ω is related to the kinetic energy E by $E = \hbar\omega = p_0^2/2m = \hbar^2 k_0^2/2\mathrm{m}$.

The center of the Gaussian wave packet will move by an amount $<v>t$. Considering these conditions, we may approximate the wave packet ψ at time $t = (1/2)\Delta t$ by changing the phase in the Gaussian wave packet by replacing $[ik_0(x - x_0)]$ with $[ik_0(x - x_0) - i\omega(1/2)\Delta t]$

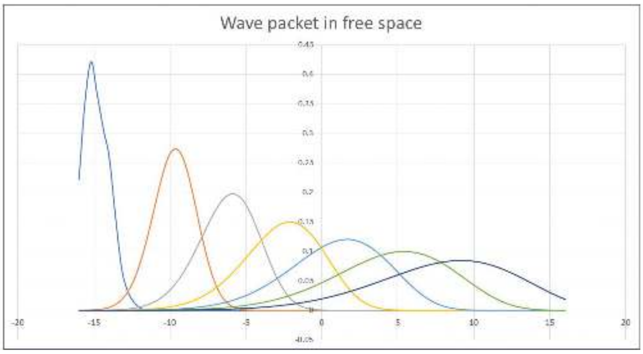


FIGURE 7.6 A wave packet in free space using the method of Visscher et al.

= [$ik_0(x - x_0) - i\hbar k_0^2\Delta t/(4m)$], and the argument of the Gaussian curve by replacing [$x - x_0$] with [$x - x_0 - \langle v\rangle\Delta t/2$] = [$x - x_0 - \hbar k_0\Delta t/(2m)$]. The result is not exact because these changes require a small correction in the overall normalization factor.

7.2.2 Wave Packet in Free Space Using the Visscher Algorithm

Figure 7.5 lists the VBA code to calculate the motion of a wave packet in free space. Although the potential V(x) = 0 in this case, the VBA code has a definition of `Function V(x, V0, a) = 0` so that the potential form may be changed for more applications. Figure 7.6 shows the computed wave packet in free space by the algorithm by Visscher et al. The initial wave packet is somewhat distorted from a Gaussian curve due to the approximate algorithm. The motion of the wave packet is comparable to the one shown in Figure 7.1.

7.2.3 Wave Packet at a Potential Step

Assume that there is a potential step of height 2 at $0 \le x$. We use $\hbar = 1$ and $m = 1$. The VBA code is the same except the Function statement for the step potential is

```
Function V(x, V0, a) 'Step potential
If x > a Then
V = V0
Else
V = 0
End If
End Function
```

Figure 7.7 shows the wave packets approaching the potential step. At $t = 9$, the wave packet is bumping the edge of the potential step and at $t = 15$, the reflective wave and the transmitted wave are both observed. At $t = 21$, both the reflection and the transmission are moving far away from the potential step at $x = 0$.

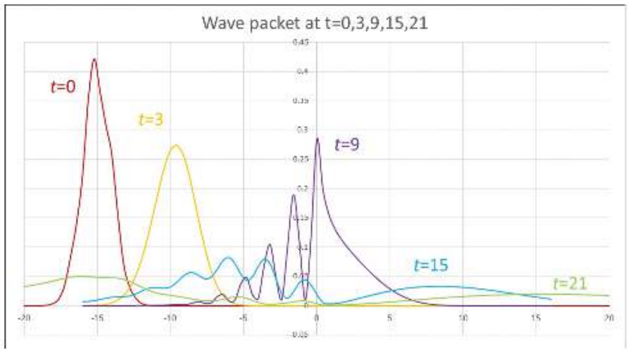


FIGURE 7.7 Time dependence of a wave packet against potential step.

7.3 ASYMPTOTIC BEHAVIOR OF WAVE FUNCTIONS NEAR THE TRUE EIGENVALUE

7.3.1 Standing Wave on a String

There are so-called "shooting methods" to solve time-independent Schrödinger equations and boundary value problems in general [7]. Here is an example of a one-dimensional standing wave.

$$\text{Problem}: \frac{d^2\psi(x)}{dx^2} + \omega^2\psi(x) = 0 \text{ where } 0 \le x \le 1 \text{ and } \psi(0) = \psi(1) = 0. \tag{7.28}$$

Analytical solution: $\psi_n(x) \sim \sin(n\pi x)$ and $\omega = n\pi$, $n = 1, 2, 3, \ldots$

The procedure of the shooting method for finding $\omega = \pi$ is:

1) Guess an eigenvalue. For example, ω would be between 3.0 and 3.2;
2) Obtain the differential equation with the trial ω-values. For solving the differential equation numerically, select an appropriate method such as the Euler method or the Runge-Kutta method. In this case, the Runge-Kutta method should be better;
3) If the resulting solution does not satisfy the boundary condition, change the trial eigenvalue and find the corresponding solution again; and
4) Repeat the process until a trial eigenvalue is found for which the boundary condition satisfies within a pre-determined tolerance.

Note: If the trial eigenvalue is not the true value, the solution for the trial eigenvalue does not satisfy the boundary condition. In the above problem, $\psi(1) > 0$ if $\omega_{\text{trial}} < \pi$, whereas $\psi(1) < 0$ if $\omega_{\text{trial}} > \pi$. In other boundary value problems, the solution with a trial eigenvalue tends to diverge in one direction if the trial eigenvalue is made slightly smaller and tends to diverge in the opposite direction if the trial eigenvalue is made slightly larger.

Figure 7.8 lists a VBA code to calculate $\psi(x)$'s with the same initial condition of $\psi(0) = 0$ and $d\psi(0)/dx = 1$ for $\omega_{\text{trial}} = 3.05$ to 3.25 with increments of 0.05.

```
Sub StandingWave ()
Cells(1, 1) = "Standing wave by shooting method"
'Phi is a trial eigen function to be found for a trail eigen values.
' Dphi=d(Phi)/dt is the 1st derivative of Phi.
' DDphi=d(Dphi)/dt=omega^2phi  is the 2nd derivative of Phi
'Write labels and initial values in cells:
        Cells(3, 1) = "Initial t": t = 0: Cells(4, 1) = t
        Cells(3, 2) = "Initial Phi": Phi = 0: Cells(4, 2) = Phi
        Cells(3, 3) = "Initial Dphi": Dphi = 1: Cells(4, 3) = Dphi
        Cells(3, 4) = "delta t": h = 0.01: Cells(4, 4) = h                'Time increment
        Cells(5, 1) = "Trial eigen value"
        Cells(6, 2) = "t"
For j = 1 To 5
   t = 0
    Cells(6, 2 + j) = "Phi": Phi = 0: Dphi = 1
    omega = 2.99 + j / 20: Cells(5, 2 + j) = omega: GoTo RK
'Runge-Kutta parameters:
RK:     n = 120  ' # of Iteration (n*h = range of Phi; n*h=1):
        For i = 0 To n
          Cells(i + 7, 2) = t
          Cells(i + 7, 2 + j) = Phi
              k1 = f(t, Phi, Dphi)
              l1 = g(omega, t, Phi, Dphi)
              k2 = f(t + h / 2, Phi + h * k1 / 2, Dphi + h * l1 / 2)
              l2 = g(omega, t + h / 2, Phi + h * k1 / 2, Dphi + h * l1 / 2)
              k3 = f(t + h / 2, Phi + h * k2 / 2, Dphi + h * l2 / 2)
              l3 = g(omega, t + h / 2, Phi + h * k2 / 2, Dphi + h * l2 / 2)
              k4 = f(t + h, Phi + h * k3, Dphi + h * l3)
              l4 = g(omega, t + h, Phi + h * k3, Dphi + h * l3)
           Phi = Phi + h * (k1 + 2 * k2 + 2 * k3 + k4) / 6
           Dphi = Dphi + h * (l1 + 2 * l2 + 2 * l3 + l4) / 6
        t = t + h
      Next i
Next j
End Sub
_____________________________________________________________
Function g(omega, t, Phi, Dphi)
'g=d(Dphi)/dt  ' The 2nd derivative of Phi.
   g = -omega ^ 2 * Phi
End Function
_____________________________________________________________
Function f(t, Phi, Dphi)
'f=d(phi)/dt
   f = Dphi
End Function
```

FIGURE 7.8 Finding the eigenvalue of a standing wave by the shooting method.

Figure 7.9 illustrates the solutions of the differential equation 7.26 of the first mode $\omega_1 = \pi$. When $\omega_{\text{trial}} = 3.15$, the solution is the closest to satisfying the boundary condition at $x = 1$: $\psi(1) = 0$.

Figure 7.10 shows the solutions of the differential equation 7.28 for the second mode $\omega_2 = 2\pi$. When $\omega_{\text{trial}} = 6.28$, the solution is the closest to satisfy the boundary condition $\psi(1) = 0$.

For the standing wave problem, only one boundary condition at $x = 0$ was used. The other boundary condition at $x = 1$ may be implemented by incorporating a fake potential well of $V(x) = 0$ for $0 \leq x \leq 1$ and otherwise $V_0 >>1$. This creates a one-dimensional Schrödinger equation of a deep potential well.

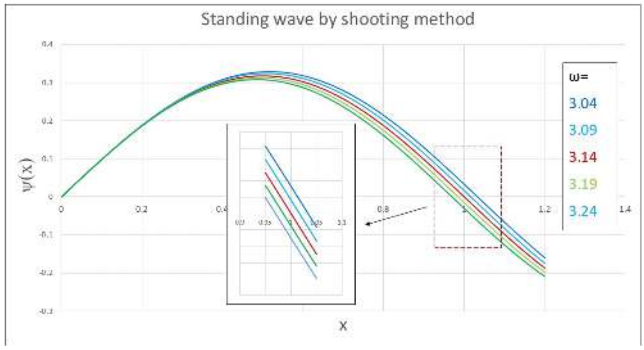


FIGURE 7.9 Behavior of solutions near $x = 1$ with ω around 3.14.

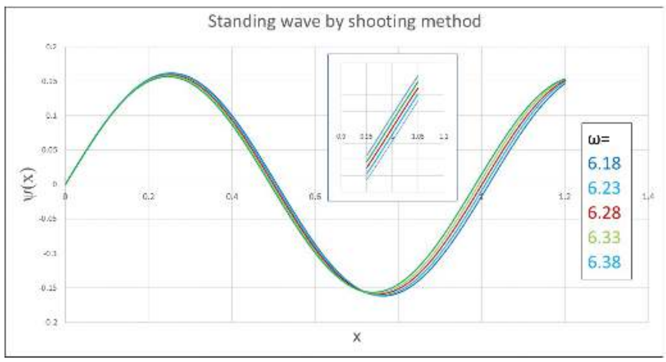


FIGURE 7.10 Behavior of solutions near $x = 1$ with ω around 6.28.

7.3.2 Euler-Cromer Algorithm for a Particle in an Infinite Potential Well

The Euler-Cromer algorithm is a shooting method for finding the eigenvalues of a bound state Schrödinger equation [8, 9]. Here is a brief description of the algorithm.

1) In the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x), \tag{7.29}$$

if the potential function is real and even: $V(x) = V(-x)$, then the wave function will be either even $\psi(x) = \psi(-x)$ or odd $\psi(x) = -\psi(-x)$.

2) For an even wave function, choose $\psi(0) = 1$ and $d\psi(0)/dx = 0$; and

For an odd wave function, choose $\psi(0) = 0$ and $d\psi(0)/dx = 1$.

3) Guess a value of E.

4) Define $x_n = n\Delta x$.

5) Compute $\psi'_{n+1} = \psi'_n+\psi''_n\Delta x$ and $\psi_{n+1} = \psi_n+\psi'_n\Delta x$.

6) Iterate $\psi(x)$ by increasing x until $\psi(x)$ diverges.

7) Change E and repeat steps 6 and 7.

8) Observe the diverting direction. Find the E-value when the direction changes.

9) Narrow the range of E-values and repeat steps 6 and 7.

Figure 7.11 lists a VBA code to perform the Euler-Cromer algorithm for a potential well where $V(x) = 0$ for $|x| \leq 1$ and V_0 otherwise where V_0 may be set to a large value such as $V_0 = 200$. The trial eigenvalues are from 1.20 to 1.24 with increments of 0.01.

Figure 7.12 shows the asymptotic behavior of wave functions with several trial eigenvalues. Due to the computational error of the Euler method, the accumulation of the error makes wave functions diverge. In Figure 7.10, the solution of the trial eigenvalue of 1.22 has the least diverging property, and one of the trial eigenvalues, 1.23, is the closest to $\psi(1) = 0$. The exact eigenvalue is $\pi^2/8 = 1.233$.

```
Sub Qbound()
Cells(1, 1) = "Time-independent Schrödinger eq."
V0 = 200
a = 1
h = 0.05
xmax = 2
Parity = 1
'Change E to see divergences
 For k = 1 To 6
      E = 1.2 + 0.01 * (k - 1)
      Cells(2, k + 1) = E
   If Parity = -1 Then                        'Odd parity
      Phi = 0                                 'Initial value at x =0
      Dphi = 1                                '1st derivative
   Else
      Phi = 1                                  'Even parity
      Dphi = 0
   End If
i = 0
x = 0
    Do Until x > xmax
           xOld = x
           PhiOld = Phi
          Cells(5 + i, 1) = xOld
          Cells(5 + i, k + 1) = PhiOld
                  x = x + h
          DDphi = 2 * (V(x, V0, a) - E) * Phi    ' Schrödinger eq.
          Dphi = Dphi + DDphi * h                ' Euker-Cromer algorithm
         Phi = Phi + Dphi * h
             i = i + 1
    Loop
Next k
End Sub
________________________________________________________________
Function V(x, V0, a)
    If Abs(x) > a Then
         V = V0
    Else
         V = 0
    End If
End Function
```

FIGURE 7.11 VBA code of Euler-Cromer algorithm applied to a potential well problem.

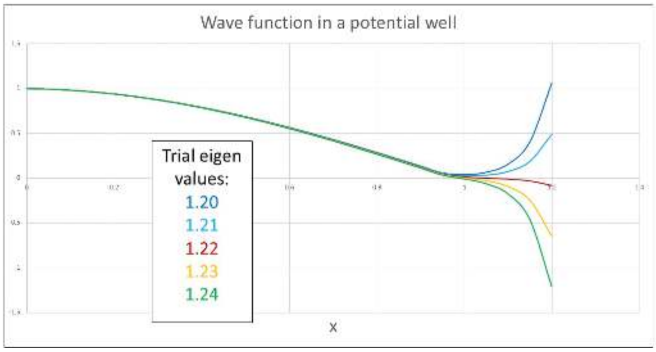


FIGURE 7.12 Asymptotic behavior of wave functions near the boundary with several trial eigenvalues.

Note that the numerical value of potential height V_0 affects the eigenvalue. Proper implementation of the boundary condition is required to obtain accurate eigenvalues for the shooting method.

7.3.3 Harmonic Oscillator

Let us start with the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+\frac{1}{2}k^2x^2\psi(x)=E\psi(x). \tag{7.30}$$

Let $\xi = \alpha x$, where $\alpha^4 = mk/\hbar^2$ to obtain

$$\frac{d^2\psi(\xi)}{d\xi^2}+\left(\lambda-\xi^2\right)\psi(\xi)=0 \text{ where } \lambda=\frac{2m}{\alpha^2\hbar^2}=\frac{2E}{\hbar}\sqrt{\frac{m}{k}}. \tag{7.31}$$

The exact eigenvalue $\lambda = 1$ from the ground state energy $E_0 = (1/2)\ \hbar$. We solve the above equation using the Runge-Kutta method while changing the trial value of λ. Preliminary calculation indicates that divergence is very fast and we narrow down the range of the trial value to 0.999, 1.000, and 1.0001. Figure 7.13 lists the VBA code for the solution of differential Equation 7.29 with given λ-values.

Figure 7.14 shows that the asymptotic behavior of wave functions is observed as positively diverging if λ_{trial} <1 and negatively diverging if λ_{trial} >1. When λ_{trial} = 1, the wave function appears to be approaching zero.

The above approach does not include the boundary condition at $\xi = \pm\infty$. One may incorporate the boundary conditions at $\xi = \pm\infty$, where Equation 7.31 asymptotically becomes

$$\frac{d^2\psi(\xi)}{d\xi^2}-\xi^2\psi(\xi)=0. \tag{7.32}$$

Thus, the solution of Equation 7.32, i.e., the asymptotic wave function should be $\psi(\xi)\sim\exp(-\xi^2/2)$, which is finite at $\xi = \pm\infty$. Let $\psi(\xi) = f(\xi)\exp(-\xi^2/2)$, then we obtain

```
Sub QuantumOsci()
Cells(1, 1) = "Harmonic oscillator in quantum mechanics"
'Phi is the wave function.
' Dphi=d(Phi)/dx is the 1st derivative of Phi.
' DDphi=d(Dphi)/dx=-(lambda-x^2)*phi=0  is the 2nd derivative of Phi
'lambda = (2*E/Dirac h)*Sqrt(m/k)
'Write labels and initial values in cells:
        Cells(3, 1) = "Initial x": x = 0: Cells(4, 1) = x
        Cells(3, 2) = "Initial Phi": Phi = 1: Cells(4, 2) = Phi
        Cells(3, 3) = "Initial Dphi": Dphi = 0: Cells(4, 3) = Dphi
        Cells(3, 4) = "delta x": h = 0.04: Cells(4, 4) = h              'Position increment
        Cells(6, 2) = "x"
        Cells(5, 1) = "lambda"
' Change lambda 0.000, 1.000, and 1.001 to observe the behavior of phi at larger x.
For j = 0 To 2
   Cells(6, 3 + j) = "Phi": Phi = 1: Dphi = 0: x = 0
      If j = 0 Then lambda = 0.999: Cells(5, 3 + j) = lambda: GoTo RK
      If j = 1 Then lambda = 1#: Cells(5, 3 + j) = lambda: GoTo RK
      If j = 2 Then lambda = 1.001: Cells(5, 3 + j) = lambda
'Runge-Kutta parameters:
RK:     n = 100  ' Iteration # (n*h = range of Phi; n*h=5):
        For i = 0 To n
          Cells(i + 7, 2) = x
          Cells(i + 7, 3 + j) = Phi
             k1 = f(x, Phi, Dphi)
             l1 = g(lambda, x, Phi, Dphi)
             k2 = f(x + h / 2, Phi + h * k1 / 2, Dphi + h * l1 / 2)
             l2 = g(lambda, x+ h / 2, Phi + h * k1 / 2, Dphi + h * l1 / 2)
             k3 = f(x + h / 2, Phi + h * k2 / 2, Dphi + h * l2 / 2)
             l3 = g(lambda, x + h / 2, Phi + h * k2 / 2, Dphi + h * l2 / 2)
             k4 = f(x + h, Phi + h * k3, Dphi + h * l3)
             l4 = g(lambda, x + h, Phi + h * k3, Dphi + h * l3)
                 Phi = Phi + h * (k1 + 2 * k2 + 2 * k3 + k4) / 6
                 Dphi = Dphi + h * (l1 + 2 * l2 + 2 * l3 + l4) / 6
            x = x + h
       Next i
Next j
End Sub
________________________________________________________________
Function g(lambda, x, Phi, Dphi)
'g=d(Dphi)/dx  ' The 2nd derivative of Phi.
     g = (x ^ 2 - lambda) * Phi
End Function
________________________________________________________________
Function f(x, Phi, Dphi)
'f=d(phi)/dx
     f = Dphi
End Function
```

FIGURE 7.13 VBA code for calculating wave functions for different eigenvalues.

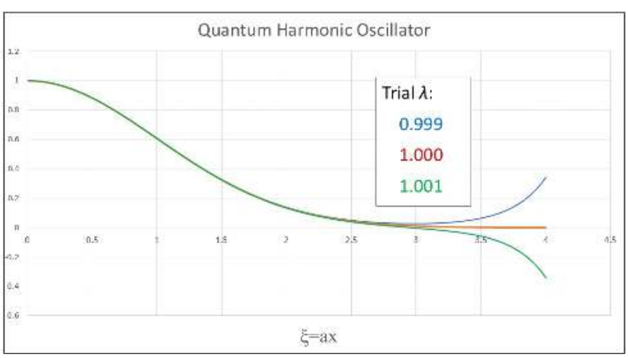


FIGURE 7.14 Asymptotic behavior of wave functions with trial eigenvalues.

$$\frac{d^2 f(\xi)}{d\xi^2} - 2\xi \frac{df(\xi)}{d\xi} + (\lambda - 1) f(\xi) = 0 \tag{7.33}$$

where $f(\xi)\exp(-\xi^2/2)$ must vanish at $\xi = \pm\infty$.

Equation 7.33 is a Hermite differential equation (6.22) with $2n = \lambda - 1$. From Section 6.2.3, the Hermite polynomial of the zeroth order is $H_0(x) = 1$. Thus, $f(\xi)$ is expected to be 1 when $\lambda = 1$.

The VBA code created for using the differential equation 7.33 is similar to the one listed in Figure 7.12 with a different definition of `Function g(lambda, x, Phi, Dphi)`. In this case,

```
g = 2 * x * Dphi - (lambda - 1) * Phi
```

Figure 7.15 shows the result of the shooting method. As shown when $\lambda > 1$, $f(\xi)$ tends to exhibit a negative divergence, and when $\lambda < 1$, $f(\xi)$ tends to be a positive divergence. For the first excited state, $n = 1$ or $\lambda = 3$. The initial condition should be $f(\xi) = 0$ and $df(\xi)/d\xi = 1$ at $\xi = 0$ for an odd function. Figure 7.16 shows the result for $\lambda = 2.9$, 3.0, and 3.1 for around $n = 1$. Recall that the Hermite polynomial of the first order is $H_1(x) = 2x$, and the result shown here is consistent with $H_1(x)$.

7.3.4 Hydrogen Atom

The radial wave function $R(r)$ of the Schrödinger equation for a hydrogen-like atom is

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) - k_e\frac{Ze^2}{r}R(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}R(r) = ER(r) \tag{7.34}$$

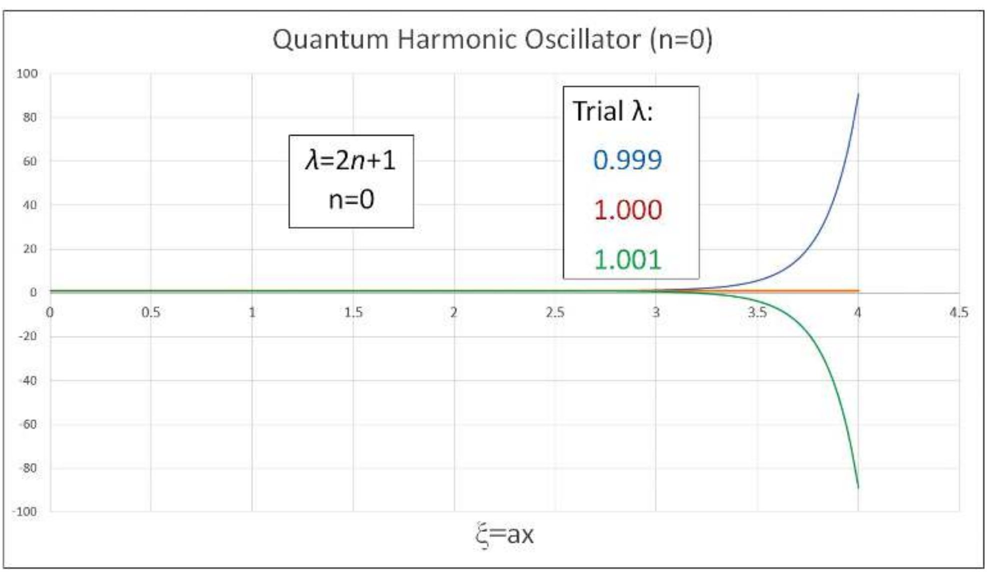


FIGURE 7.15 Asymptotic behavior of a wave function of a harmonic oscillator in the ground state.

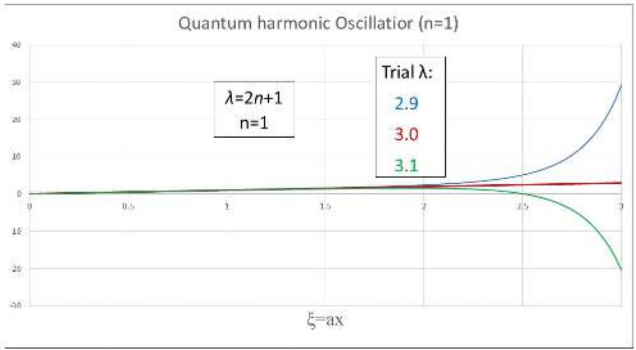


FIGURE 7.16 Asymptotic behavior of a wave function of a harmonic oscillator of the first excited state.

where μ is the reduced mass, $k_e = 1/4\pi\varepsilon_0$, and ℓ is the angular momentum quantum number [5]. Let

$$\rho = \alpha r \text{ where } \alpha = \frac{8\mu|E|}{\hbar^2} \text{ and } \lambda = \frac{2\mu k_e Ze^2}{\alpha\hbar^2} = \frac{k_e Ze^2}{\hbar^2}\sqrt{\frac{\mu}{2|E|}}. \tag{7.35}$$

So that Equation 7.34 is rewritten to

$$\frac{1}{\rho^2}\frac{d}{dr}\left(\rho^2\frac{dR(\rho)}{d\rho}\right) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{\ell(\ell+1)}{\rho^2}\right]R(\rho) = 0 \tag{7.36}$$

where the particular choice of the number 1/4 for the eigenvalue term is arbitrary but convenient for the following development.

We incorporate the boundary conditions at $\rho\to\infty$ with Equation 7.34. With the limit of $\rho\to\infty$, Equation 7.36 is approximately

$$\frac{d^2R(\rho)}{d\rho^2} - \frac{1}{4}R(\rho) \approx 0. \tag{7.37}$$

Let $R(\rho) = \rho^n \exp(\pm\rho/2)$ then

$$\frac{d^2R}{d\rho^2} = \pm\frac{1}{2}n\rho^{n-1}\exp\left(\pm\frac{1}{2}\rho\right) + \frac{1}{4}\rho^n\,\mathrm{xp}\left(\pm\frac{1}{2}\rho\right) \approx \frac{1}{4}\rho^n\,\mathrm{xp}\left(\pm\frac{1}{2}\rho\right).$$

Thus, $R(\rho) = \rho^n\exp(\pm\rho/2)$ satisfies the above equation for any n. However, since $R(\rho) \to 0$ as $\rho \to \infty$, $\exp(\rho/2)$ is not allowed and n must be finite. We may look for an exact solution of Equation 7.36 of the form $R(\rho) = F(\rho)\exp(-\rho/2)$ where $F(\rho)$ may be a finite polynomial function. From Equation 7.36, $F(\rho)$ satisfies

$$\frac{d^2F(\rho)}{d\rho^2} + \left(\frac{2}{\rho} - 1\right)\frac{dF(\rho)}{d\rho} + \left[\frac{\lambda-1}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]F(\rho) = 0. \tag{7.38}$$

Find the solution of Equation 7.38 in the form

$$F(\rho) = \rho^s f(\rho) \text{ where } f(\rho) = a_0 + a_1 p + a_2\rho^2 + \cdots + a_k\rho^k, a_0 \neq 0, \tag{7.39}$$

and $s > 0$ for the boundary condition at $\rho = 0$. Substitute Equation 7.39 with Equation 7.38 and obtain

$$\rho^2 \frac{d^2 f(\rho)}{d\rho^2} + \rho\left[2(s+1) - \rho\right]\frac{df(\rho)}{d\rho} + \left[\rho(\lambda - s - 1) + s(s+1) - \ell(\ell+1)\right]f(\rho) = 0. \tag{7.40}$$

Setting $\rho = 0$ in Equation 7.40 gives $s(s + 1) - \ell(\ell + 1) = 0$, and $s = \ell$ for $s > 0$. Equation 7.38 now becomes

$$\rho\frac{d^2 f(\rho)}{d\rho^2} + \left[2(\ell+1) - \rho\right]\frac{df(\rho)}{d\rho} + \left[\lambda - \ell - 1\right]f(\rho) = 0. \tag{7.41}$$

Substituting the power series 7.39 into Equation 7.41, we obtain

$$\left(k+1\right)\left(k+2+2\ell\right)a_{k+1} + \left\{1 - \lambda\left(k+1+\ell\right)\right\}a_k = 0,$$

or

$$a_{k+1} = -\frac{k+\ell+1-\lambda}{(k+1)(k+2+2\ell)}a_k. \tag{7.42}$$

Note that the series solution 7.39 cannot be infinite for satisfying the boundary condition when $r \to \infty$. There must be an integer k such that $a_k \neq 0$ but $a_{k+1} = 0$. Thus, $k + \ell + 1 - \lambda = 0$ from the numerator of Equation 7.42, and we obtain

$$\lambda = k + \ell + 1 \equiv n \text{ where } n = k + \ell + 1 = 1, 2, 3, \ldots. \tag{7.43}$$

The energy E can be obtained from the definition 7.35,

$$E = -\frac{k_e^2 Z^2 e^2}{2a}\frac{1}{n^2} \text{ where } n = 1, 2, 3, \ldots; \text{ and } n > \ell. \tag{7.42}$$

Note: Equation 7.41 with $\lambda = n$ is an associated Laguerre differential equation (6.38), and the polynomial solutions are the associated Laguerre polynomials. The radial wave function is of the form $e^{-\frac{1}{2}\rho}\rho^\ell L_{n+\ell}^{2\ell+1}(\rho)$. Refer to advanced books on quantum physics [10] for explicit radial functions.

For the ground state, $n = 1$ and $\ell = 0$, Equation 7.41 has the eigenvalue $\lambda = n = 1$. Figure 7.15 lists the VBA code to demonstrate the behavior of the eigenfunction of Equation 7.41 with

```
Sub Hatom()
Cells(1, 1) = "Ground state of H-atom"
'Phi is the wave function.
'Dphi=d(Phi)/dt is the 1st derivative of Phi.
'DDphi=d(Dphi)/dt=(1-2 / r - 1) * Dphi + (1-lambda) * Phi / r  is the 2nd derivative of Phi
'Write labels and initial values in cells:
        Cells(3, 1) = "Initial r": r = 0: Cells(4, 1) = r
        Cells(3, 2) = "Initial Phi": Phi = 0: Cells(4, 2) = Phi
        Cells(3, 3) = "Initial Dphi": Dphi = -1: Cells(4, 3) = Dphi
        Cells(3, 4) = "dr": h = 0.1: Cells(4, 4) = h                    'Radial increment
        Cells(6, 2) = "r"
        Cells(5, 1) = "lambda"
'Change lambda value around the true eigen value (lambda=1)
For j = 1 To 3
   r = 0: Cells(7, 2) = r
   Cells(6, 2 + j) = "Phi": Phi = 1: Dphi = 0
  If j = 1 Then lambda = 0.99: Cells(5, 2 + j) = lambda: GoTo RK
  If j = 2 Then lambda = 1: Cells(5, 2 + j) = lambda: GoTo RK
  If j = 3 Then lambda = 1.01: Cells(5, 2 + j) = lambda: GoTo RK
 'Runge-Kutta parameters:
RK:     maxN = 100  ' Iteration # (n*h = range of Phi; n*h=5):
        For i = 1 To maxN
        r = r + h
          Cells(i + 7, 2) = r
          Cells(i + 6, 2 + j) = Phi
             k1 = f(lambda, r, Phi, Dphi)
             l1 = g(lambda, r, Phi, Dphi)
             k2 = f(lambda, r + h / 2, Phi + h * k1 / 2, Dphi + h * l1 / 2)
             l2 = g(lambda, r + h / 2, Phi + h * k1 / 2, Dphi + h * l1 / 2)
             k3 = f(lambda, r + h / 2, Phi + h * k2 / 2, Dphi + h * l2 / 2)
             l3 = g(lambda, r + h / 2, Phi + h * k2 / 2, Dphi + h * l2 / 2)
             k4 = f(lambda, r + h, Phi + h * k3, Dphi + h * l3)
             l4 = g(lambda, r + h, Phi + h * k3, Dphi + h * l3)
          Phi = Phi + h * (k1 + 2 * k2 + 2 * k3 + k4) / 6
          Dphi = Dphi + h * (l1 + 2 * l2 + 2 * l3 + l4) / 6
      Next i
Next j
End Sub
_____________________________________________________________
Function g(lambda, r, Phi, Dphi)
'g=d(Dphi)/dt  ' The 2nd derivative of  Phi.
     g = (1 - 2 / r) * Dphi + (1 - lambda) * Phi / r          From equation (7.39)
End Function
_____________________________________________________________
Function f(lambda, r, Phi, Dphi)
'f=d(phi)/dt
     f = Dphi
End Function
```

FIGURE 7.17 VBA code for seeking eigenvalue E by the shooting method.

a few λ-values around $\lambda = 1$. The eigenfunction of Equation 7.41 is constant, $f(\rho) = a_0 = 1$ if $\lambda = 1$. The VBA code calculates $a_0 = 1$.

Figure 7.18 shows the computed behaviors of the radial wave functions near $\lambda = 1$ ($n = 1$ and $\ell = 0$). Because the Laguerre polynomial of the zero-th order is 1, the solution $f(\rho)$ is expected to be 1 when $\lambda = 1$. When n is smaller than 1, $f(\rho)$ exhibits a positive deviation from the constant $a_0 = 1$, and when n is larger than 1, $f(\rho)$ exhibits a negative deviation from the constant.

Figure 7.19 shows the computed behaviors of the radial wave functions near $\lambda = 2$ ($n = 2$ and $\ell = 0$). The solution $f(\rho)$ is expected to be linear when $\lambda = 1$.

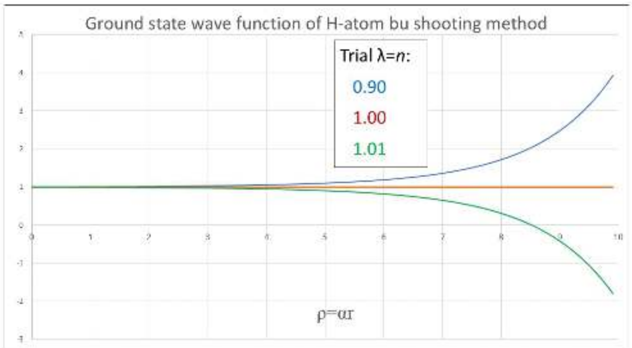


FIGURE 7.18 Asymptotic behavior of the radial wave function (n = 1).

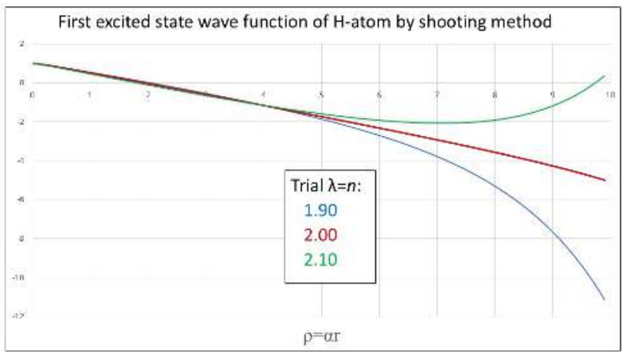


FIGURE 7.19 Asymptotic behavior of the radial wave function (n = 1).

SUGGESTED FURTHER STUDY

For learning advanced computational algorithms to solve boundary value problems, there are many lecture notes [11–13] and books [14, 15]. For general knowledge of computational physics, one needs to recommend creating and running examples of advanced computational books [6, 16–18].

REFERENCES

1. Merzbacher E, *Quantum Mechanics*, John Wiley & Sons, Inc., 1970. https://archive.org/details/quantummechanics0000merz_y3q4/page/n643/mode/2up.
2. Bohm D, *Quantum Theory*, Dover Books on Physics, Dover Publications, 1951.
3. The group velocity was defined as the electromagnetic signal velocity. See Stratton A, *Electromagnetic Theory*, McGraw Hill Book Company, 1941. https://archive.org/details/electromagnetict031016mbp/page/n3/mode/2up.
4. Liboff RL, *Introduction to Quantum Mechanics*, Addison-Wesly, 2003.
5. Schiff LI, *Quantum Mechanics*, McGraw Hill Book Company, 1968. https://archive.org/details/ost-physics-schiff-quantummechanics.
6. Gould H and Tobochnik J, *An Introduction to Computer Simulation Methods*, Addison-Wesly, 1996.
7. *Euler-Cromer Method – Physics 481*, University of Redlands. http://facweb1.redlands.edu/fac/eric_hill/Phys331/P331-Euler-Cromer%20(Python%20only).pdf.

8. *The Shooting Method (Application to Energy Levels of the Simple Harmonic Oscillator and Other Problems of a Particle in a Potential Minimum)*, University of California Santa Cruz. https://young.physics.ucsc.edu/242/shooting2.pdf.
9. Reis VE, *Application of Shooting Method to Solve the Schrödinger Equation*, The Ohio State University. https://people.ohio.edu/elster/phys5071/extras/Quantum_Mechanics_II_Vitor_Reis.pdf.
10. *Radial Wave Functions from the Solution of the Radial Equation*, Washington University. https://faculty.washington.edu/seattle/physics441/ch10b.pdf.
11. Venturi D, *Numerical Methods to Solve Boundary Value Problems for ODEs*, Duke Mathematical Department. https://services.math.duke.edu/~jtwong/math563-2020/lectures/Lec9-BVPs.pdf.
12. Adams A, *The Evolution and Schrödinger Equation*, MIT OpenCourseWare, 2013. https://ocw.mit.edu/courses/8-04-quantum-physics-i-spring-2013/resources/lecture-6/.
13. Wong J, *Lecture Notes Numerical Methods for Boundary Value Problems*, Duke Mathematic Department, 2020. https://services.math.duke.edu/~jtwong/math563-2020/lectures/Lec9-BVPs.pdf.
14. Boyce WE and DiPrima RC, *Elementary Differential Equations and Boundary Value Problems*, John Wiley & Sons, Inc., 2003.
15. Atkinson K, Han W, and Stewart D, *Numerical Solution of Ordinary Differential Equations*, John Wiley & Sons, Inc., 2009. https://onlinelibrary.wiley.com/doi/book/10.1002/9781118164495.
16. DeVries PL and Hasbun JW, *A First Course in Computational Physics*, Jones and Bartlett Publishers, 2011.
17. Cho S, *Monte Carlo Simulations using Microsoft Excel*Springer, 2023.
18. Giordano NJ, *Computational Physics*, Printes Hall, 1997.

Interdisciplinary Topics

INTERDISCIPLINARY TOPICS ARE ALWAYS bringing opportunities to be aware of how physics and mathematics are applied in other fields. There are two topics selected from polymer and population dynamics:

1) Polymers give us interesting topics in conjunction with entropy change and self-avoiding random walks. We apply a model similar to the examples discussed in Chapter 5 to demonstrate the entropic elasticity of polymers. A model to calculate the polymer length is self-avoiding random walks. We demonstrate it by placing a polymer chain in a two-dimensional square lattice.
2) There are many natural phenomena which can be modeled with differential equations. Differential equations to describe population change exhibit very curious predictions. Numerical computation and visualization of several models are considered. The dynamics of biological systems where species interact as prey and predator are also portrayed.

8.1 POLYMERS

8.1.1 Entropic Elasticity

The elasticity of rubber is caused by the entropy change [1]. Let the number of possible configurations of monomers in a polymer chain be Ω. Once Ω is found, entropy, which is given by $S = k_B \ln\Omega$ from the description in Section 5.1, can be calculated where k_B is the Boltzmann constant. Figure 8.1 depicts two different states of a polymer chain. Let $\Omega = \Omega_1$ when the polymer is unstretched and $\Omega = \Omega_2$ when the polymer is stretched. As we calculate below, because $\Omega_1 > \Omega_2$, $S_1 > S_2$ and $S_2 - S_1 < 0$. From a stretched state, the polymer tends to return to an unstretched state where the polymer has larger entropy, producing the restoring elastic force.

Consider a one-dimensional polymer chain that is made of N monomers. The joints between the two monomers freely point to the right or left. Figure 8.2 depicts the polymer chain model. This model is very similar to the one-dimensional random walk.

DOI: 10.1201/9781003516347-8

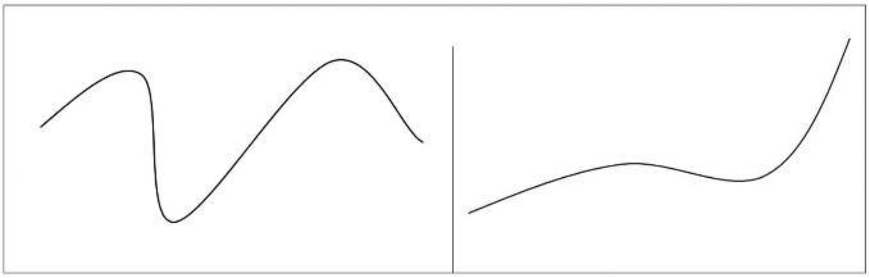


FIGURE 8.1 Unstretched and stretched states of the polymer.

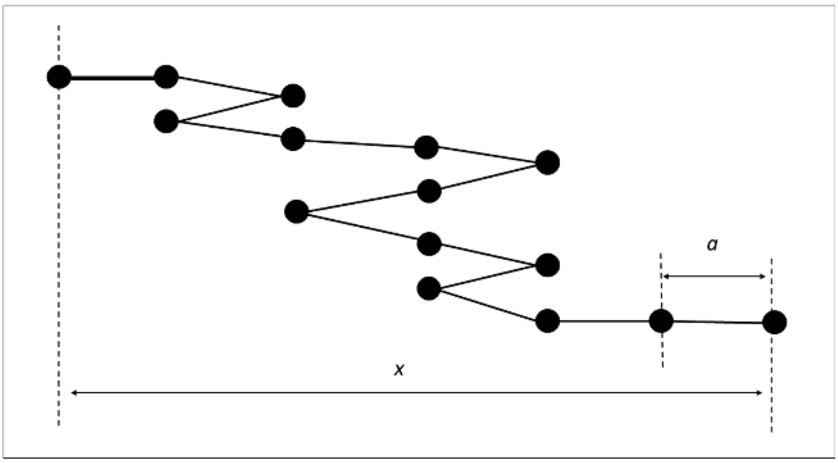


FIGURE 8.2 A one-dimensional polymer chain.

Suppose the length of monomers is a, the length of the polymer chain is x, the number of right-pointing monomers is N_R, and the number of left-pointing monomers is N_L, then the length of the polymer chain is given by

$$x = (N_R - N_L)a \text{ where } N = N_R + N_L, \tag{8.1}$$

and the number of possible orientations of monomers to yield x is

$$\Omega(x) = \frac{N!}{N_R!N_L!} = \frac{N!}{\left(\frac{Na+x}{2a}\right)!\left(\frac{Na-x}{2a}\right)!}. \tag{8.2}$$

where we used $N_R = \frac{Na+x}{2a}$ and $N_L = \frac{Na+x}{2a}$.

Using the Stirling formula, entropy is

$$S = k_B \ln\Omega(x) = Nk_B\left[\ln 2 - \frac{1}{2}\left(1+\frac{x}{Na}\right)\ln\left(1+\frac{x}{Na}\right) - \frac{1}{2}\left(1-\frac{x}{Na}\right)\ln\left(1-\frac{x}{Na}\right)\right], \tag{8.3}$$

and the tension in the polymer chain is given by

$$
\begin{aligned}
X = \left(\frac{\partial F}{\partial x}\right)_T = -T\left(\frac{\partial S}{\partial x}\right)_T &= \frac{k_B T}{a}\ln\frac{1+(x/Na)}{1-(x/Na)} \\
&= \frac{k_B T}{a}\left[\ln\{1+(x/Na)\} - \ln\{1-(x/Na)\}\right].
\end{aligned}
\tag{8.4}
$$

Using the Taylor expansions, $\ln(1\pm\xi)2 = \pm\xi - \frac{1}{2}\xi^2 \pm \frac{1}{3}\xi^3 - \frac{1}{4}\xi_4 \pm \ldots$, we obtain

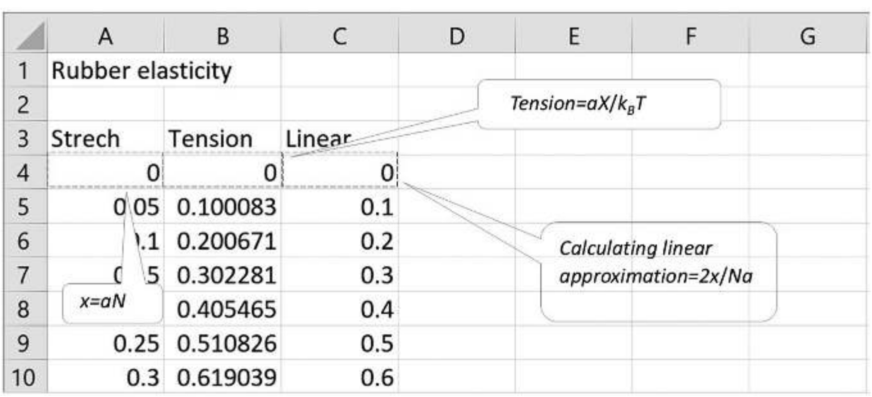
$$
\frac{aX}{k_B T} = 2\left[\frac{x}{Na} + \frac{1}{3}\left(\frac{x}{Na}\right)^3 + O(x^5)\right]. \tag{8.5}
$$

Therefore, tension X is proportional to the length of the polymer to the first order, following Hooke's law. Figure 8.3 is a screenshot of the numerical calculation including the third-order term.

Figure 8.4 shows the length dependence of tension [a$X/k_\mathrm{B}T$], where the horizontal axis is the stretched length [x/Na]. When the stretched length is short, Hooke's law follows the first order. As the stretched length becomes longer, higher-order nonlinear terms appear in the entropic elasticity.

8.1.2 Polymer Length and Self-Avoiding Walk

Assume that a polymer chain is placed on an upstretched two-dimensional surface. How can we calculate the length of the two-dimensional polymer chain? Assume there are N monomers in a polymer chain and the joints between monomers are freely pointing and there is no correlation between the two monomers. We use a square lattice model where the lattice constant is the monomer length [2]. In this model, each monomer can take four different directions (up, down, right, and left), but two monomers cannot take the same lattice segment. Starting with the monomer at one end placed on the square lattice, the second monomer can be randomly placed, avoiding the first monomer, and so forth. This



	A	B	C	D	E	F	G
1	Rubber elasticity						
2							
3	Strech	Tension	Linear				
4	0	0	0				
5	0.05	0.100083	0.1				
6	0.1	0.200671	0.2				
7	0.15	0.302281	0.3				
8		0.405465	0.4				
9	0.25	0.510826	0.5				
10	0.3	0.619039	0.6				

FIGURE 8.3 Calculation of tension.

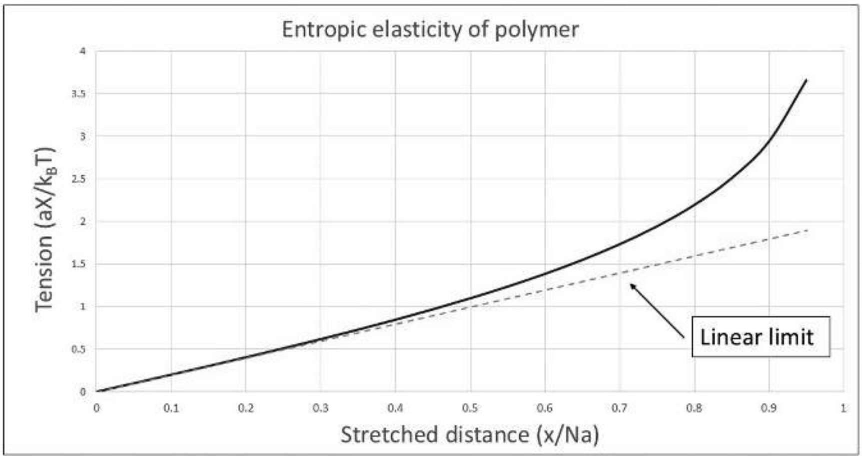


FIGURE 8.4 Entropic elasticity.

configuration is equivalent to the self-avoiding walk on the two-dimensional square lattice [3]. Figure 8.5 lists the VBA code to place a polymer of 120 monomers of unit length to a square lattice of unit lattice constant.

Figure 8.6 shows a typical result of 120 consecutive self-avoiding walks to represent 120 monomers.

Note: Although there are more efficient computation algorithms for self-avoiding random walks [4], personal computers today may be fast enough to apply the simple algorithm we applied here.

8.2 POPULATION DYNAMICS

Population dynamics is a description of the size and age composition of a group of individuals of a single species and how the number and age composition of individuals in a population change over time. Differential equations are used to model the dynamics with pre-determined conditions [5]. It is interesting to get an idea of how several factors are to be implemented in a basic differential equation.

8.2.1 Malthus's Law of Population and Logistic Equation

Imagine a bacterial growth. If the bacteria do not die, the equation to describe the bacterial growth is given by

$$\frac{dN}{dt} = nN \tag{8.6}$$

where n is the growth (birth) rate. The radioactive decay has the same differential equation with the negative coefficient n.

Malthus's law includes the death rate, which states that the time dependence of the population of a species can be given by a differential equation,

```
Sub SAW2D()
Cells(1, 1) = "Self-avoiding walk (SAW) on the two-dimensional square lattice."
GridSize = 21
WalkLength = 120
Dim grid(GridSize, GridSize) As Integer
Dim pathX(WalkLength) As Integer
Dim pathY(WalkLength) As Integer
    For i = 0 To WalkLength
        pathX(i) = 0
        pathY(i) = 0
    Next i
'Initialize the grid and starting position
    For x = 1 To GridSize
        For Y = 1 To GridSize
            grid(x, Y) = 0
        Next Y
    Next x
'Set the origin (the mid-point of the lattice) as the starting point:
    x = (GridSize + 1) / 2
    Y = (GridSize + 1) / 2
    grid(x, Y) = 1        'Footprinted
    pathX(0) = x
    pathY(0) = Y
' Directions: right (1,0), left (-1,0), down (0,1), up (0, -1)
  Dim dx(3) As Integer
  Dim dy(3) As Integer
    dx(0) = 1: dy(0) = 0
    dx(1) = -1: dy(1) = 0
    dx(2) = 0: dy(2) = 1
    dx(3) = 0: dy(3) = -1
ii = 0
    For i = 1 To WalkLength
      ii = ii + 1
       'Check for possible moves
         Dim possibleMoves(3) As Integer
          Count = 0
            For k = 0 To 3
              newX = x + dx(k)
              newY = Y + dy(k)
               If newX > 0 And newX <= GridSize And newY > 0 And newY <= GridSize  Then
                  If grid(newX, newY) = 0 Then
                     possibleMoves(Count) = k
                     Count = Count + 1
                  End If
               End If
            Next k
        'If there are no possible moves, exit the loop
            If Count = 0 Then Exit For
        'Choose a random move from the possible moves
            d = possibleMoves(Int(Rnd * Count))
              x = x + dx(d)
              Y = Y + dy(d)
         'Mark the new position on the grid and add to the path
              grid(x, Y) = 1
              pathX(i) = x
              pathY(i) = Y
     Next i
        Cells(2, 1) = ii
         For i = 0 To ii
            If pathX(i) <> 0 Then
              Cells(i + 4, 1) = i: Cells(i + 4, 2) = pathX(i): Cells(i + 4, 3) = pathY(i)
            Else
              Exit For
            End If
          Next i
            R = Sqr((pathX(ii) - pathX(0)) ^ 2 + (pathY(ii) - pathY(0)) ^ 2)
            C ells(3, 1) = R
End Sub
```

FIGURE 8.5 VBA code of self-avoiding walks on a square lattice.

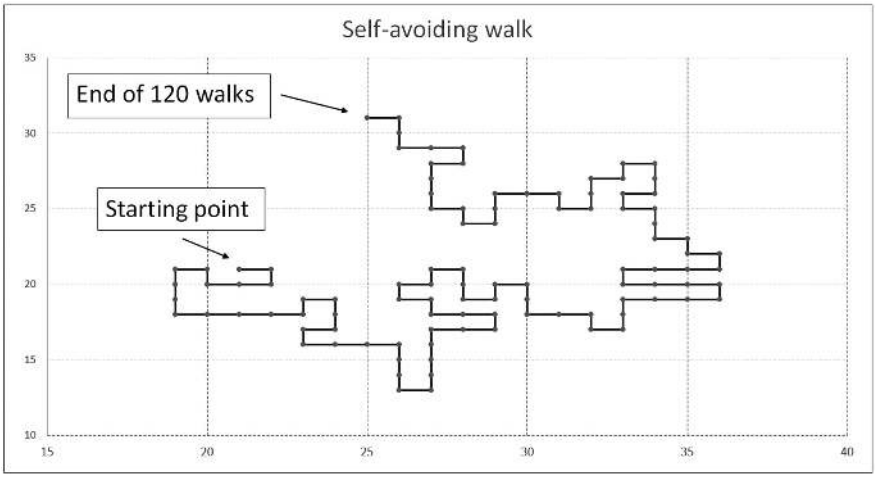


FIGURE 8.6 A polymer chain on a square lattice.

$$\frac{dN}{dt} = nN - mN = \varepsilon N \tag{8.7}$$

where n is the birth rate, m is the death rate, and $\varepsilon = n - m$ is called the Malthus coefficient [6]. The solution of Equation 8.7 is

$N(t) = N_0\exp(\varepsilon t)$ where N_0 is the population at $t = 0$.

The solution indicates the exponential increase when $\varepsilon > 0$, and the exponential decrease when $\varepsilon < 0$. If $\varepsilon = 0$, there is no change in the population.

More realistically, increasing and/or decreasing rates of the population are not steady because the birth and death rates are not constant over time. Logistic equation models growth and saturation of population,

$$\frac{dN}{dt} = (\varepsilon - \lambda N)N. \tag{8.8}$$

where $\varepsilon > 0$ is called the Malthus coefficient and λ is called the crowdedness constant [7]. The solution of Equation 8.8 can be obtained in the following manner. Let

$$G(N) = \int_{N_0}^{N} \frac{dx}{x(\varepsilon - \lambda x)} \text{ where } N_0 = N \text{ at } t = 0. \tag{8.9}$$

Evaluating the integral of $G(N)$ to obtain

$$G(N) = \frac{1}{\varepsilon}\left[\ln\left(\frac{N}{N_0}\right) - \ln\left(\frac{\varepsilon - \lambda N}{\varepsilon - \lambda N_0}\right)\right] = \frac{1}{\varepsilon}\ln\left(\frac{N}{\varepsilon - \lambda N}\frac{\varepsilon - \lambda N_0}{N_0}\right). \tag{8.10}$$

Using Equation 8.8, Equation 8.9 yields

$$G(N) = \int_{N_0}^{N} \frac{dx}{(dx/dt)} = \int_{t_0}^{t} dt = t - t_0. \tag{8.11}$$

Combining Equations 8.10 and 8.11,

$$\frac{N}{\varepsilon-\lambda N}\frac{\varepsilon-\lambda N_0}{N_0}=\exp[\varepsilon(t-t_0)].$$

Thus,

$$\frac{N}{\varepsilon-\lambda N}=\frac{N_0}{\varepsilon-\lambda N_0}\exp[\varepsilon(t-t_0)]\equiv C\exp[\varepsilon(t-t_0)] \text{ where } C=\frac{N_0}{\varepsilon-\lambda N_0}. \tag{8.12}$$

Solving Equation 8.12 for $N(t)$, we obtain

$$N(t)=\frac{\varepsilon C\exp[\varepsilon(t-t_0)]}{1+\lambda C\exp[\varepsilon(t-t_0)]}=\frac{\varepsilon N_0\, e^{\varepsilon(t-t_0)}}{\varepsilon+\lambda N_0[e^{\varepsilon(t-t_0)}-1]}. \tag{8.13}$$

Assuming appropriate numerical values of N_0, ε , and λ, one may draw a graph of $N(t)$. Alternatively, one may numerically solve the differential Equation 8.8. Figure 8.7 shows the VBA code to solve Equation 8.8 by applying the Runge-Kutta method (Appendix A3). In this code, $\varepsilon = 3$, $\lambda = 0.1$, and $N_0 = 1$. Figure 8.8 shows its result where $t = 0$ to 5 with increments of 0.05. The graph indicates a growth followed by saturation. Such a curve is called a sigmoid curve.

```
Sub LogisticEq()
Cells(1, 1) = "Population dynamics by Logistic equation"
'Parameters in the Logistic eq:
   Cells(3, 1) = "Malthus":  epsilon = 3: Cells(4, 1) = epsilon             'Malthus coefficient
   Cells(3, 2) = "Crowdedness": lambda = 0.1: Cells(4, 2) = lambda   'Crowdedness constant
'Writing labels and initial value in cells:
   Cells(3, 3) = "Initial t": t = 0: Cells(4, 3) = t
   Cells(3, 4) = "delta t": h = 0.05: Cells(4, 4) = h
   Cells(3, 5) = "Initial Population": population = 1: Cells(4, 5) = population
'Runge-Kutta method:
   n = 100 ' Iteration #
   Cells(6, 2) = "t"
   Cells(6, 3) = "Population"
     For i = 0 To n
        Cells(7 + i, 2) = t
        Cells(7 + i, 3) = population
             L1 = g(epsilon, lambda, t, population)
             L2 = g(epsilon, lambda, t + h * L1 / 2, population + h * L1 / 2)
             L3 = g(epsilon, lambda, t + h * L2 / 2, population + h * L2 / 2)
             L4 = g(epsilon, lambda, t + h * L3, population + h * L3)
        t = t + h
        population = population + h * (L1 + 2 *  L2 + 2 * L3 + L4) / 6
      Next i
End Sub
_______________________________________________________________________
Function g(epsilon, lambda, t, population)
'd(Population)/dt=g
      g = (epsilon - lambda * population) * population
End Function
```

FIGURE 8.7 VBA code for solving the Logistic equation.

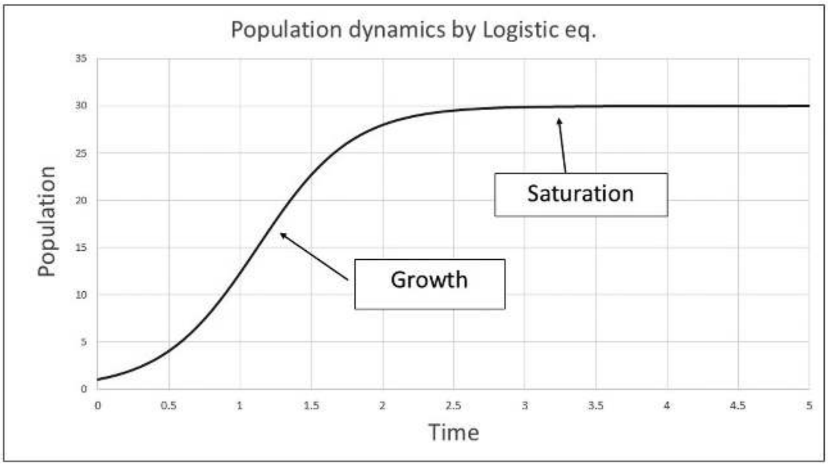


FIGURE 8.8 Population $N(t)$ from the Logistic equation.

8.2.2 Lotka-Volterra Equations

The Lotka-Volterra equations are a pair of equations used to describe the dynamics of biological systems where two species interact as prey (N_1) and predator (N_2) [8]. The Lotka-Volterra equation modified Equation 8.8 to make a pair of equations for properly considering the interaction of two species.

$$\begin{cases} \dfrac{dN_1}{dt} = \left(\varepsilon_1 - \lambda_1 N_2\right) N_1 \text{ and} \\ \dfrac{dN_2}{dt} = \left(\varepsilon_2 - \lambda_2 N_1\right) N_2. \end{cases} \tag{8.14\&8.15}$$

The analytical solution of the pair of differential equations can be found in the following way:

(1) Calculate [Equation 8.14•λ_2]+[Equation 8.15•λ_1] to obtain

$$\lambda_2 \frac{dN_1}{dt} + \lambda_1 \frac{dN_2}{dt} = \lambda_2 \varepsilon_1 N_1 - \lambda_1 \varepsilon_2 N_2. \tag{8.16}$$

(2) Calculate [Equation 8.14•ε_2/N_1]+ [Equation 8.15•ε_1/N_2] to obtain

$$\varepsilon_2 \frac{dN_1/dt}{N_1} + \varepsilon_1 \frac{dN_2/dt}{N_2} = -\lambda_2 \varepsilon_1 N_1 + \lambda_1 \varepsilon_2 N_2. \tag{8.17}$$

(3) From Equations 8.16 and 8.17,

$$\varepsilon_2 \frac{dN_1/dt}{N_1} + \varepsilon_1 \frac{dN_2/dt}{N_2} = \lambda_2 \frac{dN_1}{dt} + \lambda_1 \frac{dN_2}{dt}. \tag{8.18}$$

(4) Calculate the integrals of Equation 8.18 to obtain

$\varepsilon_2 \ln N_1 + \varepsilon_1 \ln N_2 - \lambda_2 N_1 + \lambda_1 N_2 =$ constant, and therefore,

$$N_1^{\varepsilon_2} N_2^{\varepsilon_1} e^{-\lambda_2 N_1 + \lambda_1 N_2} = C. \tag{8.19}$$

It is difficult to make a graph of $N_1(t)$ and $N_2(t)$ from the analytical solution 8.19 to observe $N_1(t)$ and $N_2(t)$, but one may numerically solve the pair of differential equations 8.14 and 8.15. Figure 8.9 lists the VBA code to solve the pair of equations using the Runge-Kutta method. In this code, $\varepsilon_1 = \varepsilon_2 = \lambda_1 = \lambda_2 = 1$ and $N_1 = 1$ and $N_2 = 2$ at $t = 0$.

Figure 8.10 shows the time dependence of N_1 and N_2, and the population of predator vs the population of prey. Note that the vertical scales are different. The computed correlation

```
Sub LotkaVolterraEq()
Cells(1, 1) = "Population dynamics between predator and prey by Lotka -Volterra equation"
'N1= Population of prey and N2=Population of predator.
'Parameters in the Lotka-Volterra eq:
   Cells(3, 1) = "Malthus1": epsilon1 = 1: Cells(4, 1) = epsilon 1            'Malthus coefficient
   Cells(3, 2) = "Crowdedness1": lambda1 = 2: Cells(4, 2) = lambda1      'Crowdedness constant
   Cells(3, 3) = "Malthus2": epsilon2 = 1: Cells(4, 3) = epsilon 2            'Malthus coefficient
   Cells(3, 4) = "Crowdedness2": lambda2 = 1: Cells(4, 4) = epsilon2      'Crowdedness constant
'Writing labels and initial value in cells:
   Cells(3, 5) = "Initial N1": N1 = 1: Cells(4, 5) = N1                          'Prey
   Cells(3, 6) = "Initial N2": N2 = 2: Cells(4, 6) = N2                          'Predator
   Cells(3, 7) = "Initial t": t = 0: Cells(4, 7) = t
   Cells(3, 8) = "delta t": h = 0.02: Cells(4, 8) = h
'Runge-Kutta method:
   n = 500 ' Iteration #
   Cells(6, 2) = "t"
   Cells(6, 3) = "Prey"
   Cells(6, 4) = "Predator"
   For i = 0 To n
        Cells(7 + i, 2) = t
        Cells(7 + i, 3) = N1
        Cells(7 + i, 4) = N2
     L1 = g(epsilon1, lambda1, epsilon2, lambda2, t, N1, N2)
     F1 = f(epsilon1, lambda1, epsilon2, lambda2, t, N1, N2)
     L2 = g(epsilon1, lambda1, epsilon2, lambda2, t + h / 2, N1 + h * L1 / 2, N2 + h * F1 / 2)
     F2 = f(epsilon1, lambda1, epsilon2, lambda2, t + h / 2, N1 + h * L1 / 2, N2 + h * F1 / 2)
     L3 = g(epsilon1, lambda1, epsilon2, lambda2, t + h / 2, N1 + h * L2 / 2, N2 + h * F2 / 2)
     F3 = f(epsilon1, lambda1, epsilon2, lambda2, t + h / 2, N1 + h * L2 / 2, N2 + h * F2 / 2)
     L4 = g(epsilon1, lambda1, epsilon2, lambda2, t + h, N1 + h * L3, N2 + h * F3)
     F4 = f(epsilon1, lambda1, epsilon2, lambda2, t + h, N1 + h * L3, N2 + h * F3)
   t = t + h
     N1 = N1 + h * (L1 + 2 * L2 + 2 * L3 + L4) / 6
     N2 = N2 + h * (F1 + 2 * F2 + 2 * F3 + F4) / 6
   Next i
End Sub
______________________________________________________________________________
Function g(epsilon1, lambda1, epsilon2, lambda2, t, N1, N2)
'dN1/dt=g
     g = (epsilon 1 - lambda1 * N2) * N1
End Function
______________________________________________________________________________

Function f(epsilon1, lambda1, epsilon2, lambda2, t, N1, N2)
'dN2/dt=f
     f = -(epsilon2 - lambda2 * N1) * N2
End Function
```

FIGURE 8.9 VBA code to solve the Lotka-Volterra equation.

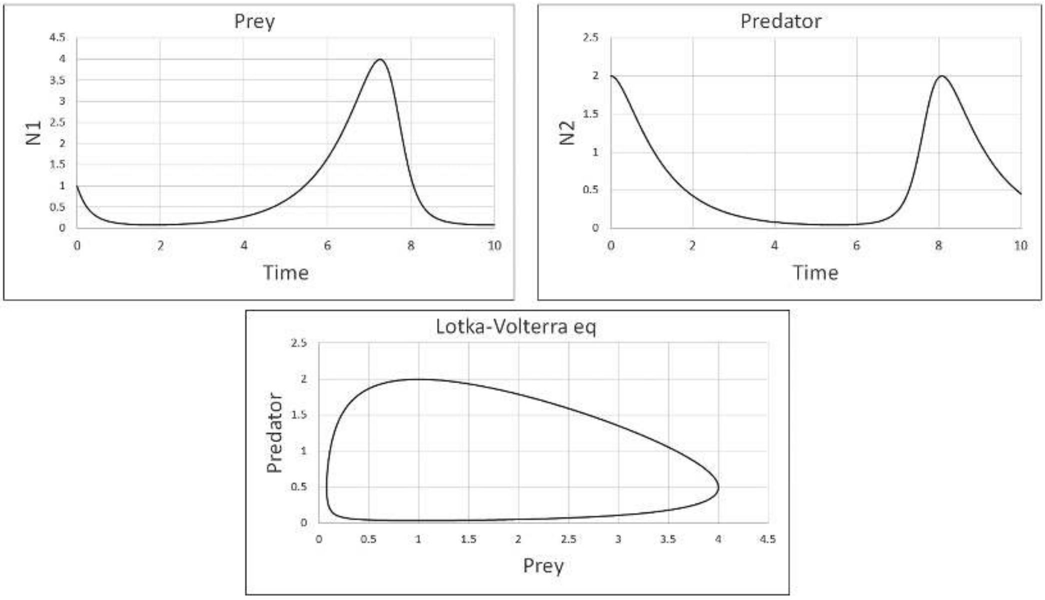


FIGURE 8.10 Prey-predator relationship described by the Lotka-Volterra equation.

between N_1 and N_2 follows the nature where the change (increase/decrease) in the population of predators tracks the change (increase/decrease) in the population of prey.

8.2.3 Population Dynamics Including Reproduction

Volterra made postulates to represent population explosion with reproduction:

1) The ratios of males and females to the total population do not change over time:

$$\frac{N_{male}}{N} = \alpha \text{ and } \frac{N_{female}}{N} = \beta \text{ are both constants} \tag{8.20}$$

where N is the total population;

2) The number of encounters with the opposite sex is proportional to

$$N_{male} \cdot N_{female} = \alpha\beta N^2; \tag{8.21}$$

3) There are n encounters per unit time and m births from the encounter, and assume m/n is constant in time;

4) With the above assumptions, the total number of births is given by

$$K\alpha\beta\left(\frac{ma}{n}\right)N^2 \equiv \lambda N^2 \text{ where } K \text{ and } \lambda \text{ are constants; and} \tag{8.22}$$

5) If there is no birth, the population satisfies

$$\frac{dN}{dt} = -\varepsilon N \text{ where } \varepsilon > 0 \tag{8.23}$$

to implement death.

Combining Equations 8.20 with 8.23, the population change is given by

$$\frac{dN}{dt} = -\varepsilon N + \lambda N^2 = (-\varepsilon + \lambda N)N = -(\varepsilon - \lambda N)N. \tag{8.24}$$

Equation 8.24 is the same as the Logistic equation (8.8) except for its negative sign.

The solution of Equation 8.24 is

$$N(t) = \frac{N_0}{(1-R)e^{\varepsilon t} + R} \text{ where } R = N_0 \frac{\lambda}{\varepsilon}. \tag{8.25}$$

There are three possibilities for the dynamics of Equation 8.25, depending on the h-value:

(i) R=1, i.e., $\varepsilon - \lambda N_0 = 0$ at t=0. $N = N_0$: no change in N;

(ii) R<1, i.e., $\varepsilon - \lambda N_0 > 0$ at t=0. As $t \rightarrow \infty$, $N \rightarrow \infty$: declining population; and

(iii) R>1, i.e., $\varepsilon - \lambda N_0 < 0$ at t=0. As $t \rightarrow t_\infty$, $(1/\varepsilon)\ln[\lambda N_0/(\lambda N_0 - \varepsilon)$, $N \rightarrow \infty$: population explosion.

One may interpret the above conditions in a different way. From the differential equation 8.24,

(i)' If $\varepsilon - \lambda N_0 = 0$ at $t = 0$, N may not change where the initial population is $N_0 - R = 0$ because $R = N_0\lambda/\varepsilon$;

(ii)' If $\varepsilon - \lambda N_0 > 0$ at $t = 0$, N may increase where the initial population is $N_0 - R = N_0(\varepsilon - \lambda)/\varepsilon > 0$; and

(iii)' If $\varepsilon - \lambda N_0 < 0$ at $t = 0$, N may decrease where the initial population is $N_0 - R = N_0(\varepsilon - \lambda)/\varepsilon < 0$;

Figure 8.11 lists the VBA code to analyze Equation 8.21 with the Runge-Kutta method for visualizing the population change on the conditions (i)' to (iii)'. Note that N_0 is the initial population only if $\lambda = \varepsilon$. This code is obtained using the VBA code listed in Figure 8.7, where $\varepsilon = 1$, $\lambda = 1$, and $N_0 = 1$. The three possible R-values are selected to set the initial populations by $N_0 - R$ to satisfy the above three conditions: 1 for case (i)'; and −0.006 for case (ii)', and 0.1 for case (iii)'.

Figure 8.12 shows the three possibilities of population change with reproduction. The numerical value of $R = \lambda N_0/\varepsilon = 1$ is the threshold. If the reproduction rate λ rate is more

```
Sub Reproduction()
Cells(1, 1) = "Population dynamics including reproduction by Lotka -Volterra eq"
'N = Population.
'Parameters in the Lotka-Volterra eq:
   Cells(3, 1) = "Epsilon": epsilon = 1: Cells(4, 1) = epsilon
   Cells(3, 2) = "Lambda": lambda = 1: Cells(4, 2) = lam bda
   N0 = 1                                                    'Initial N=N0 when R=1"
'Writing labels and initial value in cells:
   Cells(3, 7) = "Initial t": t = 0: Cells(4, 7) = t
   Cells(3, 8) = "delta t": de lt = 0.05: Cells(4, 8) = delt
   Cells(3, 6) = "N at t=0"
   Cells(7, 2) = "t"
   Cells(5, 1) = "Population dynamics"
For j = -1 To 1                                              'Creating 3 different R-values
   Cells(5, 2 + j + 2) = "R"
   Cells(7, 2 + j + 2) = "N"
      If j = 1 Then R = 0.1 * j: GoTo Population
      If j = 0 Then R = j: GoTo Population
      If j = -1 Then R = j * 0.006
Population:
   N = N0 - R: Cells(4, 6) = N
   Cells(6, 2 + j + 2) = R
   t = 0                                                     'Resetting initial time.
'Runge-Kutta method:
NN = 90 ' Iteration #
   For i = 0 To NN
        Cells(8 + i, 2) = t
        Cells(8 + i, 2 + j + 2) = N
     L1 = g(epsilon, lambda, t, N)
     L2 = g(epsilon, lambda, t + delt / 2, N + delt * L1 / 2)
     L3 = g(epsilon, lambda, t + delt / 2, N + delt * L2 / 2)
     L4 = g(epsilon, lambda, t + delt, N + delt * L3)
        N = N + delt * (L1 + 2 * L2 + 2 * L3 + L4) / 6
     t = t + delt
   Next i
Next j
End Sub
_______________________________________________________________
Function g(epsilon, lambda, t, N)
'dN/dt=g
     g = -(epsilon - lambda * N) * N
End Function
```

FIGURE 8.11 VBA code for computing population change with reproduction.

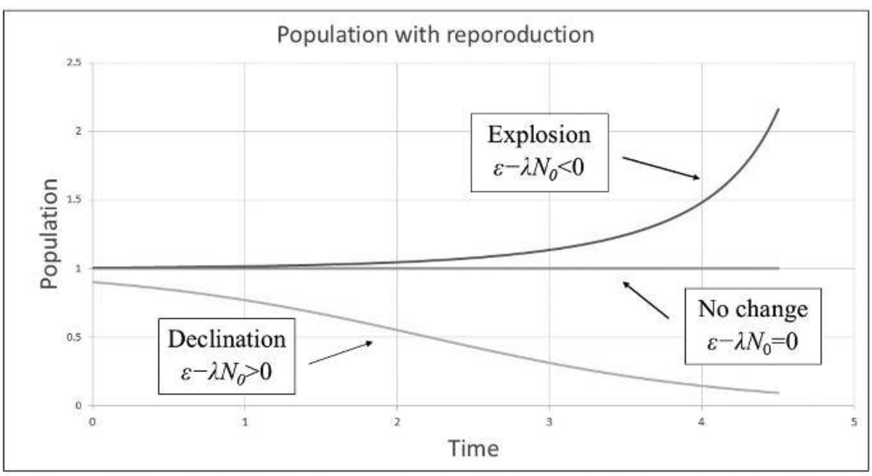


FIGURE 8.12 Population dynamics with reproduction.

than the death rate ε, or $R > 1$, the population explodes. On the other hand, if the reproduction rate λ rate is less than the death rate ε, or $R < 1$, the population decreases. These days, many countries are facing the latter case.

8.2.4 Population Dynamics with Birth, Death at Birth, and Reproduction

In the above argument, the assumption (3): There are n encounters per unit time and m births from the encounter and assume m/n is constant in time. Incorporating death at birth in population dynamics involves adjusting the model described in Section 8.2.3 to account for a portion of births that do not survive. For including death at birth, we may replace m with $m - \rho N$ where ρ is a proportional constant [9]. Equation 8.22 becomes

$$K\alpha\beta\left(\frac{m-\rho N}{n}\right)N^2 = \lambda N^2 - K\alpha\beta\frac{\rho}{n}N^3, \tag{8.26}$$

and Equation 8.24 becomes

$$\frac{dN}{dt} = \left[-\varepsilon + (\lambda - \mu)N - \gamma_0 N^2\right]N \equiv -\left(aN^2 - bN - c\right)N \tag{8.27}$$

where $\gamma_0 = K\alpha\beta\rho/n$, and $c = \varepsilon$, $b = (\lambda - \mu)$, and $a = \gamma_0$. Suppose the quadrilateral equation $aN^2 - bN + c = 0$ has two real roots p and q ($p > q > 0$), Equation 8.27 becomes

$$\frac{dN}{dt} = -a(N-p)(N-q)N \text{ where } p,q = \frac{b \pm \sqrt{b^2 - 4ac}}{2a} \text{ and } p > q. \tag{8.28}$$

The solution of Equation 8.28 can be given by

$$e^{-c_1(p-q)t} = \left(\frac{N}{N_0}\right)^{p=q}\left(\frac{N-p}{N_0-p}\right)^{q}\left(\frac{N-q}{N_0-q}\right)^{-p}. \tag{8.29}$$

From Equation 8.28, one notices dN/dt behaves differently with different initial population N_0. Let

$$\frac{dN}{dt} = -af(N)N \text{ where } f(N) = (N-p)(N-q)N \text{ and } q < p. \tag{8.30}$$

Figure 8.13(a) depicts a function $f(N)$. From the figure,

1) If $N>p$, $dN/dt<0$ and $N(t)$ decreases;
2) If $N=p$, $dN/dt=0$ and $N(t)$ does not change;
3) If $q<N<p$, $dN/dt>0$ and $N(t)$ increases;
4) If $N=q$, $dN/dt=0$ and $N(t)$ does not change; and
5) If $0<N<q$, $dN/dt<0$ and $N(t)$ decreases.

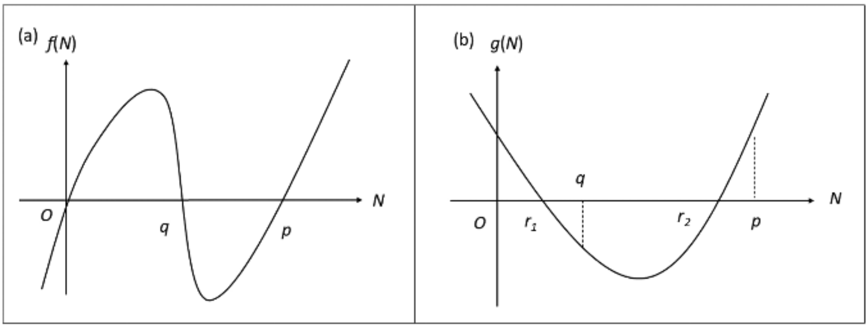


FIGURE 8.13 Functions $f(N)$ and $g(N)$.

TABLE 8.1 Population dynamics with different conditions of birth and death, and reproduction

N_0	$f(N)$	dN/dt	$g(N)$	d^2N/dt^2	Behavior of $N(t)$
$N_0 > p$	+	−	+	−	$N(t)$ decreases to asymptotically approach $N = p$.
$N_0 = p$	0	0	+	0	$N(t)$ remains the same.
$r_2 < N_0 < p$	−	+	+	+	$N(t)$ increases to asymptotically approach $N = p$.
$q < N_0 < r_2$	−	+	−	−	Although $N(t)$ increases to asymptotically approach $N = p$, the curve is sigmoid.
$N_0 = q$	0	0	−	0	$N(t)$ remains the same.
$r_1 < N_0 < q$	+	−	−	+	$N(t)$ increases to asymptotically approach $N = 0$. At $N = r_2$, there is an inflexion.
$0 < N_0 < r_1$	+	−	+	−	$N(t)$ increases to $N = 0$ without any inflexion.

In order to analyze the behavior more precisely, we examine d^2N/dt^2.

$$\begin{aligned}\frac{d^2N}{dt^2} &= \frac{d}{dt}\left(\frac{dN}{dT}\right) = -a\left(3N^2 - 2(p+q)N + pq\right)\frac{dN}{dt} \\ &= -ag(N)\frac{dN}{dt} = -aNf(N)g(N)\end{aligned} \tag{8.31}$$

where $g(N) = 3N^2 - 2(p + q)N + pq$. Figure 8.13(b) depicts a function $g(N)$. Because $g(p) > 0$, $g(q) < 0$, and $g(0) > 0$, $g(N)$ has two roots, r_1 and r_2, such that $0 < r_1 < q < r_2 < p$.

Table 8.1 shows the possible cases of $N(t)$ according to the range of initial N.

Figure 8.14 shows the five cases where $p = 2$ and $q = 1$. For the given p and q values, $r_1 = 0.427$ and $r_2 = 1.577$. The population is stable when the initial population is around $p = 2$ while it is sensitive to the initial population around q. The Runge-Kutta–based VBA code to generate the outcome is similar to the one in Figure 8.10 with the following function declaration from Equation 8.28.

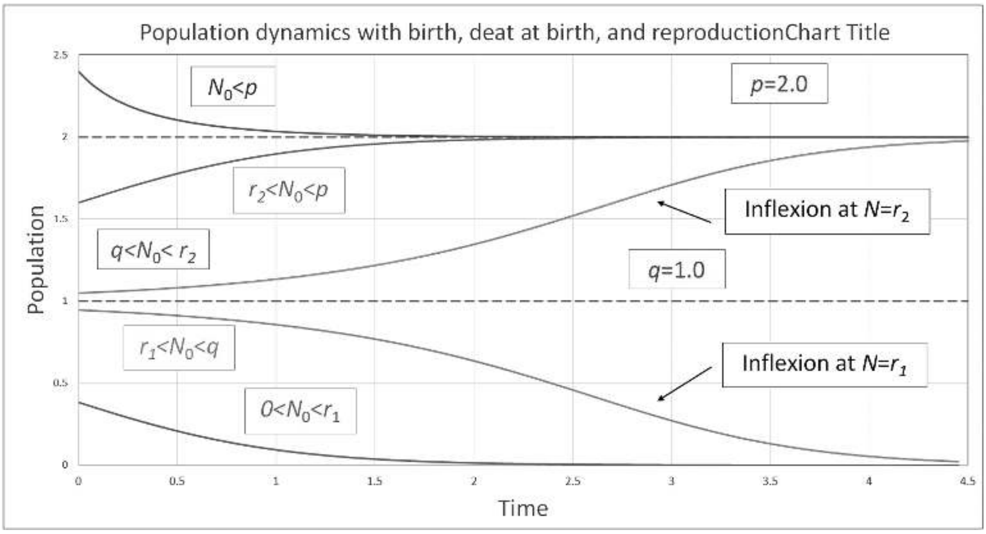


FIGURE 8.14 Population dynamics with birth, death at birth, and reproduction.

```
Function g(p, q, t, N)
'dN/dt = g
    g = -(N - p) * (N - q) * N
End Function
```

SUGGESTED FURTHER STUDY

The Galton–Watson process models family names as patrilineal (passed from father to son), while offspring are randomly either male or female, and names become extinct if the family name line dies out (holders of the family name die without male descendants) [10, 11]. This model may also be applicable to the change in the number of neutrons in a nuclear fission chain reaction. A neutron collides with a nucleus with a certain probability to produce a random number of neutrons.

Nonlinear equations exhibit many interesting phenomena around us. In particular, the Logistic equation exhibits chaotic behaviors [12]. For studying general concepts of nonlinear oscillations, refer to [13].

REFERENCES

1. *Elasticity of Single Polymer Chains*, MIT OpenCourseWare. https://ocw.mit.edu/courses/3-052-nanomechanics-of-materials-and-biomaterials-spring-2007/c54311f6d5d6249a873175fc298b87c1_lec19.pdf.
2. *Polymer Physics The Isolated Polymer Chain*, University of Cincinnati. https://www.eng.uc.edu/~beaucag/Classes/Physics/Chapter1.pdf
3. Self-Avoiding Walk – from Wolfram MathWorld. https://mathworld.wolfram.com/Self-AvoidingWalk.html.
4. Janse Van Renburg EJ, *Monte Carlo Methods for the Self-Avoiding Walk*, Oxford Academic, 2015. https://doi.org/10.1093/acprof:oso/9780199666577.003.0013.

5. How Populations Grow: The Exponential and Logistic Equations | Learn Science at Scitable (nature.com). https://www.nature.com/scitable/knowledge/library/how-populations-grow-the-exponential-and-logistic-13240157/.
6. Chasnov JR, *Malthusian Growth Model*, LibreTexts Mathematics, 2022. https://math.libretexts.org/Bookshelves/Applied_Mathematics/Mathematical_Biology_(Chasnov)/01%3A_Population_Dynamics.
7. Chasnov JR, *Logistic Population Growth*, LibreTexts Biology, 2022. https://bio.libretexts.org/Bookshelves/Introductory_and_General_Biology/General_Biology_(Boundless)/45%3A_Population_and_Community_Ecology/45.02%3A_Environmental_Limits_to_Population_Growth/45.2B%3A_Logistic_Population_Growth.
8. Chasnov JR, *Lotka-Volterra Predator-Prey Model*, LibreTexts Mathematics. https://math.libretexts.org/Bookshelves/Applied_Mathematics/Mathematical_Biology_(Chasnov)/01%3A_Population_Dynamics/1.04%3A_The_Lotka-Volterra_Predator-Prey_Model.
9. Yamaguchi M, 非線形現象の数学 (*Mathematics of Nonlinear phenomena*), Asakura Publishing Co., Ltd., 1971.
10. *Branching Processes*, Department of Statistics, University of Chicago. http://galton.uchicago.edu/~lalley/Courses/312/Branching.pdf.
11. *Branching Processes*, University of California, Berkeley. https://www.stat.berkeley.edu/~aldous/Networks/lec2.pdf.
12. Nayfeh AH, *Nonlinear Oscillations*, Wiley Open Library, 1995. https://onlinelibrary.wiley.com/doi/pdf/10.1002/9783527617586.fmatter?msockid=0a906db87d8667c3188c795f7c8166dd.
13. Hayashi C, *Nonlinear Oscillations in Physical Systems*, Princeton Legacy Library, 1986. https://www.degruyter.com/document/doi/10.1515/9781400852871/html.

Appendix

SOME DETAILS NOT EXPLAINED are collected in this appendix.

A.1 USEFUL FEATURES OF EXCEL

A.1.1 AutoFill

AutoFill is a useful Excel feature for scientific calculations. With this feature, iterative calculations can be carried out without VBA programming. Here is a simple example that enters integer 0, 1, 2, 3, …. in Column `A` (Figure A.1).

(1) Input **0** in Cell `A1`.

(2) Go to Cell `A2` and enter **=A1+1** and press `<Enter>`. The value in Cell `A2` is calculated to be 1.

(3) Place the cursor in Cell `A2` and hit `<Enter>`. The Cell is emphasized.

(4) Click on the fill handle (a small solid square at the lower right corner). The cursor becomes a plus sign (**+**). While pressing the right mouse button, drag the cursor to cells below in column `A` until reaching the desired integer value.

Note: There is a quicker method when a formula is involved. Provided there is data in a column adjacent to the one with the formula, all that is required is to right double-click the fill handle and the formula will automatically be copied to the below columns [1].

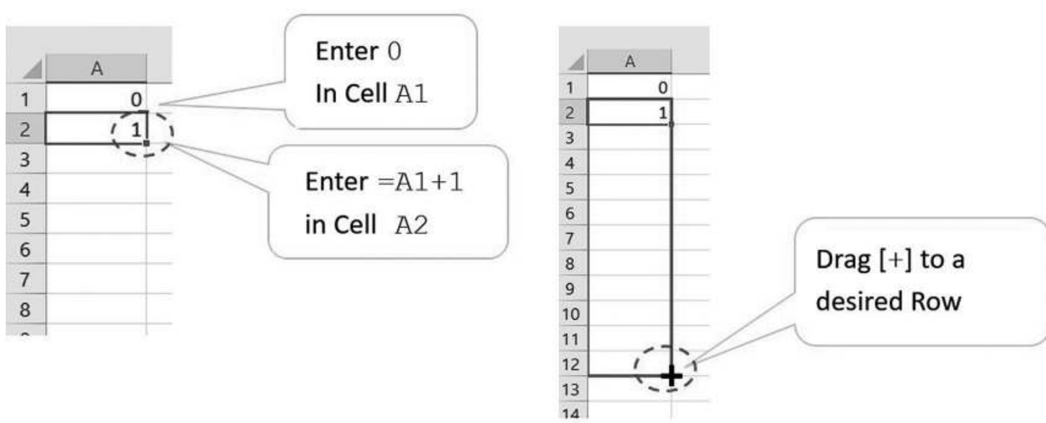


FIGURE A.1 *AutoFill* feature.

DOI: 10.1201/9781003516347-9

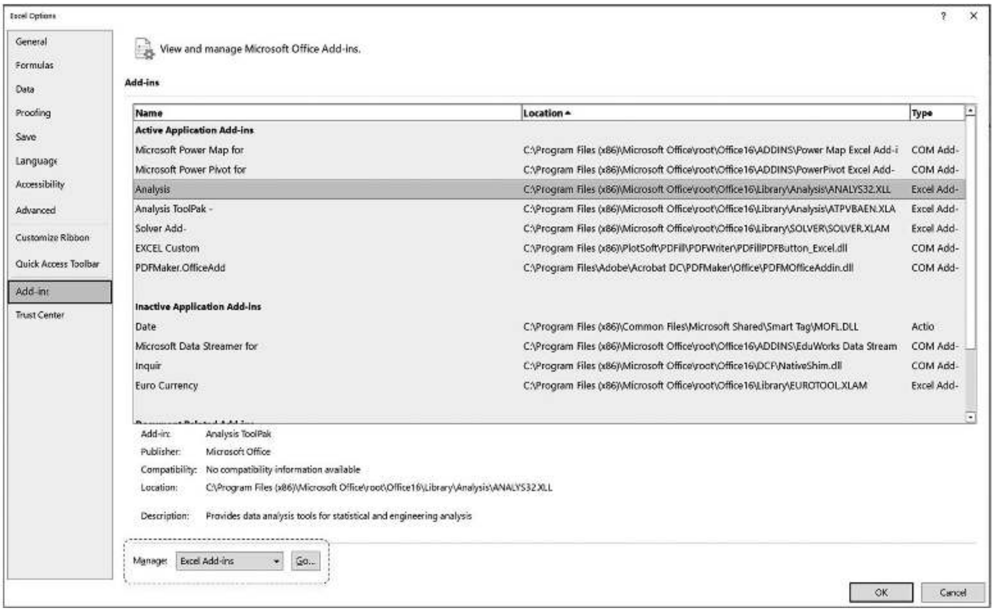


FIGURE A.2 Add-ins options screen.

A.1.2 Data Analysis

Because Excel's default setting is not for scientific computation, we need to add data analysis tools in order to add the Fourier transform option and other useful scientific calculation tools [2]. From the [`File`] menu, select [`Options`] to display the "`Excel option`" screen. Click on [`Add-Ins`] to display the following screen (Figure A.2).

Next, click on [`Go`] to display available add-ins, and then check [`Analysis ToolPak`], [`Analysis ToolPak-VBA`], and [`Solver Add-In`] (Figure A.3).

Remark: [`Solver`] is an optimization (maximizing or minimizing) routine used for applications such as linear programming. There are many scientific problems that can be computed using this feature. It would be better to install it on your computer.

A.1.3 Excel Macro (VBA)

Excel macro is a visual basic programing environment. Those who are interested in Excel macro, refer to other books [2, 3]. Take the following steps to enable Excel's macro capability:

(1) Go to [`Trust Center`] (Figure A.4).

(2) From [Option], go to [Trust Center], and click on [Trust Center Settings…] of [Excel Options] in [Microsoft Excel Trust Center].

(3) Select [`Macro Settings`] and check [`Enable All Macro (not recommended; potentially dangerous code can run)`] (Figure A.5). Click [`OK`] to complete the setting.

(4) In the pulldown menu, click on [`View`] and click on [`Macros`] to select [`View Macros`] and create a macro (visual basic) program (Figure A.6).

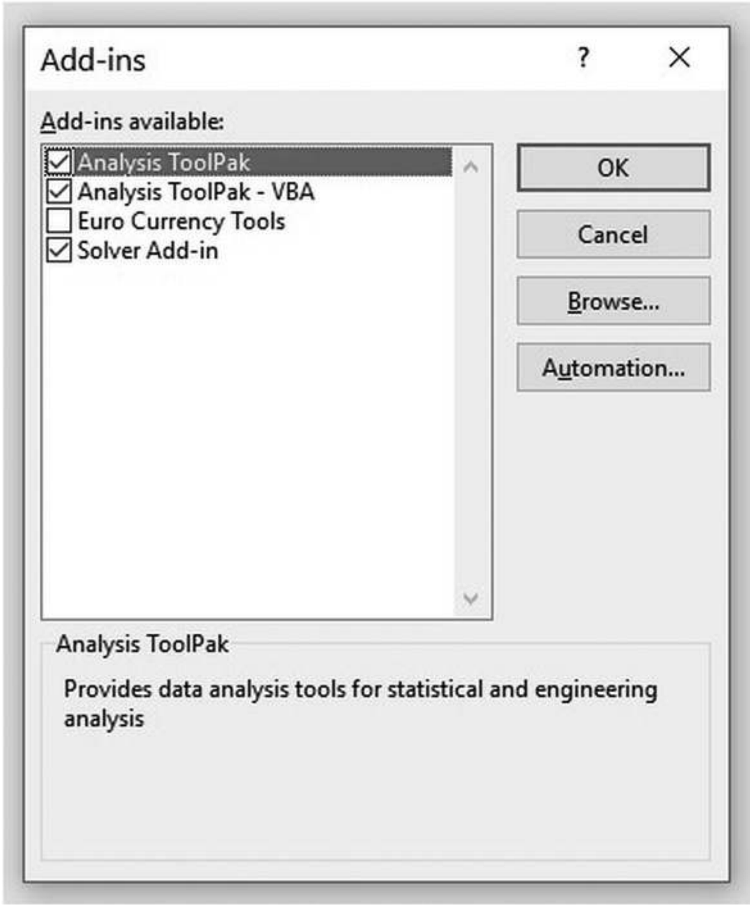


FIGURE A.3 Available add-ins.

After entering a macro name, create a source code using a built-in editor (Figure A.7). Alternatively, use MS WORD or a text-editor such as "Notepad++" to write a code and paste it to the Macro editor. When the created VBA code needs to be reviewed or edited, click on [`Edit`].

A.1.4 Iterative Calculation

From the [`File`] menu, select [`options`] to display the [`EXCEL Options`] screen. Click on [`Formulas`] to display the following screen. Figure A.8 shows the screenshot of this procedure.

A.2 EULER'S METHOD

Consider a one-dimensional motion. From the definition of the derivative of, e.g., the position $x\ (t)$ and the acceleration $a(t)$

$$\lim_{\Delta t\to 0}\frac{x(t+\Delta t)-x(t)}{\Delta t}=\frac{dx(t)}{dt}\text{ and }\lim_{\Delta t\to 0}\frac{v(t+\Delta t)-v(t)}{\Delta t}=\frac{dv(t)}{dt}=a(t). \tag{A.1}$$

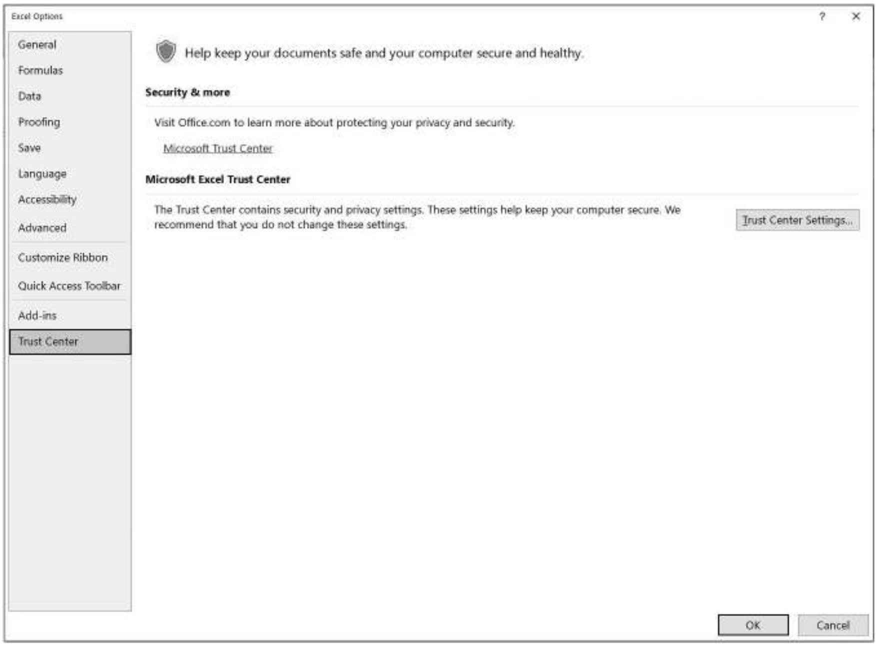


FIGURE A.4 Excel options.

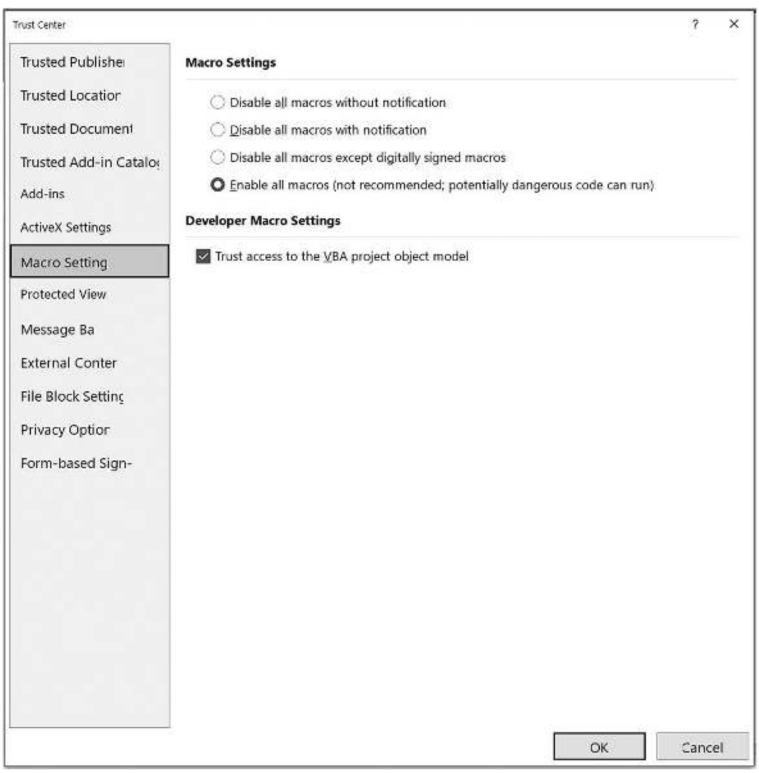


FIGURE A.5 Macro settings.

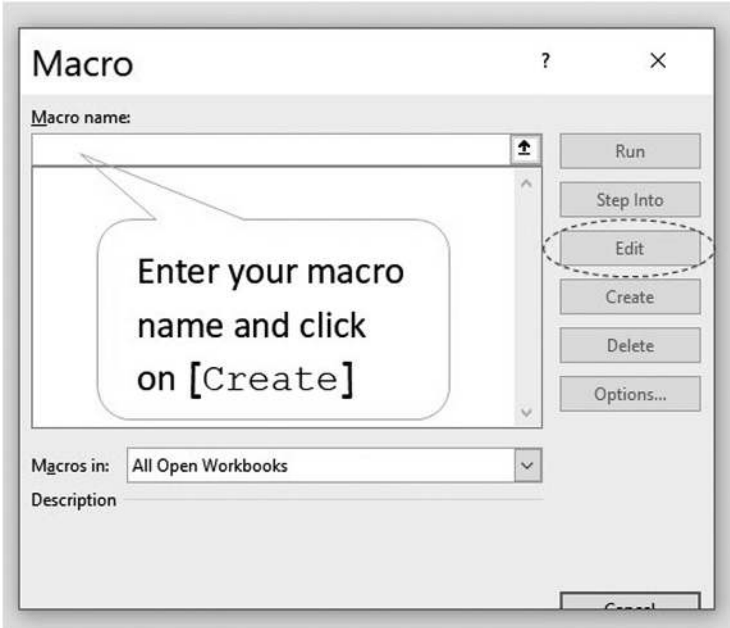


FIGURE A.6 Creating Macro (VBA) code.

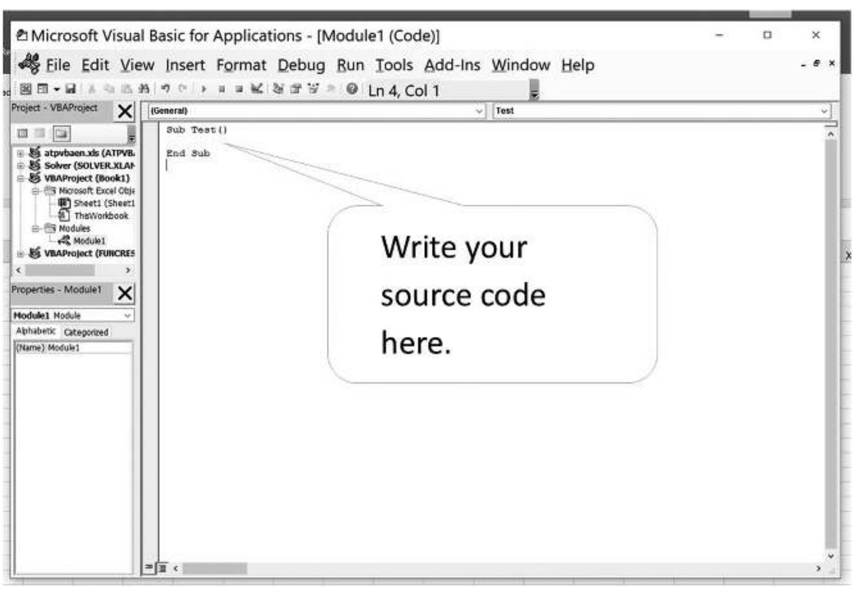


FIGURE A.7 Macro editor.

Utilizing Equation A.1, the Euler method numerically solves the differential equations such as the equation of motion, $F = ma$, by successively calculating the position $x(t + \Delta t)$ and velocity $v(t + \Delta t)$ at time $t + \Delta t$ using the position $x(t)$ and the velocity $v(t)$ at time t and the derivatives dx/dt and dv/dt at time t:

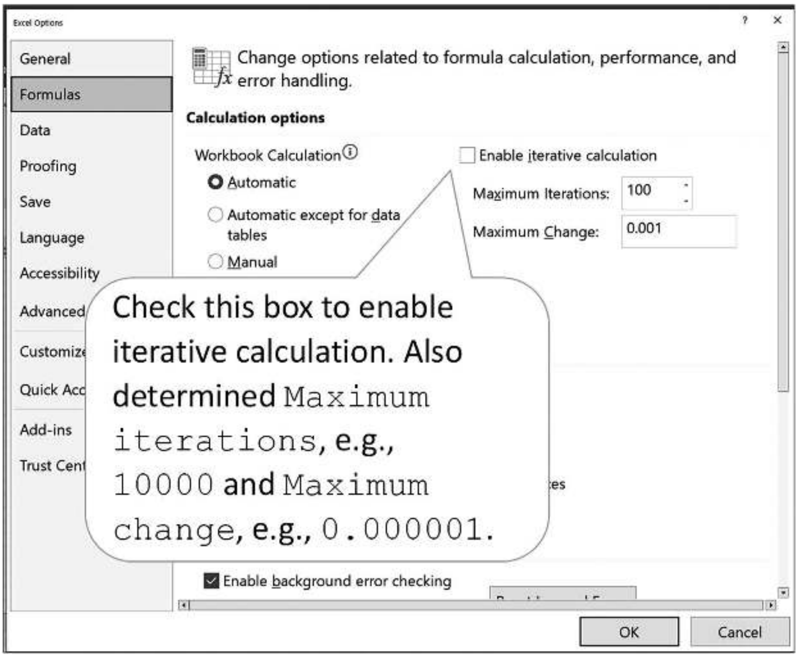


FIGURE A.8 Enable iterative calculation.

$$x(t+\Delta t) = x(t) + \left.\frac{dx}{dt}\right|_t \cdot \Delta t = x(t) + v(t)\Delta t, \tag{A.2}$$

$$v(t+\Delta t) = v(t) + \left.\frac{dv}{dt}\right|_t \cdot \Delta t = v(t) + a(t)\Delta t \text{ because } \left.\frac{dv}{dt}\right|_t = g. \quad \text{and (A.3)}$$

With the initial condition of the position and the velocity, x_0 and v_0, and the time interval, e.g., Δt = 0.01 sec, the Euler method generates the position of the trajectory using Equations A.2 and A.3. The Euler method can be carried out on a spreadsheet with the *AutoFill* feature.

This method is applicable when a motion is "slow and smooth in time" or "under a constant acceleration" such as projectile motions. However, if the motion is under a large change in acceleration such as harmonic oscillations, the Euler method may cause a large computational error.

A.3 THE RUNGE-KUTTA METHOD

Another approach to solving the equation of motion, called the Runge-Kutta method, is a better choice [2, 3]. Below is the algorithm of the fourth-order Runge-Kutta method.

First-order differential equation: $\dfrac{dx}{dt} = f(t,x)$

1) Define the size of time increment: $t_{i+1} = t_i + h$, where h is the time increment and i = 0, 1, 2, …, N.

2) Calculate the following K-values using given $t = t_i$ and $x = x_i$.

$$
\begin{aligned}
K_1 &= f(t, x) \\
K_2 &= f(t + \frac{h}{2},\ \ x + \frac{hK_1}{2}) \\
K_3 &= f(t + \frac{h}{2},\ \ x + \frac{hK_2}{2}) \\
K_4 &= f(t + h,\ \ x + hK_3).
\end{aligned}
\tag{A.4}
$$

3) Calculate the next x-value: $x_{i+1} = x_i + \Delta x$ at $t = t_{i+1}$, where the position increment is a weighted average of the K-values, i.e., $\Delta x = h(K_1 + 2K_2 + 2K_3 + K_4)/6$. (A.5).

4) Repeat the steps 9)–11) for a pre-determined N-value (e.g., 100) to obtain a table of the t-values and the x-values.

Second-order differential equation: $\dfrac{d^2x}{dt^2} = g(t, x, v)$ *where* $v = \dfrac{dx}{dt}$

5) Separate the differential equation into two equations:

$$\frac{dv}{dt} = g(t, x, v) \text{ and } v = \frac{dx}{dt} = f(t, x, v). \tag{A.6}$$

6) Define the size of time increment: $t_{i+1} = t_i + h$ where h is the time interval and $i = 0, 1, 2, \ldots, N$.

7) For solving $\dfrac{dv}{dt} = g(t, x, v)$, calculate the following L-values using given $t = t_i$, $x = x_i$, and $v = v_i$:

$$
\begin{aligned}
L_1 &= g(t, x, v); \\
L_2 &= g(t + \frac{h}{2},\ \ x + \frac{hL_1}{2},\ \ v + \frac{hL_1}{2}); \\
L_3 &= g(t + \frac{h}{2},\ \ x + \frac{hL_2}{2},\ \ v + \frac{hL_2}{2}); \\
L_4 &= g(t + \frac{h}{2},\ \ x + hL_3,\ \ v + hL_3).
\end{aligned}
\tag{A.7}
$$

$$\Delta v = h(L_1 + 2L_2 + 2L_3 + L_4)/6.$$

8) Calculate the next v-value: $v_{i+1} = v_i + \Delta v$ at $t = t_{i+1}$ where $\Delta v = h(L_1 + 2L_2 + 2L_3 + L_4)/6$. (A.8)

9) Solving $\dfrac{dx}{dt} = f(t, x, v)$ is essentially the same as the first order differential equation described earlier. In this case, there is also a velocity term. Calculate the following K-values at given $t = t_i$, $x = x_i$, and $v = v_i$:

$$\begin{aligned} K_1 &= f(t,x,v) \\ K_2 &= f(t+\frac{h}{2},\ x+\frac{hK_1}{2},\ v+\frac{hK_1}{2}) \\ K_3 &= f(t+\frac{h}{2},\ x+\frac{hK_2}{2},\ v+\frac{hK_2}{2}) \\ K_4 &= f(t+\frac{h}{2},\ x+hK_3,\ v+\frac{hK_3}{2}). \end{aligned} \tag{A.9}$$

10) Calculate the next x-value: $x_{i+1} = x_i + \Delta x$ at $t = t_{i+1}$, where $\Delta x = h(K_1 + 2K_2 + 2K_3 + K_4)/6$. (A.10)
11) Repeat the above steps for a pre-determined N (e.g., 100) to obtain a table of the t-values, the x-values, and the v-values.

The Runge-Kutta method is much easier to implement with Excel's VBA (Visual Basic for Applications). Refer to Appendix A1.3 for enabling the VBA capability. Remember that the VBA code for the Runge-Kutta method applies to many other second-order differential equation problems because the mathematical function, $g(t, x, v)$, is the only part that needs to be changed.

A.4 SIMPSON'S METHOD FOR DEFINITE INTEGRAL

Consider an integral $I = \int_a^b f(x)dx$ where the integral interval $[a, b]$ is finite (e.g., $a = 0$ and $b = 1$). If the integrant f(x)n is too complicated to perform the integral, we approximate $f(x)$ to make the integral easier.
Denote the Taylor expansion of f(x) as

$$f(x) = f_0 = xf' + \frac{x^2}{2!}f'' + \frac{x^3}{3!}f''' + \cdots \tag{A.11}$$

where all derivatives are evaluated at $x = 0$. It can be shown that

$$f_{\pm 1} \equiv f(x = \pm h) = f_0 \pm hf' + \frac{h^2}{2}f'' \pm \frac{h^3}{6}f''' + O(h^4). \tag{A.12}$$

The first derivative of f(x) can be approximated by

$$f' \approx \frac{f_1 - f_{-1}}{2h}, \tag{A.13}$$

and the second derivative can be approximated by

$$f'' \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}. \tag{A.14}$$

Thus, Equation A.11 can be improved using Equations A.13 and A.17:

$$f(x) = f_0 + \frac{f_1 - f_{-1}}{2h}x + \frac{f_1 - 2f_0 + f_{-1}}{2h^2}x^2 + O(x^3). \tag{A.15}$$

Using Equation A.15, the following integral can be approximated by

$$\int_{-h}^{+h} f(x)dx = \frac{h}{3}\left(f_1 + 4f_0 + f_{-1}\right) + O(h^5),$$

The integral to be evaluated can be approximated by

$$\begin{aligned} I &= \int_a^b f(x)dx \\ &= \frac{h}{3}\left[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \cdots + 4f(b-h) + f(b)\right]. \end{aligned} \tag{A.16}$$

Figure A.9 lists a VBA code of Simpson's methods to evaluate $\int_0^1 \exp(-x)dx = 1 - e^{-1}$ = 0.632121. Simpson's method outputs 0.632121 to this significant figure.

How can we evaluate the integral like $I = \int_0^\infty f(x)dx$? If the integrant f(x) monotonically decreases quickly and becomes nearly zero at a certain x-value (say, b), then $f(x)$ ~0 for $b \leq x$ and we may have

$$I = \int_0^\infty f(x)dx \approx \int_0^b f(x)dx. \tag{A.17}$$

```
Sub Simpson()
Cells(1, 1) = "Simpson's rule doe definite integrals"
   a = 0 ' a>=0
   b = 1
   N = 64
   h = (b - a) / N
  Sum = 0
  Sum = F(a)
  coeff = 2
For i = 1 To N - 1
   If coeff = 2 Then coeff = 4 Else coeff = 2
      x = i * h
      Cells(4 + i, 1) = x
      Cells(4 + i, 2) = coeff
         Sum = Sum + coeff * F(x)
         Cells(4 + i, 3) = Sum
Next i
  Sum = Sum + F(b)
  Integral = Sum * h / 3
 Cells(3, 1) = "Integral=": Cells(3, 2) = integral
End Sub
________________________________________________
Function F(x)
F = Exp(-x)
End Function
```

FIGURE A.9 Simpson's method for evaluating the integral.

For example, $\int_0^{\infty} e^{-x}\, dx = 1$. By applying Simpson's method,

$$\int_0^{5} e^{-x}\, dx = 0.99326 \text{ and } \int_0^{10} e^{-x}\, dx = 0.99996!$$

Another approach is to split the integration region into two segments,

$$I = \int_0^{\infty} f(x)dx = \int_0^{a} f(x)dx + \int_a^{\infty} f(x)dx, \tag{A.18}$$

and change the variable x with $1/y$ for the second integral.

$$\int_a^{\infty} f(x)dx = \int_{1/a}^{0} f(y^{-1})dy\frac{dx}{dy} = \int_0^{1/a} \frac{f(y^{-1})}{y^2}dy. \tag{A.19}$$

$$\text{Thus, } I = \int_0^{\infty} f(x)dx = \int_0^{a} f(x)dx + \int_0^{1/a} \frac{f(y^{-1})}{y^2}dx. \tag{A.20}$$

If the change of variable has not introduced an additional singularity into the integrand, this integral can often be evaluated by one of the standard numerical methods.

A.5 EULER'S ANGLES

Euler's angles are a set of three angles $\{\alpha, \beta, \gamma\}$ that rotate a coordinate frame (x, y, z) to another frame (X, Y, Z) [4]. Figure A.10 depicts the Euler angles where the rotational order of coordinates is

$$(x, y, z) \underset{\alpha}{\rightarrow} (x,', y', z') \underset{\beta}{\rightarrow} (x'', y'', z'') \underset{\gamma}{\rightarrow} (X, Y, Z).$$

Using matrix representation, rotational matrices are:

1) Rotation about the z-axis by angle α is given by $M_z(\alpha) = \begin{bmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}$ (A.21)

Coordinates: $xyz \rightarrow x'y'z'$ where $z'=z$.

2) Rotation about the y'-axis by angle ß is given by $M_{y'}(\beta) = \begin{bmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{bmatrix}$ (A.22)

Coordinates: $x'y'z' \rightarrow x''y''z''$ where $y''=y'$.

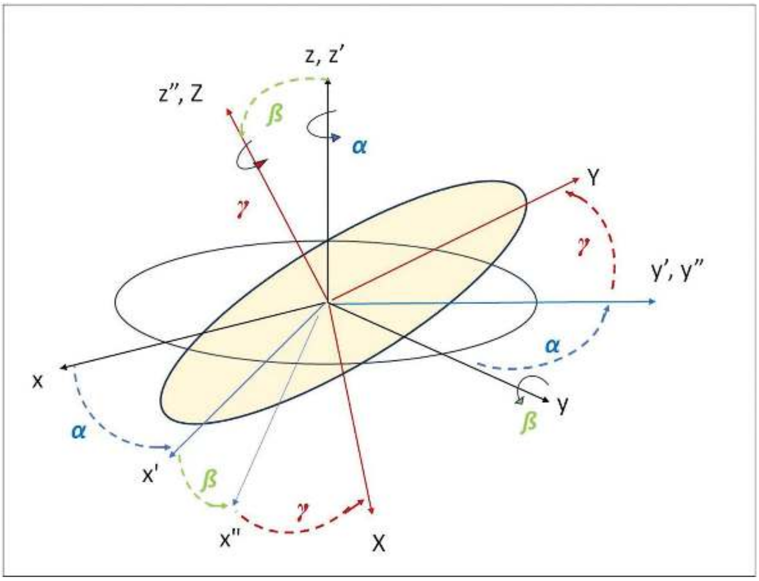


FIGURE A.10 Euler's angles.

3) Rotation about the z"-axis by angle γ is given by $M_{y'}(\gamma) = \begin{bmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix}$ (A.23).

Coordinates: $x"y"z" \rightarrow XYZ$ where Z = z".

Combining them, the rotation from xyz to XYZ is given by

$$M(\alpha,\beta,\gamma) = M_{z"}(\gamma)M_{y'}(\beta)M_z(\alpha) = \begin{bmatrix} \cos\beta\cos\alpha\cos\gamma \\ -\sin\alpha\sin\gamma & \cos\beta\sin\alpha\cos\gamma \\ +\cos\alpha\sin\gamma & -\sin\beta\cos\gamma \\ -\cos\beta\cos\alpha\sin\gamma \\ -\sin\alpha\sin\gamma & -\cos\beta\sin\alpha\cos\gamma \\ +\cos\alpha\sin\gamma & \sin\beta\sin\gamma \\ \sin\beta\sin\alpha & \sin\beta\cos & \cos\beta \end{bmatrix}. \tag{A.24}$$

Figure A.11 lists the VBA code for rotating unit vectors $e_1 = (1, 0, 0)$, $e_2 = (0, 1, 0)$, $e_3 = (0, 0, 1)$} of the xyz-frame to another set of {`R1,R2,R3`} of the XYZ-frame using specified angle values of {α, β, γ}. Unit vectors are defined by specifying the coordinates of their tips and tails. This code reads Euler's angles from the spreadsheet: α = 45°, ß = –30°, and γ = 0°.

```
Sub UnitVector3D()
Cells(1, 1) = "Rotation of unit vectors using  Euler angles"
  Pi = 3.14159265358979
  Alpha = 0: Beta = 0: Gamma = 0
'Euler angles
  Cells(3, 1) = "Alpha": Alpha = Cells(4, 1): Alpha = Alpha * Pi / 180: Cells(5, 1) = Alpha
  Cells(3, 2) = "Beta": Beta = Cells(4, 2): Beta = Beta * Pi / 180: Cells(5, 2) = Beta
  Cells(3, 3) = "Gamma": Gamma = Cells(4, 3): Gamma = Gamma * Pi / 180: Cells(5, 3) = Gamma
  Cells(4, 4) = "degrees": Cells(5, 4) = "radians"
'Unit vectors fixed with space
   Cells(6, 2) = "Tail": Cells(6, 3) = "Tip": Cells(6, 6) = "Tail": Cells(6, 7) = "Tip"
   'Unit vector along x-axis.
   Cells(6, 1) = "e1"
   Cells(7, 1) = "x1": Cells(7, 2) = 0: x1 = 1: Cells(7, 3) = x1
   Cells(8, 1) = "y1": Cells(8, 2) = 0 : y1 = 0: Cells(8, 3) = y1
   Cells(9, 1) = "z1": Cells(9, 2) = 0: z1 = 0: Cells(9, 3) = z1
    'Unit vector along y-axis.
   Cells(10, 1) = "e2"
   Cells(11, 1) = "x2": Cells(11, 2) = 0: x2 = 0: Cells(11, 3) = x2
   Cells(12, 1) = "y2": Cells(12, 2)  = 0: y2 = 1: Cells(12, 3) = y2
   Cells(13, 1) = "z2": Cells(13, 2) = 0: z2 = 0: Cells(13, 3) = z2
   'Unit vector along z-axis.
   Cells(14, 1) = "e3"
   Cells(15, 1) = "x3": Cells(15, 2) = 0: x3 = 0: Cells(15, 3) = x3
   Cells(16, 1) = "y3": Cells(16, 2) = 0: y3 = 0: Cells(16, 3) = y3
   Cells(17, 1) = "z3": Cells(17, 2) = 0: z3 = 1: Cells(17, 3) = z3
'Rotated unit vectors
    'Unit vector along X-axis.
   Rx1 = FX(x1, y1, z1, Alpha, Beta, Gamma)
   Ry1 = FY(x1, y1, z1, Alpha, Beta, Gamma)
   Rz1 = FZ(x1, y1, z1, Alpha, Beta, Gamma)
      Cells(7, 5) = "Rx1": Cells(7, 6) = 0: Cells(7, 7) = Rx1
      Cells(8, 5) = "Ry1": Cells(8, 6) = 0: Cells(8, 7) = Ry1
      Cells(9, 5) = "Rz1": Cells(9, 6) = 0: Cells(9, 7) = Rz1
   'Unit vector along Y-axis.
   Rx2 = FX(x2, y2, z2, Alpha, Beta, Gamma)
   Ry2 = FY(x2, y2, z2, Alpha, Beta, Gamma)
   Rz2 = FZ(x2, y2, z2, Alpha, Beta, Gamma)
      Cells(11, 5) = "Rx2": Cells(11, 6) = 0: Cells(11, 7) = Rx2
      Cells(12, 5) = "Ry2": Cells(12, 6)  = 0: Cells(12, 7) = Ry2
      Cells(13, 5) = "Rz2": Cells(13, 6) = 0: Cells(13, 7) = Rz2
   'Unit vector along x-axis.
   Rx3 = FX(x3, y3, z3, Alpha, Beta, Gamma)
   Ry3 = FY(x3, y3, z3, Alpha, Beta, Gamma)
   Rz3 = FX(x3, y3, z3, Alpha, Beta, Gamma)
      Cells(15, 5) = "Rx3": Cells(15, 6) = 0: Cells(15, 7) = Rx3
      Cells(16, 5) = "Ry3": Cells(16, 6) = 0: Cells(16, 7) = Ry3
      Cells(17, 5) = "Rz3": Cells(17, 6) = 0: Cells(17, 7) = Rz3
End Sub
____________________________________________________________________________________________

Function FX(x, y, z, Alpha, Beta, Gamma)
FX = x * (Cos(Beta) * Cos(Alpha) * Cos(Gamma)  - Sin(Alpha) * Sin(Gamma)) + y * (Cos(Beta) * Sin(Alpha) * Cos(Gamma) + Cos  (Alpha) *
Sin(Gamma)) - z * Sin(Beta) * Cos(Gamma)
End Function
____________________________________________________________________________________________

Function FY(x, y, z, Alpha, Beta, Gamma)
FY = -x * (Cos(Beta) * Cos(Alpha) * Sin(Gamma) +  Sin(Alpha) * Cos(Gamma))  - y * (Cos(Beta) * Sin(Alpha) * Sin(Gamma)  - Cos(Alpha) *
Cos(Gamma)) + z * Sin(Beta) * Sin(Gamma)
End Function
____________________________________________________________________________________________

Function FZ(x, y, z, Alpha, Beta, Gamma)
FZ = x * Sin(Beta) * Cos(Alpha) + y * Sin(Beta) * Sin(Alpha) + z * Cos(Beta)
End Function
```

FIGURE A.11 VBA code for rotating unit vectors using Euler's angles.

	A	B	C	D	E	F	G
1	Rotation of unit vectors using Euler angles						
2							
3	Alpha	Beta	Gamma				
4	45	-30	0	degrees			
5	0.785398	-0.5236	0	radians			
6	e1	Tail	Tip			Tail	Tip
7	x1	0	1		Rx1	0	0.612372
8	y1	0	0		Ry1	0	-0.70711
9	z1	0	0		Rz1	0	-0.35355
10	e2						
11	x2	0	0		Rx2	0	0.612372
12	y2	0	1		Ry2	0	0.707107
13	z2	0	0		Rz2	0	-0.35355
14	e3						
15	x3	0	0		Rx3	0	0.5
16	y3	0	0		Ry3	0	0
17	z3	0	1		Rz3	0	0.5
18							

FIGURE A.12 Screenshot of rotation of unit vectors.

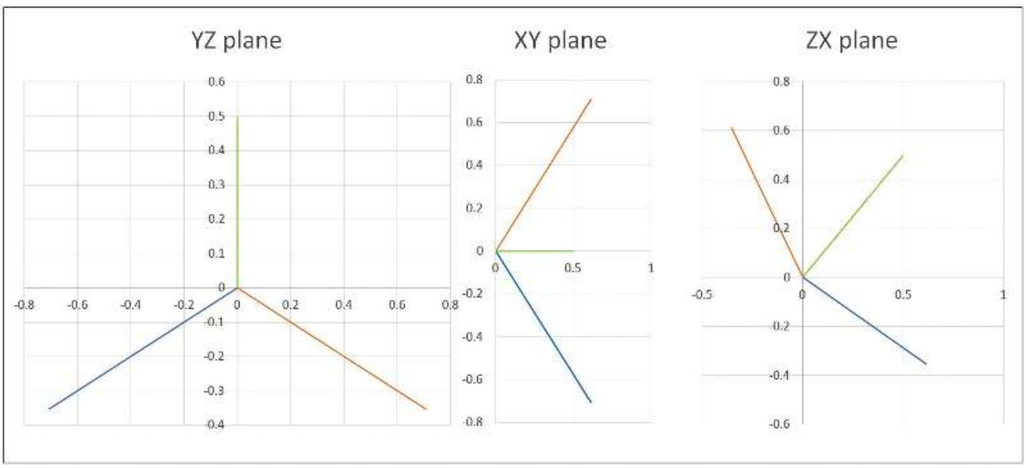


FIGURE A.13 Unit vectors as observed from the rotated coordinates XYZ.

Figure A.12 is a screenshot of unit vectors. Coloring was done manually for illustration purposes.

Figure A.13 shows rotated unit vectors projected on YZ, XY, and ZX planes.

A.6 SERIES EXPANSION USING ORTHONORMAL BASES

For complicated integrals, we applied Simpson's method.

A.6.1 Hermite Expansion

$$f(x) = \sum_{n=0} c_n h_n(x)$$

where $c_n = \int_{-\infty}^{\infty} f(x)h_n(x)dx = \frac{1}{\left[\sqrt{\pi}2^n n!\right]^{1/2}} \int_{-\infty}^{\infty} f(x)H_n(x)e^{-x^2/2}dx,$

and

$$h_n(x) = \frac{1}{\left[\sqrt{\pi}2^n n!\right]^{1/2}} H_n(x)e^{-x^2/2}.$$

Example 1: $f(x) = x$ where $-\infty < x < +\infty$.

Note: $\int_0^{\infty} x^{2n+1}e^{-ax^2}dx = \frac{n!}{2a^{n+1}}.$

$$c_0 = \int_{-\infty}^{\infty} f(x)h_0(x)dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} xe^{-x^2/2}dx = 0.$$

$$c_2 = c_4 = c_6 = 0.$$

$$c_1 = \frac{1}{\left[2\sqrt{\pi}\right]^{1/2}} \int_{-\infty}^{\infty} x(2x)e^{-x^2/2}dx = \frac{2}{\left[2\sqrt{\pi}\right]^{1/2}} \int_0^{\infty} x^2e^{-x^2/2}dx = 2.6264.$$

$$c_3 = \int_{-\infty}^{\infty} f(x)h_3(x)dx = \frac{1}{\left[\sqrt{\pi}\cdot 2^3\cdot 3!\right]^{1/2}} \int_{-\infty}^{\infty} x(8x^4 - 12x^2)e^{-x^2/2}dx = 3.26041.$$

$$c_5 = \int_{-\infty}^{\infty} f(x)h_5(x)dx = \frac{2}{\left[\sqrt{\pi}\cdot 2^5\cdot 5!\right]^{1/2}} \int_{-\infty}^{\infty} f(x)(32x^5 - 160x^3 + 120x)e^{-x^2/2}dx = 3.63863.$$

Thus,

$$f(x) \equiv x = 2.66264h_1(x) + 3.26041h_3(x) + 3.63863h_5(x) + \ldots$$

Figure 6.5 shows the graph of the final result.

Example 2: $f(x) = \sin x$ where $-\pi < x < +\pi$.

$$c_0 = c_2 = c_4 = c_6 = 0.$$

$$c_1 = 2\int_0^{\infty} f(x)h_1(x)dx = \frac{2}{\left[2\sqrt{\pi}\right]^{1/2}} \int_0^{\infty} (\sin x)(2x)e^{-x^2/2}dx$$

$$\approx \frac{2}{\left[2\sqrt{\pi}\right]^{1/2}} \int_0^{+10} (\sin x)(2x)e^{-x^2/2}dx = 1.615$$

$$c_3 = 2\int_0^{\infty} f(x)h_3(x)dx = \frac{2}{\left[\sqrt{\pi}\cdot 2^3\cdot 3!\right]^{1/2}}\int_0^{\infty}(\sin x)(8x^3 - 12x)e^{-x^2/2}dx$$

$$\approx \frac{2}{\left[2\sqrt{\pi}\right]^{1/2}}\int_0^{+10}(\sin x)(8x^3 - 12x)e^{-x^2/2}dx = 0.6594$$

$$c_5 = 2\int_0^{\infty} f(x)h_5(x)dx = \frac{2}{\left[\sqrt{\pi}\cdot 2^5\cdot 5!\right]^{1/2}}\int_0^{\infty}(\sin x)(32x^5 - 160x^3 + 120x)e^{-x^2/2}dx$$

$$\approx \frac{2}{\left[2\sqrt{\pi}\right]^{1/2}}\int_0^{+10}(\sin x)(32x^5 - 160x^3 + 120x)e^{-x^2/2}dx = -0.1463$$

Thus,

$$f(x) \equiv \sin x = 1.615h_1(x) + 0.594h_3(x) - 0.1463h_5(x) + \ldots$$

Figure 6.5 shows the graph of the final result.

A.6.2 Bessel Expansion

$$f(x) = \sum_{n=1}^{\infty} c_n J_n(k_n x)$$

where the k_n are chose so that $Jn(k_n a) = 0$, and the coefficients are given by

$$c_n = \frac{\int_0^a f(x)J_m(k_n x)x dx}{(a^2/2)\left[J_{m+1}(k_n a)\right]^2}.$$

Bessel's zeros [5]:

	J0	J1	J2	J3	J4	J5
1	2.4048	3.8317	5.1356	6.3802	7.5883	8.7715
2	5.5201	7.0156	8.4172	9.7610	11.0647	12.3386
3	8.6537	10.1735	11.6198	13.0152	14.3725	15.7002
4	11.7915	13.3237	14.7960	16.2235	17.6160	18.9801
5	14.9309	16.4706	17.9598	19.4094	20.8269	22.2178

	A	B	C	D	E	F	G	H	I	J
1	f(x)=x by Bessle functions									
2										
3	x	J1/J2	Exact							
4	0	0	0							
5	0.01	0.036555								
6	0.02	0.072472	0.0							
7	0.03	0.107132	0.03							
8	0.04	0.139946	0.04							
9	0.05	0.170374	0.05							
10	0.06	0.197937	0.06							
11	0.07	0.22223	0.07							
12	0.08	0.242933	0.08							
13	0.09	0.259816	0.09							
14	0.1	0.27275	0.1							
15	0.11	0.281705	0.11							

```
=2*(BESSELJ(3.8317*A4,1)/(3.8317
*BESSELJ(3.8317,2))+BESSELJ(7.01
56*A4,1)/(7.0156*BESSELJ(7.0156,
2))+BESSELJ(10.1735*A4,1)/(10.17
35*BESSELJ(10.1735,2))+BESSELJ(1
3.3237*A4,1)/13.3237*BESSELJ(13.
3237,2))+BESSELJ(16.471*A4,1)/(1
6.471*BESSELJ(16.471,2)))
```

in Cell `B4`.

FIGURE A.14 Calculation table of Bessel expansion of $f(x) = x$.

Example: $f(x) = x$ where $0 \leq x \leq 1$.

$$x = 2\sum_{k=1} \frac{J_1(a_{1k}x)}{a_{1k}J_2(a_{1k})} = 2\left[\frac{J_1(3.8317x)}{3.8317J_2(3.8317)} + \frac{J_1(7.0156x)}{7.0156J_2(7.0156)} + \right]$$

$$\frac{1}{2}x = \sum_{k=1} \frac{J_1(a_{1k}x)}{a_{1k}J_2(a_{1k})} = \frac{J_1(3.8317x)}{3.8317 \cdot J_2(3.8317)} + \frac{J_1(7.0156x)}{7.0156 \cdot J_2(7.0156)}$$
$$+ \frac{J_1(10.1735x)}{10.1735 \cdot J_2(10.1735)} + \frac{J_1(13.3237x)}{13.3237 \cdot J_2(13.3237)} + \cdots$$

Note: The built-in $J_n(x)$ in Excel is `BESSELJ(x,n)`. Figure A.14 is a screenshot of the calculation table of the $x = 2\sum_{k=1} \frac{J_1(a_{1k}x)}{a_{1k}J_2(a_{1k})}$ up to 4 terms where $0 \leq x \leq 1$. Excel's *AutoFill* feature is used for the calculation.

Figure 6.6 shows the series expansion of the four terms.

A.6.3 Legendre Expansion

$$f(x) = \sum_{\ell=1} c_\ell P_\ell(x) = c_1P_1(x) + c_3P_3(x) + c_5P_5(x)$$

where $c_\ell = \frac{2\ell+1}{2}\int_{-1}^{1} f(x)P_\ell(x)dx$.

Example: $f(x) = \sin x$ where $-1 \leq x \leq 1$.

Figure A.15 lists a VBA code to calculate the coefficients c_ℓ where $\ell = 1, 2, 3, 4, 5, 6$ using Simpson's method. Note that $c_2 = c_4 = c_6 = 0$. Once the coefficients are calculated, we evaluate

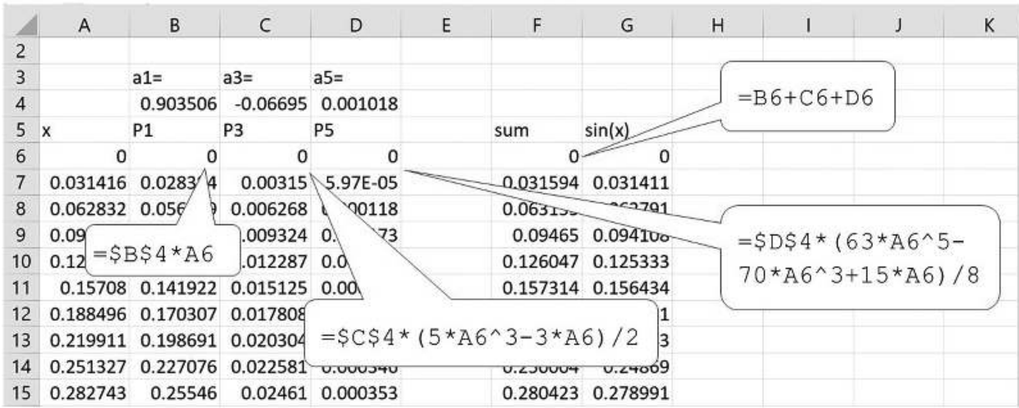
```
Sub SimpsonLegendre()
Cells(1, 1) = "Sin(x) by Legendre polynomials"
Pi = 3.14159254
a = 0  'a>=0
b = 1
N = 500
h = (b - a) / N
Weight = 2                  'Weight (2 or 4)  in the Simpson's formula
 sum1 = F1(a)                'Integral of xsin(x)exp( -x^2/2) where F1(0) = 0
'Integral of xsin(x)
For i = 1 To N - 1
  If Weight = 2 Then Weight = 4 Else Weight = 2
    x = i * h
       sum1 = sum1 + Weight * F1(x)
Next i
  sum1 = (sum1 + F1(b)) * h / 3    'Complete the integral
    a1 = 3 * sum1
    Cells(3, 2) = "a1=": Cells(4, 2) = a1
'Integral of (5*x^3-3*x)/2 where F3(0)=0.
 sum3 = F3(a)
For i = 1 To N - 1
  If Weight = 2 Then Weight = 4 Else Weight = 2
    x = i * h
       sum3 = sum3 + Weight * F3(x)
Next i
  sum3 = (sum3 + F3(b)) * h / 3     'Complete the integral
    a3 = 7 * sum3
    Cells(3, 3) = "a3=": Cells(4, 3) = a3
'Integral of (x^5)*sin(x)*exp(-x^2/2) where F5(0)=0.
 sum5 = F5(a)
For i = 1 To N - 1
  If Weight = 2 Then Weight = 4 Else Weight = 2
    x = i * h
       sum5 = sum5 + Weight * F5(x)
Next i
  sum5 = (sum5 + F5(b)) * h / 3      'Complete the integral
    a5 = 11 * sum5
    Cells(3, 4) = "a5=": Cells(4, 4) = a5
End Sub
_______________________________________________________________
Function F1(x)
F1 = Sin(x) * x
End Function
_______________________________________________________________

Function F3(x)
F3 = Sin(x) * (5 * x ^ 3 - 3 * x) / 2
End Function
_______________________________________________________________

Function F5(x)
F5 = Sin(x) * (63 * x ^ 5 - 70 * x ^ 3 + 15 * x) / 8
End Function
```

FIGURE A.15 VBA code for calculating the coefficient c.

$$f(x) = \sum_{\ell=1} c_\ell P_\ell(x) = c_1 P_1(x) + c_3 P_3(x) + c_5 P_5(x)$$

for $0 \leq x \leq \pi$ beyond $x = 1$ using *AutoFill* to see if the series fits well.

Figure A.16 shows the series expansion where we extend the result to $x = \pi$. The series expansion deviates from the exact value near $x = \pi$. Figure A.22 is a screenshot to obtain the final result as shown in Figure 6.13.



	A	B	C	D	E	F	G
3		a1=	a3=	a5=			
4		0.903506	-0.06695	0.001018			
5	x	P1	P3	P5		sum	sin(x)
6	0	0	0	0		0	0
7	0.031416	[illegible]	0.00315	5.97E-05		0.031594	0.031411
8	0.062832	[illegible]	0.006268	[illegible]		[illegible]	[illegible]
9	[illegible]	[illegible]	[illegible]	[illegible]		0.09465	[illegible]
10	[illegible]	[illegible]	[illegible]	[illegible]		0.126047	0.125333
11	0.15708	0.141922	0.015125	[illegible]		0.157314	0.156434
12	0.188496	0.170307	[illegible]	[illegible]		[illegible]	[illegible]
13	0.219911	0.198691	[illegible]	[illegible]		[illegible]	[illegible]
14	0.251327	0.227076	0.022581	[illegible]		[illegible]	[illegible]
15	0.282743	0.25546	0.02461	0.000353		0.280423	0.278991

FIGURE A.16 Screenshot of series expansion of sin$x$ with the Legendre polynomials.

A.7 KINEMATICS OF WAVE PACKET IN FREE SPACE

The detailed calculation of Equation 7.11 is shown below.

$$F(k)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\psi(x,0)e^{-ikx}dx \text{ where } \psi(x,0)=\frac{1}{\left(2\pi\sigma^2\right)^{1/4}}\exp\left[-\frac{x^2}{4\sigma^2}\right]\exp\left[ik_0x\right].$$

Using the integral formula shown in Appendix A9,

$$F(k)=\frac{1}{2\pi}\left(\frac{2\sigma^2}{\pi}\right)^{1/4}\int_{-\infty}^{+\infty}\mathrm{e}^{-\frac{x^2}{4\sigma^2}+ik_0x-ikx}dx=\frac{1}{2\pi}\left(\frac{2\sigma^2}{\pi}\right)^{1/4}\sqrt{\pi}\sqrt{4\sigma^2}\,e^{-\sigma^2(k-k_0)^2}=\sqrt{\frac{\sigma}{\pi}}e^{-\sigma^2(k-k_0)^2}.$$

Equation 7.1 becomes

$$\psi(x,t)=\int_{-\infty}^{+\infty}F(k)e^{i(kx-\omega t)}dk=\sqrt{\frac{\sigma}{\pi}}\int_{-\infty}^{+\infty}e^{-\sigma^2(k-k_0)^2}e^{i(kx-\omega t)}dk$$

$$=\sqrt{\frac{\sigma}{\pi}}\int_{-\infty}^{+\infty}\exp[-\sigma^2(k-k_0)^2+i(kx-\frac{\hbar k^2}{2m}t)]dk$$

where $\omega=\hbar k^2/2m$.

$$\psi(x,t)=\sqrt{\frac{\sigma}{\pi}}\int_{-\infty}^{+\infty}\exp[-(\sigma^2+i\frac{\hbar t}{2m})k^2+(ix+2\sigma^2k_0)k-\sigma^2k_0^2]dk$$

$$=\sqrt{\frac{\sigma}{\pi}}\exp(-\sigma^2k_0^2)\int_{-\infty}^{+\infty}\exp[-ak^2+bk]dk$$

where $a=\sigma^2+i\dfrac{\hbar t}{2m}$ and $b=ix+2\sigma^2k_0$.

Using the integral formula again,

$$\psi(x,t)=\sqrt{\frac{\sigma}{\pi}}\exp(-\sigma^2k_0^2)\sqrt{\frac{\pi}{a}}\exp\left(\frac{4b^2}{a}\right)$$

$$\psi(x,t)=\sqrt{\frac{\sigma}{\pi}}\exp(-\sigma^2k_0^2)\sqrt{\frac{\pi}{a}}\exp\left(\frac{4b^2}{a}\right)=\frac{\sqrt{\sigma}\exp(-\sigma^2k_0^2)}{\sqrt{\sigma^2+i\frac{\hbar t}{2m}}}\exp\left[-\frac{4(x-i2\sigma^2k_0)^2}{\left(\sigma^2+i\frac{\hbar t}{2m}\right)}\right]$$

$$=\frac{1}{\sqrt{1+i\alpha t}}\exp\left[-\left\{\frac{(x-i2\sigma^2k_0)^2}{4\sigma^2\left(1+i\alpha t\right)}+\sigma^2k_0^2\right\}\right]=\frac{1}{\sqrt{1+i\alpha t}}\exp\left[-\left\{\frac{4(x-i2\sigma^2k_0)^2}{\sigma^2\left(1-\alpha^2t^2\right)}(1-i\alpha t)+\sigma^2k_0^2\right\}\right]$$

A.8 INTEGRAL FORMULA $I=\int_{-\infty}^{\infty}\exp[-ax^2+bx]dx=\sqrt{\frac{\pi}{a}}\exp\left(\frac{b^2}{4a}\right)$

1) $I=\int_{-\infty}^{\infty}\exp\left(-ax^2\right)dx=\sqrt{\frac{\pi}{a}}$ where $\mathrm{Re}[a]\geq 0$.

If the coefficient is real, the integral can be proved by replacing $\sqrt{a}x$ with *y*. If *a* is a complex number, let $a = re^{i\theta}$ where Re[a]≥0 ($|\theta|\leq\pi/2$). Consider the following complex integral along the path as shown in Figure A.17.

From the Cauchy's integral theorem, $\int_C e^{-z^2}dz=0$.

Thus, $\int_0^R e^{-ax^2}a^{1/2}dx=\int_0^R e^{-x^2}dx+\int_0^{\theta/2}e^{-R^2e^{2i\varphi}}i\mathrm{R}e^{i\varphi}d\varphi$ where $\sqrt{a}=\sqrt{r}e^{i\theta/2}$.

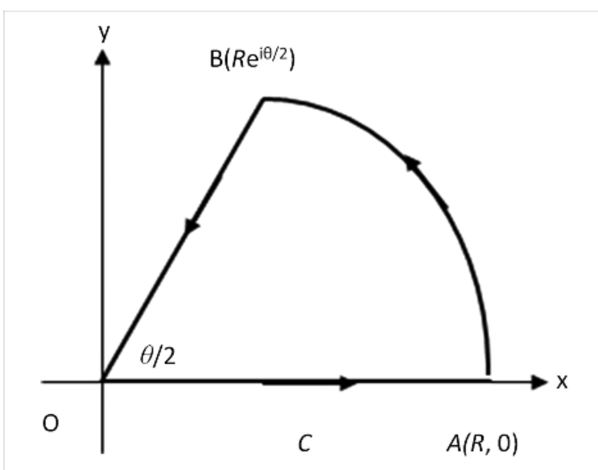


FIGURE A.17 Integral path *C* for the complex integral of $\exp(-ax^2/2)$.

Because $\left|\int_0^{\theta/2} e^{-R^2 e^{2i\varphi}} i\,\mathrm{R}e^{i\varphi} d\varphi\right| \le \int_0^{\theta/2} e^{-R^2 e^{2i\varphi}} i\,\mathrm{R}e^{i\varphi} d\varphi \to 0$ as $R \to \infty$, the integral along the arc vanishes and we obtain $\int_0^{\infty} e^{-ax^2} dx = \frac{1}{a^{1/2}} \int_0^{\infty} e^{-x^2} dx = \frac{1}{2a^{1/2}} \sqrt{\pi}$ where $\mathrm{Re}[a] \ge 0$.

If the coefficient a is a pure imaginary number, let $a = \pm i\alpha = e^{\pm i\pi/2}\alpha$ ($\alpha > 0$), then

$$\int_{-\infty}^{+\infty} e^{\pm i\alpha x^2} dx = e^{\pm i\pi/4} \sqrt{\frac{\pi}{\alpha}} \text{ where } \alpha > 0.$$

2) $I = \int_{-\infty}^{\infty} \exp\left(-ax^2 + bx\right) dx = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a}\right)$.

If both a and b are real numbers,

$$I = \int_{-\infty}^{\infty} \exp\left(-ax^2 + bx\right) dx = \int_{-\infty}^{\infty} \exp\left[-a\left(x - \frac{b}{2a}\right)^2 + \frac{b^2}{4a}\right] dx$$
$$= \exp\left(\frac{b^2}{4a}\right) \cdot \int_{-\infty}^{\infty} \exp\left[-a\left(x - \frac{b}{2a}\right)^2\right] dx = \sqrt{\frac{\pi}{a}} \cdot \exp\left(\frac{b^2}{4a}\right).$$

If a is a complex number, let $a = re^{i\theta}$, where Re[a]≥0 ($|\theta| \le \pi/2$) and b an arbitrary complex number. Consider the following complex integral along the path as shown in Figure A.18.

From Cauchy's integral theorem, $\int_{C'} e^{-az^2} dz = 0$. Thus,

$$\int_{-R}^{R} e^{-a(x+b)^2} a^{1/2} dx = \int_{-R}^{R} e^{-ax^2} dx + \int_0^{\mathrm{Im}[b]} e^{-a(R+it)^2} i dt + \int_{\mathrm{Im}[b]}^{0} e^{-a(-R+it)^2} i dt.$$

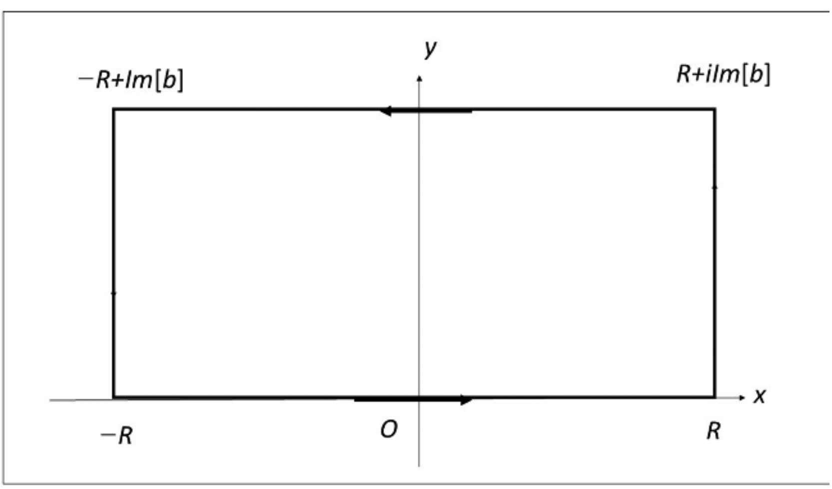


FIGURE A.18 Integral path C' for the complex integral of $\exp[-a(x+b)x^2]$.

The last two terms on the right side become zero when R → ∞, and we obtain

$$\int_{-R}^{R} e^{-a(x+b)^2} a^{1/2} dx = \int_{-R}^{R} e^{-ax^2} dx = \frac{\sqrt{\pi}}{a^{1/2}} \text{ where } \mathrm{Re}\left[\mathrm{a}\right] > 0.$$

Therefore,

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = e^{\frac{b^2}{4a}} \cdot \int_{-\infty}^{\infty} e^{-a\left(x-\frac{b}{2a}\right)^2} dx = e^{\frac{b^2}{4a}} \cdot \frac{\sqrt{\pi}}{a^{1/2}}.$$

A.9 EXPANSION COEFFICIENTS OF WAVE FUNCTION OF A HARMONIC OSCILLATOR

Let the Hamiltonian $\breve{H}$, its eigen vector $|\varphi_n\rangle$, and eigenvalue E_n: $\breve{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$, $n = 0, 1, 2, \ldots$

The time-dependent wave function of the system is given by

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n \varphi_n(x) \exp\left(-\frac{i}{\hbar} E_n t\right).$$

Using the above wave function at $t = 0$, the coefficient c_n can be calculated.

$$\langle \varphi_n(x) | \psi(0) \rangle = \sum_{m=0} c_m \langle \varphi_n(x) | \varphi_m(x) \rangle = \sum_{m=0} c_m \delta_{m,n} = c_n$$

For the harmonic oscillator, the inner product is

$$c_n = \langle \varphi_n(x) | \psi(0) \rangle = \int_{-\infty}^{+\infty} \varphi_n^*(x) \psi(x,0) dx.$$

The initial wave function is given by Equation 7.18,

$$\psi(x,0) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \exp\left[-\frac{\alpha^2}{2}(x-x_0)^2\right] \text{ where } \alpha = \left(\frac{m\omega_0}{\hbar}\right)^{1/2},$$

the normalized eigenvector is given by

$$\varphi_n(x) = N_n H_n(\alpha x) \exp(-\alpha^2 x^2) \text{ where } N_n = \left(\frac{\alpha}{\pi^{1/2} 2^n n!}\right),$$

and H_n is the Hermite polynomial discussed in section 6.3.

$$c_n = \frac{N_n^*}{\pi^{1/4}\alpha^{1/2}} \int_{-\infty}^{+\infty} H_n(\xi) \exp\left(-\frac{1}{2}\xi^2\right) \exp\left(-\frac{1}{2}(\xi-\xi_0)^2\right) d\xi$$

$$= \frac{N_n^*}{\pi^{1/4}\alpha^{1/2}} \int_{-\infty}^{+\infty} H_n(\xi) \exp\left[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^2)\right] d\xi$$

where $\xi = \alpha x$ and $\xi_0 = \alpha x_0$.

Using the generating function of Hermite polynomial Equation 6.34, consider the following two integrals:

$$\int_{-\infty}^{+\infty} \exp\left(-s^2+2s\xi\right)\exp\left[-(\xi^2-\xi_0\xi+\frac{1}{2}\xi_0^2)\right]d\xi=\sum_{k=0}^{\infty}\frac{s^k}{k!}\int_{-\infty}^{\infty}H_k(\xi)\exp\left[-(\xi^2-\xi_0\xi+\frac{1}{2}\xi_0^2)\right]d\xi,$$

and

$$\pi^{1/2}\exp\left(-\frac{1}{4}\xi_0^2+s\xi_0\right)=\pi^{1/2}\exp\left(-\frac{1}{4}\xi_0^2\right)\sum_{k=0}^{\infty}\frac{(s\xi_0)^k}{k!}.$$

we obtain

$$c_n=\frac{\xi_0^n}{(2^n n!)^{1/2}}\exp\left[-\frac{\xi_0^2}{4}\right]=\frac{(\alpha x_0)^n}{\sqrt{2^n n!}}\exp\left[-\frac{(\alpha x_0)^2}{4}\right].$$

Refer to [Shiff] for this calculation.

REFERENCES

1. AutoFill in Excel. https://www.excel-easy.com/examples/autofill.html.
2. Bloch SC, *Excel for Engineers and Scientists*, Wiley, 2003.
3. Liengme BV, *Excel*® VBA for Physicist A Primer IOP Concise Physics: Morgan & Claypool, 2016.
4. Euler Angles – from Wolfram MathWorld. https://mathworld.wolfram.com/EulerAngles.html.
5. Bessel Function Zeros – from Wolfram MathWorld. https://mathworld.wolfram.com/BesselFunctionZeros.html.
6. Schiff LI, 1968 *Quantum Mechanics*, McGraw Hill Book Company, 1968. https://archive.org/details/ost-physics-schiff-quantummechanics.

Index

S

T

V

W