

# Chapter 1

## Introduction

### 1.1 Quantum mechanics and real life

Quantum mechanics, we might think, is a strange subject, one that does not matter for daily life. Only a few people, therefore, should need to worry about its difficult details. These few, we might imagine, run about in the small dark corners of science, at the edge of human knowledge. In this unusual group, we would expect to find only physicists making ever larger machines to look at ever smaller objects, chemists examining the last details of tiny atoms and molecules, and perhaps a few philosophers absently looking out the window as they wonder about free will. Surely, quantum mechanics therefore should not matter for our everyday experience. It could not be important for designing and making real things that make real money and change real lives. Of course, we would be wrong.

Quantum mechanics is everywhere. We do not have to look far to find it. We only have to open our eyes. Look at some object, say a flowerpot or a tennis ball. Why is the flowerpot a soothing terra-cotta orange color and the tennis ball a glaring fluorescent yellow? We could say each object contains some appropriately colored pigment or dye, based on a material with an intrinsic color, but we are not much further forward in understanding. (Our color technology would also be stuck in medieval times, when artists had to find all their pigments in the colors in natural objects, sometimes at great cost.<sup>1</sup>) The particularly bright yellow of our modern tennis ball would also be quite impossible if we restricted our pigments to naturally occurring materials.

Why does each such pigment have its color? We have no answer from the “classical” physics and chemistry developed before 1900. But quantum mechanics answers such questions precisely and completely.<sup>2</sup> Indeed, the beginning of quantum mechanics comes from one

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<sup>1</sup> They had to pay particularly dearly for their ultramarine blue, a pigment made by grinding up the gemstone *lapis lazuli*. The Spanish word for blue, *azul*, and the English word *azure* both derive from this root. The word *ultramarine* refers to the fact that the material had to be brought from “beyond (ultra) the sea (marine)” – i.e., imported, presumably also at some additional cost. Modern blue coloring is more typically based on copper phthalocyanine, a relatively cheap, manmade chemical.

<sup>2</sup> In quantum mechanics, photons, the quantum mechanical particles of light, have different colors depending on their tiny energies; materials have energy levels determined by the quantum mechanics of electrons, energy levels separated by similarly tiny amounts. We can change the electrons from one energy level to another by absorbing or emitting photons. The specific color of an object comes from the specific separations of the energy levels in the material. A few aspects of color can be explained without quantum mechanics. Color can sometimes result from scattering (e.g., the blue of the sky or the white of

particular aspect of color. Classical physics famously failed to explain the color of hot objects,<sup>3</sup> such as the warm yellow of the filament in a light bulb or the glowing red of hot metal in a blacksmith's shop. Max Planck realized in 1900 that if the energy in light existed only in discrete steps, or quanta, he could get the right answer for these colors. And so, quantum mechanics was born.

The impact of quantum mechanics in explaining our world does not end with color. We have to use quantum mechanics in explaining most properties of materials. Why are some materials hard and others soft? For example, why can a diamond scratch almost anything, but a pencil lead will slide smoothly, leaving a black line behind it?<sup>4</sup> Why do metals conduct electricity and heat easily but glass does not? Why is glass transparent? Why do metals reflect light? Why is one substance heavy and another light? Why is one material strong and another brittle? Why are some metals magnetic and others are not? We need, of course, a good deal of other science, such as chemistry, materials science, and other branches of physics, to answer such questions in any detail; but, in doing so, all of these sciences will rely on our quantum mechanical view of how materials are put together.

So, we might now believe, the consequences of quantum mechanics are essential for understanding the ordinary world around us. But is quantum mechanics useful? If we devote our precious time to learning it, will it let us make things we could not make before? One science in which the quantum mechanical view is obviously essential is chemistry, the science that enables most of our modern materials. No one could deny that chemistry is useful.

Suppose even that we set chemistry and materials themselves aside and ask a harder question: Do we need quantum mechanics when we design devices – objects intended to perform some worthwhile function? After all, the washing machines, eyeglasses, staplers, and automobiles of everyday life need only nineteenth century physics for their basic mechanical design, even if we employ the latest alloys, plastics, or paints to make them. Perhaps we can concede such macroscopic mechanisms to the classical world. But when, for example, we look at the technology to communicate and process information, we have simply been forced to move to quantum mechanics. Without quantum theory as a practical technique, we would not be able to design the devices that run our computers and our Internet connections.

The mathematical ideas of computing and information had begun to take their modern shape in the 1930s, 1940s and 1950s. By the 1950s, telephones and broadcast communication were well established and the first primitive electronic computers had been demonstrated. The transistor and integrated circuit were the next key breakthroughs. These devices made complex computers and information switching and processing practical. These devices relied heavily on the quantum mechanical physics of crystalline materials.

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some paints), diffraction (e.g., by a finely ruled grating or a hologram), or interference (e.g., the varied colors of a thin layer of oil on the surface of water), all of which can be explained by classical wave effects. All such classical wave effects are also explained as limiting cases of quantum mechanics, of course.

<sup>3</sup> This problem was known as the “ultraviolet catastrophe” because classical thermal and statistical physics predicted that any warm object would emit ever-increasing amounts of light at ever shorter wavelengths. The colors associated with such wavelengths would necessarily extend past the blue into the ultraviolet – hence, the name.

<sup>4</sup> Even more surprising here is that diamonds and pencil lead are both made from exactly the same element, carbon.

A well-informed devil's advocate could still argue, though, that the design of transistors and integrated circuits themselves was initially still an activity using classical physics. Designers would still use the idea of resistance from nineteenth-century electricity, even if they added the ideas of charged electrons as particles carrying the current, and would add various electrical barriers (or “potentials”) to persuade electrons to go one way or another. No modern transistor designer can ignore quantum mechanics, however. For example, when we make small transistors, we must also make very thin electrical insulators. Electrons can manage to penetrate through the insulators because of a purely quantum mechanical process known as *tunneling*. At the very least, we have to account for that tunneling current as an undesired, parasitic process in our design.

As we try to shrink transistors to ever smaller sizes, quantum mechanical effects become progressively more important. Naively extrapolating the historical trend in miniaturization would lead to devices the size of small molecules in the first few decades of the twenty-first century. Of course, the shrinkage of electronic devices as we know them cannot continue to that point. But, as we make ever tinier devices, quantum mechanical processes become ever more important. Eventually, we may need new device concepts beyond the semiclassical transistor; it is difficult to imagine how such devices would not involve yet more quantum mechanics.

We might argue, at least historically, about the importance of quantum mechanics in the design of transistors. We could have no comparable debate when we consider two other technologies crucial for handling information: optical communications and magnetic data storage.

Today, nearly all the information we send over long distances is carried on optical fibers – strands of glass about the thickness of a human hair. We very carefully put a very small light just at one end of that fiber. We send the “ones” and “zeros” of digital signals by rapidly turning that light on and off and looking for the pattern of flashes at the fiber's other end. To send and receive these flashes, we need optoelectronic devices – devices that will change electrical signals into optical pulses and vice versa. All of these optoelectronic devices are quantum mechanical on many different levels. First, they mostly are made of crystalline semiconductor materials, just like transistors, and hence rely on the same underlying quantum mechanics of such materials. Second, they send and receive photons, the particles of light Einstein proposed to expand upon Planck's original idea of quanta. Here, these devices are exploiting one of the first of many strange phenomena of quantum mechanics, the photoelectric effect. Third, most modern semiconductor optoelectronic devices used in telecommunications employ very thin layers of material, layers called *quantum wells*. The properties of these thin layers depend exquisitely on their thicknesses through a textbook piece of quantum mechanics known as the “particle-in-a-box” problem. That physics allows us to optimize some of the physical processes we already had in thicker layers of material and also to create some new mechanisms only seen in thin layers. For such devices, engineering using quantum mechanics is both essential and very useful.

When we try to pack more information onto the magnetic hard disk drives in our computers, we first have to understand exactly how the magnetism of materials works. That magnetism is almost entirely based on a quantum mechanical attribute called *spin* – a phenomenon with no real classical analog. The sensors that read the information off the drives are also often now based on sophisticated structures with multiple thin layers that are designed completely with quantum mechanics.

Quantum mechanics is, then, a subject increasingly necessary for engineering devices, especially as we make small devices or exploit quantum mechanical properties that only occur

in small structures. The examples given here are only a few from a broad and growing field that can be called *nanotechnology*. Nanotechnology exploits our expanding abilities to make very small structures or patterns. The benefits of nanotechnology come from the new properties that appear at these very small scales. We get most of those new properties from quantum mechanical effects of one kind or another. Quantum mechanics is, therefore, essential for nanotechnology.

## 1.2 Quantum mechanics as an intellectual achievement

Any new scientific theory has to give the same answers as the old theories everywhere these previous models worked and yet successfully describe phenomena that previously we could not understand. The prior theories of mechanics, Newton's Laws, worked very well in a broad range of situations. Our models for light similarly were quite deep and had achieved a remarkable unification of electricity and magnetism (in Maxwell's equations). But, when we would try to make a model of the atom, for example, with electrons circling around some charged nucleus like satellites in orbit around the earth, we would meet major contradictions. Existing mechanics and electromagnetic theory would predict that any such orbiting electron would constantly be emitting light; but, atoms simply do not do that.

The challenge for quantum mechanics was not an easy one. To resolve these problems of light and the structure of matter, we actually had to tear down much of our view of the way the world works, to a degree never seen since the introduction of natural philosophy and the modern scientific method in the Renaissance. We were forced to construct a completely new set of principles for the physical world. These were, and still are in many cases, completely bizarre and certainly different from our intuition. Many of these principles simply have no analogs in our normal view of reality.

We mentioned previously one of the bizarre aspects of quantum mechanics: the process of tunneling allows particles to penetrate barriers that are classically too high for them to overcome. This process is, however, actually nothing like the act of digging a tunnel; we are confronting here the common difficulty in quantum mechanics of finding words or analogies from everyday experience to describe quantum mechanical ideas. We will often fail.

There are many other surprising aspects of quantum mechanics. The typical student starting quantum mechanics is confused when told, as he or she often will be, that some question simply does not have an answer. The student will, for example, think it perfectly reasonable to ask what are the position and momentum (or, more loosely, speed) of some particle, such as an electron. Quantum mechanics (or, in practice, its human oracle, the professor) will enigmatically reply that there is no answer to that question. We can know one or the other precisely but not both at once. This particular enigma is an example of Heisenberg's uncertainty principle.

Quantum mechanics does raise more than its share of deep questions, and it is arguable that we still do not understand quantum mechanics. In particular, there are still major questions about what a measurement really is in the quantum world. Erwin Schrödinger famously dramatized the difficulty with the paradox of his cat. According to quantum mechanics, an object may exist in a superposition state, in which it is, for example, neither definitely on the left nor on the right. Such superposition states are not at all unusual – in fact, they occur all the time for electrons in any atom or molecule. Though a particle might be in a superposition state, when we try to measure it, we always find that the object is at some specific position (e.g., definitely on the left or on the right). This mystical phenomenon is known as “collapse of the

wavefunction.” We might find that to be a bizarre idea, but one that – for something really tiny like an electron – we could perhaps accept.

But now Schrödinger proposes that we think not about an electron but instead about his cat. We are likely to care much more about the welfare of this “object” than we did about some electron. An electron is, after all, easily replaced with another just the same<sup>5</sup>; there are plenty of them – in fact, something like  $10^{24}$  electrons in every cubic centimeter of any solid material. And Schrödinger constructs a dramatic scenario. His cat is sealed in a box with a lethal mechanism that may go off as a result of, for example, radioactive decay. Before we open the box to check on it, is the cat alive, dead, or, as quantum mechanics might seem to suggest, in some “superposition” of the two?

The superposition hypothesis now seems absurd. In truth, we cannot check it here; we do not know how to set up an experiment to test such quantum mechanical notions with macroscopic objects. In trying to repeat such an experiment, we cannot set up the same starting state exactly enough for something as complex as a cat. Physicists disagree about the resolution of this paradox. It is an example of a core problem of quantum mechanics: the process of measurement, with its mysterious “collapse of the wavefunction,” cannot be explained by quantum mechanics.<sup>6</sup> The proposed solutions to this measurement problem can be extremely bizarre; in the “many worlds” hypothesis, for example, the world is supposed continually to split into multiple realities, one for each possible outcome of each possible measurement.

Another important discussion centers around whether quantum mechanics is complete. When we measure a quantum mechanical system, there is at least in practice some randomness in the result. If, for example, we tried to measure the position of an electron in an atom, we would keep getting different results. Or, if we measured how long it took a radioactive nucleus to decay, we would get different numbers each time. Quantum mechanics would correctly predict the average position we would measure for the electron and the average decay time of the nucleus, but it would not tell us the specific position or time yielded by any particular measurement.

We are, of course, quite used to randomness in our ordinary classical world. The outcome of many lotteries is decided by which numbered ball appears out of a chute in a machine. The various different balls are all bouncing around inside the machine, driven probably by some air blower. The process is sufficiently complicated that we cannot practically predict which ball will emerge, and all have equal chance. But we do tend to believe classically that if we knew the initial positions and velocities of all the air molecules and the balls in the machine, we could, in principle, predict which ball would emerge. Those variables are, in practice, hidden from us, but we do believe they exist. Behind the apparent randomness of quantum mechanics, then, are there just similarly some hidden variables? Could we actually predict outcomes precisely if we knew what those hidden variables were? Is the apparent randomness of quantum mechanics just because of our lack of understanding of some deeper theory and its starting conditions, some “complete” theory that would supersede quantum mechanics?

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<sup>5</sup> Indeed, in quantum mechanics, electrons can be absolutely identical, much more identical than the so-called “identical” toys from an assembly line or “identical” twins in a baby carriage.

<sup>6</sup> If, at this point, the reader raises an objection that there is an inconsistency in saying that quantum mechanics will only answer questions about things we can measure but quantum mechanics cannot explain the process of measurement, the reader would be quite justified in doing so!

Einstein believed that, indeed, quantum mechanics was not complete, that there were some hidden variables that, once we understood them, would resolve and remove its apparent randomness. Relatively recent work, centered around a set of relations called Bell's inequalities, shows rather surprisingly that there are no such hidden variables (or, at least, not local ones that propagate with the particles) and that, despite its apparent absurdities, quantum mechanics may well be a complete theory in this sense.

It also appears that quantum mechanics is “nonlocal”: two particles can be so “entangled” quantum mechanically that measuring one of them can apparently instantaneously change the state of the other one, no matter how far away it is (though it is not apparently possible to use such a phenomenon to communicate information faster than the velocity of light).<sup>7</sup>

Despite all its absurdities and contradictions of common sense, and despite the initial disbelief and astonishment of each new generation of students, quantum mechanics works. As far as we know, it is never wrong; we have made no experimental measurement that is known to contradict quantum mechanics, and there have been many exacting tests. Quantum mechanics is both stunningly radical and remarkably right. It is an astonishing intellectual achievement.

The story of quantum mechanics itself is far from over. We are still trying to understand exactly what are all the elementary particles and just what are the implications of such theories for the nature of the universe.<sup>8</sup> Many researchers are working on the possibility of using some of the strange possibilities of quantum mechanics for applications in handling information transmission. One example would send messages whose secrecy was protected by the laws of quantum physics, not just the practical difficulty of cracking classical codes. Another example is the field of quantum computing, in which quantum mechanics might allow us to solve problems that would be too hard ever to be solved by any conventional machine.

### 1.3 Using quantum mechanics

At this point, the poor student may be about to give up in despair. How can one ever understand such a bizarre theory? And, if one cannot understand it, how can one even think of using it? Here is the good news: whether we think we understand quantum mechanics, and whether there is yet more to discover about how it works, quantum mechanics is surprisingly easy to use.

The prescriptions for using quantum mechanics in a broad range of practical problems and engineering designs are relatively straightforward. They use the same mathematical techniques most engineering and science students will already have mastered to deal with the “classical” world.<sup>9</sup> Because of a particular elegance in its mathematics,<sup>10</sup> quantum mechanical calculations can actually be easier than those in many other fields.

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<sup>7</sup> This nonlocality is often known through the original “EPR” thought experiment or paradox proposed by Einstein, Podolsky, and Rosen.

<sup>8</sup> Such theories require relativistic approaches that are, unfortunately, beyond the scope of this book.

<sup>9</sup> In the end, most calculations require performing integrals or manipulating matrices. Many of the underlying mathematical concepts are ones that are quite familiar to engineers used to Fourier analysis, e.g., or other linear transforms.

<sup>10</sup> Quantum mechanics is based entirely and exactly on linear algebra. Unlike most other uses of linear algebra, the fundamental linearity of quantum mechanics is apparently *not* an approximation.



The main difficulty the beginning student has with quantum mechanics lies in knowing which of our classical notions of the world have to be discarded, and what new notions we have to use to replace them.<sup>11</sup> The student should expect to spend some time in disbelief and conflict with what is being asserted in quantum mechanics – that is entirely normal! In fact, a good fight with these propositions is perhaps psychologically necessary, like the clarifying catharsis of an old-fashioned barroom brawl.

And, there is a key point that simplifies all the absurdities and apparent contradictions: provided we only ask questions about quantities that can be measured, there are no philosophical problems that need worry us or, at least, that would prevent us from calculating anything that we could measure.<sup>12</sup> As we use quantum mechanical principles in tangible applications, such as electronic or optical devices and systems, the apparently bizarre aspects become simply commonplace and routine. The student may soon stop worrying about quantum mechanical tunneling and Heisenberg's uncertainty principle. In the foreseeable future, such routine comprehension and acceptance may also extend to concepts such as nonlocality and entanglement as we press them increasingly into practical use.

Understanding quantum mechanics does certainly mark a qualitative change in one's view of how the world actually works.<sup>13</sup> That understanding gives students the opportunity to apply this knowledge in ways that others cannot begin to comprehend.<sup>14</sup> Whether the goal is basic understanding or practical exploitation, learning quantum mechanics is, in this author's opinion, certainly one of the most fascinating things one can do with one's brain.

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<sup>11</sup> The associated teaching technique of breaking down the student's beliefs and replacing them with the professor's "correct" answers has a lot in common with brainwashing!

<sup>12</sup> This philosophical approach of dealing only with questions that can be answered by measurement (or that are purely logical questions within some formal system of logic) and regarding all other questions as meaningless is essentially what is known in the philosophical world as "logical positivism." It is the most common approach taken in dealing with quantum mechanics, at least at the elementary philosophical level, and, by allowing university professors to dismiss most student questions as meaningless, saves a lot of time in teaching the subject!

<sup>13</sup> It is undoubtedly true that if one does not understand quantum mechanics, one does not understand how the world actually works. It may also, however, be true that even if one does understand quantum mechanics, one still may not understand how the world works.

<sup>14</sup> Despite the inherent sense of superiority such an understanding may give the student, it is, however – as many physicists have already regrettably found – not particularly useful to point this out at parties.

# Chapter 2

## Waves and quantum mechanics – Schrödinger's equation

Prerequisites: Appendix A Background mathematics; Appendix B Background physics.

If the world of quantum mechanics is so different from everything we have been taught before, how can we even begin to understand it? Miniscule electrons seem so remote from what we see in the world around us that we do not know what concepts from our everyday experience we could use to get started. There is, however, one lever from our existing intellectual toolkit that we can use to pry open this apparently impenetrable subject, and that lever is the idea of waves. If we just allow ourselves to suppose that electrons might be describable as waves and follow the consequences of that radical idea, the subject can open up before us. Astonishingly, we will find we can then understand a large fraction of those aspects of our everyday experience that can only be explained by quantum mechanics, such as color and the properties of materials. We will also be able to engineer novel phenomena and devices for quite practical applications.

On the face of it, proposing that we describe particles as waves is a strange intellectual leap in the dark. There is apparently nothing in our everyday view of the world to suggest we should do so. Nevertheless, it was exactly such a proposal historically (i.e., de Broglie's hypothesis) that opened up much of quantum mechanics. That proposal was made before there was direct experimental evidence of wave behavior of electrons. Once that hypothesis was embodied in the precise mathematical form of Schrödinger's wave equation, quantum mechanics took off.

Schrödinger's equation remains to the present day one of the most useful relations in quantum mechanics. Its most basic application is to model simple particles that have mass, such as a single electron, though the extensions of it go much further than that. It is also a good example of quantum mechanics, exposing many of the more general concepts. We use these concepts as we go on to more complicated systems, such as atoms, or to other quite different kinds of particles and applications, such as photons and the quantum mechanics of light. Understanding Schrödinger's equation, therefore, is a very good way to start understanding quantum mechanics. In this chapter, we introduce the simplest version of Schrödinger's equation – the time-independent form – and explore some of the remarkable consequences of this wave view of matter.

### 2.1 Rationalization of Schrödinger's equation

Why do we have to propose wave behavior and Schrödinger's equation for particles such as electrons? After all, we are quite sure electrons are particles because we know that they have definite mass and charge. And we do not see directly any wave-like behavior of matter in our



everyday experience. It is, however, now a simple and incontrovertible experimental fact that electrons can behave like waves or, at least, in some way are “guided” by waves. We know this for the same reasons we know that light is a wave – we can see the interference and diffraction that are so characteristic of waves. At least in the laboratory, we see this behavior routinely.

We can, for example, make a beam of electrons by applying a large electric field in a vacuum to a metal, pulling electrons out of the metal to create a monoenergetic electron beam (i.e., all with the same energy). We can then see the wave-like character of electrons by looking for the effects of diffraction and interference, especially the patterns that can result from waves interacting with particular kinds or shapes of objects.

One common situation in the laboratory is, for example, to shine such a beam of electrons at a crystal in a vacuum. Davisson and Germer did exactly this in their famous experiment<sup>1</sup> in 1927, diffracting electrons off a crystal of nickel. We can see the resulting diffraction if, for example, we let the scattered electrons land on a phosphor screen as in a television tube (cathode ray tube); we will see a pattern of dots on the screen. We would find that this diffraction pattern behaved rather similarly to the diffraction pattern we might get in some optical experiment; we could shine a monochromatic (i.e., single frequency) light beam at some periodic structure<sup>2</sup> whose periodicity was of a scale comparable to the wavelength of the waves (e.g., a diffraction grating). The fact that electrons behave both as particles (e.g., they have a specific mass and a specific charge) and as waves is known as a *wave-particle duality*.<sup>3</sup>

The electrons in such wave diffraction experiments behave as if they have a wavelength

$$\lambda = \frac{h}{p} \quad (2.1)$$

where  $p$  is the electron momentum and  $h$  is Planck's constant

$$h \cong 6.626 \times 10^{-34} \text{ Joule} \cdot \text{seconds}$$

(This relation, Eq. (2.1), is known as de Broglie's hypothesis). For example, the electron can behave as if it were a plane wave, with a wavefunction  $\psi$ , propagating in the  $z$  direction, and of the form<sup>4</sup>

$$\psi \propto \exp(2\pi iz / \lambda) \quad (2.2)$$

If it is a wave, or is behaving as such, we need a wave equation to describe the electron. We find empirically<sup>5</sup> that the electron behaves like a simple scalar wave (i.e., not like a vector wave, such as electric field,  $\mathbf{E}$ , but like a simple acoustic [sound] wave with a scalar amplitude; in acoustics, the scalar amplitude could be the air pressure). We therefore propose that the

<sup>1</sup> C. Davisson and L. H. Germer, “Diffraction of Electrons by a Crystal of Nickel,” *Phys. Rev.* **30**, 705 – 740 (1927)

<sup>2</sup> That is, a structure whose shape repeats itself in space, with some spatial “period” or length.

<sup>3</sup> This wave-particle duality is the first and one of the most profound of the apparently bizarre aspects of quantum mechanics that we will encounter.

<sup>4</sup> We have chosen a complex wave here,  $\exp(2\pi iz / \lambda)$ , rather than a simpler real wave, e.g.,  $\sin(2\pi z / \lambda)$  or  $\cos(2\pi z / \lambda)$ , because the mathematics of quantum mechanics is set up to require the use of complex numbers. The choice does also make the algebra easier.

<sup>5</sup> At least in the absence of magnetic fields or other magnetic effects.

electron wave obeys a scalar wave equation, and we choose the simplest one we know: the *Helmholtz wave equation* for a monochromatic wave. In one dimension, the Helmholtz equation is

$$\frac{d^2\psi}{dz^2} = -k^2\psi \quad (2.3)$$

This equation has solutions such as  $\sin(kz)$ ,  $\cos(kz)$ , and  $\exp(ikz)$  (and  $\sin(-kz)$ ,  $\cos(-kz)$ , and  $\exp(-ikz)$ ) that all describe the spatial variation in a simple wave. In three dimensions, we can write this as

$$\nabla^2\psi = -k^2\psi \quad (2.4)$$

where the symbol  $\nabla^2$  (known variously as the *Laplacian operator*, *del squared*, and *nabla squared*, and sometimes written  $\Delta$ ) means

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \quad (2.5)$$

where  $x$ ,  $y$ , and  $z$  are the usual Cartesian coordinates, all at right angles to one another. This has solutions such as  $\sin(\mathbf{k}\cdot\mathbf{r})$ ,  $\cos(\mathbf{k}\cdot\mathbf{r})$ , and  $\exp(i\mathbf{k}\cdot\mathbf{r})$  (and  $\sin(-\mathbf{k}\cdot\mathbf{r})$ ,  $\cos(-\mathbf{k}\cdot\mathbf{r})$ , and  $\exp(-i\mathbf{k}\cdot\mathbf{r})$ ), where  $\mathbf{k}$  and  $\mathbf{r}$  are vectors. The wavevector magnitude,  $k$ , is defined as

$$k = 2\pi / \lambda \quad (2.6)$$

or, equivalently, given the empirical wavelength exhibited by the electrons (i.e., de Broglie's hypothesis, Eq. (2.1))

$$k = p / \hbar \quad (2.7)$$

where

$$\hbar = h / 2\pi \cong 1.055 \times 10^{-34} \text{ Joule} \cdot \text{seconds}$$

(a quantity referred to as *h bar*). With our expression for  $k$  (Eq. (2.7)), we can rewrite our simple wave equation (Eq. (2.4)) as

$$-\hbar^2 \nabla^2 \psi = p^2 \psi \quad (2.8)$$

We can now choose to divide both sides by  $2m_o$ , where, for the case of the electron,  $m_o$  is the free electron rest mass

$$m_o \cong 9.11 \times 10^{-31} \text{ kg}$$

to obtain

$$-\frac{\hbar^2}{2m_o} \nabla^2 \psi = \frac{p^2}{2m_o} \psi \quad (2.9)$$

But we know for Newtonian classical mechanics, where  $p = m_o v$  (with  $v$  as the velocity), that

$$\frac{p^2}{2m_o} \equiv \text{kinetic energy of an electron} \quad (2.10)$$

and, in general,