6.5 THE FINITE SQUARE WELL	6.5 HỐ THẾ CÓ BỀ SÂU HỮU HẠN
The "box" potential is an	Hố thế dạng "hộp" là một mô hình

oversimplification that is never realized in practice. Given sufficient energy, a particle can escape the confines of any well. The potential energy for a more realistic situation—the finite square well—is shown in Figure 6.15, and essentially is that depicted in Figure 6.6b before taking the limit V: <» . A classical particle with energy E greater than the well height U can penetrate the gaps at x = 0 and x = L to enter the outer region. Here it moves freely, but with reduced speed corresponding to a diminished kinetic energy E — U.

A classical particle with energy E less than U is permanently bound to the region 0 < x < L. Quantum mechanics asserts, however, that there is some probability that the particle can be found outside this region! That is, the wavefunction generally is nonzero outside the well, and so the probability of finding the particle here also is nonzero. For stationary states, the wavefunction p(x) is found from the time- independent Schrodinger equation. Outside the well where U(x) = U, this is

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with a2 = 2m(U — E)/h2 a constant. Because U > E, a2 necessarily is positive and the independent solutions to this equation are the real exponentials e+ax and e—ax. The positive exponential must be rejected in region III where x > L to keep p(x) finite as x : <»; likewise, the negative exponential must be rejected in region I where x < 0 to keep p(x)

đơn giản hóa quá mức không tồn tại trong thực tế. Khi có đủ năng lượng, một hạt có thể thoát ra khỏi bất kỳ hố thế nào. Thế năng ứng với trường hợp thực tế hơn-hố thế có bề sâu hữu hạn-được biểu diễn trong Hình 6.15, về cơ bản, thế này tương tự như Hình 6.6b tại giới hạn….Một hạt cổ điển có năng lượng E lớn hơn độ cao hố thế U có thể xuyên qua các khoảng trống tại x=0 hoặc x=L để đi ra vùng bên ngoài. Lúc đó nó sẽ chuyển động tự do nhưng vận tốc giảm do động năng giảm còn ….

<mark>checked</mark>

Một hạt cổ điển có năng lượng E nhỏ hơn U bị giam cầm mãi mãi trong vùng 0 < x < L. Tuy nhiên, cơ học lượng tử khẳng định rằng có một xác xuất nhất định để tìm thấy hạt nằm bên ngoài vùng này! Tức là, nói chung hàm sóng sẽ khác không bên ngoài giếng, và do đó xác suất tìm thấy hạt tại đó cũng khác không. Để tìm các hàm sóng ứng với các trạng thái dừng…., chúng ta dùng phương trình Schrodinger độc lập thời gian. Bên ngoài giếng U(x) = U, phương trình này có dạng

Trong đó a2 = 2m(U — E)/h2 là một hằng số. Vì U > E, a2 phải dương và các nghiệm độc lập của phương trình này là hãm e mũ thực e+ax và e—ax. Hàm e mũ dương này phải bằng không trong vùng III ứng với x > L để p(x) hữu hạn khi x : <»; Tương tự, hàm e mũ âm phải bằng không trong vùng I ứng với x < 0 để p(x) hữu hạn khi x : —<». Vì thế, sóng bên ngoài có dạng

finite as x : —<». Thus, the exterior wave takes the form

....

....

The coefficients A and B are determined by matching this wave smoothly onto the wavefunction in the well interior. Specifically, we require p(x) and its first derivative dp/dx to be continuous at x = 0 and again at x = L. This can be done only for certain values of E, corresponding to the allowed energies for the bound particle. For these energies, the matching conditions specify the entire wavefunction except for a multiplicative constant, which then is determined by normalization. Figure 6.16 shows the wavefunctions and probability densities that result for the three lowest allowed particle energies. Note that in each case the waveforms join smoothly at the boundaries of the potential well.

The fact that p is nonzero at the walls increases the de Broglie wavelength in the well (compared with that in the infinite well), and this in turn lowers the energy and momentum of the particle. This observation can be used to approximate the

Figure 6.16 (a) Wavefunctions for the lowest three energy states for a particle in a potential well of finite height. (b) Probability densities for the lowest three energy states for a
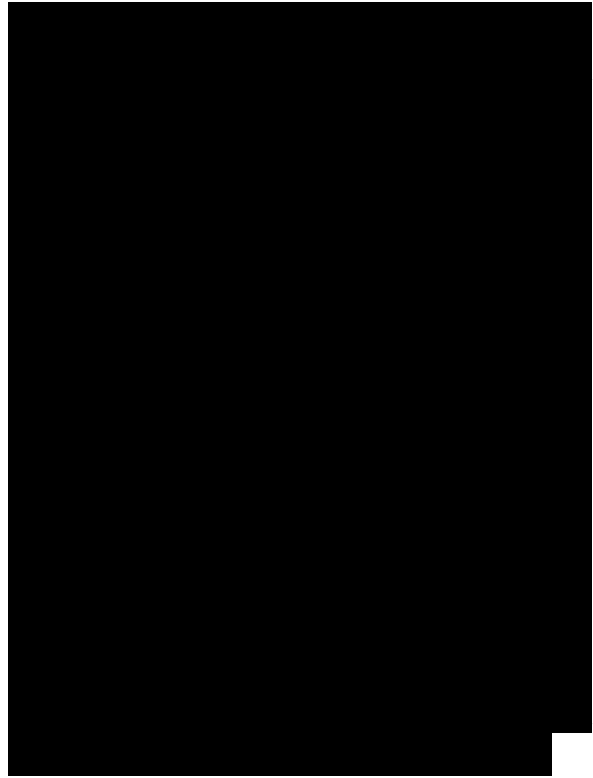
particle in a potential well of finite height.

allowed energies for the bound particle. The wavefunction penetrates the exterior region on a scale of length set by the penetration depth S, given by

 (6.21)

Specifically, at a distance S beyond the well edge, the wave amplitude has fallen to 1/e of its value at the edge and approaches zero exponentially in the exterior region. That is, the exterior wave is essentially zero beyond a distance S on either side of the potential well. If it were truly zero beyond this distance, the allowed energies would be those for an infinite well of length L + 2S (compare Equation 6.17), or

The allowed energies for a particle bound to the finite well are given approximately by Equation 6.22 so long as S is small compared with L. But S itself is energy dependent according to Equation 6.21. Thus, Equation 6.22 becomes an implicit relation for E that must be solved numerically for a given value of n. The approximation is best for the lowest-lying states and breaks down completely as E approaches U, where S becomes infinite. From this we infer (correctly) that the number of bound states is limited by the height U of our potential well. Particles with energies E exceeding U are not bound to the well, that is, they may be found with comparable probability in the

exterior regions. The case of unbound states will be taken up in the following chapter.

EXAMPLE 6.8 A Bound Electron
Estimate the ground-state energy for an electron confined to a potential well of width 0.200 nm and height 100 eV.

Solution We solve Equations 6.21 and 6.22 together, using an iterative procedure. Because we expect $E \ll U(= 100 \text{ eV})$, we estimate the decay length S by first neglecting E to get

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Thus, the effective width of the (infinite) well is $L + 2S = 0.239$ nm, for which we calculate the ground-state energy:

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From this Ewe calculate U- E= 93.42 eV and a new decay length

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This, in turn, increases the effective well width to 0.240 nm and lowers the ground- state energy to E= 6.53 eV. The iterative process is repeated until the desired accuracy is achieved. Another iteration gives the same result to the accuracy reported. This is in excellent agreement with the exact value, about 6.52 eV for this case.

Exercise 3 Bound-state waveforms and allowed energies for the finite square well also can be found using purely numerical methods. Go to our companion Web site (http://info.brookscole.com/mp3e)

and select QMTools Simulations : Exercise 6.3. The applet shows the potential energy for an electron confined to a finite well of width 0.200 nm and height 100 eV. Follow the on-site instructions to add a stationary wave and determine the energy of the ground state. Repeat the procedure for the first excited state. Compare the symmetry and the number of nodes for these two wavefunctions. Find the highest-lying bound state for this finite well. Count nodes to determine which excited state this is, and thus deduce the total number of bound states this well supports.

EXAMPLE 6.9 Energy of a Finite Well: Exact Treatment

Impose matching conditions on the interior and exterior wavefunctions and show how these lead to energy quantization for the finite square well.

Solution The exterior wavefunctions are the decaying exponential functions given by Equation 6.20 with decay constant a = [2m(U — E)/h2]1/2. The interior wave is an oscillation with wavenumber k = (2mE/h2)1/2 having the same form as that for the infinite well, Equation 6.15; here we write it as

rf/(x) = C sin kx + D cos kx for 0 < x < L

To join this smoothly onto the exterior wave, we insist that the wavefunction and its slope be
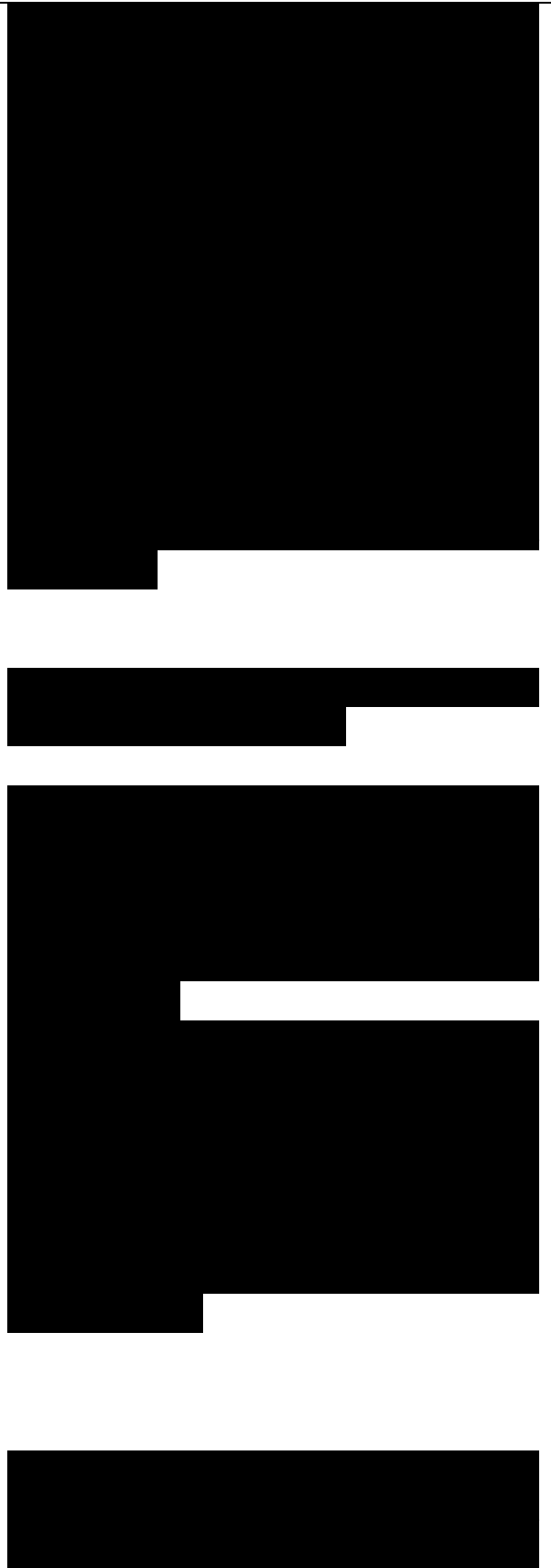
continuous at the well edges $x = 0$ and $x = L$. At $x = 0$ the conditions for smooth joining require

....

Dividing the second equation by the first eliminates A, leaving

C a ~D = ~k

In the same way, smooth joining at x = L requires

....

Again dividing the second equation by the first eliminates B. Then replacing C/D with a/k gives

....

For a specified well height U and width L, this last relation can only be satisfied for special values of E (E is contained in both k and a). For any other energies, the waveform will not match smoothly at the well edges, leaving a wavefunction that is physically inadmissable. (Note that the equation cannot be solved explicitly for E; rather, solutions must be obtained using numerical or graphical methods.)

Exercise 4 Use the result of Example 6.9 to verify that the ground-state energy for an electron confined to a square well of width 0.200 nm and height 100 eV is about 6.52 eV.

6.6 THE QUANTUM OSCILLATOR

Figure 6.17 A general potential function U(x). The points labeled a and c are positions of stable equilibrium, for which dU/dx = 0 and d2U/dx2 > 0. Point b

is a position of unstable equilibrium, for which

$dU/dx = 0$ and $d2U/dx2 < 0$.

As a final example of a potential well for which exact results can be obtained, let us examine the problem of a particle subject to a linear restoring force $F = —Kx$. Here x is the displacement of the particle from equilibrium $(x = 0)$ and K is the force constant. The corresponding potential energy is given by $U(x) = jKx2$. The prototype physical system fitting this description is a mass on a spring, but the mathematical description actually applies to any object limited to small excursions about a point of stable equilibrium.

Consider the general potential function sketched in Figure 6.17. The positions a, b, and c all label equilibrium points where the force $F = —dU/dx$ is zero. Further, positions a and c are examples of stable equilibria, but b is unstable. The stability of equilibrium is decided by examining the forces in the immediate neighborhood of the equilibrium point. Just to the left of a, for example, $F = —dU/dx$ is positive, that is, the force is directed to the right; conversely, to the right of a the force is directed to the left. Therefore, a particle displaced slightly from equilibrium at a encounters a force driving it back to the equilibrium point (restoring force). Similar arguments show that the equi-librium at c also is stable. On the other hand, a particle displaced in either direction
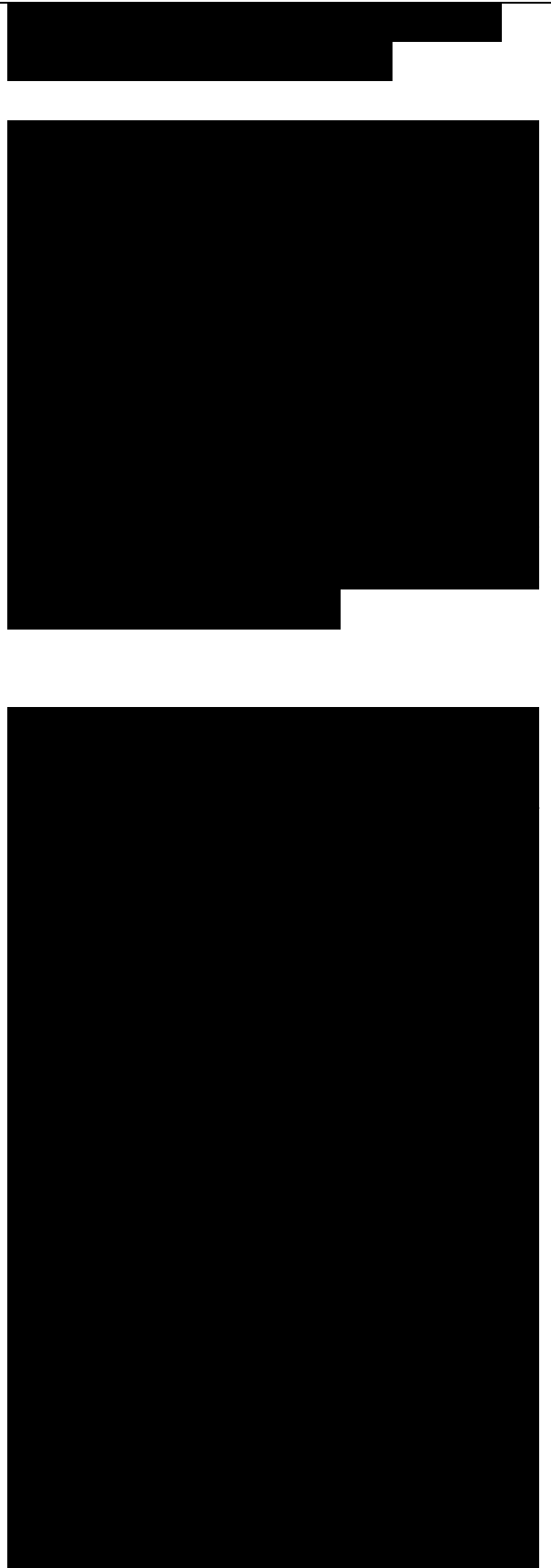
from point b experiences a force that drives it further away from equilibrium—an unstable condition. In general, stable and unstable equilibria are marked by potential curves that are concave or convex, respectively, at the equilibrium point. To put it another way, the curvature of U(x) is positive ($d2Uldx2 > 0$) at a point of stable equilibrium, and negative ($d2Uldx2 < 0$) at a point of unstable equilibrium.

Near a point of stable equilibrium such as a (or c), U(x) can be fit quite well by a parabola:

$$U (x) = U (a) + |k (x — a)2 \qquad (6.23)$$

Of course, the curvature of this parabola (= K) must match that of U(x) at the equilibrium point x = a:

Further, U(a), the potential energy at equilibrium, may be taken as zero if we agree to make this our energy reference, that is, if we subsequently measure all energies from this level. In the same spirit, the coordinate origin may be placed at x = a, in effect allowing us to set a = 0. With U(a) = 0 and a = 0, Equation 6.23 becomes the spring potential once again; in other words, a particle limited to small excursions about any stable equilibrium point behaves as if it were attached to a spring with a force constant K prescribed by the curvature of the true potential at equilibrium. In this way the oscillator becomes a first approximation to the vibrations occurring in many real systems.

The motion of a classical oscillator

with mass m is simple harmonic vibration at the angular frequency w = VK/to. If the particle is removed from equilibrium a distance A and released, it oscillates between the points x = — A and x = +A (A is the amplitude of vibration), with total energy E = ^KA2. By changing the initial point of release A, the classical particle can in principle be given any (nonnegative) energy whatsoever, including zero.

The quantum oscillator is described by the potential energy U (x) = \Kx2 = 2mw2x2 in the Schrodinger equation. After a little rearrangement we get

as the equation for the stationary states of the oscillator. The mathematical technique for solving this equation is beyond the level of this text. (The exponential and trigonometric forms for ^ employed previously will not work here because of the presence of x2 in the potential.) It is instructive, however, to make some intelligent guesses and verify their accuracy by direct substitution. The ground-state wavefunction should possess the following attributes:

1. ^ should be symmetric about the midpoint of the potential well x = 0.

2. <{J should be nodeless, but approaching zero for | x| large.

Both expectations are derived from our experience with the lowest energy states of the infinite and finite square

wells, which you might want to review at this time. The symmetry condition (1) requires ^ to be some function of x2; further, the function must have no zeros (other than at infinity) to meet the nodeless requirement (2). The simplest choice fulfilling both demands is the Gaussian form

(6.26)
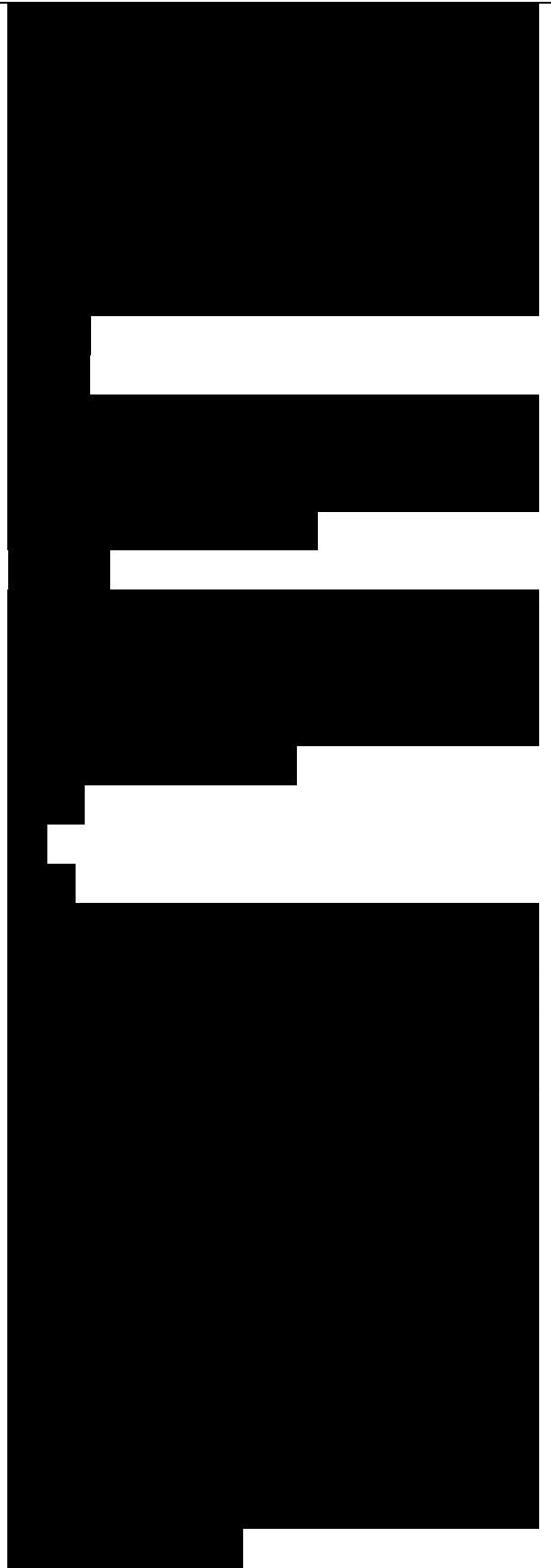
EXAMPLE 6.10 Normalizing the Oscillator Ground State Wavefunction

Normalize the oscillator ground-state wavefunction found in the preceding paragraph.

Solution With $p_0(x) = C_0 e^{-mmx^2/2h}$, the integrated probability is

$\int p_0(x)^2 dx = C_0 \int e^{-mmx^2/h} dx$

Evaluation of the integral requires advanced techniques. We shall be content here simply to quote the formula

$\int e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad a > 0$

Limits of Vibration for a Classical Oscillator

EXAMPLE 6.11

Obtain the limits of vibration for a classical oscillator having the same total energy as the quantum oscillator in its ground state.

Solution The ground-state energy of the quantum oscillator is $E_0^0 = \frac{1}{2}hm$. At its limits of vibration $x = \pm A$, the classical oscillator has transformed all this energy into elastic potential energy of the spring, given by $\frac{1}{2}KA^2 = \frac{1}{2}mm^2A^2$. Therefore,

In our case we identify a with mm/h and obtain

The classical oscillator vibrates in the interval given by $-A < x < A$, having insufficient energy to exceed these limits.

Normalization requires this integrated probability to be 1, leading to

...................

EXAMPLE 6.12 The Quantum

Oscillator in the Nonclassical Region Calculate the probability that a quantum oscillator in its ground state will be found outside the range permitted for a classical oscillator with the same energy.

Solution Because the classical oscillator is confined to the interval —A < x < A, where A is its amplitude of vibration, the question is one of finding the quantum oscillator outside this interval. From the previous example we have A = Vh/mM for a classical oscillator with energy |h(». The quantum oscillator with this energy is described by the wavefunction ipo(x) = Cgexp(— mMx2/2h), with Co = (mffl/wft)1/4 from Example 6.10. The probability in question is found by integrating the probability density 10o|2 in the region beyond the classical limits of vibration, or | ^o |2 dx + | ^o |2 dx ”A From the symmetry of ^q, the two integrals contribute equally to P, so I mw\1/2 f’ 2/h P = 2 I — I I e—mwx /h dx

Changing variables from x to z = Vmw/h x and using A = Vh/mw (corresponding to z = 1) leads to ....

Expressions of this sort are encountered frequently in probability studies. With the lower limit of integration changed to a variable— say, y—the result for P defines the complementary error function erfc(y). Values of the error function may be found in tables. In this way we obtain P = erfc(1) = 0.157, or about 16%.
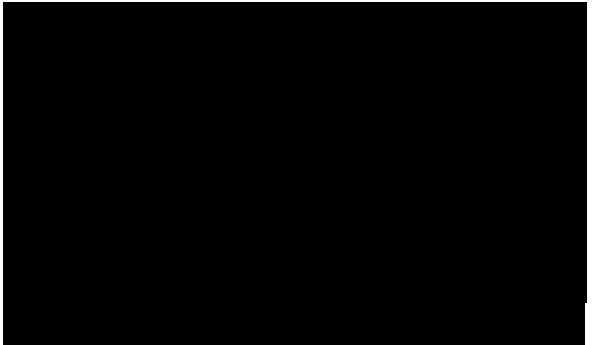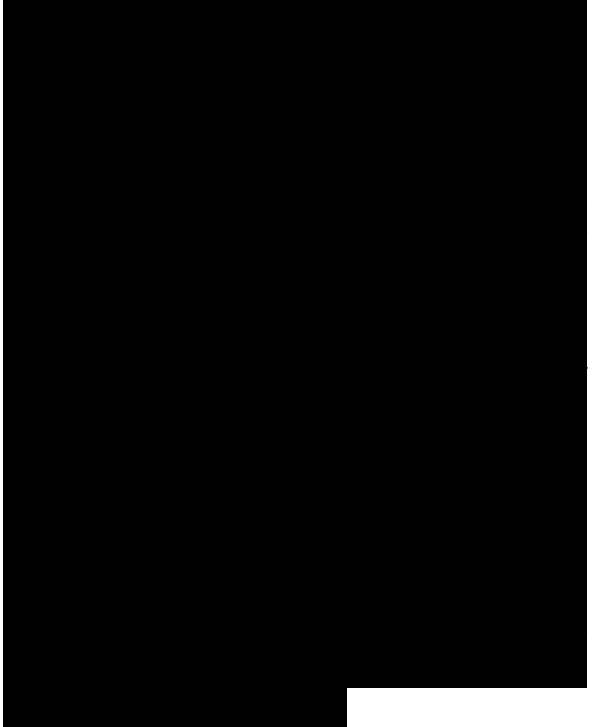
To obtain excited states of the oscillator, a procedure can be followed similar to that for the ground state. The first excited state should be antisymmetric about the midpoint of the oscillator well (x = 0) and display exactly one node. By virtue of the antisymmetry, this node must occur at the origin, so that a suitable trial solution would be i^(x) = x exp(—ax2). Substituting this form into Equation 6.25 yields the same a as before, along with the first excited-state energy E1 = |hw.

Continuing in this manner, we could generate ever-higher-lying oscillator states with their respective energies, but the procedure rapidly becomes too laborious to be practical. What is needed is a systematic approach, such as that provided by the method of power series expansion.11 Pursuing this method would take us too far afield, but the result for the allowed oscillator energies is quite simple and sufficiently important that it be included here:

....

The energy-level diagram following from Equation 6.29 is given in Figure 6.19. Note the uniform spacing of levels, widely recognized as the hallmark of the harmonic oscillator spectrum. The energy difference between adjacent levels is just AE = hw. In these results we find the quantum justification for Planck's revolutionary hypothesis concerning his cavity resonators (see Section
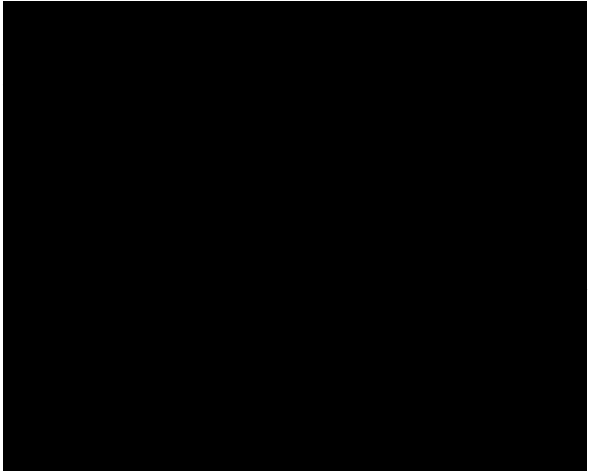
3.2). In deriving his blackbody radiation formula, Planck assumed that these resonators (oscillators), which made up the cavity walls, could possess only those energies that were multiples of hf = hw. Although Planck could not have foreseen the zero-point energy hw/2, it would make no difference: His resonators still would emit or absorb light energy in the bundles AE = hf necessary to reproduce the blackbody spectrum.

nThe method of power series expansion as applied to the problem of the quantum oscillator is developed in any more advanced quantum mechanics text. See, for example, E. E. Anderson, Modern Physics and Quantum Mechanics, Philadelphia, W. B. Saunders Company, 1971.

…………………

Figure 6.19 Energy-level diagram for the quantum oscillator. Note that the levels are equally spaced, with a separation equal to hw. The ground state energy is E0.

Figure 6.20 Probability densities for a few states of the quantum oscillator. The dashed curves represent the classical probabilities corresponding to the same energies.

The probability densities for some of the oscillator states are plotted in Figure 6.20. The dashed lines, representing the classical probability densities for the same energy, are provided for comparison (see Problem 28 for the calculation of
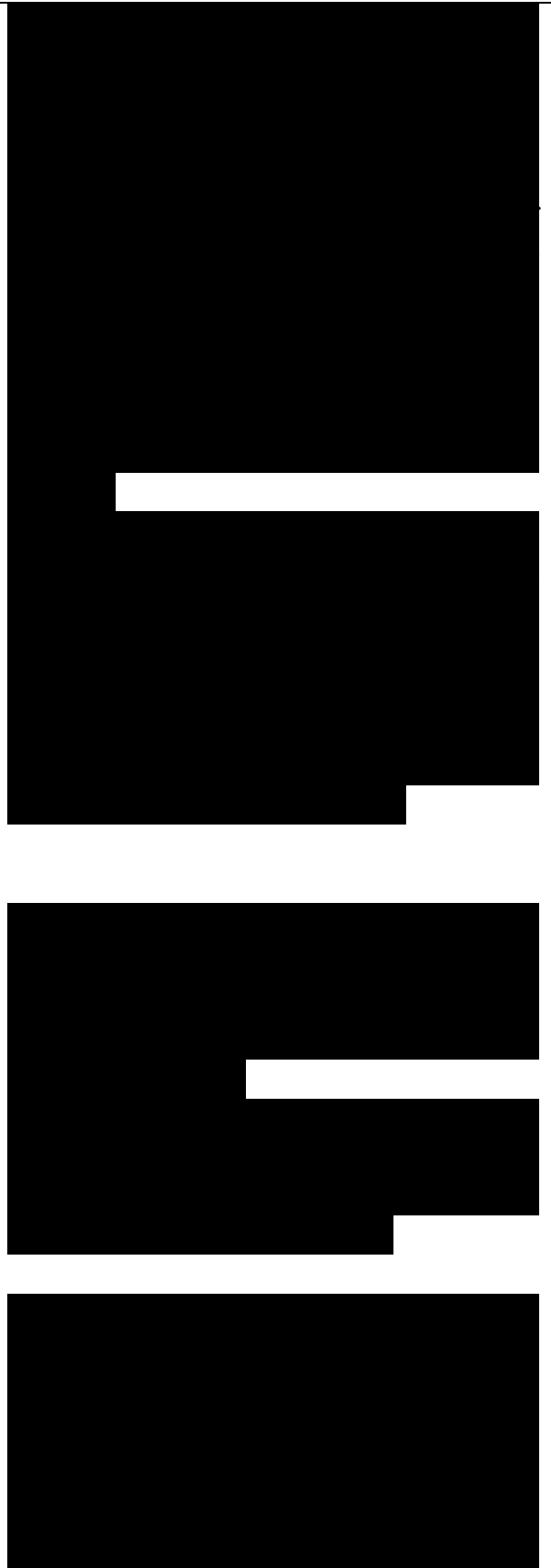
classical probabilities). Note that as n increases, agreement between the classical and quantum probabilities improves, as expected from the correspondence principle.

EXAMPLE 6.13 Quantization of Vibrational Energy

The energy of a quantum oscillator is restricted to be one of the values (n + 2) ho. How can this quantization apply to the motion of a mass on a spring, which seemingly can vibrate with any amplitude (energy) whatever?

Solution The discrete values for the allowed energies of the oscillator would go unnoticed if the spacing between adjacent levels were too small to be detected. At the macroscopic level, a laboratory mass m of, say, 0.0100 kg on a spring having force constant K = 0.100 N/m (a typical value) would oscillate with angular frequency o = VK/m = 3.16 rad/s. The corresponding period of vibration is T = 2-n/o = 1.99 s. In this case the quantum level spacing is only
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Such small energies are far below present limits of detection.

At the atomic level, however, much higher frequencies are commonplace. Consider the vibrational frequency of the hydrogen molecule. This behaves as an oscillator with K = 510.5 N/m and reduced mass x = 8.37 X 10~28 kg. The angular frequency of oscillation is therefore

510.5 N/m 8.37 X l0~28 kg = 7.8l X l0l4 rad/s

At such frequencies, the quantum of energy ho is 0.5l3 eV, which can be measured easily!

6.8 OBSERVABLES AND OPERATORS

An observable is any particle property that can be measured. The position and momentum of a particle are observables, as are its kinetic and potential energies. In quantum mechanics, we associate an operator with each of these observables. Using this operator, one can calculate the average value of the corresponding observable. An operator here refers to an operation to be performed on whatever function follows the operator. The quantity operated on is called the operand. In this language a constant c becomes an operator, whose meaning is understood by supplying any function f (x) to obtain cf(x). Here the operator c means "multiplication by the constant c." A more complicated operator is d/dx, which, after supplying an operand f(x), means "take the derivative of f(x) with respect to x." Still another example is $(d/dx)^2 = (d/dx)(d/dx)$. Supplying the operand f(x) gives $(d/dx)^2 f(x) = (d/dx)(df/dx) = d^2f/dx^2$. Hence, $(d/dx)^2$ means "take the second derivative with respect to x, that is, take the indicated derivative twice."

The operator concept is useful in quantum mechanics because all expectation values we have

encountered so far can be written in the same general form, namely,

(6.37)

In this expression, Q is the observable and [Q] is the associated operator. The order of terms in Equation 6.37 is important; it indicates that the operand for [Q] always is ¥. Comparing the general form with that for (p) in Equation 6.36 shows that the momentum operator is [p] = (ti/i)(d/dx). Similarly, writing x|¥|2 = ¥*x¥ in Equation 6.31 implies that the operator for position is [x] = x. From [x] and [p] the operator for any other observable can be found. For instance, the operator for x2 is just [x2] = [x]2 = x2. For that matter, the operator for potential energy is simply [U] = U([x]) = U(x), meaning that average potential energy is computed as

Still another example is the kinetic energy K. Classically, K is a function of p: K = p2/2m. Then the kinetic energy operator is [K] = ([p])2/2m = (— ti/2m)d2/dx2, and average kinetic energy is found from

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To find the average total energy for a particle, we sum the average kinetic and potential energies to get

Table 6.2 Common Observables and Associated Operators

The form of this result suggests that the term in the braces is the operator for total energy. This operator is called the Hamiltonian, symbolized by [H]:

The designation [E] is reserved for

another operator, which arises as follows: Inspection of Schrodinger's equation (Equation 6.10) shows that it can be written neatly as [H]^ = ihd^/dt. Using this in Equation 6.38 gives an equivalent expression for (E) and leads to the identification of the energy operator:

Notice that [H] is an operation involving only the spatial coordinate x, whereas [E] depends only on the time t. That is, [H] and [E] really are two different operators, but they produce identical results when applied to any solution of Schrodinger's equation. This is because the LHS of Schrodinger's equation is simply [H]^, while the RHS is none other than [E]^ (compare Equation 6.10)! Table 6.2 summarizes the observables we have discussed and their associated operators.

OPTIONAL

Quantum uncertainty for any observable Q

QUANTUM UNCERTAINTY AND THE EIGENVALUE PROPERTY

In Section 6.7 we showed how Ax, the quantum uncertainty in position, could be found from the expectation values (x2) and (x). But the argument given there applies to any observable, that is, the quantum uncertainty AQ for any observable Q is calculated as ....

Again, if AQ = 0, Qis said to be a sharp observable and all

measurements of Q yield the same value. More often, however, AQ > 0 and repeated measurements reveal a distribution of values—as in Table 6.1 for the observable x. In such cases, we say the observable is fuzzy, suggesting that, prior to actual measurement, the particle cannot be said to possess a unique value of Q.

In classical physics all observables are sharp. The extent to which sharp observables can be specified in quantum physics is limited by uncertainty principles, such as

(6.42)

The uncertainties here are to be calculated from Equation 6.41. Equation 6.42 says that no matter what the state of the particle, the spread in distributions obtained in measurements of x and of p will be inversely related: when one is small, the other will be large. Alternatively, if the position of the particle is quite "fuzzy," its momentum can be relatively "sharp," and vice versa. The degree to which both may be simultaneously sharp is limited by the size of h. The incredibly small value of h in SI units is an indication that quantum ideas are unnecessary at the macroscopic level.

Despite restrictions imposed by uncertainty principles, some observables in quantum physics may still be sharp. The energy E of all stationary states is one example. In the free particle plane waves of Section 6.2 we have another: The

plane wave with wavenumber k,

$W_k(x, t) = e^{(kx \sim ai)}$

describes a particle with momentum p = hk. Evidently, momentum is a sharp observable for this wavefunction. We find that the action of the momentum operator in this instance is especially simple:

……………..

that is, the operation [p] returns the original function multiplied by a constant. This is an example of an eigenvalue problem for the operator [p]. The wavefunction ^k is the eigenfunction, and the constant, in this case hk, is the eigenvalue. Notice that the eigenvalue is just the sharp value of particle momentum for this wave. This connection between sharp observables and eigenvalues is a general one: For an observable Q to be sharp, the wavefunction must be an eigenfunction of the operator for Q. Further, the sharp value for Q in this state is the eigenvalue. In this way the eigenvalue property can serve as a simple test for sharp observables, as the following examples illustrate.

EXAMPLE 6.16 Plane Waves and Sharp Observables

Use the eigenvalue test to show that the plane wave $^k(x, t) = e^{i(kx-wt)}$ is one for which total energy is a sharp observable. What value does the energy take in this case?

Solution To decide the issue we examine the action of the energy operator [E] on the candidate function $e^{i(kx-a)t}K$ Since taking a derivative
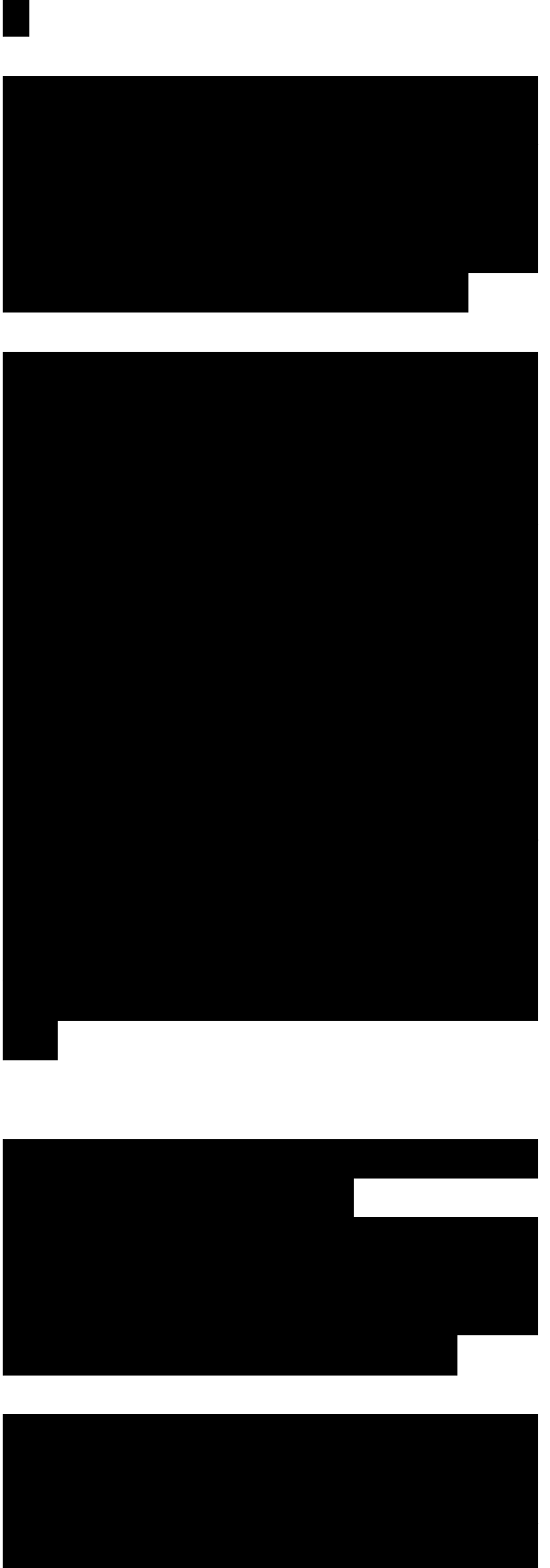
with respect to t of this function is equivalent to multiplying the function by — i«, we have

………………

showing that ei(kx—wt) is an eigenfunction of the energy operator [E] and the eigenvalue is tiw. Thus, energy is a sharp observable and has the value tiw in this state.

It is instructive to compare this result with the outcome found by using the other energy operator, [H]. The Hamiltonian for a free particle is simply the kinetic energy operator [K], because the potential energy is zero in this case. Then

....

Again, the operation returns the original function with a multiplier, so that ei(kx—wt'> also is an eigenfunction of [H]. The eigenvalue in this case is ti2k2/2m, which also must be the sharp value of particle energy. The equivalence with hrn follows from the dispersion relation for free particles (see footnote 1).

Exercise 6 Show that total energy is a sharp observable for any stationary state.

EXAMPLE 6.17 Sharp Observables for a Particle in a Box

Are the stationary states of the infinite square well eigenfunctions of [p]? of [p]2? If so, what are the eigenvalues? Discuss the implications of these results.

Solution The candidate function in this case is any one of the square well wave- functions ¥(x, t) = ^2/L

sin(nvx/L)e—iEnt/ti. Because the first derivative gives (d/dx)sin(n^x/L) = (nv/L)cos(nvx/L), we see at once that the operator [p] will not return the original function ¥, and so these are not eigenfunctions of the momentum operator. They are, however, eigenfunctions of [p]2. In particular, we have (d2/dx2)sin(n^x/L) = —(n^/L)2sin(nvx/L), so that

....

The eigenvalue is the multiplier (nnti/L)2. Thus, the squared momentum (or magnitude of momentum) is sharp for such states, and repeated measurements of p2 (or |p|) for the state labeled by n will give identical results equal to (nnti/L)2 (or nwh/L). By contrast, the momentum itself is not sharp, meaning that different values for p will be obtained in successive measurements. In particular, it is the sign or direction of momentum that is fuzzy, consistent with the classical notion of a particle bouncing back and forth between the walls of the "box."

SUMMARY

In quantum mechanics, matter waves (or de Broglie waves) are represented by a wavefunction ¥(x, t). The probability that a particle constrained to move along the x-axis will be found in an interval dx at time t is given by |¥|2dx. These probabilities summed over all values of x must total 1 (certainty). That is,

This is called the normalization condition. Furthermore, the
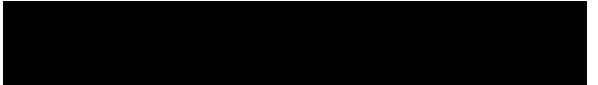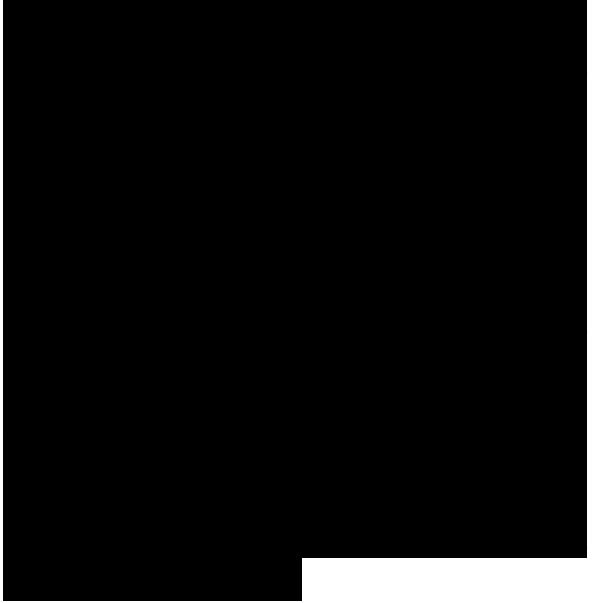
probability that the particle will be found in any interval a < x < b is obtained by integrating the probability density | ^ |2 over this interval.

Aside from furnishing probabilities, the wavefunction can be used to find the average, or expectation value, of any dynamical quantity. The average position of a particle at any time t is
(6.31)

In general, the average value of any observable Q at time t is

(6.37)
where [Q] is the associated operator. The operator for position is just [x] = x, and that for particle momentum is [p] = (h/i)3/3x.

The wavefunction ^ must satisfy the Schrodinger equation,
(6.10)

Separable solutions to this equation, called stationary states, are ^(x, t) = p(x)e—mt, with p(x) a time-independent wavefunction satisfying the time- independent Schrodinger equation
(6.13)

The approach of quantum mechanics is to solve Equation 6.13 for p and E, given the potential energy U(x) for the system. In doing so, we must require
•   that p(x) be continuous
•   that p(x) be finite for all x, including x = ±TO
•   that p(x) be single valued

• that dp/ dx be continuous wherever U(x) is finite

Explicit solutions to Schrodinger's equation can be found for several potentials of special importance. For a free particle the stationary states are the plane waves $p(x) = e^{ikx}$ of wavenumber k and energy $E = h^2k^2/2m$. The particle momentum in such states is $p = hk$, but the location of the particle is completely unknown. A free particle known to be in some range Ax is described not by a plane wave, but by a wave packet, or group, formed from a superposition of plane waves. The momentum of such a particle is not known precisely, but only to some accuracy Ap that is related to Ax by the uncertainty principle,

AxAp > 2h

For a particle confined to a one-dimensional box of length L, the stationary-state waves are those for which an integral number of half-wavelengths can be fit inside, that is, $L = nA/2$. In this case the energies are quantized as

and the wavefunctions within the box are given by

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$^n(x) = 4 L \sin j$ n = 1' 2, 3 • • •(6.18)

For the harmonic oscillator the potential energy function is $U(x) = |ma^2x^2$, and the total particle energy is quantized according to the relation

En = + —j ha n = 0, 1, 2, • • • (6.29)

The lowest energy is E0 = 2>ha; the separation between adjacent energy

levels is uniform and equal to ha. The wavefunction for the oscillator ground state is

 (6.26)

where a = ma/2h and C0 is a normalizing constant. The oscillator results apply to any system executing small-amplitude vibrations about a point of stable equilibrium. The effective spring constant in the general case is

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with the derivative of the potential evaluated at the equilibrium point a. The stationary state waves for any potential share the following attributes:

• Their time dependence is e—iat.

• They yield probabilities that are time independent.

• All average values obtained from stationary states are time independent.

• The energy in any stationary state is a sharp observable; that is, repeated measurements of particle energy performed on identical systems always yield the same result, E = ha. For other observables, such as position, repeated measurements usually yield different results. We say these observables are fuzzy. Their inherent "fuzziness" is reflected by the spread in results about the average value, as measured by the standard deviation, or uncertainty. The uncertainty in any observable Q can be calculated from expectation values

| as
  (6.41) | |