1 Introduction

1.1 Motivation

You may ask why one needs to know about quantum mechanics. Possibly the simplest answer is that we live in a quantum world! Engineers would like to make and control electronic, opto-electronic, and optical devices on an atomic scale. In biology there are molecules and cells we wish to understand and modify on an atomic scale. The same is true in chemistry, where an important goal is the synthesis of both organic and inorganic compounds with precise atomic composition and structure. Quantum mechanics gives the engineer, the biologist, and the chemist the tools with which to study and control objects on an atomic scale.

As an example, consider the deoxyribonucleic acid (DNA) molecule shown in Fig. 1.1. The number of atoms in DNA can be so great that it is impossible to track the position and activity of every atom. However, suppose we wish to know the effect a particular site (or neighborhood of an atom) in a single molecule has on a chemical reaction. Making use of quantum mechanics, engineers, biologists, and chemists can work together to solve this problem. In one approach, laser-induced fluorescence of a fluorophore attached to a specific site of a large molecule can be used to study the dynamics of that individual molecule. The light emitted from the fluorophore acts as a small beacon that provides information about the state of the molecule. This technique, which relies on quantum mechanical

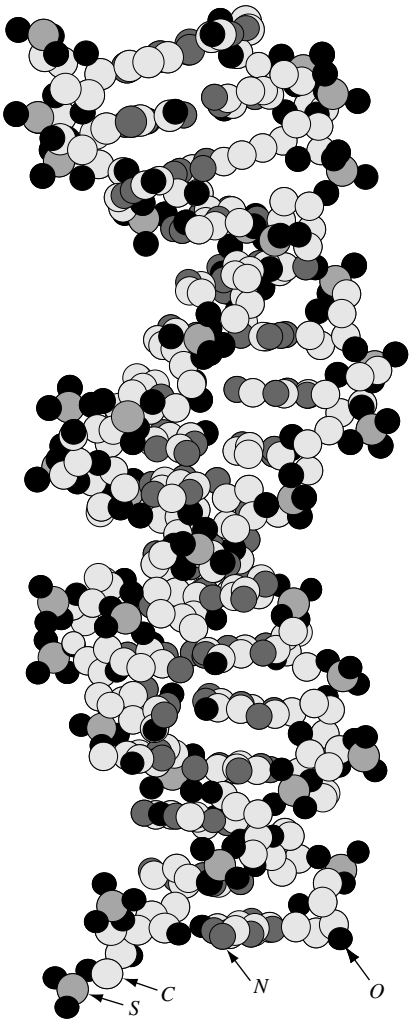

Fig. 1.1 Ball and stick model of a DNA molecule. Atom types are indicated.

photon stimulation and photon emission from atomic states, has been used to track the behavior of single DNA molecules.[1]

Interdisciplinary research that uses quantum mechanics to study and control the behavior of atoms is, in itself, a very interesting subject. However, even within a given discipline such as electrical engineering, there are important reasons to study quantum mechanics. In the case of electrical engineering, one simple motivation is the fact that transistor dimensions will soon approach a size where single-electron and quantum effects determine device performance. Over the last few decades advances in the complexity and performance of complementary metal-oxide-semiconductor (CMOS) circuits have been carefully managed by the microelectronics industry to follow what has become known as "Moore's Law."[2] This rule-of-thumb states that the number of transistors in silicon integrated circuits increases by a factor of two every eighteen months. Associated with this law is an increase in the performance of computers. The Semiconductor Industry Association (SIA) has institutionalized Moore's Law via the "SIA Roadmap," which tracks and identifies advances needed in most of the electronics industry's technologies.[3] Remarkably, reductions in the size of transistors and related technology have allowed Moore's Law to be sustained for over 35 years (see Fig. 1.2). Nevertheless, the impossibility of continued reduction in transistor device dimensions is well illustrated by the fact that Moore's law predicts that dynamic random access memory (DRAM) cell size will be *less* than that of an atom by the year 2030. Well before this end-point is reached, quantum effects will dominate device performance, and conventional electronic circuits will fail to function.

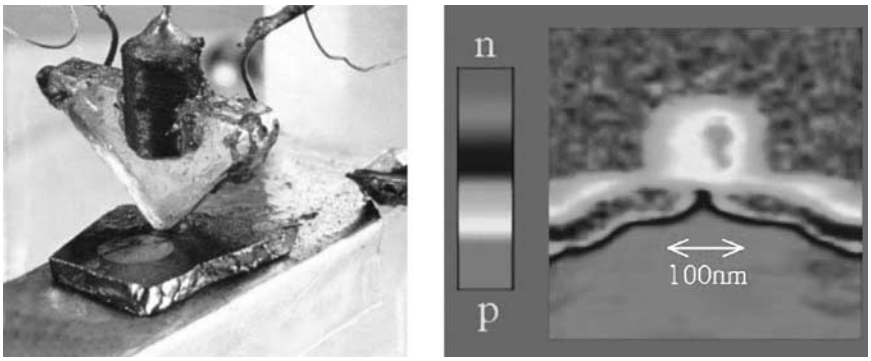

Fig. 1.2 Photograph (left) of the first transistor. Brattain and Bardeen's *p-n-p* point-contact germanium transistor operated as a speech amplifier with a power gain of 18 on December 23, 1947. The device is a few mm in size. On the right is a scanning capacitance microscope cross-section image of a silicon *p*-type metal-oxide-semiconductor field-effect transistor (*p*-MOSFET) with an effective channel length of about 20 nm, or about 60 atoms.[4] This image of a small transistor was published in 1998, 50 years after Brattain and Bardeen's device. Image courtesy of G. Timp, University of Illinois.

1. S. Weiss, *Science* **283**, 1676 (1999).
2. G. E. Moore, *Electronics* **38**, 114 (1965). Also reprinted in *Proc. IEEE* **86**, 82 (1998).
3. http://www.sematech.org.
4. Also see G. Timp *et al. IEEE International Electron Devices Meeting (IEDM) Technical Digest* p. 615, Dec. 6–9, San Francisco, California, 1998 (ISBN 078034779).

We need to learn to use quantum mechanics to make sure that we can create the smallest, highest-performance devices possible.

Quantum mechanics is the basis for our present understanding of physical phenomena on an atomic scale. Today, quantum mechanics has numerous applications in engineering, including semiconductor transistors, lasers, and quantum optics. As technology advances, an increasing number of new electronic and opto-electronic devices will operate in ways that can only be understood using quantum mechanics. Over the next 20 years, fundamentally quantum devices such as single-electron memory cells and photonic signal processing systems may well become commonplace. It is also likely that entirely new devices, with functionality based on the principles of quantum mechanics, will be invented. The purpose and intent of this book is to provide the reader with a level of understanding and insight that will enable him or her to appreciate and to make contributions to the development of these future, as yet unknown, applications of quantum phenomena.

The small glimpse of our quantum world that this book provides reveals significant differences from our everyday experience. Often we will discover that the motion of objects does not behave according to our (classical) expectations. A simple, but hopefully motivating, example is what happens when you throw a ball against a wall. Of course, we expect the ball to bounce right back. Quantum mechanics has something different to say. There is, under certain special circumstances, a finite chance that the ball will appear on the other side of the wall! This effect, known as tunneling, is fundamentally quantum mechanical and arises due to the fact that on appropriate time and length scales particles can be described as waves. Situations in which *elementary* particles such as electrons and photons tunnel are, in fact, relatively common. However, quantum mechanical tunneling is not always limited to atomic-scale and elementary particles. Tunneling of *large* (macroscopic) objects can also occur! Large objects, such as a ball, are made up of many atomic-scale particles. The possibility that such large objects can tunnel is one of the more amazing facts that emerges as we explore our quantum world.

However, before diving in and learning about quantum mechanics it is worth spending a little time and effort reviewing some of the basics of classical mechanics and classical electromagnetics. We do this in the next two sections. The first deals with classical mechanics, which was first placed on a solid theoretical basis by the work of Newton and Leibniz published at the end of the seventeenth century. The survey includes reminders about the concepts of potential and kinetic energy and the conservation of energy in a closed system. The important example of the one-dimensional harmonic oscillator is then considered. The simple harmonic oscillator is extended to the case of the diatomic linear chain, and the concept of dispersion is introduced. Going beyond mechanics, in the following section classical electromagnetism is explored. We start by stating the coulomb potential for charged particles, and then we use the equations that describe electrostatics to solve practical problems. The classical concepts of capacitance and the coulomb blockade are used as examples. Continuing our review, Maxwell's equations are used to study electrodynamics. The first example discussed is electromagnetic wave propagation at the speed of light in free space, c. The key result – that power and momentum are carried by an electromagnetic wave – is also introduced.

Following our survey of classical concepts, in Chapter 2 we touch on the experimental basis for quantum mechanics. This includes observation of the interference phenomenon with light, which is described in terms of the linear superposition of waves. We then

discuss the important early work aimed at understanding the measured power spectrum of black-body radiation as a function of wavelength, λ, or frequency, $\omega = 2\pi c/\lambda$. Next, we treat the photoelectric effect, which is best explained by requiring that light be quantized into particles (called photons) of energy $E = \hbar\omega$. Planck's constant $\hbar = 1.0545 \times 10^{-34}$ J s, which appears in the expression $E = \hbar\omega$, is a small number that sets the absolute scale for which quantum effects usually dominate behavior.[5] Since the typical length scale for which electron energy quantization is important usually turns out to be the size of an atom, the observation of discrete spectra for light emitted from excited atoms is an effect that can only be explained using quantum mechanics. The energy of photons emitted from excited hydrogen atoms is discussed in terms of the solutions of the Schrödinger equation. Because historically the experimental facts suggested a wave nature for electrons, the relationships among the wavelength, energy, and momentum of an electron are introduced. This section concludes with some examples of the behavior of electrons, including the description of an electron in free space, the concept of a wave packet and dispersion of a wave packet, and electronic configurations for atoms in the ground state.

Since we will later apply our knowledge of quantum mechanics to semiconductors and semiconductor devices, there is also a brief introduction to crystal structure, the concept of a semiconductor energy band gap, and the device physics of a unipolar heterostructure semiconductor diode.

1.2 Classical mechanics

1.2.1 Introduction

The problem classical mechanics sets out to solve is predicting the motion of large (macroscopic) objects. On the face of it, this could be a very difficult subject simply because large objects tend to have a large number of degrees of freedom[6] and so, in principle, should be described by a large number of parameters. In fact, the number of parameters could be so enormous as to be unmanageable. The remarkable success of classical mechanics is due to the fact that powerful concepts can be exploited to simplify the problem. Constants of the motion and constraints may be used to reduce the description of motion to a simple set of differential equations. Examples of constants of the motion often include conservation of energy and momentum.[7] Describing an object as rigid is an example of a constraint being placed on the object.

Consider a rock dropped from a tower. Classical mechanics initially ignores the internal degrees of freedom of the rock (it is assumed to be rigid), but instead defines a center of mass so that the rock can be described as a point particle of mass, m. Angular momentum is decoupled from the center of mass motion. Why is this all possible? The answer is neither simple nor obvious.

5. Sometimes $\hbar$ is called Planck's *reduced* constant to distinguish it from $h = 2\pi\hbar$.
6. For example, an object may be able to vibrate in many different ways.
7. Emmy Noether showed in 1915 that the existence of a symmetry due to a local interaction gives rise to a conserved quantity. For example, conservation of energy is due to time translation symmetry, conservation of linear momentum is due to space translational symmetry, and angular momentum conservation is due to rotational symmetry.

It is known from experiments that atomic-scale particle motion can be very different from the predictions of classical mechanics. Because large objects are made up of many atoms, one approach is to suggest that quantum effects are somehow averaged out in large objects. In fact, classical mechanics is often assumed to be the macroscopic (large-scale) limit of quantum mechanics. The underlying notion of finding a means to link quantum mechanics to classical mechanics is so important it is called the *correspondence principle*. Formally, one requires that the results of classical mechanics be obtained in the limit $\hbar \to 0$. While a simple and convenient test, this approach misses the point. The results of classical mechanics are obtained because the quantum mechanical wave nature of objects is averaged out by a mechanism called *decoherence*. In this picture, quantum mechanical effects are *usually* averaged out in large objects to give the classical result. However, this is not always the case. We should remember that sometimes even large (macroscopic) objects can show quantum effects. A well-known example of a macroscopic quantum effect is superconductivity and the tunneling of flux quanta in a device called a SQUID.[8] The tunneling of flux quanta is the quantum-mechanical equivalent of throwing a ball against a wall and having it sometimes tunnel through to the other side! Quantum mechanics allows large objects to tunnel through a thin potential barrier if the constituents of the object are prepared in a special quantum-mechanical state. The wave nature of the entire object must be maintained if it is to tunnel through a potential barrier. One way to achieve this is to have a coherent superposition of constituent particle wave functions.

Returning to classical mechanics, we can now say that the motion of macroscopic material bodies is *usually* described by classical mechanics. In this approach, the linear momentum of a rigid object with mass m is $\mathbf{p} = m\, d\mathbf{x}/dt$, where $\mathbf{v} = d\mathbf{x}/dt$ is the velocity of the object moving in the direction of the unit vector $\mathbf{x}^{\sim} = \mathbf{x}/|\mathbf{x}|$. Time is measured in units of seconds (s), and distance is measured in units of meters (m). The magnitude of momentum is measured in units of kilogram meters per second (kg m s^{-1}), and the magnitude of velocity (speed) is measured in units of meters per second (m s^{-1}). Classical mechanics assumes that there exists an inertial frame of reference for which the motion of the object is described by the differential equation

$$\mathbf{F} = d\mathbf{p}/dt = m\, d^2\mathbf{x}/dt^2 \tag{1.1}$$

where the vector $\mathbf{F}$ is the force. The magnitude of force is measured in units of newtons (N). Force is a vector field. What this means is that the particle can be subject to a force the magnitude and direction of which are different in different parts of space.

We need a new concept to obtain a measure of the forces experienced by the particle moving from position $\mathbf{r}_1$ to $\mathbf{r}_2$ in space. The approach taken is to introduce the idea of *work*. The work done moving the object from point 1 to point 2 in space along a path is *defined* as

$$W_{12} = \int_{\mathbf{r}=\mathbf{r}_1}^{\mathbf{r}=\mathbf{r}_2} \mathbf{F} \cdot d\mathbf{r} \tag{1.2}$$

8. For an introduction to this see A. J. Leggett, *Physics World* **12**, 73 (1999).

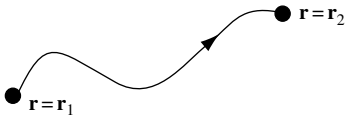

Fig. 1.3 Illustration of a classical particle trajectory from position $\mathbf{r}_1$ to $\mathbf{r}_2$.

where $\mathbf{r}$ is a spatial vector coordinate. Figure 1.3 illustrates one possible trajectory for a particle moving from position $\mathbf{r}_1$ to $\mathbf{r}_2$.

The definition of work is simply the integral of the force applied multiplied by the infinitesimal distance moved in the direction of the force for the complete path from point 1 to point 2. For a *conservative* force field, the work W_{12} is the same for any path between points 1 and 2. Hence, making use of the fact $\mathbf{F} = d\mathbf{p}/dt = m\, d\mathbf{v}/dt$, one may write

$$W_{12} = \int_{\mathbf{r}=\mathbf{r}_1}^{\mathbf{r}=\mathbf{r}_2} \mathbf{F}\cdot d\mathbf{r} = m\int d\mathbf{v}/dt\cdot\mathbf{v}dt = \frac{m}{2}\int \frac{d}{dt}(v^2)dt \tag{1.3}$$

so that $W_{12} = m(v_2^2 - v_1^2)/2 = T_2 - T_1$, where $v^2 = \mathbf{v}\cdot\mathbf{v}$ and the scalar $T = mv^2/2$ is called the kinetic energy of the object.

For conservative forces, because the work done is the same for any path between points 1 and 2, the work done around any *closed path*, such as the one illustrated in Fig. 1.4, is always zero, or

$$\oint \mathbf{F}\cdot d\mathbf{r} = 0 \tag{1.4}$$

This is always true if force is the gradient of a *single-valued* spatial scalar field where

$$\mathbf{F} = -\nabla V(\mathbf{r}) \tag{1.5}$$

since $\oint \mathbf{F}\cdot d\mathbf{r} = -\oint \nabla V\cdot d\mathbf{r} = -\oint dV = 0$. In our expression, $V(\mathbf{r})$ is called the potential. Potential is measured in volts (V), and potential energy is measured in joules (J) or electron volts (eV). If the forces acting on the object are conservative, then total energy, which is the sum of kinetic and potential energy, is a constant of the motion. In other words, total energy $T + V$ is conserved.

Since kinetic and potential energy can be expressed as functions of the variable's position and time, it is possible to define a *Hamiltonian* function for the system, which is $H = T + V$. The Hamiltonian function may then be used to describe the dynamics of particles in the system.

For a nonconservative force, such as a particle subject to frictional forces, the work done around any closed path is not zero, and $\oint \mathbf{F}\cdot d\mathbf{r} \neq 0$.

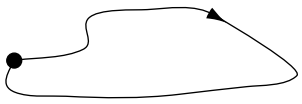

Fig. 1.4 Illustration of a closed-path classical particle trajectory.

Let us pause here for a moment and consider some of what has just been introduced. We think of objects moving due to something. Forces cause objects to move. We have introduced the concept of force to help ensure that the motion of objects can be described as a simple process of *cause and effect*. We imagine a force-field in three-dimensional space that is represented mathematically as a continuous, integrable vector field, $\mathbf{F}(\mathbf{r})$. Assuming that time is also continuous and integrable, we quickly discover that in a conservative force-field energy is conveniently partitioned between a kinetic and potential term and total energy is conserved. By simply representing the total energy as a function or Hamiltonian, $H = T + V$, we can find a differential equation that describes the dynamics of the object. Integration of the differential equation of motion gives the trajectory of the object as it moves through space.

In practice, these ideas are very powerful and may be applied to many problems involving the motion of macroscopic objects. As an example, let us consider the problem of finding the motion of a particle mass, m, attached to a spring. Of course, we know from experience that the solution will be oscillatory and so characterized by a frequency and amplitude of oscillation. However, the power of the theory is that we can obtain relationships among all the parameters that govern the behavior of the system.

In the next section, the motion of a classical particle mass m attached to a spring and constrained to move in one dimension is discussed. The type of model we will be considering is called the simple harmonic oscillator.

1.2.2 The one-dimensional simple harmonic oscillator

Figure 1.5 illustrates a classical particle mass m constrained to motion in one dimension and attached to a lightweight spring that obeys Hooke's law. Hooke's law states that the displacement, x, from the equilibrium position, $x = 0$, is proportional to the force on the particle such that $F = -\kappa x$ where the proportionality constant is κ and is called the spring constant. In this example, we ignore any effect due to the finite mass of the spring by assuming its mass is small relative to the particle mass, m.

To calculate the frequency and amplitude of vibration, we start by noting that the total energy function or Hamiltonian for the system is

$$H = T + V \tag{1.6}$$

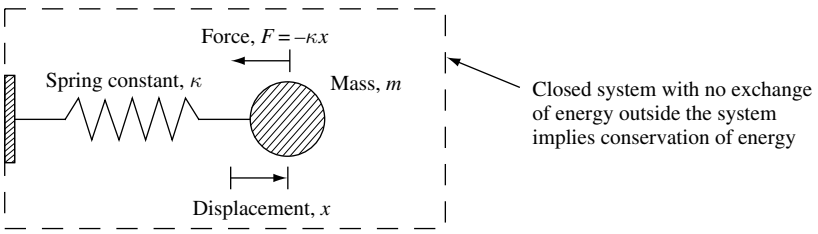

Fig. 1.5 Illustration showing a classical particle mass m attached to a spring and constrained to move in one dimension. The displacement of the particle from its equilibrium position is x and the force on the particle is $F = -\kappa x$ where κ is the spring constant. The box drawn with a broken line indicates a closed system.

where potential energy, obtained by integrating Eq. (1.5), is $V = \frac{1}{2}\kappa x^2 = \int_0^x \kappa x' dx'$ and kinetic energy is $T = m(dx/dt)^2/2$, so that

$$H = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 + \frac{1}{2}\kappa x^2 \tag{1.7}$$

The system is *closed*, so there is no exchange of energy outside the system. There is no dissipation, total energy in the system is a constant, and

$$\frac{dH}{dt} = 0 = m\frac{dx}{dt}\frac{d^2x}{dt^2} + \kappa x\frac{dx}{dt} \tag{1.8}$$

so that the *equation of motion* can be written as

$$\boxed{\kappa x + m\frac{d^2x}{dt^2} = 0} \tag{1.9}$$

The solutions for this second-order linear differential equation are

$$x(t) = A\cos(\omega_0 t + \phi) \tag{1.10}$$

$$\frac{dx(t)}{dt} = -\omega_0 A\sin(\omega_0 t + \phi) \tag{1.11}$$

$$\frac{d^2x(t)}{dt^2} = -\omega_0^2 A\cos(\omega_0 t + \phi) \tag{1.12}$$

where A is the amplitude of oscillation, ω_0 is the angular frequency of oscillation measured in radians per second (rad s^{-1}), and ϕ is a fixed phase. The velocity leads the displacement in phase by $\pi/2$ and the acceleration is in antiphase with the displacement.

We may now write the potential energy and kinetic energy as

$$V = \frac{1}{2}\kappa^2 A^2\cos^2(\omega_0 t + \phi) \tag{1.13}$$

and

$$T = \frac{1}{2}m\omega_0^2 A^2\sin^2(\omega_0 t + \phi) \tag{1.14}$$

respectively. Total energy

$$E = T + V = m\omega_0^2 A^2/2 = \kappa A^2/2 \tag{1.15}$$

since $\sin^2(\theta) + \cos^2(\theta) = 1$ and $\kappa = m\omega_0^2$. Clearly, an increase in total energy increases amplitude $A = \sqrt{2E/\kappa} = \sqrt{2E/m\omega_0^2}$, and an increase in κ, corresponding to an increase in the stiffness of the spring, decreases A. The theory gives us the relationships among all the parameters of the classical harmonic oscillator: κ, m, A, and total energy.

We have shown that the classical simple harmonic oscillator vibrates in a single *mode* with frequency ω_0. The vibrational energy stored in the mode can be changed continuously by varying the amplitude of vibration, A.

Suppose we have a particle mass $m = 0.1\,\text{kg}$ attached to a lightweight spring with spring constant $\kappa = 360\,\text{N m}^{-1}$. Particle motion is constrained to one dimension, and the amplitude of oscillation is observed to be $A = 0.01\,\text{m}$. In this case, the angular frequency of oscillation is just $\omega_0 = \sqrt{\kappa/m} = 60\,\text{rad s}^{-1}$. Since angular frequency $\omega = 2\pi\nu$ where $\nu = 1/\tau$ is the oscillation frequency measured in cycles per second or hertz (Hz) and τ is the oscillation period measured in seconds (s), in this case $\nu \sim 9.5\,\text{Hz}$ and $\tau \sim 0.1\,\text{s}$. The total energy in the system is $E = \kappa A^2/2 = 18\,\text{mJ}$. We can solve the equation of motion and obtain position, $x(t)$, velocity, $dx(t)/dt$, and acceleration, $d^2x(t)/dt^2$, as a function of time. Velocity is zero when $x = \pm A$ and the particle changes its direction of motion and starts moving back towards the equilibrium position $x = 0$. The position $x = \pm A$, where velocity is zero, is called the *classical turning point* of the motion. Peak velocity, $v_{\max} = \pm A\omega_0$, occurs as the particle crosses its equilibrium position, $x = 0$. In this case $v_{\max} = \pm A\ \omega_0 = \pm 0.6\,\text{m s}^{-1}$. Maximum acceleration, $a_{\max} = \pm A\omega_0^2$, occurs when $x = \pm A$. In this case $a_{\max} = \pm A\omega_0^2 = \pm 36\,\text{m s}^{-2}$. Figure 1.6 illustrates these results.

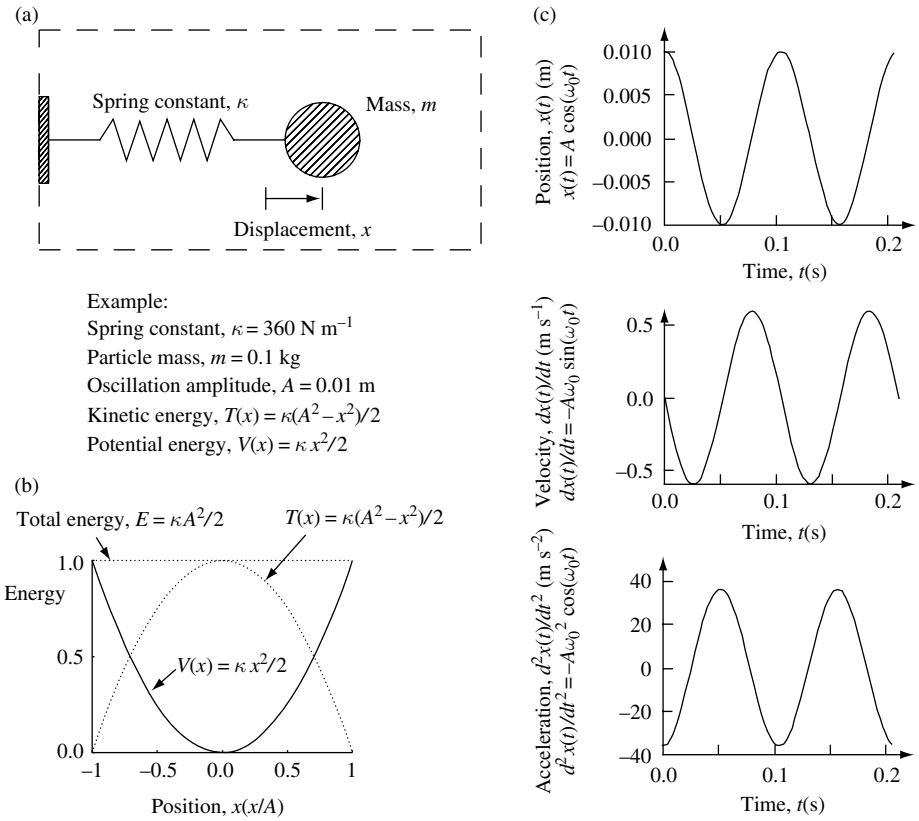

Fig. 1.6 Example predictions for the classical one-dimensional harmonic oscillator involving motion of a particle mass m attached to a lightweight spring with spring constant κ. In this case, the spring constant is $\kappa = 360\,\text{N m}^{-1}$, particle mass, $m = 0.1\,\text{kg}$, and the oscillation amplitude is $A = 0.01\,\text{m}$. (a) Illustration of the closed system showing displacement of the particle from its equilibrium position at $x = 0$. (b) Kinetic energy T and potential energy V functions of position, x. (c) Position, velocity, and acceleration functions of time, t.

1.2.3 Harmonic oscillation of a diatomic molecule

Consider the vibrational motion of a diatomic molecule illustrated in Fig. 1.7. We will show that the Hamiltonian can be separated into center of mass motion and relative motion of the two atoms. If the potential for relative atom motion is harmonic then the frequency of oscillation about their equilibrium position is just $\omega = \sqrt{\kappa/m_r}$ where κ is the spring constant and m_r is the *reduced mass* such that $1/m_r = 1/m_1 + 1/m_2$.

The molecule sketched in Fig. 1.7 consists of two atoms mass m_1 and mass m_2 with position $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively. The center of mass coordinate is $\mathbf{R}$ and relative position vector is $\mathbf{r}$. We assume that the forces, and hence the potential, governing relative motion depend only on the magnitude of the difference vector so that $|\mathbf{r}| = |\mathbf{r}_2 - \mathbf{r}_1|$. If we choose the origin as the center of mass then $m_1\mathbf{r}_1 + m_2\mathbf{r}_2 = 0$, so that

$$\mathbf{r}_1 = \frac{m_2}{(m_1 + m_2)}\mathbf{r} \tag{1.16}$$

and

$$\mathbf{r}_2 = \frac{m_1}{(m_1 + m_2)}\mathbf{r} \tag{1.17}$$

That this is so is easy to see since, for example,

$$\mathbf{r}_1 = \frac{-m_2}{m_1}\mathbf{r}_2 = \frac{-m_2}{m_1}(\mathbf{r}_1 - \mathbf{r}) \tag{1.18}$$

$$\mathbf{r}_1\left(1 + \frac{m_2}{m_1}\right) = \frac{m_2}{m_1}\mathbf{r} \tag{1.19}$$

$$\mathbf{r}_1(m_1 + m_2) = m_2\mathbf{r} \tag{1.20}$$

$$\mathbf{r}_1 = \frac{m_2}{(m_1 + m_2)}\mathbf{r} \tag{1.21}$$

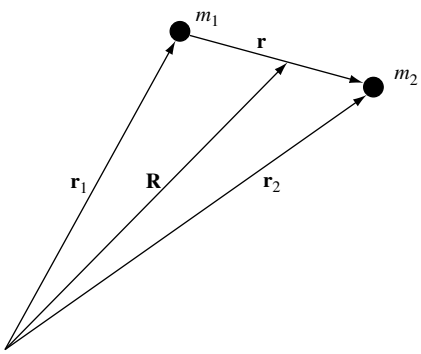

Fig. 1.7 Illustration of a diatomic molecule consisting of two atoms with mass m_1 and m_2 and position $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively. The relative position vector is $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and the center of mass coordinate is $\mathbf{R}$.