Introduction

This book is based on notes prepared for a graduate course "Scientific Foundations of Engineering" in the Gordon Engineering Leadership Program at Northeastern University. The elevator speech on why such a course is needed goes as follows: (1) most engineering students take all of their basic science courses during freshman year, (2) they don't like those freshman courses very much, and (3) they forget the material as quickly as they can and concentrate on the specifics of electrical engineering, or mechanical engineering, or other engineering discipline where their interests and enthusiasm lies.

This summary may be unfair to some engineering students, but most engineering students (and their professors) at least grudgingly admit that it isn't terribly far off. And, in general, this approach serves the students well through their undergraduate education process and in their industrial careers – as long as they remain specialized in their specific engineering discipline. However, consider the case where an electrical engineer is leading a multidisciplinary project. One day a mechanical engineer who reports to her walks into her office and says, "Boss, this isn't going to work – we can't get the heat out!" A conventionally trained electrical engineer isn't likely to be able to frame a single substantive question about the problem. She hasn't studied heat transport or thermodynamics since the freshman year (if at all!), and likely has forgotten anything she ever knew about the subject. The ability to frame questions which put fundamental boundaries on the problem, "What is the power load? How hot will the device get? How much blackbody emission is there at that temperature? What is the thermal conductivity of the substrate?", will not only enable an engineering leader to quickly frame the gravity of the problem, but will undoubtedly earn her a reputation as someone with whom you want to have done your homework carefully before making rash statements about engineering limits!

Science curricula often employ a "spiral curriculum" model. In physics for example, mechanics, thermal physics, and electromagnetics are surveyed in freshman year, revisited in specialized courses in sophomore or junior year, and often studied again from a quantum statistical viewpoint in a senior class. Engineering education more often selects a "breadth" coverage of the vast range of engineering applications, rather than the depth of understanding that the spiral curriculum seeks to impart.

Among the topics that the typical quick pass through scientific fundamentals causes to be neglected or skipped in most engineering educations is the entire field of quantum science. Despite the critical and growing importance of nanoscale quantum science on

nearly every electronic device we use or carry on us, I suspect that most engineering professors would be surprised by how few engineering students or professional engineers can give even a rudimentary description of the source of semiconductor band gaps, the distinction between metals and insulators and semiconductors, or how a p-n junction or micro-mechanical device works.

This lack of depth of understanding of fundamental scientific principles and lack of any formal instruction in the science of quantum systems is what we intended the "Scientific Foundations of Engineering" course in the Gordon Engineering Leadership Program to address. Our model was the confidence with which a well-trained scientist can approach an unfamiliar problem and quickly understand the fundamental principles and make "back-of-the-envelope" calculations about how large an effect each of these fundamentals may play in the problem. Even a little bit of this ability to understand the basic physical laws underlying a phenomenon, to place a problem in context, and to estimate the size of various influences on a system can give an engineering leader an ability to direct a project through proof-of-principle experiments and make-or-break decision points to an operating marketable product. Our goal in the Gordon program is to develop engineers with gravitas to whom no area of engineering is outside of the sphere of understanding in the "here be dragons" area of the unknown, and developing knowledge of scientific fundamentals in the "Scientific Foundations" course is part of that goal.

In looking for a book to teach the "Scientific Foundations" course, however, the authors found freshman survey texts that did not make use of advanced mathematics and were intended for readers who were new to the study of science and engineering, and highly theoretical books for professional physicists, which lacked examples meaningful to engineers, but no book suitable for the intended audience. In this book, we have combined a unified treatment of classical and quantum physics with a wealth of worked examples with an engineering flavor. We typically begin each chapter with a question about physical phenomena that engineers may know and have wondered about. This helps put the treatment of the physics in a context of what the implications of the theory are and why anyone would want to know about it.

In Chapters 1 and 2, we address kinematics and dynamics in the broadest framework to understand the limits of reaching for the "d-equals-one-half-a-t-squared" solution, and how this low-order solution can be used iteratively to find solutions even outside the limits of constant acceleration problems. In these chapters and throughout the book we consider examples primarily in Cartesian x–y–z space. While many real problems are best addressed in cylindrical or spherical coordinates, the concepts are fundamentally the same and we have opted for conceptual clarity over computational completeness whenever possible.

In Chapter 3, we discuss rotational motion and use the generalization of the scalar mass in linear motion into moment of inertia in rotational motion as a way to introduce the concept of tensor quantities. The linear motion concepts of force, momentum, and energy are similarly generalized into torque, angular momentum, and rotational kinetic energy with the fundamental principles of conservation of momentum (always!) and conservation of mechanical energy (in ideal systems that do not generate heat) reinforced.

Chapter 4 introduces rotation matrices to deal with cases where tensor quantities are not aligned with the principal axes. As an example, the generalization of an isotropic mass into an effective mass tensor for electrons in anisotropic materials is considered.

With the fundamental mechanical laws established, the role of materials is introduced in the fundamental property of elasticity in Chapter 5. Shear and compressive stress and strain are shown to be elements of the 3×3 second-order stress and strain tensors, making elasticity that links stress and strain a fourth-order elastic tensor which can be reduced by symmetries to a 6×6 symmetric tensor with 21 independent material parameters. This is further reduced in cubic materials to an elastic tensor with three parameters: the Young's modulus, the shear modulus, and the Poisson ratio.

In Chapter 6, simple harmonic motion of a system with a linear restoring force and a velocity-dependent loss mechanism is discussed with and without a harmonic driving force. The use of Euler's relation to describe oscillatory motion with amplitude and phase by a complex exponential is introduced, allowing the inclusion of a small imaginary part to model the loss mechanism. The identical form and solution of an LCR electrical circuit with the spring–mass system is shown with complex exponentials representing the charge and current, leading to the electrical engineering method of complex impedance.

In Chapter 7, harmonic motion in time is extended to systems with spatial coupling, creating the phenomenon of waves in mechanical systems: one-dimensional waves in strings and three-dimensional sound waves in fluids. By continuing the complex exponential notation for the wave oscillation we can model lossy media, interference in films or from multiple sources, and diffraction phenomena with a complex exponential wave form with a complex wave vector k.

Chapters 8, 9, 10, and 11 provide an introduction to quantum physics and chemistry. In Chapter 8, we discuss the historical origins of quantum theory, why it was such a radical departure from classical physics, why it became necessary to accept such a totally different approach to understand the world, and why the "quantum picture" continues to be anti-intuitive and difficult to accept. In Chapter 9, we examine the postulates of quantum mechanics and how we can "shut up and calculate" everything that is determinable for quantum systems, including tunneling, and low-dimensional quantum systems, such as 1D and 2D quantum wells. In Chapter 10, we extend the quantum analysis to real systems from quantum dots to the hydrogen atom and touch on the chemistry of the "spdf" quantum states and hybridized outer orbitals. In Chapter 11, we look at electrons in extended lattices and band states with both direct and indirect band gaps, and how these are reflected in the electronic properties of metals, insulators, and semiconductors and optical interactions, such as in light-emitting diodes.

In Chapter 12, we look at thermal physics from the perspective of random equipartition of particles into energy states, extending into thermal transport, thermal equilibrium, heat capacity, and thermodynamics. In Chapter 13, we look at thermal effects through the mathematics of quantum statistics: Maxwell–Boltzmann statistics for classical distinguishable particles, Fermi–Dirac statistics for quantum indistinguishable particles that obey the exclusion principle ("fermions") and Bose–Einstein statistics

for quantum particles such as photons that do not have any restrictions on the occupancy of a single quantum state ("bosons"). The differences in the occupation of states for the three different statistical models is demonstrated though a simple "thought experiment" and the different statistical models are developed in the examples of blackbody radiation (photon/boson statistics) and semiconductor occupancy and p-n junctions (electron/fermion statistics).

In Chapters 14, 15, and 16, we look at electromagnetic theory, effects, and materials. Chapter 14 develops Maxwell's equations in the mathematics of vector calculus ("div, grad, curl"), using Gauss's and Stokes' integral relations to move from the four Maxwell's equations and the electromagnetic Lorentz force equation to understand a wide variety of electromagnetic effects: Faraday effect, electrical generation, eddy currents, transformers, and electromagnetic motors. Starting from the four Maxwell's equations, Chapter 15 develops the electromagnetic wave equation and applies it to examine wave propagation in uniform, lossy, and anisotropic materials. The electromagnetic boundary conditions are derived and applied to plane-wave reflection at surfaces for both normal and non-normal incidence, and to interference effects in thin films. In Chapter 16, electromagnetic wave propagation in materials is studied from the viewpoint of the constitutive relations and the material-dependent tensor permittivity, conductivity, and permeability. Physical models are used to develop examples including the plasma edge in gases, semiconductors, and metals, Lorentzian oscillators in the infrared properties in polar crystals, quantum absorption in transparent gases, and ferromagnetic resonance in magnetic materials.

Chapter 17 provides an introduction to the physics of fluids, using mechanical concepts for static fluid effects, such as buoyancy, and vector calculus from electromagnetics to develop the continuity equation, Euler equation, Bernoulli equation, and Navier–Stokes equation for moving fluids. The transition from laminar to turbulent flow with increasing Reynolds number, still one of the most important unsolved scientific problems, is presented.

Throughout, we have emphasized the connections between concepts and phenomena in different fields and the similarity of the mathematics used to describe them: how a spring–mass harmonic oscillator described by a complex exponential leads to familiar expressions in AC electrical circuits, in infrared properties in crystals with optical phonons, and in quantum-energy-level absorption lines in gases and transparent solids. Or how anisotropic materials effects in elasticity, electrical permittivity, or magnetic resonance can be described by tensor properties similar to a general description of rotational motion with a tensor moment of inertia. The ability of a scientist or engineer to apply models and concepts from their area of specialization to new phenomena in different limits can serve to demystify unfamiliar technologies and allow them to apply their knowledge to novel systems.

The authors would like to express their gratitude to Professors George Adams and John Cipolla for their assistance in Chapters 5 and 17, and to the classes of students from the Gordon Engineering Leadership Program who, with their questions and comments, have helped move this project from a set of cryptic notes to a text which we trust will be comprehensible and useful to engineering and science students and professionals.

1 Kinematics and vectors

The foundation of much of engineering concerns the location of stationary and moving objects in three dimensions, and it is critical to have the mathematical tools to quantify the position of those objects and predict their movement. In fact, although we are surrounded by moving objects every day, relatively few people have a conceptual framework and vocabulary to describe motion. In addition, simple three-dimensional problems such as finding the volume of a parallelepiped defined by its three edges are hard to visualize and calculate. In this chapter we will develop the mathematical framework for motion, for describing the three-dimensional position of objects, and for calculating their non-uniform motion.

1.1 Kinematics

Kinematics is the mathematical description of motion, of how position changes with time. In one dimension, motion is completely described by the function f where

$$x = f(t). \tag{1.1}$$

In general, $f(t)$ is a complicated function. Even what we might consider to be simple motion, someone running at a more or less constant speed for example, is likely to be quite complicated if we look in detail. And the motion of the hand of that runner, as she moves it back in forth in stride, is likely to be extremely complex and unlikely to be described by any closed-form mathematical expression. How can one describe motion, especially if it is complex? One could ask, for example, if there is any mathematical way to describe the one-dimensional motion of the graph shown in Figure 1.1.

Commonly in science and engineering, we can only make progress if we apply some level of approximation to the problem. Appropriately approximated, the problem may be conceptually straightforward and mathematically tractable. One mathematical technique that is convenient for approximation is expansion of the function describing the motion in a *Taylor series*. The Taylor series expansion of a function $x(t)$ around a particular time t_o is:

$$\boldsymbol{x} = \boldsymbol{x_o} + \left.\frac{\boldsymbol{dx}}{\boldsymbol{dt}}\right|_{t=t_o}(\boldsymbol{t}-\boldsymbol{t_o}) + \frac{1}{2!}\left.\frac{\boldsymbol{d^2x}}{\boldsymbol{dt^2}}\right|_{t=t_o}(\boldsymbol{t}-\boldsymbol{t_o})^2 + \frac{1}{3!}\left.\frac{\boldsymbol{d^3x}}{\boldsymbol{dt^3}}\right|_{t=t_o}(\boldsymbol{t}-\boldsymbol{t_o})^3 + \ldots \tag{1.2}$$

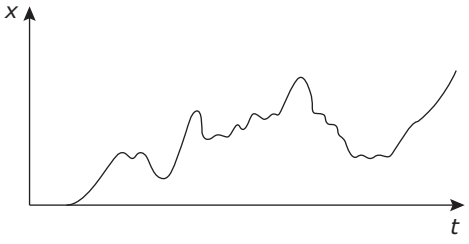


Figure 1.1 Position vs. time for complex one-dimensional motion.

Question 1.1

What would the general expression for the *n*th term of the series be?

A Taylor series allows us to predict the position at time Δt later if we know the initial position and all orders of rates of change of the function at the initial position. Mathematically this series is expected to converge because of the $1/n!$ prefactor – the factorial function $n!$ exceeds even the exponential function e^n for large n. Practically, given an appropriate time scale where the motion is reasonably smooth, the higher-order derivatives tend to be progressively smaller, and we can approximate the motion with a few terms. Letting $t_o \to 0$, which is equivalent to starting our clock at $t = t_o$ or setting $t = \Delta t = (t - t_o)$, we find an series expansion for $x(t)$ as below, where we have indicated the usual names given to the time derivatives of distance: *velocity* = $v = dx/dt$, *acceleration* = $a = dv/dt = d^2x/dt^2$, and *jerk* = $da/dt = d^3x/dt^3$.

$$x = x_o + \underbrace{\left.\frac{dx}{dt}\right|_{t=t_o}}_{v\ \text{(velocity)}} t + \frac{1}{2!}\underbrace{\left.\frac{d^2x}{dt^2}\right|_{t=t_o}}_{a\ \text{(acceleration)}} t^2 + \frac{1}{3!}\underbrace{\left.\frac{d^3x}{dt^3}\right|_{t=t_o}}_{da/dt\ \text{(jerk)}} t^3 + \frac{1}{4!}\left.\frac{d^4x}{dt^4}\right|_{t=t_o} t^4 + \ldots \tag{1.3}$$

Note that there is no reason to truncate this series at any term except the expectation that the higher-order derivatives will be negligible compared to $1/n!$ since higher-order derivatives correspond to rapidly changing forces. Nevertheless, freshman physics books are so filled with examples of constant acceleration that it is not surprising that engineers often assume that distance is always found from

$$x = x_o + v_o t + \frac{1}{2}at^2. \tag{1.4}$$

In fact, for constant acceleration, when a = constant and we have

$$0 = \frac{da}{dt} = \frac{d^2x}{dt^2} = \frac{d^3x}{dt^3} = \frac{d^4x}{dt^4} \quad (\ldots \text{and all higher orders}),$$

we can recover our familiar freshman physics equations by integration:

$$a = \frac{dv}{dt} = \frac{d^2x}{dt^2} = \text{constant} \Rightarrow$$

(1) $v = \int a dt = at + v_o$

Constant of integration = initial velocity

(2) $x = \int v dt = \int (at + v_o) dt = \frac{1}{2} a t^2 + v_o t + x_o$ (1.5)

(3) Eliminating t by algebra from (1) and (2) $\left(t = \frac{v - v_o}{a}\right)$

$$\text{gives} \quad v^2 = v_o^2 + 2a(x - x_o)$$

$$\text{or} \quad v = \sqrt{v_o^2 + 2a(x - x_o)}.$$

In the more difficult (and more common) case where the acceleration is not constant, but depends on *t* or *v* or *x*, the equations for constant acceleration are not accurate. In this case, we can solve the problem numerically by taking steps in time or distance that are small enough that the acceleration can be considered as constant within the time interval Δt considered. (For Δt small, $\Delta t \gg \Delta t^2 \gg \Delta t^3$ and terms beyond constant acceleration are negligible.) The new position, velocity, and acceleration are calculated at the end of the small interval Δt, and then the next Δt interval is solved with these new initial values.

Such an iterative solution for a problem with non-constant acceleration can be diagramed as in Figure 1.2.

Question 1.2

Consider the case of a car slowing down and coming to a stop at a traffic light. Can this be represented with a constant acceleration? Why or why not?

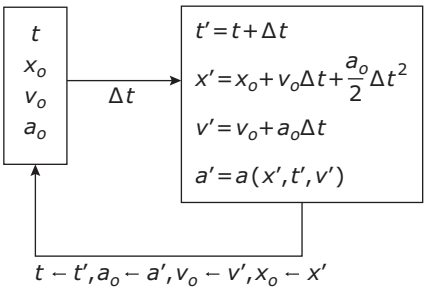


Figure 1.2 Block diagram of iterative solution for non-constant acceleration.

Iterative solutions are the basis of numerical differential equations solvers such as the second-and-third-order and third-and-fourth-order Runge–Kutta methods that are the basis of the MATLAB differential equation solvers `ode23` and `ode45`.

Example 1.1 If the effects of air resistance are ignored, a falling object near the Earth's surface experiences a constant acceleration due to the force of gravity g = 9.8 m/s^2 downward (toward the center of the Earth). This is a good approximation at low velocities for dense heavy objects – a bowling ball, for example – but is completely inadequate to describe a falling piece of paper. The effect of air resistance is to create a *non-uniform* acceleration that decreases as the square of the velocity

$$a = -9.8 - \gamma|v|v$$

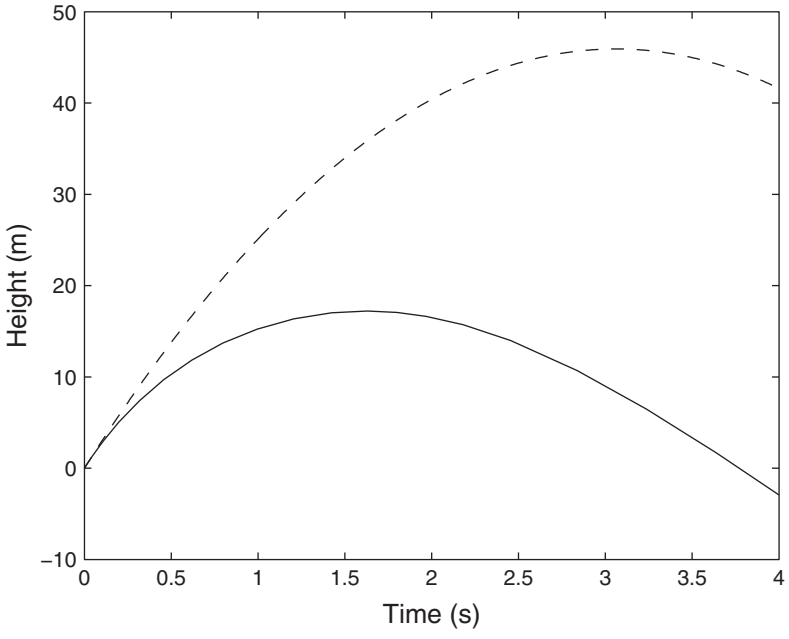
where the constant γ depends on the mass and shape of the object and the air density. The air resistance component of the acceleration in the second term is the product of number of air molecules that the object collides with in a given time interval (proportional to the velocity) multiplied by the retarding force due to a collision with an air molecule which also increases with the velocity as we will see in Chapter 2, giving the velocity-squared dependence. The minus sign in the equation indicates that the gravitational acceleration is downward, and the absolute value of the velocity multiplied by the velocity guarantees that the air friction opposes the motion: the acceleration is more negative when the velocity is up (positive) and less negative when the velocity is down (negative). The MATLAB solution for an object with γ = 0.05 projected directly upward with an initial velocity of 30 m/s from t = 0 to t = 4 s is shown in the figure below (solid line) compared to the no-friction result from Eq. (1.4) (dashed):

```
>> type air_friction.m
function [ Ydot ] = air_friction(t, Y )
%AIR_FRICTION Function to find acceleration and velocity
  with air friction
% Input vector Y=[y, v_y] ; output vector Ydot= dY/dt=[v_y, a_y}
v_y=Y(2);
a_y=-9.8-0.05*abs(v_y)*v_y;
Ydot=[v_y, a_y]';
end

>>[ t,y]=ode23(@air_friction,[0,4],[0,30]);
>> plot(t, y(:,1))
>> hold on
>> tnf=[0:.01:4];
>> ynf=30*tnf - 0.5*9.8*tnf.^2;
>> plot(tnf, ynf, '--')
>> ylabel('Height (m)'); xlabel('Time (s)')
```

Continued

Example 1.1 (*cont.*)



1.2 Vectors

A vector is an ordered group of n numbers that follow particular rules under the operations of addition, subtraction, and multiplication. The individual components of the vector are added or subtracted independently and not mixed when the vectors are added or subtracted, and multiplication by a scalar number multiplies each component equally. A vector equation represents n independent scalar equations.

The mathematical properties of vectors make them appropriate to describe displacements in two- ($n = 2$) or three- ($n = 3$) dimensional space, if the components of the vector represent distances in orthogonal directions. Addition of two vectors represents the effect of two successive displacements of an object, and subtraction of two vectors represents the change in position of an object. It is often useful to define a unit vector in the direction of a given vector $\vec{V}$. A vector of length 1 in the direction of $\vec{V}$ is given by $\hat{V} = \vec{V}/|\vec{V}|$, where $|\vec{V}|$ indicates the magnitude (length) of the vector. By simple geometry we find the length of a vector $\vec{V} = [x, y, z]$ is given by $|\vec{V}| = \sqrt{x^2 + y^2 + z^2}$.

Question 1.3

Why does the $\hat{V}$ vector have length=1? What is the unit vector in the direction [2, 1]?}

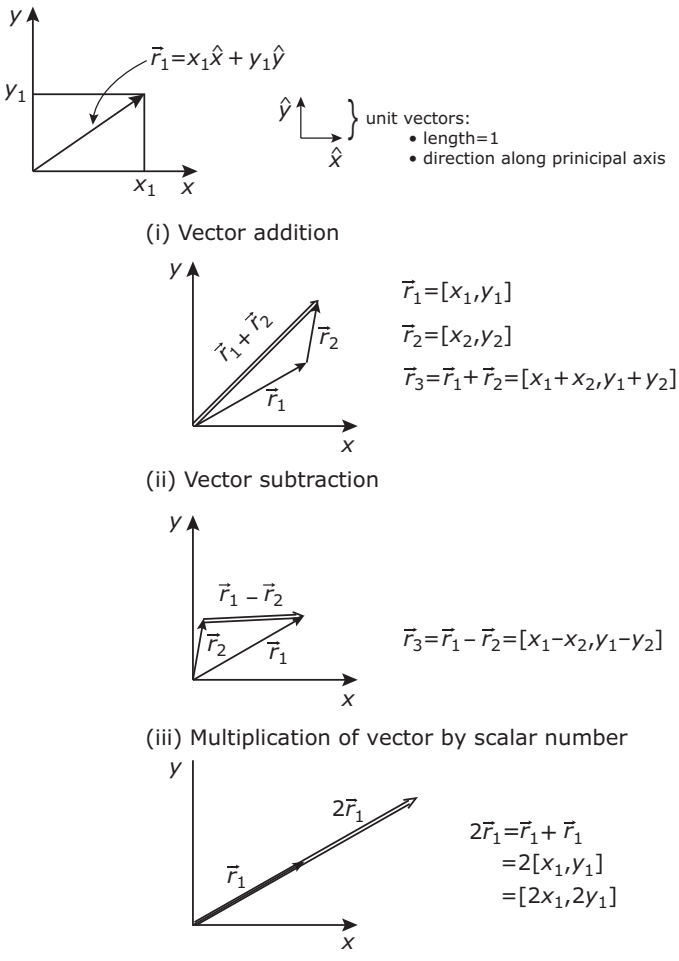


Figure 1.3 Expression of a vector in terms of *unit vectors* and rules for vector addition, subtraction, and multiplication by a scalar, illustrated for two dimensions. (Generalization to three dimensions is straightforward: $\vec{r}_3 = \vec{r}_1 + \vec{r}_2 = [x_1 + x_2, y_1 + y_2, z_1 + z_2]$, etc.)

The rules for vector addition, subtraction, and multiplication by a scalar number are summarized in Figure 1.3 for vectors $\vec{r}_1 = x_1\,\hat{x} + y_1\,\hat{y}$ and $\vec{r}_2 = x_2\,\hat{x} + y_2\,\hat{y}$ indicating positions in two dimensions.

1.3 Vector kinematics

Since position in two or three dimensions can be represented by vectors, motion which is the displacement of position in a time interval Δt can also be represented by vectors: