Applied Quantum Mechanics

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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 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)

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[1] S. Weiss, *Science* **283**, 1676 (1999).

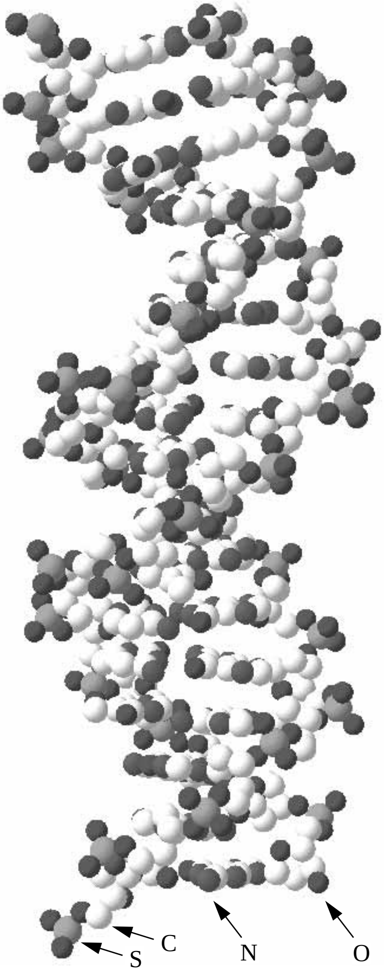

Fig. 1.1. Ball and stick model of a DNA molecule. Atom types are indicated.

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 2 every 18 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)

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[2] G. E. Moore, *Electronics* **38**, 114 (1965). Also reprinted in *Proc. IEEE* **86**, 82 (1998).

[3] http://www.sematech.org.

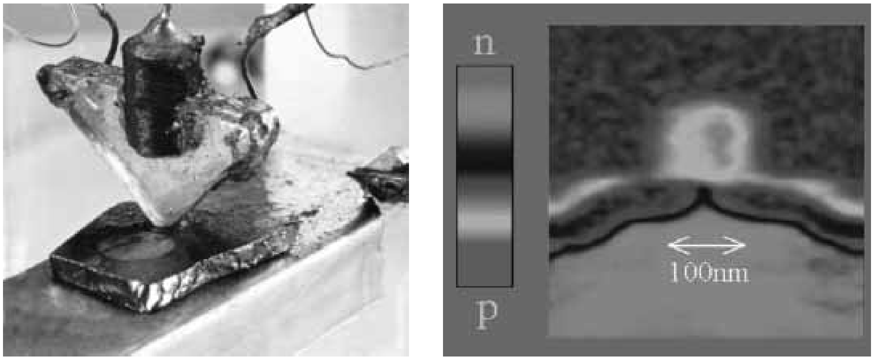

Fig. 1.2. Photograph (left) of the first transistor. Brattain and Bardeen's *p*–*n*–*p* point-contact germanium transistor operated as a speech amplifier with a power gain of 18 on December 23, 1947. The device is a few millimeters in size. On the right is a scanning capacitance microscope cross-section 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.

cell size will be *less* than that of an atom by the year 2030. Well before this endpoint is reached, quantum effects will dominate device performance, and conventional electronic circuits will fail to function.

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 available. It is also likely that entirely new devices, with functionality based on the principles of quantum mechanics, will be invented. The purpose 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.

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[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 0780 3477 9).

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 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.

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[5] Sometimes $\hbar$ is called Planck's *reduced* constant to distinguish it from $h = 2\pi\hbar$.

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 include conservation of energy and momentum. 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.

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 $\hbar \rightarrow 0$. While a simple and convenient test, this approach misses

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[6] For example, an object may be able to vibrate in many different ways.

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.[7] 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 $\mathbf{p} = m \cdot d\mathbf{x}/dt$, where $\mathbf{v} = d\mathbf{x}/dt$ is the velocity of the object moving in the direction of the unit vector $\hat{\mathbf{x}}$. 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

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

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 position $\mathbf{r}_2$ 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

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

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

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

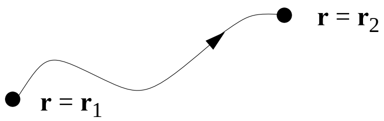


Fig. 1.3. Illustration of a classical particle trajectory from position $\mathbf{r}_1$ to position $\mathbf{r}_2$.

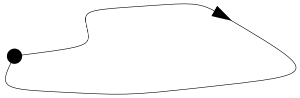


Fig. 1.4. Illustration of a closed-path classical particle trajectory.

the fact $\mathbf{F} = d\mathbf{p}/dt = m \cdot d\mathbf{v}/dt$, 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 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 $\mathbf{F} = -\nabla V(\mathbf{r})$, 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 $\oint \mathbf{F} \cdot d\mathbf{r} \neq 0$.

Let's 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 a 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's 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 use the formalism to 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 considered. The type of model we will be considering is called the simple harmonic oscillator.

1.2.2 The one-dimensional simple harmonic oscillator

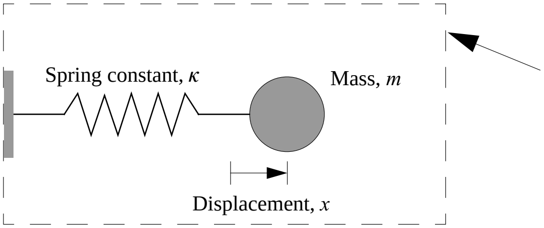
Figure 1.5 illustrates a classical particle mass m attached to a lightweight spring that obeys Hooke's law. Hooke's law states that the displacement, x, from the equilibrium position, $x = 0$, is proportional to the force on the particle. The proportionality constant is κ and is called the spring constant. 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

$$H = T + V \tag{1.5}$$

where potential energy 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

$$H = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 + \frac{1}{2}\kappa x^2 \tag{1.6}$$



Closed system with no exchange of energy outside the system implies conservation of energy.

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. The box drawn with a broken line indicates a closed system.

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

$$\frac{dH}{dt} = 0 = m\frac{dx}{dt}\frac{d^2x}{dt^2} + \kappa x\frac{dx}{dt} \tag{1.7}$$

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

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

The solutions for this second-order linear differential equation are

$$x(t) = A\cos(\omega_0 t + \phi) \tag{1.9}$$

$$\frac{dx(t)}{dt} = -\omega_0 A\sin(\omega_0 t + \phi) \tag{1.10}$$

$$\frac{d^2x(t)}{dt^2} = -\omega_0^2 A\cos(\omega_0 t + \phi) \tag{1.11}$$

where A is the amplitude of oscillation, ω_0 is the frequency of oscillation measured in radians per second (rad s^{-1}), and ϕ is a fixed phase. We may now write the potential energy and kinetic energy as

$$V = \frac{1}{2}\kappa A^2\cos^2(\omega_0 t + \phi) \tag{1.12}$$

and

$$T = \frac{1}{2}m\omega_0^2 A^2\sin^2(\omega_0 t + \phi) \tag{1.13}$$

respectively. Total energy $E = T + V = m\omega_0^2 A^2/2 = \kappa A^2/2$ 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 $m = 0.1$ kg attached to a lightweight spring with spring constant $\kappa = 360\ \mathrm{N\ m^{-1}}$. Particle motion is constrained to one dimension, and the amplitude of oscillation is observed to be $A = 0.01$ m. In this case, the frequency of oscillation is just $\omega_0 = \sqrt{\kappa/m} = 60\ \mathrm{rad\ s^{-1}}$, which is about 9.5 oscillations per second, and the total energy in the system is $E = \kappa A^2/2 = 18$ 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

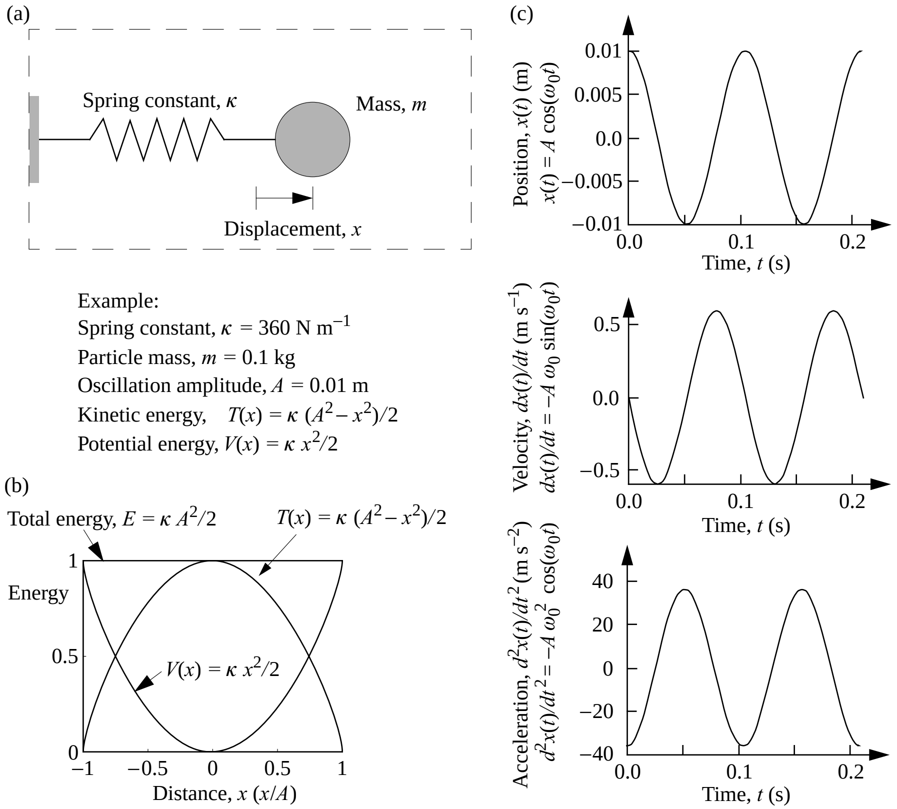


Fig. 1.6. Example predictions for the classical one-dimensional harmonic oscillator involving motion of a particle mass m attached to a lightweight spring with spring constant κ. In this case, the spring constant is $\kappa = 360$ N m^{-1}, particle mass, $m = 0.1$ kg, and the oscillation amplitude is $A = 0.01$ 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.

$x = \pm A$, 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 $v_{\max} = \pm A\omega_0 = \pm 0.6$ m s^{-1}. Maximum acceleration, $a_{\max} = \pm A\omega_0^2$, occurs when $x = \pm A$. In this case $a_{\max} = \pm A\omega_0^2 = \pm 36$ m s^{-2}. Figure 1.6 illustrates these results.

Now let's use what we have learned and move on to a more complex system. In the next example we want to solve the equations of motion of an isolated linear chain of particles, each with mass m, connected by identical springs. This particular problem is a common starting-point for the study of lattice vibrations in crystals. The methods used, and the results obtained, are applicable to other problems such as solving for the vibrational motion of atoms in molecules.

We should be clear why we are going to this effort now. We want to introduce the concept of a *dispersion relation*. It turns out that this is an important way of simplifying the description of an otherwise complex system.

The motion of coupled oscillators can be described using the idea that a given frequency of oscillation corresponds to definite wavelengths of vibration. In practice, one plots frequency of oscillation, ω, with inverse wavelength or wave vector of magnitude $q = 2\pi/\lambda$. Hence, the dispersion relationship is $\omega = \omega(\mathbf{q})$. With this relationship, one can determine how vibration waves and pulses propagate through the system. For example, the phase velocity of a wave is $v_q = \omega/q$ and a pulse made up of wave components near a value q_0 often propagates at the group velocity,

$$v_{\mathrm{g}} = \left.\frac{\partial\omega}{\partial q}\right|_{q=q_0} \tag{1.14}$$

If the dispersion relation is known then we can determine quantities of practical importance such as v_q and v_{g}.

1.2.3 The monatomic linear chain

Figure 1.7 shows part of an isolated linear chain of particles, each of mass m, connected by springs. The site of each particle is labeled with an integer, j. Each particle occupies a lattice site with equilibrium position jL, where L is the lattice constant. Displacement from equilibrium of the j-th particle is u_j, and there are a large number of particles in the chain.

Assuming small deviations u_j from equilibrium, the Hamiltonian of the linear chain is

$$H = \sum_j \frac{m}{2}\left(\frac{du_j}{dt}\right)^2 + V_0(0) + \frac{1}{2!}\sum_{jk}\frac{\partial^2 V_0}{\partial u_j u_k}u_j u_k + \frac{1}{3!}\sum_{jkl}\frac{\partial^3 V_0}{\partial u_j u_k u_l}u_j u_k u_l + \cdots \tag{1.15}$$

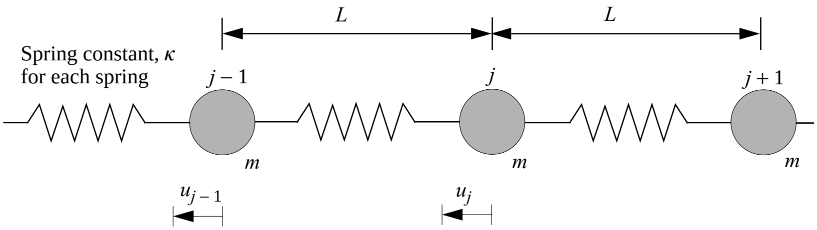


Fig. 1.7. Illustration of part of an isolated linear chain of particles, each of mass m, connected by identical springs with spring constant κ. The site of each particle is labeled relative to the site, j. Each particle occupies a lattice site with equilibrium position jL, where L is the lattice constant. Displacement from equilibrium of the j-th particle is u_j. It is assumed that there are a large number of particles in the linear chain.

The first term on the right-hand side is a sum over kinetic energy of each particle, and $V_0(0)$ is the potential energy when all particles are stationary in the equilibrium position. The remaining terms come from a Taylor expansion of the potential about the equilibrium positions. Each particle oscillates about its equilibrium position and is coupled to other oscillators via the potential.

In the harmonic approximation, the force constant $\kappa_{jk} = (\partial^2 E_0/\partial u_j \partial u_k)|_0$ is real and symmetric so that $\kappa_{jk} = \kappa_{kj}$, and if all springs are identical then $\kappa = \kappa_{jk}$. Restricting the sum in Eqn (1.15) to nearest neighbors and setting $V_0(0) = 0$, the Hamiltonian becomes

$$H = \sum_j \frac{m}{2}\left(\frac{du_j}{dt}\right)^2 + \frac{\kappa}{2}\sum_j \left(2u_j^2 - u_j u_{j+1} - u_j u_{j-1}\right) \tag{1.16}$$

This equation assumes that motion of one particle is from forces due to the relative position of its nearest neighbors.

The displacement from equilibrium at site j is u_j and is related to that of its nearest neighbor by

$$u_{j\pm1} = u_j e^{\pm iqL} \tag{1.17}$$

where $q = 2\pi/\lambda$ is the wave vector of a vibration of wavelength, λ. Using Eqn (1.16) and assuming no dissipation in the system, so that $dH/dt = 0$, the equation of motion is

$$m\frac{d^2u_j}{dt^2} = \kappa(u_{j+1} + u_{j-1} - 2u_j) \tag{1.18}$$

Second-order differential equations of this type have time dependence of the form $e^{-i\omega t}$, which, on substitution into Eqn (1.18), gives

$$-m\omega^2 u_j = \kappa(e^{iqL} + e^{-iqL} - 2)u_j = -4\kappa \sin^2\left(\frac{qL}{2}\right)u_j \tag{1.19}$$

From Eqn (1.19) it follows that

$$\omega(q) = \sqrt{\frac{4\kappa}{m}}\sin\left(\frac{qL}{2}\right) \tag{1.20}$$

This equation tells us that there is a unique nonlinear relationship between the frequency of vibration, ω, and the magnitude of the wave vector, q. This is an example of a *dispersion relation*, $\omega = \omega(\mathbf{q})$.

The dispersion relation for the monatomic linear chain is plotted in Fig. 1.8(a). It consists of a single *acoustic branch*, $\omega = \omega_{\text{acoustic}}(q)$, with maximum frequency $\omega_{\max} = (4\kappa/m)^{1/2}$. Notice that vibration frequency approaches $\omega \to 0$ *linearly* as $q \to 0$. In the long wavelength limit ($q \to 0$), the acoustic branch dispersion relation describing lattice dynamics of a monatomic linear chain predicts that vibrational waves propagate

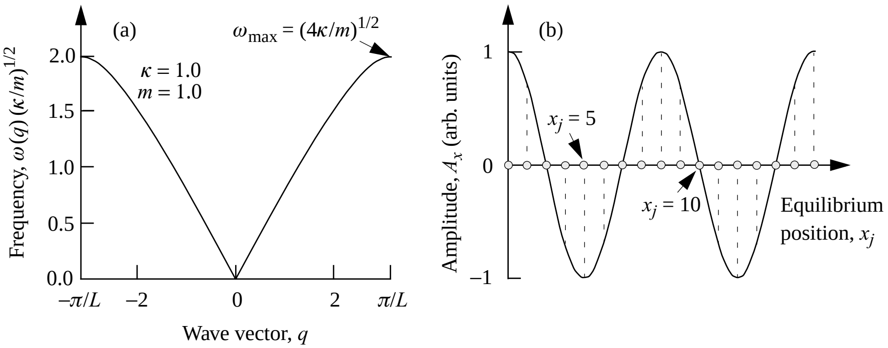


Fig. 1.8. (a) Dispersion relation for lattice vibrations of a one-dimensional monatomic linear chain. The dispersion relation is linear at low values of q. The maximum frequency of oscillation is $\omega_{\max} = (4\kappa/m)^{1/2}$. Particles have mass $m = 1.0$, and the spring constant is $\kappa = 1.0$. (b) Amplitude of vibrational motion in the x direction on a portion of the linear chain for a particular mode of frequency ω. Equilibrium position x_j is indicated.

at constant group velocity $v_g = \partial\omega/\partial q$. This is the velocity of sound waves in the system.

Each normal mode of the linear chain is a harmonic oscillator characterized by frequency ω and wave vector q. In general, each mode of frequency ω in the linear chain involves harmonic motion of all the particles in the chain that are also at frequency ω. As illustrated in Fig. 1.8(b), not all particles have the same amplitude. Total energy in a mode is proportional to the sum of the amplitudes squared of all particles in the chain.

The existence of a dispersion relation is significant, and so it is worth considering some of the underlying physics. We start by recalling that in our model there are a large number of atoms in the linear monatomic chain. At first sight, one might expect that the large number of atoms involved gives rise to all types of oscillatory motion. One might anticipate solutions to the equations of motion allowing all frequencies and wavelengths, so that no dispersion relation could exist. However, this situation does not arise in practice because of some important simplifications imposed by *symmetry*. The motion of a given atom is determined by forces due to the relative position of its nearest neighbors. Forces due to displacements of more distant neighbors are not included. The facts that there is only one spring constant and there is only one type of atom are additional constraints on the system. One may think of such constraints as imposing a type of symmetry that has the effect of eliminating all but a few of the possible solutions to the equations of motion. These solutions are conveniently summarized by the dispersion relation, $\omega = \omega(\mathbf{q})$.

1.2.4 The diatomic linear chain

Figure 1.9 illustrates a diatomic linear chain. In this example we assume a periodic array of atoms characterized by a lattice constant, L. There are two atoms per *unit cell*

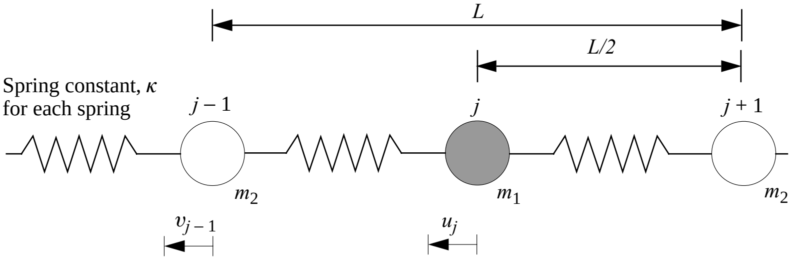


Fig. 1.9. Illustration of an isolated linear chain of particles of alternating mass m_1 and m_2 connected by identical springs with spring constant κ. There are two particles per *unit cell* spaced by $L/2$. One particle in the unit cell has mass m_1, and the other particle has mass m_2. The site of each particle is labeled relative to the site, j. The displacement from equilibrium of particles mass m_1 is u, and for particles mass m_2 it is v.

spaced by $L/2$. One atom in the unit cell has mass m_1 and the other atom has mass m_2. The site of each atom is labeled relative to the site, j. The displacement from equilibrium of particles mass m_1 is u, and for particles mass m_2 it is v. The motion of one atom is related to that of its nearest similar (equal-mass) neighbor by

$$u_{j\pm 2} = u_j e^{\pm iqL} \tag{1.21}$$

where $q = 2\pi/\lambda$ is the wave vector of a vibration of wavelength, λ. If we assume that the motion of a given atom is from forces due to the relative position of its nearest neighbors, the equations of motion for the two types of atoms are

$$m_1 \frac{d^2 u_j}{dt^2} = \kappa(v_{j+1} + v_{j-1} - 2u_j) \tag{1.22}$$

$$m_2 \frac{d^2 v_{j-1}}{dt^2} = \kappa(u_j + u_{j-2} - 2v_{j-1}) \tag{1.23}$$

or

$$m_1 \frac{d^2 u_j}{dt^2} = \kappa(1 + e^{iqL})v_{j-1} + 2\kappa u_j \tag{1.24}$$

$$m_2 \frac{d^2 v_{j-1}}{dt^2} = \kappa(1 + e^{-iqL})u_j - 2\kappa v_{j-1} \tag{1.25}$$

Solutions for u and v have time dependence of the form $e^{-i\omega t}$, giving

$$-m_1\omega^2 u_j = \kappa(1 + e^{iqL})v_{j-1} - 2\kappa u_j \tag{1.26}$$

$$-m_2\omega^2 v_{j-1} = \kappa(1 + e^{-iqL})u_j - 2\kappa v_{j-1} \tag{1.27}$$

or

$$(2\kappa - m_1\omega^2)u_j - \kappa(1 + e^{iqL})v_{j-1} = 0 \tag{1.28}$$

$$-\kappa(1 + e^{-iqL})u_j + (2\kappa - m_2\omega^2)v_{j-1} = 0 \tag{1.29}$$

This is a linear set of equations with an intrinsic or (from the German word) *eigen* solution given by the characteristic equation

$$\begin{vmatrix} 2\kappa - m_1\omega^2 & -\kappa(1+e^{iqL}) \\ -\kappa(1+e^{-iqL}) & 2\kappa - m_2\omega^2 \end{vmatrix} = 0 \tag{1.30}$$

so that the characteristic polynomial is

$$\omega^4 - 2\kappa\left(\frac{m_1+m_2}{m_1m_2}\right)\omega^2 + \frac{2\kappa^2}{m_1m_2}(1-\cos(qL)) = 0 \tag{1.31}$$

The roots of this polynomial give the characteristic values, or *eigenvalues*, ω_q.

To understand further details of the dispersion relation for our particular linear chain of particles, it is convenient to look for solutions that are extreme limiting cases. The extremes we look for are $q \to 0$, which is the long wavelength limit ($\lambda \to \infty$), and $q \to \pi/L$, which is the short wavelength limit ($\lambda \to 2L$).

In the *long wavelength limit* $q \to 0$

$$\omega^2\left(\omega^2 - 2\kappa\left(\frac{m_1+m_2}{m_1m_2}\right)\right) = 0 \tag{1.32}$$

and solutions are

$$\omega = 0 \quad \text{and} \quad \omega = \left(2\kappa\left(\frac{m_1+m_2}{m_1m_2}\right)\right)^{1/2}$$

with the latter corresponding to both atom types beating against each other.

In the *short wavelength limit* $q \to \pi/L$

$$\omega^4 - 2\kappa\left(\frac{m_1+m_2}{m_1m_2}\right)\omega^2 + \frac{4\kappa^2}{m_1m_2} = 0 \tag{1.33}$$

and solutions are

$$\omega_1 = (2\kappa/m_1)^{1/2}$$

corresponding to only atoms of mass m_1 vibrating, and

$$\omega_2 = (2\kappa/m_2)^{1/2}$$

corresponding to only atoms mass m_2 vibrating.

With these limits, it is now possible to sketch a *dispersion relation* for the lattice vibrations. In Fig. 1.10 the dispersion relation $\omega = \omega(q)$ is given for the case $m_1 < m_2$, with $m_1 = 0.5$, $m_2 = 1.0$, and $\kappa = 1.0$. There is an *acoustic branch* $\omega = \omega_{\text{acoustic}}(q)$ for which vibration frequency linearly approaches $\omega \to 0$ as $q \to 0$, and there is an *optic branch* $\omega = \omega_{\text{optic}}(q)$ for which $\omega \neq 0$ as $q \to 0$.

As one can see from Fig. 1.10, the acoustic branch is capable of propagating low-frequency sound waves the group velocity of which, $v_g = \partial\omega/\partial q$, is a constant for long wavelengths. Typical values for the velocity of sound waves in a semiconductor at room

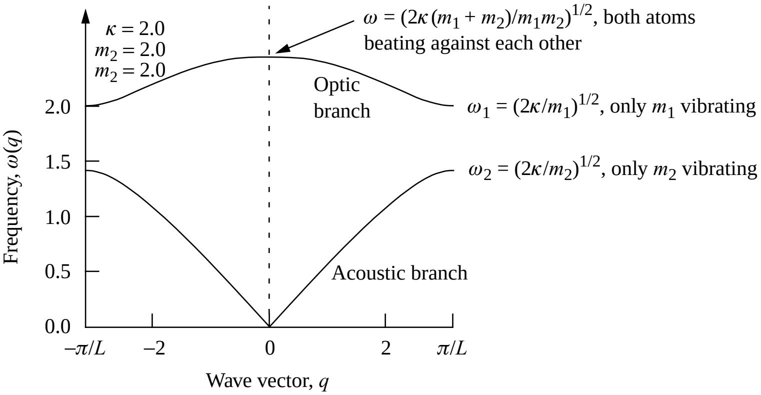


Fig. 1.10. Dispersion relation for lattice vibrations of a one-dimensional diatomic linear chain. Particles have masses $m_1 = 0.5$ and $m_2 = 1.0$. The spring constant is $\kappa = 1.0$.

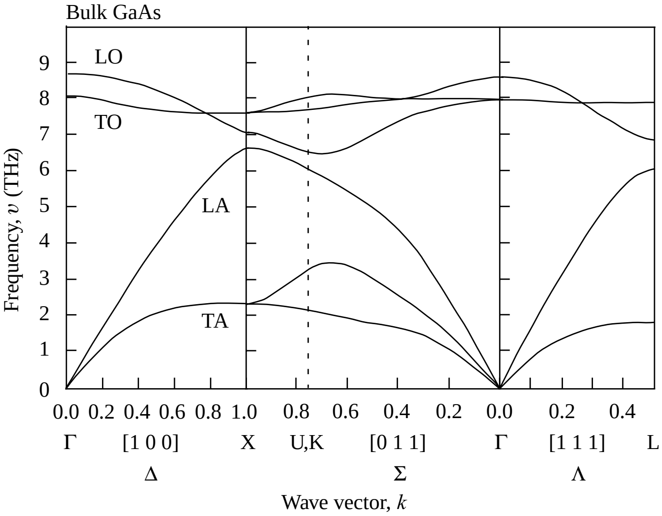


Fig. 1.11. Lattice vibration dispersion relation along principal crystal symmetry directions of bulk GaAs.[8] The longitudinal acoustic (LA), transverse acoustic (TA), longitudinal optic (LO), and transverse optic (TO) branches are indicated.

temperature are $v_g = 8.4 \times 10^3$ m s^{-1} in (100)-oriented Si and $v_g = 4.7 \times 10^3$ m s^{-1} in (100)-oriented GaAs.[9]

For the one-dimensional case, one branch of the dispersion relation occurs for each atom per unit cell of the lattice. The example we considered had two atoms per unit cell, so we had an optic and an acoustic branch. In three dimensions we add extra degrees of freedom, resulting in a total of three acoustic and three optic branches. In our example,

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[8] Lattice vibration dispersion relations for additional semiconductor crystals may be found in H. Bilz and W. Kress, *Phonon Dispersion Relations in Insulators*, Springer Series in Solid-State Sciences **10**, Springer-Verlag, Berlin, 1979 (ISBN 3 540 09399 0).

[9] For comparison, the speed of sound in air at temperature 0 °C at sea level is 331.3 m s^{-1} or 741 mph.

for a wave propagating in a given direction there is one *longitudinal acoustic* and one *longitudinal optic* branch with atom motion parallel to the wave propagation direction. There are also two *transverse acoustic* and two *transverse optic* branches with atom motion normal to the direction of wave propagation.

To get an idea of the complexity of a real lattice vibration dispersion relation, consider the example of GaAs. Device engineers are interested in GaAs because it is an example of a III-V compound semiconductor that is used to make laser diodes and high-speed transistors. GaAs has the zinc blende crystal structure with a lattice constant of $L = 0.565$ nm. Ga and As atoms have different atomic masses, and so we expect the dispersion relation to have three optic and three acoustic branches. Because the positions of the atoms in the crystal and the values of the spring constants are more complex than in the simple linear chain model we considered, it should come as no surprise that the dispersion relation is also more complex. Figure 1.11 shows the dispersion relation along the principal crystal symmetry directions of bulk GaAs.

1.3 Classical electromagnetism

We now take our ideas of fields and the tools we have developed to solve differential equations from classical mechanics and apply them to electromagnetism. In the following, we divide our discussion between electrostatics and electrodynamics.

1.3.1 Electrostatics

We will only consider stationary distributions of charges and fields. However, to obtain results it is necessary to introduce charge and to build up electric fields slowly over time to obtain the stationary charge distributions we are interested in. This type of adiabatic integration is a standard approach that is used to find solutions to many practical problems.

A basic starting point is the experimental observation that the electrostatic force due to a point charge Q in vacuum (free space) separated by a distance r from charge $-Q$ is

$$\mathbf{F}(\mathbf{r}) = \frac{-Q^2}{4\pi\varepsilon_0 r^2}\hat{\mathbf{r}} \tag{1.34}$$

where $\varepsilon_0 = 8.8541878 \times 10^{-12}$ F m^{-1} is the permittivity of free space measured in units of farads per meter. Force is an example of a vector field the direction of which, in this case, is given by the unit vector $\hat{\mathbf{r}}$. It is a central force because it has no angular dependence. Electrostatic force is measured in units of newtons (N), and charge is measured in coulombs (C). We will be interested in the force experienced by an electron with charge $Q = -e = -1.6021765 \times 10^{-19}$ C.

The force experienced by a charge e in an electric field is $\mathbf{F} = e\mathbf{E}$, where $\mathbf{E}$ is the electric field. Electric field is an example of a vector field, and its magnitude is measured in units of volts per meter (V m^{-1}). The (negative) potential energy is just the force times the distance moved

$$-eV = \int e\mathbf{E} \cdot d\hat{\mathbf{x}} \tag{1.35}$$

Electrostatic force can be related to potential via $\mathbf{F} = -e\nabla V$, and hence the coulomb potential energy due to a point charge e in vacuum (free space) separated by a distance r from charge $-e$ is

$$eV(r) = \frac{-e^2}{4\pi\varepsilon_0 r} \tag{1.36}$$

The coulomb potential is an example of a scalar field. Because it is derived from a central force, the coulomb potential has no angular dependence and is classified as a central-force potential. The coulomb potential is measured in volts (V) and the coulomb potential energy is measured in joules (J) or electron volts (eV).

When there are no currents or time-varying magnetic fields, the Maxwell equations we will use for electric field **E** and magnetic flux density **B** are

$$\nabla \cdot \mathbf{E} = \rho/\varepsilon_0\varepsilon_\mathrm{r} \tag{1.37}$$

and

$$\nabla \cdot \mathbf{B} = 0 \tag{1.38}$$

In the first equation, ε_r is the relative permittivity of the medium, and ρ is charge density. We chose to define the electric field as $\mathbf{E} = -\nabla V$. Notice that because electric field is given by the negative gradient of the potential, only *differences* in the potential are important. The direction of electric field is positive from positive electric charge to negative electric charge. Sometimes it is useful to visualize electric field as field lines originating on positive charge and terminating on negative charge. The divergence of the electric field is the local charge density. It follows that the flux of electric field lines flowing out of a closed surface is equal to the charge enclosed. This is Gauss's law, which may be expressed as

$$\int_V \nabla \cdot \mathbf{E}\, dV = \oint_S \mathbf{E} \cdot d\mathbf{S} = \int_V (\rho/\varepsilon_0\varepsilon_\mathrm{r}) dV \tag{1.39}$$

where the two equations on the left-hand side are expressions for the net electric flux out of the region (Stokes's theorem) and the right-hand side is enclosed charge.

Maxwell's expression for the divergence of the magnetic flux density given in Eqn (1.38) is interpreted physically as there being no magnetic monopoles (leaving the possibility of dipole and higher-order magnetic fields). Magnetic flux density **B** is an example of a vector field, and its magnitude is measured in units of tesla (T).

Sometimes it is useful to define another type of electric field called the displacement vector field, $\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$. In this expression, ε_r is the average value of the relative permittivity of the material in which the electric field exists. It is also useful to define the quantity $\mathbf{H} = \mathbf{B}/\mu_0\mu_r$, which is the magnetic field vector where μ_0 is called the permeability of free space and μ_r is called the relative permeability.

1.3.1.1 The parallel-plate capacitor

Electric charge and energy can be stored by doing work to spatially separate charges Q and $-Q$ in a capacitor. Capacitance is the proportionality constant relating the potential applied to the amount of charge stored. Capacitance is defined as

$$\boxed{C = \frac{Q}{V}} \tag{1.40}$$

and is measured in units of farads (F).

A capacitor is a very useful device for storing electric charge. A capacitor is also an essential part of the field-effect transistor used in silicon integrated circuits and thus is of great interest to electrical engineers.

We can use Maxwell's equations to figure out how much charge can be stored for every volt of potential applied to a capacitor. We start by considering a very simple geometry consisting of two parallel metal plates that form the basis of a parallel-plate capacitor.

Figure 1.12 is an illustration of a parallel-plate capacitor. Two thin, square, metal plates each of area A are placed facing each other a distance d apart in such a way that $d \ll \sqrt{A}$. One plate is attached to the positive terminal of a battery, and the other plate is attached to the negative terminal of the same battery, which supplies a voltage V. We may calculate the capacitance of the device by noting that the charge per unit area on a plate is ρ and the voltage is just the integral of the electric field between the plates, so

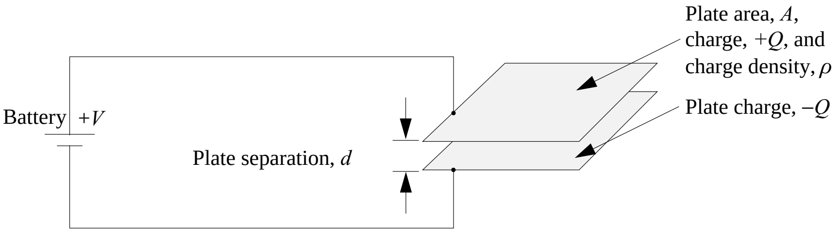

Fig. 1.12. Illustration of a parallel-plate capacitor attached to a battery supplying voltage V. The capacitor consists of two thin, square, metal plates each of area A facing each other a distance d apart.

that $V = |\mathbf{E}| \times d = \rho d/\varepsilon_0\varepsilon_r$. Hence,

$$C = \frac{Q}{V} = \frac{\rho A}{\rho d/\varepsilon_0\varepsilon_r} = \frac{\varepsilon_0\varepsilon_r A}{d} \tag{1.41}$$

where ε_r is the relative permittivity or dielectric constant of the material between the plates. This is an accurate measure of the capacitance, and errors due to fringing fields at the edges of the plates are necessarily small, since $d \ll \sqrt{A}$.

We now consider the values of numbers used in a physical device. A typical parallel-plate capacitor has $d = 100$ nm and $\varepsilon_r = 10$, so the amount of extra charge per unit area per unit volt of potential difference applied is $Q = CV = \varepsilon_0\varepsilon_r V/d = 8.8 \times 10^{-4}\ \mathrm{C\,m^{-2}}V^{-1}$ or, in terms of number of electrons per square centimeter per volt, $Q = 5.5 \times 10^{11}$ electrons $\mathrm{cm^{-2}\ V^{-1}}$. On average this corresponds to one electron per $(13.5\ \mathrm{nm})^2\ \mathrm{V^{-1}}$. In a metal, this electron charge might sit in the first 0.5 nm from the surface, giving a density of $\sim 10^{19}\ \mathrm{cm^{-3}}$ or 10^{-4} of the typical bulk charge density in a metal of $10^{23}\ \mathrm{cm^{-3}}$. A device of area 1 $\mathrm{mm^2}$ with $d = 100$ nm and $\varepsilon_r = 10$ has capacitance $C = 88$ nF.

The extra charge sitting on the metal plates creates an electric field between the plates. We may think of this electric field as storing energy in the capacitor. To figure out how much energy is stored in the electric field of the capacitor, we need to calculate the current that flows when we hook up a battery that supplies voltage V. The current flow, I, measured in amperes, is simply $dQ/dt = C \cdot dV/dt$, so the instantaneous power supplied at time t to the capacitor is IV, which is just $dQ/dt = C \cdot dV/dt$ times the voltage. Hence, the instantaneous power is $CV \cdot dV/dt$. The energy stored in the capacitor is the integral of the instantaneous power from a time when there is no extra charge on the plates, say time $t' = -\infty$ to time $t' = t$. At $t = -\infty$ the voltage is zero and so the stored energy is

$$\Delta E = \int\limits_{t'=-\infty}^{t'=t} CV\frac{dV}{dt'}dt' = \int\limits_{V'=0}^{V'=V} CV'dV' = \frac{1}{2}CV^2 \tag{1.42}$$

$$\boxed{\Delta E = \frac{1}{2}CV^2} \tag{1.43}$$

Since capacitance of the parallel-plate capacitor is $C = Q/V = \varepsilon_0\varepsilon_r A/d$ and the magnitude of the electric field is $|\mathbf{E}| = V/d$, we can rewrite the stored energy *per unit volume* in terms of the electric field to give a stored *energy density* $\Delta U = \varepsilon_0\varepsilon_r|\mathbf{E}|^2/2$. Finally, substituting in the expression $\mathbf{D} = \varepsilon_0\varepsilon_r\mathbf{E}$, one obtains the result

$$\boxed{\Delta U = \frac{1}{2}\mathbf{E} \cdot \mathbf{D}} \tag{1.44}$$