Chapter 3

The Schrödinger Equation and Its Applications

3.1 WAVE FUNCTIONS OF A SINGLE PARTICLE

In quantum mechanics, a particle is characterized by a *wave function* $\psi(\mathbf{r}, t)$, which contains information about the spatial state of the particle at time t. The wave function $\psi(\mathbf{r}, t)$ is a complex function of the three coordinates x, y, z and of the time t. The interpretation of the wave function is as follows: The probability $dP(\mathbf{r}, t)$ of the particle being at time t in a volume element $d^3r = dx\,dy\,dz$ located at the point $\mathbf{r}$ is

$$dP(\mathbf{r}, t) = C|\psi(\mathbf{r}, t)|^2 d^3r \tag{3.1}$$

where C is a normalization constant. The *total probability* of finding the particle anywhere in space, at time t, is equal to unity; therefore,

$$\int dP(\mathbf{r}, t) = 1 \tag{3.2}$$

According to (*3.1*) and (*3.2*) we conclude:

(*a*) The wave function $\psi(\mathbf{r}, t)$ must be square-integrable, i.e.,

$$\int |\psi(\mathbf{r}, t)|^2 d^3r \tag{3.3}$$

is finite.

(*b*) The normalization constant is given by the relation

$$\frac{1}{C} = \int |\psi(\mathbf{r}, t)|^2 d^3r \tag{3.4}$$

When $C = 1$ we say that the wave function is *normalized*. A wave function $\psi(\mathbf{r}, t)$ must be defined and continuous everywhere.

3.2 THE SCHRÖDINGER EQUATION

Consider a particle of mass m subjected to the potential $V(\mathbf{r}, t)$. The time evolution of the wave function is governed by the Schrödinger equation:

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t) + V(\mathbf{r}, t)\psi(\mathbf{r}, t) \tag{3.5}$$

where ∇^2 is the Laplacian operator, $\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$. Pay attention to two important properties of the Schrödinger equation:

(*a*) The Schrödinger equation is a linear and homogeneous equation in ψ. Consequently, the superposition principle holds; that is, if $\psi_1(\mathbf{r}, t), \psi_2(\mathbf{r}, t), \ldots, \psi_n(\mathbf{r}, t)$ are solutions of the Schrödinger equation, then $\psi = \sum_{i=n}^{n} \alpha_i\psi_i(\mathbf{r}, t)$ is also a solution.

(*b*) The Schrödinger equation is a first-order equation with respect to time; therefore, the state at time t_0 determines its subsequent state at all times.

3.3 PARTICLE IN A TIME-INDEPENDENT POTENTIAL

The wave function of a particle subjected to a time-independent potential $V(\mathbf{r})$ satisfies the Schrödinger equation:

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r})\psi(\mathbf{r},t) \tag{3.6}$$

Performing a separation of variables $\psi(\mathbf{r},t) = \phi(\mathbf{r})\chi(t)$, we have $\chi(t) = Ae^{-i\omega t}$ (A and ω are constants), where $\phi(\mathbf{r})$ must satisfy the equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) + V(\mathbf{r})\phi(\mathbf{r}) = \hbar\omega\phi(\mathbf{r}) \tag{3.7}$$

where $\hbar\omega$ is the energy of the state E (see Problem 3.1). This is a *stationary Schrödinger equation*, where a wave function of the form

$$\psi(\mathbf{r},t) = \phi(\mathbf{r})e^{-i\omega t} = \phi(\mathbf{r})e^{-iEt/\hbar} \tag{3.8}$$

is called a *stationary solution* of the Schrödinger equation, since the probability density in this case does not depend on time [see Problem 3.1, part (*b*)]. Suppose that at time $t = 0$ we have

$$\psi(\mathbf{r},0) = \sum_n \phi_n(\mathbf{r}) \tag{3.9}$$

where $\phi_n(\mathbf{r})$ are the spatial parts of stationary states, $\psi_n(\mathbf{r},t) = \phi(\mathbf{r})e^{-i\omega_n t}$. In this case, according to the superposition principle, the time-evolution of $\psi(\mathbf{r},0)$ is described by

$$\psi(\mathbf{r},t) = \sum_n \phi(\mathbf{r})e^{-i\omega_n t} \tag{3.10}$$

For a *free particle* we have $V(\mathbf{r},t) \equiv 0$, and the Schrödinger equation is satisfied by solutions of the form

$$\psi(\mathbf{r},t) = Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \tag{3.11}$$

where A is a constant; k and ω satisfy the relation $\omega = \hbar\mathbf{k}^2/2m$. Solutions of this form are called *plane waves.* Note that since the $\psi(\mathbf{r},t)$ are not square-integrable, they cannot rigorously represent a particle. On the other hand, a superposition of plane waves can yield an expression that is square-integrable and can therefore describe the dynamics of a particle,

$$\psi(\mathbf{r},t) = \frac{1}{(2\pi)^{3/2}}\int g(\mathbf{k})e^{i[\mathbf{k}\cdot\mathbf{r}-\omega(k)t]}\,d^3k \tag{3.12}$$

A wave function of this form is called *a wave-packet*. We often study the case of a one-dimensional wave-packet,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\mathbf{k})e^{i[kx-\omega(k)t]}\,dk \tag{3.13}$$

3.4 SCALAR PRODUCT OF WAVE FUNCTIONS: OPERATORS

With each pair of wave functions $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$, we associate a complex number defined by

$$(\phi,\psi) = \int \phi^*(\mathbf{r})\psi(\mathbf{r})\,d^3r \tag{3.14}$$

where (ϕ,ψ) is the *scalar product* of $\phi(\mathbf{r})$ and $\psi(\mathbf{r})$ (see Chapter 2).

An operator A acting on a wave function $\psi(\mathbf{r})$ creates another wave function $\psi'(\mathbf{r})$. An operator is called a linear operator if this correspondence is linear, i.e., if for every complex number α_1 and α_2,

$$A[\alpha_1\psi_1(\mathbf{r}) + \alpha_2\psi_2(\mathbf{r})] = \alpha_1 A\psi_1(\mathbf{r}) + \alpha_2 A\psi_2(\mathbf{r}) \tag{3.15}$$

There are two sets of operators that are important:

(*a*) The *spatial operators* X, Y, and Z are defined by

$$\begin{cases} X\psi(x, y, z, t) = x\psi(x, y, z, t) \\ Y\psi(x, y, z, t) = y\psi(x, y, z, t) \\ Z\psi(x, y, z, t) = z\psi(x, y, z, t) \end{cases} \tag{3.16}$$

(*b*) The *momentum operators* p_x, p_y, and p_z are defined by

$$\begin{cases} p_x\psi(x, y, z, t) = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\psi(x, y, z, t) \\ p_y\psi(x, y, z, t) = \dfrac{\hbar}{i}\dfrac{\partial}{\partial y}\psi(x, y, z, t) \\ p_z\psi(x, y, z, t) = \dfrac{\hbar}{i}\dfrac{\partial}{\partial z}\psi(x, y, z, t) \end{cases} \tag{3.17}$$

The *mean value* of an operator A in the state $\psi(\mathbf{r})$ is defined by

$$\langle A \rangle = \int \psi^*(\mathbf{r})\,[A\psi(\mathbf{r})]\,d^3r \tag{3.18}$$

The *root-mean-square deviation* is defined by

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2} \tag{3.19}$$

where A^2 is the operator $A \cdot A$.

Consider the operator called the *Hamiltonian* of the particle. It is defined by

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t) \equiv \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t) \tag{3.20}$$

where $\mathbf{p}^2$ is a condensed notation of the operator $p_x^2 + p_y^2 + p_z^2$. Using the operator formulation, the Schrödinger equation is written in the form

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = H\psi(\mathbf{r}, t) \tag{3.21}$$

If the potential energy is time-independent, a stationary solution must satisfy the equation

$$H\phi(\mathbf{r}) = E\phi(\mathbf{r}) \tag{3.22}$$

where E is a real number called the energy of state. Equation (*3.22*) is the eigenvalue equation of the operator H; the application of H on the eigenfunction $\phi(\mathbf{r})$ yields the same function, multiplied by the corresponding eigenvalue E. The allowed energies are therefore the eigenvalues of the operator H.

3.5 PROBABILITY DENSITY AND PROBABILITY CURRENT

Consider a particle described by a normalized wave function $\psi(\mathbf{r}, t)$. The *probability density* is defined by

$$\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \tag{3.23}$$

At time t, the probability $dP(\mathbf{r}, t)$ of finding the particle in an infinitesimal volume d^3r located at $\mathbf{r}$ is equal to

$$dP(\mathbf{r}, t) = \rho(\mathbf{r}, t)\,d^3r \tag{3.24}$$

The integral of $\rho(\mathbf{r}, t)$ over all space remains constant at all times. Note that this does not mean that $\rho(\mathbf{r}, t)$ must be time-independent at every point $\mathbf{r}$. Nevertheless, we can express a local *conservation of probability* in the form of a *continuity equation,*

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0 \tag{3.25}$$

where $\mathbf{J}(\mathbf{r}, t)$ is the *probability current,* defined by

$$\mathbf{J}(\mathbf{r}, t) = \frac{\hbar}{2mi}[\psi^*(\nabla\psi) - \psi(\nabla\psi^*)] = \frac{1}{m}\mathrm{Re}\left[\psi^*\left(\frac{\hbar}{i}\nabla\psi\right)\right] \tag{3.26}$$

Consider two regions in a space where their constant potentials are separated by a potential step or barrier, see Fig. 3-1.

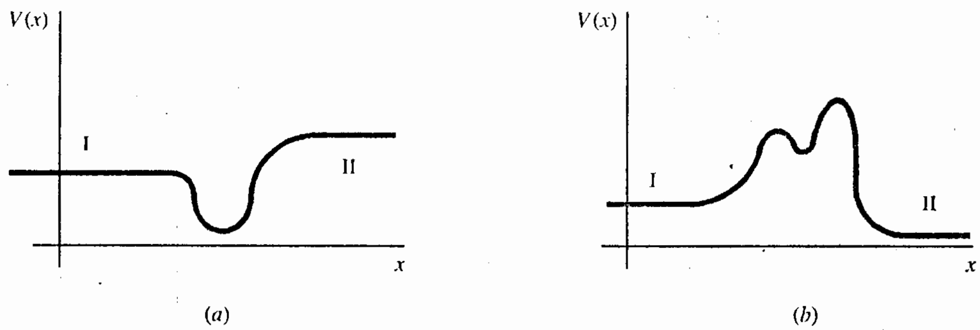

Fig. 3-1 (*a*) Potential step; (*b*) potential barrier.

We define transmission and reflection coefficients as follows. Suppose that a particle (or a stream of particles) is moving from region I through the potential step (or barrier) to region II. In the general case, a stationary state describing this situation will contain three parts. In region I the state is composed of the incoming wave with probability current J_I and a reflected wave of probability current J_R. In region II there is a transmitted wave of probability current J_T.

The *reflection coefficient* is defined by

$$R = \left|\frac{J_R}{J_I}\right| \tag{3.27}$$

The *transmission coefficient* is defined by

$$T = \left|\frac{J_T}{J_I}\right| \tag{3.28}$$

Solved Problems

3.1. Consider a particle subjected to a time-independent potential $V(\mathbf{r})$. (*a*) Assume that a state of the particle is described by a wave function of the form $\psi(\mathbf{r}, t) = \phi(\mathbf{r})\chi(t)$. Show that $\chi(t) = Ae^{-i\omega t}$ (A is constant) and that $\phi(\mathbf{r})$ must satisfy the equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) + V(\mathbf{r})\phi(\mathbf{r}) = \hbar\omega\phi(\mathbf{r}) \tag{3.1.1}$$

where m is the mass of the particle. (*b*) Prove that the solutions of the Schrödinger equation of part (*a*) lead to a time-independent probability density.

(*a*) We substitute $\psi(\mathbf{r}, t) = \phi(\mathbf{r})\chi(t)$ in the Schrödinger equation:

$$i\hbar\phi(\mathbf{r})\frac{d\chi(t)}{dt} = \chi(t)\left[-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r})\right] + \chi(t)V(\mathbf{r})\phi(\mathbf{r}) \tag{3.1.2}$$

In the regions in which the wave function $\psi(\mathbf{r}, t)$ does not vanish, we divide both sides of *(3.1.2)* by $\phi(\mathbf{r})\chi(t)$; so we obtain

$$\frac{i\hbar}{\chi(t)}\frac{d\chi(t)}{dt} = \frac{1}{\phi(\mathbf{r})}\left[-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r})\right] + V(\mathbf{r}) \tag{3.1.3}$$

The left-hand side of *(3.1.3)* is a function of t only, and does not depend on $\mathbf{r}$. On the other hand, the right-hand side is a function of $\mathbf{r}$ only. Therefore, both sides of (3.1.3) depend neither on $\mathbf{r}$ nor on t, and are thus constants that we will set equal to $\hbar\omega$ for convenience. Hence,

$$i\hbar\frac{1}{\chi(t)}\frac{d\chi(t)}{dt} = i\hbar\frac{d[\ln\chi(t)]}{dt} = \hbar\omega \tag{3.1.4}$$

Therefore,

$$\ln\chi(t) = \int -i\omega\, dt = -i\omega t + C \Rightarrow \chi(t) = Ae^{-i\omega t} \tag{3.1.5}$$

where A is constant. Substituting in *(3.1.3)*, we see that $\phi(\mathbf{r})$ must satisfy the equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) + V(\mathbf{r})\phi(\mathbf{r}) = \hbar\omega\phi(\mathbf{r}) \tag{3.1.6}$$

(*b*) For a function of the form $\psi(\mathbf{r}, t) = \phi(\mathbf{r})e^{-i\omega t}$, the probability density is by definition

$$\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 = [\phi(\mathbf{r})e^{-i\omega t}]\,[\phi(\mathbf{r})e^{-i\omega t}]^* = \phi(\mathbf{r})e^{-i\omega t}\phi^*(\mathbf{r})e^{i\omega t} = |\phi(\mathbf{r})|^2 \tag{3.1.7}$$

We see that the probability density does not depend on time. This is why this kind of solution is called "stationary."

3.2. Consider the Hamiltonian for a one-dimensional system of two particles of masses m_1 and m_2 subjected to a potential that depends only on the distance between the particles $x_1 - x_2$,

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_1 - x_2) \tag{3.2.1}$$

(*a*) Write the Schrödinger equation using the new variables x and X, where

$$x = x_1 - x_2 \quad \text{(relative distance)} \qquad X = \frac{m_1x_1 + m_2x_2}{m_1 + m_2} \quad \text{(center of mass)} \tag{3.2.2}$$

(*b*) Use a separation of variables to find the equations governing the evolution of the center of mass and the relative distance of the particles. Interpret your results.

(*a*) In terms of x_1 and x_2, the wave function of the two particles is governed by the Schrödinger equation:

$$i\hbar\frac{\partial\psi(x_1, x_2, t)}{\partial t} = H\psi(x_1, x_2, t) = -\frac{\hbar^2}{2m_1}\frac{\partial^2\psi(x_1, x_2, t)}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2\psi(x_1, x_2, t)}{\partial x_2^2} + V(x_1 - x_2)\,\psi(x_1, x_2, t) \tag{3.2.3}$$

In order to transform to the variables x and X, we have to express the differentiations $\partial^2/\partial x_1^2$ and $\partial^2/\partial x_2^2$ in terms of the new variables. We have

$$\frac{\partial x}{\partial x_1} = 1 \qquad \frac{\partial x}{\partial x_2} = -1 \qquad \frac{\partial X}{\partial x_1} = \frac{m_1}{m_1 + m_2} \qquad \frac{\partial X}{\partial x_2} = \frac{m_2}{m_1 + m_2} \tag{3.2.4}$$

Thus, for an arbitrary function $f(x_1, x_2)$ we obtain

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = \frac{\partial f(x, X)}{\partial x}\frac{\partial x}{\partial x_1} + \frac{\partial f(x, X)}{\partial X}\frac{\partial X}{\partial x_1} = \frac{\partial f(x, X)}{\partial x} + \frac{m_1}{m_1 + m_2}\frac{\partial f(x, X)}{\partial X} \tag{3.2.5}$$

Similarly,

$$\frac{\partial f(x_1, x_2)}{\partial x_2} = \frac{\partial f(x, X)}{\partial x}\frac{\partial x}{\partial x_2} + \frac{\partial f(x, X)}{\partial X}\frac{\partial X}{\partial x_2} = -\frac{\partial f(x, X)}{\partial x} + \frac{m_2}{m_1 + m_2}\frac{\partial f(x, X)}{\partial X} \tag{3.2.6}$$

or

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial x} + \frac{m_1}{m_1 + m_2}\frac{\partial}{\partial X} \qquad \frac{\partial}{\partial x_2} = -\frac{\partial}{\partial x} + \frac{m_2}{m_1 + m_2}\frac{\partial}{\partial X} \tag{3.2.7}$$

For the second derivatives in x_1 and x_2 we have

$$\begin{aligned}\frac{\partial^2}{\partial x_1^2} &= \left(\frac{\partial}{\partial x} + \frac{m_1}{m_1 + m_2}\frac{\partial}{\partial X}\right)\left(\frac{\partial}{\partial x} + \frac{m_1}{m_1 + m_2}\frac{\partial}{\partial X}\right) \\ &= \frac{\partial^2}{\partial x^2} + \frac{m_1}{m_1 + m_2}\frac{\partial}{\partial x}\frac{\partial}{\partial X} + \frac{m_1}{m_1 + m_2}\frac{\partial}{\partial X}\frac{\partial}{\partial x} + \left(\frac{m_1}{m_1 + m_2}\right)^2\frac{\partial^2}{\partial X^2}\end{aligned} \tag{3.2.8}$$

The wave function must be a smooth function for both x_1 and x_2, so we can interchange the order of differentiation and obtain

$$\frac{\partial^2}{\partial x_1^2} = \frac{\partial^2}{\partial x^2} + \left(\frac{m_1}{m_1 + m_2}\right)^2\frac{\partial^2}{\partial X^2} + \frac{2m_1}{m_1 + m_2}\frac{\partial}{\partial X}\frac{\partial}{\partial x} \tag{3.2.9}$$

For x_2 we have

$$\frac{\partial^2}{\partial x_2^2} = \left(-\frac{\partial}{\partial x} + \frac{m_2}{m_1 + m_2}\frac{\partial}{\partial X}\right)\left(-\frac{\partial}{\partial x} + \frac{m_2}{m_1 + m_2}\frac{\partial}{\partial X}\right) = \frac{\partial^2}{\partial x^2} + \left(\frac{m_2}{m_1 + m_2}\right)^2\frac{\partial^2}{\partial X^2} - \frac{2m_2}{m_1 + m_2}\frac{\partial}{\partial X}\frac{\partial}{\partial x} \tag{3.2.10}$$

Substituting (*3.2.9*) and (*3.2.10*) in (*3.2.3*), we get

$$\begin{aligned}i\hbar\frac{\partial\psi(x, X, t)}{\partial t} &= -\frac{\hbar^2}{2m_1}\left[\frac{\partial^2}{\partial x^2} + \left(\frac{m_1}{m_1 + m_2}\right)^2\frac{\partial^2}{\partial X^2} + \frac{2m_1}{m_1 + m_2}\frac{\partial}{\partial X}\frac{\partial}{\partial x}\right]\psi(x, X, t) \\ &\quad -\frac{\hbar^2}{2m_2}\left[\frac{\partial^2}{\partial x^2} + \left(\frac{m_2}{m_1 + m_2}\right)^2\frac{\partial^2}{\partial X^2} - \frac{2m_2}{m_1 + m_2}\frac{\partial}{\partial X}\frac{\partial}{\partial x}\right]\psi(x, X, t) + V(x)\psi(x, X, t) \\ &= -\frac{\hbar^2}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\frac{\partial^2\psi(x, X, t)}{\partial x^2} + V(x)\psi(x, X, t) - \frac{\hbar^2}{2}\left(\frac{1}{m_1 + m_2}\right)\frac{\partial^2}{\partial X^2}\psi(x, X, t)\end{aligned} \tag{3.2.11}$$

(*b*) Since the Hamiltonian is time-independent, $\psi(x, X, t) = \phi(x, X)\chi(t)$ (we separate the time and the spatial variables; see Problem 3.1). The equation governing the stationary part $\phi(x, X)$ is $H\phi(x, X) = E_{\text{total}}\phi(x, X)$, where E_{total} is the total energy. Substituting in (*3.2.11*) we arrive at

$$-\frac{\hbar^2}{2}\left(\frac{m_1 + m_2}{m_1 m_2}\right)\frac{\partial^2\phi(x, X)}{\partial x^2} + V(x)\phi(x, X) - \frac{\hbar^2}{2}\left(\frac{1}{m_1 + m_2}\right)\frac{\partial^2\phi(x, X)}{\partial X^2} = E_{\text{total}}\phi(x, X) \tag{3.2.12}$$

Performing a separation of the variables $\phi(x, X) = \xi(x)\eta(X)$, (*3.2.12*) becomes

$$-\frac{\hbar^2}{2}\frac{1}{\xi(x)}\left(\frac{m_1 + m_2}{m_1 m_2}\right)\frac{\partial^2\xi(x)}{\partial x^2} + V(x) = \frac{\hbar^2}{2}\frac{1}{\eta(X)}\frac{1}{m_1 + m_2}\frac{\partial^2\eta(X)}{\partial X^2} + E_{\text{total}} \tag{3.2.13}$$

The left-hand side of (*3.2.13*) depends only on x; on the other hand, the right-hand side is a function only of X. Therefore, neither side can depend on x or on X, and both are thus equal to a constant. We set

$$-\frac{\hbar^2}{2}\frac{1}{\eta(X)}\frac{1}{m_1 + m_2}\frac{\partial^2\eta(x)}{\partial X^2} = E_{\text{cm}} \tag{3.2.14}$$

By inspection, we conclude that (*3.2.14*) is the equation governing the stationary wave function of a free particle of mass $m_1 + m_2$, i.e.,

$$-\frac{\hbar^2}{2}\frac{1}{m_1 + m_2}\frac{\partial^2\eta(X)}{\partial X^2} = E_{\text{cm}}\eta(X) \tag{3.2.15}$$

Note that the wave function corresponding to the center of mass of the two particles behaves as a free particle of mass $m_1 + m_2$ and energy E_{cm}. This result is completely analogous to the classical case. Returning to

(*3.2.13*), the equation for the relative position of the two particles is

$$-\frac{\hbar^2}{2}\left(\frac{m_1+m_2}{m_1 m_2}\right)\frac{\partial^2\xi(x)}{\partial x^2}+V(x)\xi(x) = E_{\text{total}}-E_{\text{cm}} \tag{3.2.16}$$

Equation (*3.2.16*) governs the stationary wave function of a particle of mass $(m_1+m_2)/m_1m_2$ held in a potential $V(x)$ and having a total energy $E_{\text{total}}-E_{\text{cm}}$. Thus the relative position of the two particles behaves as a particle with an effective mass $(m_1+m_2)/m_1m_2$ and of energy $E_{\text{total}}-E_{\text{cm}}$ held in an effective potential $V(x)$. This is also analogous to the classical case.

3.3. Consider a particle of mass m confined in a finite one-dimensional potential well $V(x)$; see Fig. 3-2.

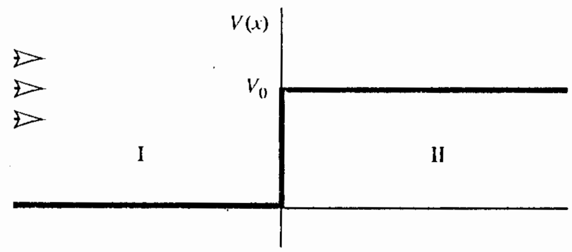

Fig. 3-2

Prove that (*a*) $\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}$, and (*b*) $\frac{d\langle p\rangle}{dt} = \left\langle -\frac{dV}{dx}\right\rangle$, where $\langle x\rangle$ and $\langle p\rangle$ are the mean values of the coordinate and momentum of the particle, respectively, and $\left\langle -\frac{dV}{dx}\right\rangle$ is the mean value of the force acting on the particle. This result can be generalized to other kinds of operators and is called *Ehrenfest's theorem.*

(*a*) Suppose that the wave function $\psi(x,t)$ refers to a particle. The Schrödinger equation is

$$\frac{\partial\psi(x,t)}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}-\frac{i}{\hbar}V(x)\psi(x,t) \tag{3.3.1}$$

and its conjugate equation is $\frac{\partial\psi^*(x,t)}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2}+\frac{i}{\hbar}V(x)\psi^*(x,t)$. [Notice that we assume $V(x)$ to be real.] The integral $\int_{-\infty}^{\infty}|\psi(x,t)|^2\,dx$ must be finite; so we get

$$\lim_{x\to\infty}|\psi(x,t)|^2 = \lim_{x\to-\infty}|\psi(x,t)|^2 = 0 \qquad\text{and}\qquad \lim_{x\to\infty}\frac{\partial\psi(x,t)}{\partial x} = \lim_{x\to-\infty}\frac{\partial\psi(x,t)}{\partial x} = 0 \tag{3.3.2}$$

Hence, the time derivative of $\langle x\rangle$ is

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty}\psi^*(x,t)x\psi(x,t)\,dx = \int_{-\infty}^{\infty}\frac{\partial\psi^*(x,t)}{\partial t}x\psi(x,t)\,dx+\int_{-\infty}^{\infty}\psi^*(x,t)x\frac{\partial\psi(x,t)}{\partial t}\,dx \tag{3.3.3}$$

Substituting the Schrödinger equation and its conjugate gives

$$\begin{aligned}\frac{d\langle x\rangle}{dt} &= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial^2\psi^*(x,t)}{\partial x^2}x\psi(x,t)\,dx+\frac{i}{\hbar}\int_{-\infty}^{\infty}\psi^*(x,t)V(x)\psi(x,t)\,dx\\ &\quad+\frac{i\hbar}{2m}\left[\int_{-\infty}^{\infty}\psi^*(x,t)x\frac{\partial^2\psi(x,t)}{\partial x^2}\,dx\right]-\frac{i}{\hbar}\int_{-\infty}^{\infty}\psi^*(x,t)V(x)\psi(x,t)\,dx\\ &= -\frac{i\hbar}{2m}\lim_{\xi\to\infty}\left[\int_{-\xi}^{\xi}\frac{\partial^2\psi^*(x,t)}{\partial x^2}x\psi(x,t)\,dx-\int_{-\xi}^{\xi}\psi^*(x,t)x\frac{\partial^2\psi(x,t)}{\partial x^2}\,dx\right]\end{aligned} \tag{3.3.4}$$

Integration by parts gives

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\lim_{\xi\to\infty}\left\{\left[\frac{\partial\psi^*(x,t)}{\partial x}x\psi(x,t)\right]_{-\xi}^{\xi} - \int_{-\xi}^{\xi}\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial}{\partial x}[x\psi(x,t)]\,dx\right.$$
$$\left. -\left[\psi^*(x,t)x\frac{\partial\psi(x,t)}{\partial x}\right]_{-\xi}^{\xi} + \int_{-\xi}^{\xi}\frac{\partial}{\partial x}[\psi^*(x,t)x]\frac{\partial\psi(x,t)}{\partial x}\,dx\right\} \tag{3.3.5}$$

Using (*3.3.2*), the first and third terms equal to zero; so we have

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\lim_{\xi\to\infty}\left[-\int_{-\xi}^{\xi}\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)\,dx - \int_{-\xi}^{\xi}\frac{\partial\psi^*(x,t)}{\partial x}x\frac{\partial\psi(x,t)}{\partial x}\,dx\right.$$
$$\left. + \int_{-\xi}^{\xi}\frac{\partial\psi^*(x,t)}{\partial x}x\frac{\partial\psi(x,t)}{\partial x}\,dx + \int_{-\xi}^{\xi}\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\,dx\right] \tag{3.3.6}$$

Eventually, integration by parts of the first term gives

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\lim_{\xi\to\infty}\left[\int_{-\xi}^{\xi} - [\psi^*(x,t)\psi(x,t)]_{-\xi}^{\xi} + 2\int_{-\xi}^{\xi}\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\,dx\right]$$
$$= \frac{1}{m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\hbar}{i}\frac{\partial\psi(x,t)}{\partial x}\,dx = \frac{1}{m}\langle p\rangle \tag{3.3.7}$$

(*b*) Consider the time derivative of $\langle p\rangle$:

$$\frac{d\langle p\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\hbar}{i}\frac{\partial\psi(x,t)}{\partial x}\,dx = \frac{\hbar}{i}\int_{-\infty}^{\infty}\frac{\partial\psi^*(x,t)}{\partial t}\frac{\partial\psi(x,t)}{\partial x}\,dx + \frac{\hbar}{i}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial}{\partial t}\frac{\partial\psi(x,t)}{\partial x}\,dx \tag{3.3.8}$$

Since $\psi(x, t)$ has smooth derivatives, we can interchange the time and spatial derivatives in the second term. Using the Schrödinger equation, (*3.3.8*) becomes

$$\frac{d\langle p\rangle}{dt} = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{\partial^2\psi^*(x,t)}{\partial x^2}\frac{\partial\psi(x,t)}{\partial x}\,dx + \int_{-\infty}^{\infty}V(x)\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\,dx$$
$$+ \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial^3\psi(x,t)}{\partial x^3}\,dx - \int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial}{\partial x}[V(x)\psi(x,t)]\,dx \tag{3.3.9}$$

Integration by parts of the first term gives

$$I \equiv \int_{-\infty}^{\infty}\frac{\partial^2\psi^*(x,t)}{\partial x^2}\frac{\partial\psi(x,t)}{\partial x}\,dx = \lim_{\xi\to\infty}\left\{\left[\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial\psi(x,t)}{\partial x}\right]_{-\xi}^{\xi} - \int_{-\xi}^{\xi}\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial^2\psi(x,t)}{\partial x^2}\,dx\right\} \tag{3.3.10}$$

Using (*3.3.2*), we arrive at

$$I = \lim_{\xi\to\infty}\left[-\int_{-\xi}^{\xi}\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial^2\psi(x,t)}{\partial x^2}\,dx\right] \tag{3.3.11}$$

Again, integration by parts gives

$$I = \lim_{\xi\to\infty}\left\{-\left[\psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2}\right]_{-\xi}^{\xi} + \int_{-\xi}^{\xi}\psi^*(x,t)\frac{\partial^3\psi(x,t)}{\partial x^3}\,dx\right\} = \int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial^3\psi(x,t)}{\partial x^3}\,dx \tag{3.3.12}$$

Returning to (*3.3.9*), we finally have

$$\frac{d\langle p\rangle}{dp} = \int_{-\infty}^{\infty}V(x)\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\,dx - \int_{-\infty}^{\infty}\psi^*(x,t)\frac{dV(x)}{dx}\psi(x,t)\,dx$$
$$- \int_{-\infty}^{\infty}\psi^*(x,t)V(x)\frac{\partial\psi(x,t)}{\partial x}\,dx = \left\langle -\frac{dV}{dx}\right\rangle \tag{3.3.13}$$

3.4. Consider a particle described by a wave function $\psi(\mathbf{r}, t)$. Calculate the time-derivative $\frac{\partial\rho(\mathbf{r}, t)}{\partial t}$, where $\rho(\mathbf{r}, t)$ is the probability density, and show that the continuity equation $\frac{\partial\rho(\mathbf{r}, t)}{\partial t} + \nabla\cdot\mathbf{J}(\mathbf{r}, t) = 0$ is valid, where $\mathbf{J}(\mathbf{r}, t)$ is the probability current, equal to $\frac{1}{m}\operatorname{Re}\left[\psi^*\left(\frac{\hbar}{i}\nabla\psi\right)\right]$.

Using the Schrödinger equation,

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t) + V(\mathbf{r}, t)\psi(\mathbf{r}, t) \tag{3.4.1}$$

Assuming $V(x)$ is real, the conjugate expression is $-i\hbar\frac{\partial\psi^*(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\mathbf{r}, t) + V(\mathbf{r}, t)\psi^*(\mathbf{r}, t)$. According to the definition of $\rho(\mathbf{r}, t)$, $\rho(\mathbf{r}, t) = \psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t)$; hence,

$$\frac{\partial\rho(\mathbf{r}, t)}{\partial t} = \frac{\partial\psi^*(\mathbf{r}, t)}{\partial t}\psi(\mathbf{r}, t) + \psi^*(\mathbf{r}, t)\frac{\partial\psi(\mathbf{r}, t)}{\partial t} \tag{3.4.2}$$

Using (*3.4.1*) and its conjugate, we arrive at

$$\frac{\rho(\mathbf{r}, t)}{\partial t} = \left[\frac{\hbar}{2mi}\nabla^2\psi^*(\mathbf{r}, t)\right]\psi(\mathbf{r}, t) - \frac{1}{i\hbar}V(\mathbf{r}, t)\psi^*(\mathbf{r}, t)\psi(\mathbf{r}, t) - \psi^*(\mathbf{r}, t)\left[\frac{\hbar}{2mi}\nabla^2\psi(\mathbf{r}, t)\right]$$
$$+\frac{1}{i\hbar}\psi^*(\mathbf{r}, t)V(\mathbf{r}, t)\psi(\mathbf{r}, t) = -\frac{\hbar}{2mi}[\psi^*(\mathbf{r}, t)\nabla^2\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\nabla^2\psi^*(\mathbf{r}, t)] \tag{3.4.3}$$

We set

$$\mathbf{J}(\mathbf{r}, t) = \frac{1}{m}\operatorname{Re}\left[\psi^*\left(\frac{\hbar}{i}\nabla\psi\right)\right] = \frac{\hbar}{2mi}[\psi^*(\mathbf{r}, t)\nabla\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\nabla\psi^*(\mathbf{r}, t)] \tag{3.4.4}$$

Using the theorem $\nabla\cdot(U\mathbf{A}) = (\nabla U)\cdot\mathbf{A} + U(\nabla\cdot\mathbf{A})$, we have

$$\nabla\cdot\mathbf{J}(\mathbf{r}, t) = \frac{\hbar}{2mi}[(\nabla\psi^*)\cdot(\nabla\psi) + \psi^*(\nabla^2\psi) - (\nabla\psi)\cdot(\nabla\psi^*) - \psi(\nabla^2\psi^*)]$$
$$= \frac{\hbar}{2mi}[\psi^*\nabla^2\psi - \psi\nabla^2\psi^*] \tag{3.4.5}$$

so

$$\frac{\partial\rho(\mathbf{r}, t)}{\partial t} + \nabla\cdot\mathbf{J}(\mathbf{r}, t) = 0 \tag{3.4.6}$$

3.5. Consider the wave function

$$\psi(x, t) = [Ae^{ipx/\hbar} + Be^{-ipx/\hbar}]\,e^{-ip^2t/2m\hbar} \tag{3.5.1}$$

Find the probability current corresponding to this wave function.

The probability current is by definition

$$j(x, t) = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right) \tag{3.5.2}$$

The complex conjugate of ψ is $\psi^*(x, t) = (A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar})\,e^{ip^2t/2m\hbar}$; so a direct calculation yields

$$j(x, t) = \frac{\hbar}{2mi}\left[(A^*e^{-ipx/\hbar} + B^*e^{ipx/\hbar})\left(\frac{ip}{\hbar}Ae^{ipx/\hbar} - \frac{ip}{\hbar}Be^{-ipx/\hbar}\right) - \left(-\frac{ip}{\hbar}A^*e^{-ipx/\hbar} + \frac{ip}{\hbar}B^*e^{ipx/\hbar}\right)(Ae^{ipx/\hbar} + Be^{-ipx/\hbar})\right]$$
$$= \frac{p}{2m}\left[(|A|^2 - A^*Be^{-2ipx/\hbar} + AB^*e^{2ipx/\hbar} - |B|^2) - (-|A|^2 - A^*Be^{-2ipx/\hbar} + AB^*e^{2ipx/\hbar} + |B|^2)\right]$$
$$= \frac{p}{m}\left(|A|^2 - |B|^2\right) \tag{3.5.3}$$

Note that the wave function $\psi(x, t)$ expresses a superposition of two currents of particles moving in opposite directions. Each of the currents is constant and time-independent in its magnitude. The term $e^{-ip^2t/2m\hbar}$ implies that the particles are of energy $p^2/2m$. The amplitudes of the currents are A and B.

3.6. Show that for a one-dimensional square-integrable wave-packet,

$$\int_{-\infty}^{\infty} j(x)\,dx = \frac{\langle p\rangle}{m} \tag{3.6.1}$$

where $j(x)$ is the probability current.

Consider the integral $\int_{-\infty}^{\infty} |\psi(x,t)|^2\,dx$. This integral is finite, so we have $\lim_{x\to\pm\infty} |\psi(x,t)|^2 = 0$. Hence,

$$\int_{-\infty}^{\infty} j(x)\,dx = \frac{\hbar}{2im}\int_{-\infty}^{\infty}\left[\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}\right]dx \tag{3.6.2}$$

Integration by parts gives

$$\int_{-\infty}^{\infty}\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}\,dx = \lim_{\xi\to\infty}\left\{\left[\psi(x,t)\psi^*(x,t)\right]_{-\xi}^{\xi} - \int_{-\xi}^{\xi}\frac{\partial\psi(x,t)}{\partial x}\psi^*(x,t)\,dx\right\} = -\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\,dx \tag{3.6.3}$$

Therefore, we have

$$\int_{-\infty}^{\infty} j(x)\,dx = \frac{1}{m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)\,dx = \frac{\langle p\rangle}{m} \tag{3.6.4}$$

3.7. Consider a particle of mass m held in a one-dimensional potential $V(x)$. Suppose that in some region $V(x)$ is constant, $V(x) = V$. For this region, find the stationary states of the particle when (*a*) $E > V$, (*b*) $E < V$, and (*c*) $E = V$, where E is the energy of the particle.

(*a*) The stationary states are the solutions of

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2} + V\phi(x) = E\phi(x) \tag{3.7.1}$$

For $E > V$, we introduce the positive constant k defined by $\hbar^2k^2/2m = E - V$, so that

$$\frac{\partial^2\phi(x)}{\partial x^2} + k^2\phi(x) = 0 \tag{3.7.2}$$

The solution of this equation can be written in the form

$$\phi(x) = Ae^{ikx} + A'e^{-ikx} \tag{3.7.3}$$

where A and A' are arbitrary complex constants.

(*b*) We introduce the positive constant ρ defined by $\hbar^2\rho^2/2m = V - E$; so (*3.7.1*) can be written as

$$\frac{\partial^2\phi(x)}{\partial x^2} - \rho^2\phi(x) = 0 \tag{3.7.4}$$

The general solution of (*3.7.4*) is $\phi(x) = Be^{\rho x} + B'e^{-\rho x}$ where B and B' are arbitrary complex constants.

(c) When $E = V$ we have $\dfrac{\partial^2\phi(x)}{\partial x^2} = 0$; so $\phi(x)$ is a linear function of x, $\phi(x) = Cx + C'$ where C and C' are complex constants.

3.8. Consider a particle of mass m confined in an infinite one-dimensional potential well of width a:

$$V(x) = \begin{cases} 0 & -\frac{a}{2} \le x \le \frac{a}{2} \\ \infty & \text{otherwise} \end{cases} \tag{3.8.1}$$

Find the eigenstates of the Hamiltonian (i.e., the stationary states) and the corresponding eigenenergies.

For $x > a/2$ and $x < -a/2$ the potential is infinite, so there is no possibility of finding the particle outside the well. This means that

$$\psi\left(x > \frac{a}{2}\right) = 0 \qquad \psi\left(x < \frac{a}{2}\right) = 0 \tag{3.8.2}$$

Since the wave function must be continuous, we also have $\psi(a/2) = \psi(-a/2) = 0$. For $-a/2 \le x \le a/2$ the potential is constant, $V(x) = 0$; therefore, we can rely on the results of Problem 3.7. We distinguish between three possibilities concerning the energy E. As in Problem 3.7, part (a), for $E > 0$ we define the positive constant k, $\hbar^2 k^2/2m = E$; so we obtain $\phi(x) = Ae^{ikx} + A'e^{-ikx}$. Imposing the continuous conditions, we arrive at

$$\text{I} \quad Ae^{ika/2} + A'e^{-ika/2} = 0 \qquad \text{II} \quad Ae^{-ika/2} + A'e^{ika/2} = 0 \tag{3.8.3}$$

Multiplying (3.8.3I) by $e^{ika/2}$ we obtain $A' = -Ae^{ika}$. Substituting A' into (3.8.3II) yields

$$Ae^{-ika/2} - Ae^{ika}e^{ika/2} = 0 \tag{3.8.4}$$

Multiplying (3.8.4) by $e^{-ika/2}$ and dividing by A [if $A = 0$ then $\psi(x) \equiv 0$] we obtain $e^{-ika} - e^{ika} = 0$. Using the relation $e^{i\alpha} = \cos\alpha + i\sin\alpha$ we have $-2i\sin(ka) = 0$. The last relation is valid only if $ka = n\pi$, where n is an integer. Also, since k must be positive, n must also be positive. We see that the possible positive eigenenergies of the particle are

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 = \frac{\pi^2\hbar^2 n^2}{2ma^2} \tag{3.8.5}$$

The corresponding eigenfunctions are

$$\psi_n(x) = Ae^{ik_n x} - Ae^{ik_n a}e^{-ik_n x} = Ae^{in\pi x/a} - e^{in\pi(a-x)/a} = Ae^{in\pi/2}\left[e^{in\pi(x/a-1/2)} - e^{-in\pi(x/a-1/2)}\right]$$

$$= C\sin\left[n\pi\left(\frac{x}{a} - \frac{1}{2}\right)\right] \qquad (n = 1, 2, \ldots) \tag{3.8.6}$$

where C is a normalization constant obtained by

$$\frac{1}{C^2} = \int_{-a/2}^{a/2} \sin^2\left[n\pi\left(\frac{x}{a} - \frac{1}{2}\right)\right]dx \tag{3.8.7}$$

Defining $y = \frac{x}{a} - \frac{1}{2}$ and $dy = \frac{dx}{a}$, (3.8.7) becomes

$$\frac{1}{C^2} = a\int_{-1}^{0} \sin^2(n\pi y)\,dy = \frac{a}{2}\int_{-1}^{0} [1 - \cos(2\pi ny)]\,dy = \frac{a}{2}\left[y - \frac{\sin(2\pi ny)}{2\pi n}\right]_{-1}^{0} = \frac{a}{2} \tag{3.8.8}$$

Therefore, $C = \sqrt{2/a}$. Finally,

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left[n\pi\left(\frac{x}{a} - \frac{1}{2}\right)\right] \tag{3.8.9}$$

Consider now the case when $E < 0$. As in Problem 3.7, part (b), we introduce the positive constant ρ, $\hbar^2\rho^2/2m = -E$. Stationary states should be of the form $\psi(x) = Be^{\rho x} + B'e^{-\rho x}$. Imposing the boundary conditions, we obtain

$$\text{I} \quad Be^{\rho a/2} + B'e^{-\rho a/2} = 0 \qquad \text{II} \quad Be^{-\rho a/2} + B'e^{\rho a/2} = 0 \tag{3.8.10}$$

Multiplying (3.8.10I) by $e^{\rho a/2}$ yields $B' = -Be^{\rho a}$, so $Be^{-\rho a/2} - Be^{\rho a}e^{\rho a/2} = 0$. Multiplying by $e^{\rho a/2}$ and dividing by B, we obtain $1 - e^{2\rho a} = 0$. Therefore, $2\rho a = 0$. Since ρ must be positive, there are no states with corresponding negative energy.

Finally, we consider the case when $E = 0$. According to Problem 3.7, part (c), we have $\psi(x) = Cx + C'$. Imposing the boundary conditions yields

$$C\frac{a}{2} + C' = 0 \qquad -C\frac{a}{2} + C' = 0 \tag{3.8.11}$$

Solving these equations yields $C = C' = 0$, so the conclusion is that there is no possible state with $E = 0$.

3.9. Refer to Problem 3.8. At $t = 0$ the particle is in a state described by a linear combination of the two lowest stationary states:

$$\psi(x, 0) = \alpha\psi_1(x) + \beta\psi_2(x) \qquad (|\alpha|^2 + |\beta|^2 = 1) \tag{3.9.1}$$

(a) Calculate the wave function $\psi(x, t)$ and the mean value of the operators x and p_x as a function of time.
(b) Verify the Ehrenfest theorem, $md\langle x\rangle/dt = \langle p_x\rangle$.

(a) Consider part (c) of Problem 3.1. The time-evolution of the stationary states is of the form

$$\psi_n(x, t) = \psi_n(x)\exp(-iE_n t/\hbar) \tag{3.9.2}$$

Consequently, using the superposition principle gives

$$\psi(x,t) = \alpha\psi_1(x,t) + \beta\psi_2(x,t)$$
$$= \alpha\left[\sqrt{\frac{2}{a}}\sin\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\exp\left(\frac{-\pi^2 i\hbar t}{2ma^2}\right)\right] + \beta\left[\sqrt{\frac{2}{a}}\sin\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\exp\left(\frac{-\pi^2 i\hbar t}{2ma^2}\right)\right] \tag{3.9.3}$$

We now calculate

$$\langle x\rangle = \int_{-a/2}^{a/2}\psi^*(x,t)x\psi(x,t)\,dx = \int_{-a/2}^{a/2}[\alpha^* z\psi_1^*(x,t) + \beta^*\psi_2^*(x,t)]\,x\,[\alpha\psi_1(x,t)+\beta\psi_2(x,t)]\,dx$$
$$= \alpha^2\int_{-a/2}^{a/2}x|\psi_1(x,t)|^2\,dx + \beta^2\int_{-a/2}^{a/2}x|\psi_2(x,t)|^2\,dx + 2\mathrm{Re}\left[\alpha^*\beta\int_{-a/2}^{a/2}x\psi_1^*(x,t)\psi_2(x,t)\,dx\right] \tag{3.9.4}$$

Consider each of the three elements separately:

$$I_1 \equiv \int_{-a/2}^{a/2}x|\psi_1(x,t)|^2\,dx = \frac{a}{2}\int_{-a/2}^{a/2}x\,\sin\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]dx \tag{3.9.5}$$

Defining $y = \frac{x}{a} - \frac{1}{2}$, $dy = \frac{dx}{a}$, so

$$I_1 = a\int_{-1}^{0}(2y+1)\sin^2(\pi y)\,dy = 2a\int_{-1}^{0}y\sin^2(\pi y)\,dy + a\int_{-1}^{0}\sin^2(\pi y)\,dy \tag{3.9.6}$$

Solving these integrals yields

$$I_1 = 2a\left[\frac{y^2}{4} - \frac{y\sin(2\pi y)}{4\pi} - \frac{\cos(2\pi y)}{8\pi^2}\right]_{-1}^{0} + a\left[\frac{y}{2} - \frac{\sin(2\pi y)}{4\pi}\right]_{-1}^{0} = -\frac{a}{2} + \frac{a}{2} = 0 \tag{3.9.7}$$

One can repeat this procedure to show that

$$I_2 \equiv \int_{-a/2}^{a/2}x|\psi_2(x,t)|^2\,dx = \frac{2}{a}\int_{-a/2}^{a/2}x\sin^2\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]dx = 0 \tag{3.9.8}$$

Note that this result can arise from different considerations. The function $f(x) = \sin^2\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]$ is an even function of x:

$$f(-x) = \left[\sin 2\pi\left(-\frac{x}{a}-\frac{1}{2}\right)\right]^2 = \left[-\sin 2\pi\left(\frac{x}{a}+\frac{1}{2}\right)\right]^2 = \left[-\sin\left(2\pi\left(\frac{x}{a}+\frac{1}{2}\right)+2\pi\right)\right]^2$$
$$= \left[\sin 2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]^2 = f(x) \tag{3.9.9}$$

On the other hand, $f(x) = x$ is an odd function of x; therefore, $x\sin^2[2\pi(x/a - 1/2)]$ is an even function of x, and its integral vanishes from $-a/2$ to $a/2$. Consider now the last term in (*3.9.4*):

$$I_3 \equiv \int_{-a/2}^{a/2}x\psi_1^*(x,t)\psi_2(x,t)\,dx = \frac{2}{a}\int_{-a/2}^{a/2}x\sin\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\sin\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\exp\left(-\frac{3\pi^2 i\hbar t}{2ma^2}\right)dx \tag{3.9.10}$$

Defining $y = x/a - 1/2$, $dy = dx/a$, and $\omega = 3\pi^2\hbar/2ma^2$, we obtain

$$I_3 = ae^{-i\omega t}\int_{-1}^{0}(2y+1)\sin(\pi y)\sin(2\pi y)\,dy = ae^{-i\omega t}\int_{-1}^{0}(2y+1)\frac{1}{2}[\cos(\pi y) - \cos(3\pi y)]\,dy$$
$$= \frac{16a}{9\pi^2}e^{-i\omega t} \tag{3.9.11}$$

Finally, returning to (*3.9.4*) we obtain

$$\langle x\rangle = \frac{16a}{9\pi^2}2\,\mathrm{Re}\,(\alpha^*\beta e^{-i\omega t}) = \frac{32a}{9\pi^2}[\mathrm{Re}\,(\alpha^*\beta)\cos(\omega t) + \mathrm{Re}\,(i\alpha^*\beta)\sin(\omega t)] \tag{3.9.12}$$

Consider the mean value of the momentum:

$$\langle p_x \rangle = \int_{-a/2}^{a/2} \psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)\,dx = \frac{\hbar}{i}\int_{-a/2}^{a/2} [\alpha^*\psi_1^*(x,t) + \beta^*\psi_2^*(x,t)]\left[\alpha\frac{\partial\psi_1(x,t)}{\partial x} + \beta\frac{\partial\psi_2(x,t)}{\partial x}\right]dx \tag{3.9.13}$$

We calculate separately each of the four terms in (*3.9.13*):

$$\int_{-a/2}^{a/2} \psi_1^* \frac{\partial\psi_1(x,t)}{\partial x}\,dx = \frac{2\pi}{a\,a}\int_{-a/2}^{a/2} \sin\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\cos\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]dx \tag{3.9.14}$$

$\sin\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]$ is an even function of x and $\cos\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]$ is an odd function, so their product is an odd function, and therefore the integral of the product between $x = -a/2$ and $x = a/2$ equals zero. Also,

$$\int_{-a/2}^{a/2} \psi_2^*(x,t)\frac{\partial\psi_2(x,t)}{\partial x}\,dx = \frac{2}{a}\frac{2\pi}{a}\int_{-a/2}^{a/2} \sin\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\cos\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]dx \tag{3.9.15}$$

$\sin\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]$ is an odd function of x and $\cos\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]$ is an even one; therefore, their product is an odd function, and thus the integral between $x = -a/2$ and $a = 2$ vanishes. We have

$$I \equiv \int_{-a/2}^{a/2} \psi_1^*(x,t)\frac{\partial\psi_2(x,t)}{\partial x}\,dx = \frac{4\pi}{a^2}\int_{-a/2}^{a/2} \sin\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\cos\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]e^{-i\omega t}\,dx \tag{3.9.16}$$

Defining $y = \frac{x}{a} - \frac{1}{2}$ and $dy = \frac{dx}{a}$, the integral I becomes

$$I = \frac{4\pi}{a^2}e^{-i\omega t}\int_{-1}^{0} \sin(\pi y)\cos(2\pi y)\,dy = \frac{4\pi}{a}\left[\frac{\cos(\pi y)}{2\pi} - \frac{\cos(3\pi y)}{6\pi}\right]_{-1}^{0} e^{-i\omega t} = \frac{8}{3a}e^{-i\omega t} \tag{3.9.17}$$

Finally,

$$\Gamma \equiv \int_{-a/2}^{a/2} \psi_2^*(x,t)\frac{\partial\psi_1(x,t)}{\partial x}\,dx = \frac{2\pi}{a}\int_{-a/2}^{a/2} \sin\left[2\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]\cos\left[\pi\left(\frac{x}{a}-\frac{1}{2}\right)\right]e^{i\omega t}\,dx \tag{3.9.18}$$

Using the same definitions used above, we arrive at

$$\Gamma = \frac{2\pi}{a}e^{i\omega t}\int_{-1}^{0} \sin(2\pi y)\cos(\pi y)\,dy = \frac{2\pi}{a}e^{i\omega t}\left[-\frac{\cos(\pi y)}{2\pi} - \frac{\cos(3\pi y)}{6\pi}\right]_{-1}^{0} = -\frac{8}{3a}e^{i\omega t} \tag{3.9.19}$$

Substituting the results in equation (*3.9.13*), we finally reach

$$\langle p_x \rangle = \frac{8\hbar}{3ia}\left[\alpha^*\beta e^{-i\omega t} - \alpha\beta^* e^{i\omega t}\right] \tag{3.9.20}$$

(*b*) In part (*a*) we obtain

$$\langle x(t) \rangle = \frac{16a}{9\pi^2}\left[\alpha^*\exp\left(-\frac{3i\pi^2\hbar}{2ma^2}t\right) + \alpha\beta^*\exp\left(\frac{3i\pi^2\hbar}{2ma^2}t\right)\right] \tag{3.9.21}$$

Therefore, we have

$$m\frac{d\langle x\rangle}{dt} = m\frac{16a}{9\pi^2}\frac{3i\pi^2\hbar}{2ma^2}\left[-\alpha^*\beta\exp\left(-\frac{3\pi^2 i\hbar}{2ma^2}t\right) + \alpha\beta^*\exp\left(\frac{3\pi^2 i\hbar}{2ma^2}t\right)\right] = \frac{8\hbar}{3ia}[\alpha^*\beta e^{-i\omega t} - \alpha\beta^* e^{i\omega t}] \tag{3.9.22}$$

By inspection, the last expression is identical to $\langle p_x \rangle$. Thus, for this particular case Ehrenfest's theorem is verified.

3.10. Refer again to Problem 3.8. Now suppose that the potential well is located between $x = 0$ and $x = a$:

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{otherwise} \end{cases} \tag{3.10.1}$$

Find the stationary eigenstates and the corresponding eigenenergies.

We begin by performing a formal shift of the potential well, $\tilde{x} = x - a/2$, so the problem becomes identical to Problem 3.8:

$$V(\tilde{x}) = \begin{cases} 0 & -a/2 \le x \le a/2 \\ \infty & \text{otherwise} \end{cases} \tag{3.10.2}$$

Using the solution of Problem 3.8, the possible energies are

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2} \tag{3.10.3}$$

where n is a positive integer. The corresponding eigenstates are

$$\psi_n(\tilde{x}) = \sqrt{\frac{2}{a}} \sin\left[n\pi\left(\frac{\tilde{x}}{a} - \frac{1}{2}\right)\right] \tag{3.10.4}$$

Or, in terms of the original coordinate, we have

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} - n\pi\right) \tag{3.10.5}$$

3.11. Consider the step potential (Fig. 3-3):

$$V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases} \tag{3.11.1}$$

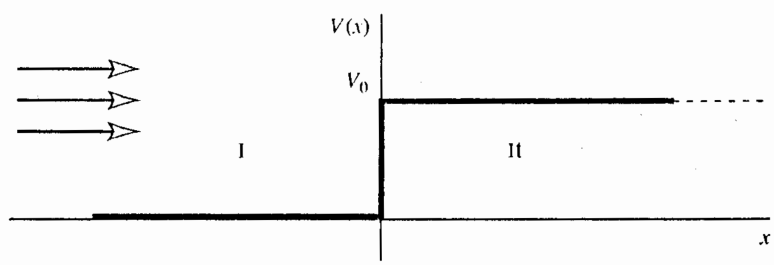

Fig. 3-3

Consider a current of particles of energy $E > V_0$ moving from $x = -\infty$ to the right. (*a*) Write the stationary solutions for each of the regions. (*b*) Express the fact that there is no current coming back from $x = +\infty$ to the left. (*c*) Use the matching conditions to express the reflected and transmitted amplitudes in terms of the incident amplitude. Note that since the potential is bounded, it can be shown that the derivative of the wave function is continuous for all x.

(*a*) Referring to Problem 3.7, part (*a*), we define

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_2 = \sqrt{\frac{2m(E-V)}{\hbar^2}} \tag{3.11.2}$$

Then the general solutions for the regions I ($x < 0$) and II ($x > 0$) are

$$\phi_I(x) = A_1 e^{ik_1x} + A'_1 e^{-ik_1x} \qquad \phi_{II}(x) = A_2 e^{ik_2x} + A'_2 e^{-ik_2x} \tag{3.11.3}$$

(*b*) The wave function of form e^{ikx} represents particles coming from $x = -\infty$ to the right, and e^{-ikx} represents particles moving from $x = +\infty$ to the left. $\phi_I(x)$ is the superposition of two waves. The first one is of incident particles propagating from left to right and is of amplitude A_1; the second wave is of amplitude A'_1 and represents reflected particles moving from right to left. Since we consider incident particles coming from $x = -\infty$ to the right, it is not possible to find in II a current that moves from $x = +\infty$ to the left. Therefore, we set $A'_2 = 0$. Thus, $\phi_{II}(x)$ represents the current of transmitted particles with corresponding amplitude A_2.

(*c*) First we apply the continuity condition of $\phi(x)$ at $x = 0$, $\phi_I(0) = \phi_{II}(0)$. So substituting in (*3.11.3*) gives

$$A_1 + A'_1 = A_2 \tag{3.11.4}$$

Secondly, $\frac{\partial\phi(x)}{\partial x}$ should also be continuous at $x = 0$; we have

$$\frac{\partial\phi_I(x)}{\partial x} = ik_1A_1e^{ik_1x} - ik_1A'_1e^{ik_1x} \qquad \frac{\partial\phi_{II}(x)}{\partial x} = ik_2A_2e^{ik_2x} \tag{3.11.5}$$

Applying $\frac{\partial\phi_I(0)}{\partial x} = \frac{\partial\phi_{II}(0)}{\partial x}$, we obtain

$$ik_1(A_1 - A'_1) = ik_2A_2 \tag{3.11.6}$$

Substituting A_2 gives $A_1 + A'_1 = (A_1 - A'_1)\,k_1/k_2$, which yields

$$\frac{A'_1}{A_1} = \frac{k_1 - k_2}{k_1 + k_2} \tag{3.11.7}$$

Eventually, substituting (*3.11.7*) in (*3.11.4*) yields $A_1\left(1 + \frac{k_1 - k_2}{k_1 + k_2}\right) = A_2$; therefore,

$$\frac{A_2}{A_1} = \frac{2k_1}{k_1 + k_2} \tag{3.11.8}$$

3.12. Refer to Problem 3.11. (*a*) Compute the probability current in the regions I and II and interpret each term. (*b*) Find the reflection and transmission coefficients.

(*a*) For a stationary state $\phi(x)$, the probability current is time-independent and equal to

$$J(x) = \frac{\hbar}{2mi}\left[\phi^*(x)\frac{\partial\phi(x)}{\partial x} - \phi(x)\frac{\partial\phi^*(x)}{\partial x}\right] \tag{3.12.1}$$

Using (*3.11.3*) for region I, we have

$$J_I(x) = \frac{\hbar}{2mi}[(A_1^*e^{-ik_1x} + A_1'^*e^{ik_1x})(ik_1A_1e^{ik_1x} - ik_1A'_1e^{-ik_1x})$$

$$-(A_1e^{ik_1x} + A'_1e^{-ik_1x})(-ik_1A_1^*e^{-ik_1x} + ik_1A_1'^*e^{ik_1x})] = \frac{\hbar k_1}{m}(|A_1|^2 - |A'_1|^2) \tag{3.12.2}$$

Similarly, for region II we have

$$J_{II}(x) = \frac{\hbar}{2mi}[A_2^*e^{-ik_2x}(ik_2)e^{ik_1x} - A_2e^{ik_2x}(-ik_2)e^{-ik_2x}] = \frac{\hbar k_2}{m}|A_2|^2 \tag{3.12.3}$$

The probability current in region I is the sum of two terms: $\hbar k_1|A_1|^2/m$ corresponds to the incoming current moving from left to right, and $-\hbar k_1|A'_1|^2/m$ corresponds to the reflected current (moving from right to left). Note that the probability current in region II represents the transmitted wave.

(*b*) Using the definition of the reflection coefficient (see Summary of Theory, refer to Eq. 3.27), it equals

$$R = \frac{|A'_1|^2\hbar k_1/m}{|A_1|^2\hbar k_1/m} = \left|\frac{A'_1}{A_1}\right|^2 \tag{3.12.4}$$

Substituting (*3.11.7*), we arrive at

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} = 1 - \frac{4k_1k_2}{(k_1 + k_2)^2} \tag{3.12.5}$$

The transmission coefficient is

$$T = \frac{|A_2|^2\hbar k_2/m}{|A_2|^2\hbar k_1/m} = \frac{k_2}{k_1}\left|\frac{A_2}{A_1}\right|^2 \tag{3.12.6}$$

Substituting (*3.11.8*), we arrive at

$$T = \frac{k_2}{k_1}\left(\frac{2k_1}{k_1 + k_2}\right)^2 = \frac{4k_1k_2}{(k_1 + k_2)^2}, \tag{3.12.7}$$

3.13. Consider a free particle of mass m whose wave function at time $t = 0$ is given by

$$\psi(x, 0) = \frac{\sqrt{a}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-a^2(k-k_0)^2/4} e^{ikx}\, dk \tag{3.13.1}$$

Calculate the time-evolution of the wave-packet $\psi(x, t)$ and the probability density $|\psi(x, t)|^2$. Sketch qualitatively the probability density for $t < 0$, $t = 0$, and $t > 0$. You may use the following identity: For any complex number α and β such that $-\pi/4 < \arg(\alpha) < \pi/4$,

$$\int_{-\infty}^{\infty} e^{-\alpha^2(y+\beta)^2}\, dy = \frac{\sqrt{\pi}}{\alpha} \tag{3.13.2}$$

The wave-packet at $t = 0$ is a superposition of plane waves e^{ikx} with coefficients $\frac{\sqrt{a}}{(2\pi)^{3/4}} e^{-a^2(k-k_0)^2/4}$; this is a Gaussian curve centered at $k = k_0$. The time-evolution of a plane wave e^{ikx} has the form $e^{ikx}e^{-iE(k)t/\hbar} = e^{ikx}e^{-i\hbar k^2 t/2m}$. We set $\omega(k) = \hbar k^2/2m$, so using the superposition principle, the time-evolution of the wave-packet $\psi(x, 0)$ is

$$\psi(x, t) = \frac{\sqrt{a}}{(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-a^2(k-k_0)^2/4} e^{i[kx-\omega(k)t]}\, dk \tag{3.13.3}$$

Our aim is to transform this integral into the form of (*3.13.2*). Therefore, we rearrange the terms in the exponent:

$$-\frac{a^2}{4}(k-k_0)^2 + i[kx - \omega(k)t] = -\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)k^2 + \left(\frac{a^2}{2}k_0 + ix\right)k - \frac{a^2}{4}k_0^2$$

$$= -\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)\left[k - \frac{\frac{a^2}{2}k_0 + ix}{2\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)}\right]^2 + \frac{\left(\frac{a^2}{2}k_0 + ix\right)^2}{4\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)} - \frac{a^2}{4}k_0^2 \tag{3.13.4}$$

Substituting in (*3.13.4*) and using (*3.13.2*) yields

$$\psi(x, t) = \frac{\sqrt{a}}{2^{3/4}\pi^{1/4}} \frac{\exp\left(-\frac{a^2k_0^2}{4}\right)}{\sqrt{\frac{a^2}{4} + \frac{i\hbar t}{2m}}} \exp\left[\frac{\left(\frac{a^2}{2}k_0 + ix\right)^2}{a^2 + \frac{2i\hbar t}{m}}\right] \tag{3.13.5}$$

The conjugate complex of (*3.13.5*) is

$$\psi^*(x, t) = \frac{\sqrt{a}}{2^{3/4}\pi^{1/4}} \frac{\exp\left(-\frac{a^2k_0^2}{4}\right)}{\sqrt{\frac{a^2}{4} - \frac{i\hbar t}{2m}}} \exp\left[\frac{\left(\frac{a^2}{2}k_0 - ix\right)^2}{a^2 - \frac{2i\hbar t}{m}}\right] \tag{3.13.6}$$

Hence,

$$|\psi(x, t)|^2 = \frac{a}{2^{3/2}\sqrt{\pi}} \frac{\exp\left(-\frac{a^2k_0^2}{2}\right)}{\sqrt{\left(\frac{a^2}{4} + \frac{i\hbar t}{2m}\right)\left(\frac{a^2}{4} - \frac{i\hbar t}{2m}\right)}} \exp\left[\frac{\left(\frac{a^2k_0}{2}\right)^2 - x^2 + ia^2k_0x}{a^2 + 2i\hbar t/m} + \frac{\left(\frac{a^2k_0}{2}\right)^2 - x^2 - ia^2k_0x}{a^2 - 2i\hbar t/m}\right]$$

$$= \sqrt{\frac{2}{\pi a^2}} \frac{1}{\sqrt{1 + 4\hbar^2t^2/m^2a^4}} \exp\left[-\frac{\frac{a^2k_0^2}{2}\left(a^4 + \frac{4\hbar^2t^2}{m^2}\right) + 2a^2\left(\frac{a^4k_0^2}{2} - x^2\right) + \frac{4\hbar k_0 a^2}{m}xt}{a^4 + 4\hbar^2t^2/m^2}\right]$$

$$= \sqrt{\frac{2}{\pi a^2}} \frac{1}{\sqrt{1 + 4\hbar^2t^2/m^2a^4}} \exp\left[-\frac{2a^2(x - \hbar k_0 t/m)^2}{a^4 + 4\hbar^2t^2/m^2}\right] \tag{3.13.7}$$

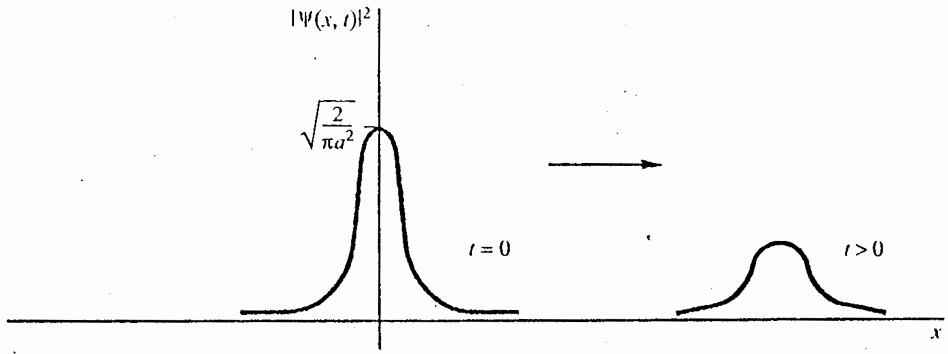

Fig. 3-4

The probability density is a Gaussian curve for every time t entered at $x_C = (\hbar k_0/m)\,t$. (i.e., the wave-packet moves with a velocity $V_0 = \hbar k_0/m$.) The value of $|\psi(x,t)|^2$ is maximal for $t = 0$ and tends to zero when $t \to \infty$. The width of the wave-packet is minimal for $t = 0$ and tends to ∞ when $t \to \infty$; see Fig. 3-4.

3.14. Consider a square potential barrier (Fig. 3-5):

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < l \\ 0 & l < x \end{cases} \tag{3.14.1}$$

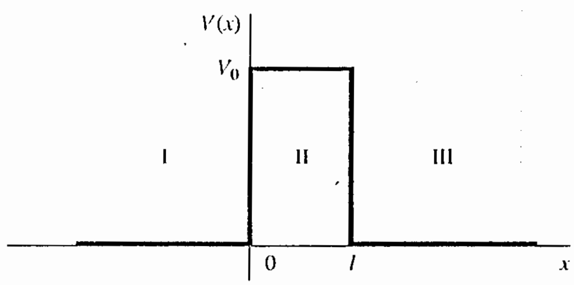

Fig. 3-5

(a) Assume that incident particles of energy $E > V_0$ are coming from $x = -\infty$. Find the stationary states. Apply the matching conditions at $x = 0$ and $x = l$. (b) Find the transmission and reflection coefficients. Sketch the transmission coefficient as a function of the barrier's width l, and discuss the results.

(a) Similar to Problem 3.7, part (a), we define

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \tag{3.14.2}$$

Thus, the stationary solutions for the three regions I ($x < 0$), II ($0 < x < l$), and III ($x > l$) are:

$$\begin{cases} \phi_I(x) = A_1 e^{ik_1x} + A'_1 e^{-ik_1x} \\ \phi_{II}(x) = A_2 e^{ik_2x} + A'_2 e^{-ik_2x} \\ \phi_{III}(x) = A_3 e^{ik_1x} + A'_3 e^{-ik_1x} \end{cases} \tag{3.14.3}$$

Each of the solutions describes a sum of terms representing movement from left to right, and from right to left. We consider incident particles from $x = -\infty$, so there should be no particles in region III moving from $x = \infty$ to the left. Therefore, we set $A'_3 = 0$. The matching conditions at $x = l$ enable us to express A_2 and A'_2 in terms of A_3. The continuity of $\phi(x)$ at $x = l$ yields $\phi_{II}(l) = \phi_{III}(l)$, so

$$A_2 e^{ik_2l} + A'_2 e^{-ik_2l} = A_3 e^{ik_1l}, \tag{3.14.4}$$

The continuity of $\phi'(x)$ yields

$$ik_2A_2e^{ik_2l} - ik_2A'_2e^{-ik_2l} = ik_1A_3e^{ik_1l} \tag{3.14.5}$$

Equations (*3.14.4*) and (*3.14.5*) give

$$\begin{cases} A_2 = \left[\dfrac{k_2+k_1}{2k_2}e^{i(k_1-k_2)l}\right]A_3 \\ A'_2 = \left[\dfrac{k_2-k_1}{2k_2}e^{i(k_1+k_2)l}\right]A_3 \end{cases} \tag{3.14.6}$$

The matching conditions at $x = 0$ yield

$$\phi_I(0) = \phi_{II}(0) \quad \Rightarrow \quad A_1 + A'_1 = A_2 + A'_2 \tag{3.14.7}$$

and

$$\phi'_I(0) = \phi'_{II}(0) \quad \Rightarrow \quad ik_1A_1 - ik_1A'_1 = ik_2A_2 - ik_2A'_2 \tag{3.14.8}$$

so we obtain

$$A_1 = \frac{k_1+k_2}{2k_1}A_2 + \frac{k_1-k_2}{2k_1}A'_2 \tag{3.14.9}$$

Using (*3.14.6*), we can express A_1 in terms of A_3:

$$\begin{aligned} A_1 &= \left[\frac{(k_1+k_2)^2}{4k_1k_2}e^{i(k_1-k_2)l} - \frac{(k_1-k_2)^2}{4k_1k_2}e^{i(k_1+k_2)l}\right]A_3 \\ &= \left[\frac{(k_1+k_2)^2-(k_1-k_2)^2}{4k_1k_2}\cos(k_2l) - i\frac{(k_1+k_2)^2+(k_1-k_2)^2}{4k_1k_2}\sin(k_2l)\right]e^{ik_1l}A_3 \\ &= \left[\cos(k_2l) - i\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2l)\right]e^{ik_1l}A_3 \end{aligned} \tag{3.14.10}$$

Similarly, we express A'_1 in terms of A_3:

$$\begin{aligned} A'_1 &= \frac{k_1-k_2}{2k_1}A_2 + \frac{k_1+k_2}{2k_1}A'_2 = \left[\frac{(k_1+k_2)(k_1-k_2)}{4k_1k_2}e^{i(k_1-k_2)l} + \frac{(k_1+k_2)(k_2-k_1)}{4k_2}e^{i(k_1+k_2)l}\right]A_3 \\ &= \left[\frac{(k_1^2-k_2^2)+(k_2^2-k_1^2)}{4k_1k_2}\cos(k_2l) + i\frac{(k_2^2-k_1^2)-(k_1^2-k_2^2)}{4k_1k_2}\sin(k_2l)\right]A_3 = i\frac{k_2^2-k_1^2}{2k_1k_2}\sin(k_2l)\,e^{ik_1l}A_3 \end{aligned} \tag{3.14.11}$$

(*b*) The reflection coefficient is the ratio of squares of the amplitudes corresponding to the incident and reflection waves (compare to Problem 3.12):

$$R = \left|\frac{A'_1}{A_1}\right|^2 \tag{3.14.12}$$

Using the results of part (*a*), we obtain

$$R = \frac{\left[\dfrac{k_2^2-k_1^2}{2k_1k_2}\sin(k_2l)\right]^2}{\cos^2(k_2l) + \left[\dfrac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2l)\right]^2} = \frac{(k_2^2-k_1^2)^2\sin^2(k_2l)}{4k_1^2k_2^2 + (k_1^2-k_2^2)^2\sin^2(k_2l)} \tag{3.14.13}$$

Finally, the transmission coefficient is

$$T = \left|\frac{A_3}{A_1}\right|^2 = \frac{1}{\cos^2(k_2l) + \left(\dfrac{k_1^2-k_2^2}{2k_1k_2}\right)^2\sin^2(k_2l)} = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 + (k_1^2-k_2^2)^2\sin^2(k_2l)} \tag{3.14.14}$$

The transmission coefficient oscillates periodically as a function of l (see Fig. 3-6) between its maximum value (one) and its minimum value $[1 + V_0^2/4E(E-V_0)]^{-1}$. When l is an integral multiple of π/k_2, there is no reflection from the barrier; this is called *resonance scattering* (see Chapter 15).

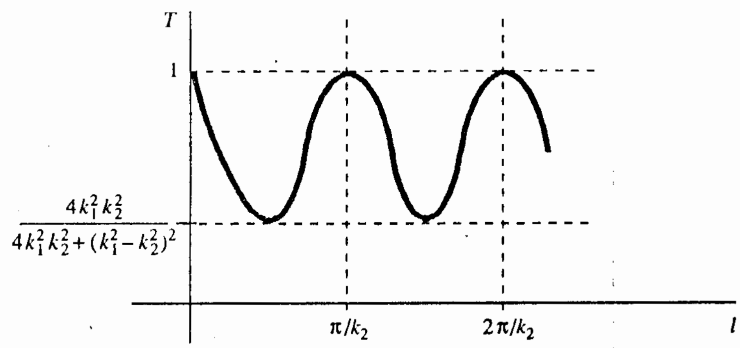

Fig. 3-6

3.15. Consider the square potential barrier of Problem 3.14. Find the stationary states describing incident particles of energy $E < V_0$. Compute the transmission coefficient and discuss the results.

The method of solution is analogous to that of Problem 3.14. Referring to Problem 3.7, we define

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad \rho = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{3.15.1}$$

The stationary solutions for the three regions I ($x < 0$), II ($0 < x < l$), and III ($x > l$) are

$$\begin{cases} \phi_I(x) = A_1 e^{ik_1x} + A_1' e^{-ik_1x} \\ \phi_{II}(x) = A_2 e^{\rho x} + A_2' e^{-\rho x} \\ \phi_{III}(x) = A_3 e^{ik_1x} + A_3' e^{-ik_1x} \end{cases} \tag{3.15.2}$$

We describe incident particles coming from $x = -\infty$, so we set $A_3' = 0$. Applying the matching conditions in $x = l$ gives

$$\phi_{II}(l) = \phi_{III}(l) \quad \Rightarrow \quad A_2 e^{\rho l} + A_2' e^{-\rho l} = A_3 e^{ik_1x} \tag{3.15.3}$$

$$\phi_{II}'(l) = \phi_{III}'(l) \quad \Rightarrow \quad A_2 \rho e^{\rho l} - A_2' e^{-\rho l} = ik_1 A_3 e^{ik_1 l} \tag{3.15.4}$$

From (*3.15.3*) and (*3.15.4*) we obtain

$$A_2 = \left[\frac{\rho + ik_1}{2\rho} e^{(ik_1 - \rho)l}\right] A_3 \qquad A_2' = \left[\frac{\rho - ik_1}{2\rho} e^{(ik_1 + \rho)l}\right] A_3 \tag{3.15.5}$$

The matching conditions at $x = 0$ yield

$$\phi_I(0) = \phi_{II}(0) \quad \Rightarrow \quad A_1 + A_1' = A_2 + A_2' \tag{3.15.6}$$

$$\phi_I'(0) = \phi_{II}'(0) \quad \Rightarrow \quad ik_1 A_1 - ik_1 A_1' = \rho A_2 - \rho A_2' \tag{3.15.7}$$

From (*3.15.6*) and (*3.15.7*) we obtain

$$A_1 = \frac{ik_1 + \rho}{2ik_1} A_2 + \frac{ik_1 - \rho}{2ik_1} A_2' \tag{3.15.8}$$

Using (*3.15.5*), we arrive at

$$A_1 = \left[\frac{(ik_1 + \rho)^2}{4ik_1\rho} e^{(ik_1 - \rho)l} - \frac{(ik_1 - \rho)^2}{4ik_1\rho} e^{(ik_1 + \rho)l}\right] A_3 = \left[-i\frac{k_1^2 - \rho^2}{2k_1\rho} \sinh(\rho l) + \cosh(\rho l)\right] e^{ik_1 l} A_3 \tag{3.15.9}$$

Finally, consider the transmission coefficient:

$$T = \left|\frac{A_3}{A_1}\right|^2 = \frac{1}{\cosh^2(\rho l) + \left(\frac{k_1^2 - \rho^2}{2k_1\rho}\right)^2 \sinh^2(\rho l)} = \frac{1}{1 + \left(\frac{k_1^2 + \rho^2}{2k_1\rho}\right)^2 \sinh^2(\rho l)} \tag{3.15.10}$$

where we used the identity $\cosh^2 \alpha - \sinh^2 \alpha = 1$. Hence,

$$T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh\left[\dfrac{\sqrt{2mV_0 - E}\,l}{\hbar}\right]^2} \tag{3.15.11}$$

We see that in contrast to the classical predictions, particles of energy $E < V_0$ have a nonzero probability of crossing the potential barrier. This phenomenon is called the *tunnel effect*.

3.16. In this problem we study the bound states for a finite square potential well (see Fig. 3-7). Consider the one-dimensional potential defined by

$$V(x) = \begin{cases} 0 & (x < -a/2) \\ -V_0 & -a/2 < x < a/2 \\ 0 & (a/2 < x) \end{cases} \tag{3.16.1}$$

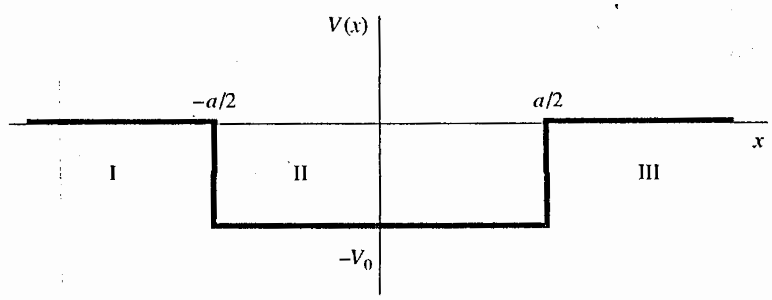

Fig. 3-7

(*a*) Write the stationary solutions for a particle of mass m and energy $-V_0 < E < 0$ for each of the regions I $(x < -a/2)$, II $(-a/2 < x < a/2)$, and III $(a/2 < x)$. (*b*) Apply the matching conditions at $x = -a/2$ and $x = a/2$. Obtain an equation for the possible energies. Draw a graphic representation of the equation in order to obtain qualitative properties of the solution.

(*a*) Referring to Problem 3.7, we define

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}} \qquad k = \sqrt{\frac{2m(E + V_0)}{\hbar^2}} \tag{3.16.2}$$

Then the stationary solutions for each of the regions are

$$\begin{cases} \phi_I(x) = Ae^{\rho x} + A'e^{-\rho x} \\ \phi_{II}(x) = Be^{ikx} + B'e^{-ikx} \\ \phi_{III}(x) = C'e^{\rho x} + Ce^{-\rho x} \end{cases} \tag{3.16.3}$$

Since $\phi(x)$ must be bounded in regions I and III, we set $A' = C' = 0$; therefore,

$$\begin{cases} \phi_I(x) = Ae^{\rho x} \\ \phi_{II}(x) = Be^{ikx} + B'e^{-ikx} \\ \phi_{III}(x) = Ce^{-\rho x} \end{cases} \tag{3.16.4}$$

(*b*) The continuity of $\phi(x)$ and $\phi'(x)$ at $x = -a/2$ yields

$$\begin{cases} Ae^{-\rho a/2} = Be^{-ika/2} + B'e^{ika/2} \\ \rho Ae^{-\rho a/2} = ikBe^{-ika/2} - ikB'e^{ika/2} \end{cases} \tag{3.16.5}$$

Similarly, the matching conditions at $x = a/2$ yield

$$\begin{cases} Ce^{-\rho a/2} = Be^{ika/2} + B'e^{-ika/2} \\ -\rho Ce^{-\rho a/2} = ikBe^{ika/2} - ikB'e^{-ika/2} \end{cases} \tag{3.16.6}$$

Hence, we can express B and B' in terms of A:

$$B = \left(\frac{\rho + ik}{2ik} e^{(-\rho + ik)a/2}\right)A \qquad B' = \left(-\frac{\rho - ik}{2ik} e^{(-\rho + ik)a/2}\right)A \tag{3.16.7}$$

We substitute (*3.16.7*) in (*3.16.6*) to obtain

$$\begin{cases} C = \left(\frac{\rho + ik}{2ik} e^{ika} - \frac{\rho - ik}{2ik} e^{-ika}\right)A \\ -\frac{\rho}{ik} C = \left(\frac{\rho + ik}{2ik} e^{ika} - \frac{\rho - ik}{2ik} e^{-ika}\right)A \end{cases} \tag{3.16.8}$$

To obtain a nonvanishing solution of (*3.16.8*), we must have

$$-\frac{\rho}{ik}\left(\frac{\rho + ik}{2ik} e^{ika} - \frac{\rho - ik}{2ik} e^{-ika}\right) = \left(\frac{\rho + ik}{2ik} e^{ika} + \frac{\rho - ik}{2ik} e^{-ika}\right) \tag{3.16.9}$$

which is equivalent to

$$\left(\frac{\rho - ik}{\rho + ik}\right)^2 = e^{2ika} \tag{3.16.10}$$

Equation (*3.16.10*) is an equation for E, since ρ and k depend only on E and on the constants of the problem. The solutions of (*3.16.10*) in terms of E are the energies corresponding to bound states of the well.

We shall transform (*3.16.10*) to express it in terms of k only. There are two possible cases. The first one is

$$\text{I} \qquad \left(\frac{\rho - ik}{\rho + ik}\right)^2 = -e^{ika} \tag{3.16.11}$$

The left-hand side of (*3.16.11*) is a complex number of modulus 1 and phase $-2\tan^{-1}(k/\rho)$. ($\rho + ik$ is the complex conjugate of $\rho - ik$.) The right-hand side of (*3.16.11*) is also a complex number of modulus 1, and its phase is $\pi + ka$ ($-e^{ika} = e^{i\pi} \cdot e^{ika} = e^{i(\pi + ka)}$). Therefore, we have

$$\tan^{-1}\left(\frac{k}{\rho}\right) = -\left(\frac{\pi}{2} + \frac{ka}{2}\right) \quad \Rightarrow \quad \frac{k}{\rho} = \tan\left[-\left(\frac{\pi}{2} + \frac{ka}{2}\right)\right] = -\tan\left(\frac{\pi}{2} + \frac{ka}{2}\right) = \cot\left(\frac{ka}{2}\right) = \frac{1}{\tan(ka/2)} \tag{3.16.12}$$

and

$$\tan\left(\frac{ka}{2}\right) = \frac{\rho}{k} \tag{3.16.13}$$

We define $k_0 = \sqrt{\frac{2mV_0}{\hbar^2}} = \sqrt{k^2 + \rho^2}$, where the parameter k_0 is E-independent. Consider

$$\frac{1}{\cos^2(ka/2)} = 1 + \tan^2\left(\frac{ka}{2}\right) = \frac{k^2 + \rho^2}{k^2} = \left(\frac{k_0}{k}\right)^2 \tag{3.16.14}$$

Equation (*3.16.11*) is thus equivalent to the following system of equations:

$$\begin{cases} \left|\cos\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0} \\ \tan\left(\frac{ka}{2}\right) > 0 \end{cases} \tag{3.16.15}$$

where we used (*3.16.13*) and (*3.16.14*) together with the fact that both ρ and k are positive.

We turn to the second possible case, i.e.,

$$\text{II} \qquad \left(\frac{\rho - ik}{\rho + ik}\right)^2 = e^{ika} \tag{3.16.16}$$

Similar arguments as in case I lead us to

$$-2\tan^{-1}\left(\frac{k}{\rho}\right) = ka \quad \Rightarrow \quad \tan\frac{ka}{2} = -\frac{k}{\rho} \tag{3.16.17}$$

Consider

$$\sin^2\left(\frac{ka}{2}\right) = \frac{\tan^2(ka/2)}{1+\tan^2(ka/2)} = \frac{k^2}{k^2+\rho^2} \tag{3.16.18}$$

Thus,

$$\begin{cases} \left|\sin\left(\dfrac{ka}{2}\right)\right| = \dfrac{k}{k_0} \\ \tan\left(\dfrac{ka}{2}\right) < 0 \end{cases} \tag{3.16.19}$$

In Fig. 3-8 we represent (*3.16.15*) and (*3.16.19*) graphically. The straight line represents the function k/k_0, and the sinusoidal arcs represent the functions $\left|\sin\left(\frac{ka}{2}\right)\right|$ and $\left|\cos\left(\frac{ka}{2}\right)\right|$. The dotted parts are the regions where the condition on $\tan\left(\frac{ka}{2}\right)$ is not fulfilled.

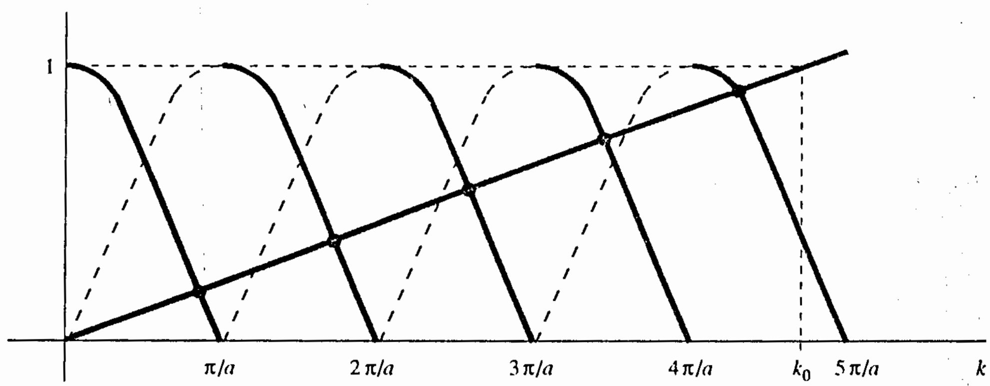

Fig. 3-8

The intersections marked with a circle represent the solutions in terms of k. From these solutions it is possible to determine the possible energies. From Fig. 3-8 we see that if $k_0 \le \pi/a$, that is, if

$$V_0 \le V_1 \equiv \frac{\pi^2\hbar^2}{2ma^2} \tag{3.16.20}$$

then there exists only one bound state of the particle. Then, if $V_1 \le V_0 < 4V_1$ there are two bound states, and so on. If $V_0 \gg V_1$, the slope $1/k_0$ of the straight line is very small. For the lowest energy levels we have approximately

$$k = \frac{n\pi}{a} \qquad (n = 1, 2, 3, \ldots) \tag{3.16.21}$$

and consequently,

$$E = \frac{\pi^2\hbar^2 n^2}{2ma^2} - V_0 \tag{3.16.22}$$

3.17. Consider a particle of mass m and energy $E > 0$ held in the one-dimensional potential $-V_0\delta(x-a)$. (*a*) Integrate the stationary Schrödinger equation between $a - \varepsilon$ and $a + \varepsilon$. Taking the limit $\varepsilon \to 0$, show that the derivative of the eigenfunction $\phi(x)$ presents a discontinuity at $x = a$ and determine it. (*b*) Relying on Problem 3.7, part (*a*), $\phi(x)$ can be written

$$\begin{cases} \phi(x) = A_1 e^{ikx} + A_1' e^{-ikx} & x < a \\ \phi(x) = A_2 e^{ikx} + A_2' e^{-ikx} & x > a \end{cases} \tag{3.17.1}$$

where $k = \sqrt{2mE/\hbar^2}$. Calculate the matrix M defined by

$$\begin{pmatrix} A_2 \\ A'_2 \end{pmatrix} = M \begin{pmatrix} A_1 \\ A'_1 \end{pmatrix} \tag{3.17.2}$$

(*a*) Using the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V_0\delta(x-a)\phi(x) = E\phi(x) \tag{3.17.3}$$

Integrating between $a - \varepsilon$ and $a + \varepsilon$ yields

$$-\frac{\hbar^2}{2m}\int_{a-\varepsilon}^{a+\varepsilon}\frac{d^2\phi(x)}{dx^2}\,dx + V_0\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)\phi(x)\,dx = E\int_{a-\varepsilon}^{a+\varepsilon}\phi(x)\,dx \tag{3.17.4}$$

According to the definition of the δ-function (see the Mathematical Appendix), the integration gives

$$-\frac{\hbar^2}{2m}\left(\left.\frac{d\phi(x)}{dx}\right|_{x=a+\varepsilon} - \left.\frac{d\phi(x)}{dx}\right|_{x=a-\varepsilon}\right) + V_0\phi(a) = E\int_{a-\varepsilon}^{a+\varepsilon}\phi(x)\,dx \tag{3.17.5}$$

Since $\phi(x)$ is continuous and finite in the interval $[a-\varepsilon, a+\varepsilon]$, in the limit $\varepsilon \to 0$,

$$-\frac{\hbar^2}{2m}\left[\lim_{\substack{x\to a \\ x>a}}\frac{d\phi(x)}{dx} - \lim_{\substack{x\to a \\ x<a}}\frac{d\phi(x)}{dx}\right] + V_0\phi(x) = 0 \tag{3.17.6}$$

We see that the derivative of $\phi(x)$ presents a discontinuity at $x = a$ that equals $2mV_0\phi(a)/\hbar^2$.

(*b*) We have two matching conditions at $x = a$. The continuity of $\phi(x)$ at $x = a$ yields

$$A_1e^{ika} + A'_1e^{-ika} = A_2e^{ika} + A'_2e^{-ika} \tag{3.17.7}$$

where the second matching condition is given in relation (*3.17.6*) and yields

$$\frac{\hbar^2}{2m}(A_1ike^{ika} - A'_1ike^{-ika} - A_2ike^{ika} + A'_2ike^{-ika}) = -V_0(A_1e^{ika} + A'_1e^{-ika}) \tag{3.17.8}$$

Equations (*3.17.6*) and (*3.17.7*) enable us to express A_2 and A'_2 in terms of A_1 and A'_1:

$$\begin{cases} A_2 = \left(1 + \dfrac{mV_0}{ik\hbar^2}\right)A_1 + \dfrac{mV_0}{ik\hbar^2}e^{-2ika}A'_1 \\[2ex] A'_2 = -\dfrac{mV_0}{ik\hbar^2}e^{2ika}A_1 + \left(1 - \dfrac{mV_0}{ik\hbar^2}\right)A'_1 \end{cases} \tag{3.17.9}$$

We therefore have

$$\begin{pmatrix} A_2 \\ A'_2 \end{pmatrix} = M \begin{pmatrix} A_1 \\ A'_1 \end{pmatrix} \tag{3.17.10}$$

where

$$M = \begin{pmatrix} 1 + \dfrac{mV_0}{ik\hbar^2} & +\dfrac{mV_0}{ik\hbar^2}e^{-2ika} \\[2ex] -\dfrac{mV_0}{ik\hbar^2}e^{2ika} & 1 - \dfrac{mV_0}{ik\hbar^2} \end{pmatrix} \tag{3.17.11}$$

3.18. In this problem we study the possible energies ($E > 0$) of a particle of mass m held in a δ-function periodic potential (see Fig. 3-9). We define a one-dimensional potential by

$$V(x) = \frac{\hbar^2\lambda}{2ma}\sum_{n=-\infty}^{\infty}\delta(x - na) \tag{3.18.1}$$

Referring to Problem 3.7, part (a), for each of the regions Ω_n $[na < x < (n+1)a]$, the stationary solution can be written in the form

$$\phi_n(x) = B_n e^{ik(x-na)} + C_n e^{-ik(x-na)} \tag{3.18.2}$$

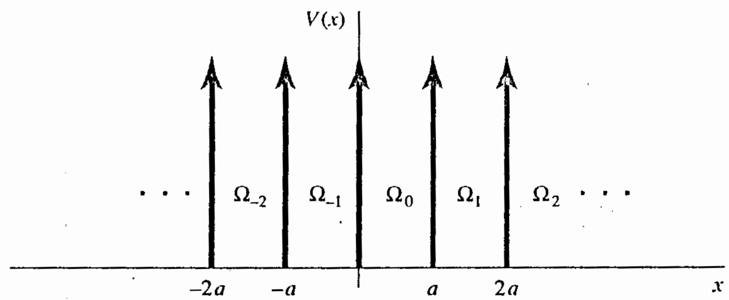

Fig. 3-9

(a) Use Problem 3.17 to find the matrix T relating the regions Ω_{n+1} and Ω_n:

$$\begin{pmatrix} B_{n+1} \\ C_{n+1} \end{pmatrix} = T \begin{pmatrix} B_n \\ C_n \end{pmatrix} \tag{3.18.3}$$

Prove that T is not a singular matrix. (b) Since T is a nonsingular matrix, we can find a basis $(\mathbf{b}_1, \mathbf{b}_2)$ of C^2 consisting of eigenvectors of the matrix T. We write

$$\begin{pmatrix} B_0 \\ C_0 \end{pmatrix} = \beta_1 \mathbf{b}_1 + \beta_2 \mathbf{b}_2 \tag{3.18.4}$$

where β_1, β_2 are complex numbers. Impose the condition that $|B_n|^2 + |C_n|^2$ does not diverge for $n \to \pm\infty$ to obtain a restriction on the eigenvalues of T. Express this restriction in terms of the possible energies E.

(a) We compare the definitions of $\phi_n(x)$ and $\phi_{n+1}(x)$ according to (3.18.2) and the definition of $\phi(x)$ in Problem 3.17, part (b). The analogy is depicted in Table 3-1.

Table 3-1

Problem 3.17	Problem 3.18
A_1	$B_n e^{-ikna}$
A_1'	$C_n e^{ikna}$
A_2	$B_{n+1} e^{-ik(n+1)a}$
A_2'	$C_{n+1} e^{ik(n+1)a}$
V_0	$\dfrac{\hbar^2 \lambda}{2ma}$

Also, the boundary between the two regions Ω_n and Ω_{n+1} is set in $x = (n+1)a$, whereas in Problem 3.17 the boundary condition is imposed at $x = a$. Using this analogy we have

$$\begin{cases} B_{n+1}e^{-ik(n+1)a} = B_n e^{-ikna}\left(1-\frac{i\lambda}{2ka}\right) - C_n e^{ikna}\left(\frac{i\lambda}{2ka}\right)e^{-2ik(n+1)a} \\ C_{n+1}e^{ik(n+1)a} = B_n e^{-ikna}\left(\frac{i\lambda}{2ka}\right)e^{2ik(n+1)a} + C_n e^{ikna}\left(1+\frac{i\lambda}{2ka}\right) \end{cases} \tag{3.18.5}$$

We therefore have

$$\begin{pmatrix} B_{n+1} \\ C_{n+1} \end{pmatrix} = T\begin{pmatrix} B_n \\ C_n \end{pmatrix} \tag{3.18.6}$$

where

$$T = \begin{pmatrix} \left(1-\frac{i\lambda}{2ka}\right)e^{ika} & -\frac{i\lambda}{2ka}e^{-ika} \\ +\frac{i\lambda}{2ka}e^{ika} & \left(1+\frac{i\lambda}{2ka}\right)e^{-ika} \end{pmatrix} \tag{3.18.7}$$

We see that T is not a singular matrix, since

$$\det T = \left(1+\frac{i\lambda}{2ka}\right)\left(1-\frac{i\lambda}{2ka}\right)+\left(\frac{i\lambda}{2ka}\right)^2 = 1 \tag{3.18.8}$$

and therefore $\det T \neq 0$.

(*b*) Since T is a nonsingular matrix, we can find a basis $(\mathbf{b}_1, \mathbf{b}_2)$ of C^2 consisting of eigenvectors of T with corresponding eigenvalues α_1 and α_2; these eigenvalues are the solutions of the cubic equation $\det(T-\alpha\mathbf{1}) = 0$ By definition,

$$\begin{cases} T\mathbf{b}_1 = \alpha_1\mathbf{b}_1 \\ T\mathbf{b}_2 = \alpha_2\mathbf{b}_2 \end{cases} \tag{3.18.9}$$

Using (*3.18.4*), we have (for $n = 1, 2, \ldots$)

$$\begin{pmatrix} B_n \\ C_n \end{pmatrix} = \underbrace{TT\cdots T}_{n\text{ times}}\begin{pmatrix} B_0 \\ C_0 \end{pmatrix} = T^n(\beta_1\mathbf{b}_1+\beta_2\mathbf{b}_2) = \beta_1\alpha_1^n\mathbf{b}_1+\beta_2\alpha_2^n\mathbf{b}_2 \tag{3.18.10}$$

Consider

$$|B_n|^2+|C_n|^2 = \left\|\begin{pmatrix} B_n \\ C_n \end{pmatrix}\right\|^2 \geq |\beta_1\alpha_1^n|^2\|\mathbf{b}_1\|^2 \tag{3.18.11}$$

Therefore, $|\alpha_1| \leq 1$; otherwise $\lim_{n\to\infty}(|B_n|^2+|C_n|^2) = \infty$. Similarly, we must have $|\alpha_2| \leq 1$. We apply a similar consideration for $n \to -\infty$:

$$\begin{pmatrix} B_0 \\ C_0 \end{pmatrix} = T^n\begin{pmatrix} B_{-n} \\ C_{-n} \end{pmatrix} \qquad \text{for } n = 1, 2 \ldots \tag{3.18.12}$$

Hence,

$$\begin{pmatrix} B_{-n} \\ C_{-n} \end{pmatrix} = T^{-n}\begin{pmatrix} B_0 \\ C_0 \end{pmatrix} = T^{-n}(\beta_1\mathbf{b}_1+\beta_2\mathbf{b}_2) = \frac{\beta_1}{\alpha_1^n}[T^{-n}(\alpha_1^n\mathbf{b}_1)] + \frac{\beta_2}{\alpha_2^n}[T^{-n}(\alpha_2^n\mathbf{b}_2)]$$

$$= \frac{\beta_1}{\alpha_1^n}[T^{-n}(T^n\mathbf{b}_1)] + \frac{\beta_2}{\alpha_2^n}[T^{-n}(T^n\mathbf{b}_2)] = \frac{\beta_n}{\alpha_1^n}\mathbf{b}_1+\frac{\beta_2}{\alpha_2^n}\mathbf{b}_2^n \tag{3.18.13}$$

Therefore,

$$|B_{-n}|^2+|C_{-n}|^2 = \left\|\begin{pmatrix} B_{-n} \\ C_{-n} \end{pmatrix}\right\|^2 \geq \left|\frac{\beta_1}{\alpha_1^n}\right|^2\|\mathbf{b}_1\|^2 \tag{3.18.14}$$

so $|\alpha_1| \geq 1$; otherwise $|\phi_n(x)|^2$ diverges for $n \to -\infty$, and similarly we must have $|\alpha_2| \geq 1$. Summing our results, we must have $|\alpha_1| = |\alpha_2| = 1$, i.e., the eigenvalues of T must be of modulus 1. Therefore, we can write

$$\det(T-e^{i\phi}\mathbf{1}) = 0 \tag{3.18.15}$$

where ϕ is a real constant. So

$$\left[\left(1-\frac{i\lambda}{2ka}\right)e^{ika}-e^{i\phi}\right]\left[\left(1+\frac{i\lambda}{2ka}\right)e^{-ika}-e^{i\phi}\right]-\frac{\lambda^2}{(2ka)^2} = 0 \tag{3.18.16}$$

A rearrangement of (*3.18.16*) gives

$$\left(1+\frac{\lambda^2}{4k^2a^2}\right)-\left[\left(1-\frac{i\lambda}{2ka}\right)e^{ika}+\left(1+\frac{i\lambda}{2ka}\right)e^{-ika}\right]e^{i\phi}+e^{2i\phi}-\frac{\lambda^2}{(2ka)^2} = 0 \tag{3.18.17}$$

or

$$1-2\left[\cos(ka)+\frac{\lambda}{2ka}\sin(ka)\right]e^{i\phi}+e^{2i\phi} = 0 \tag{3.18.18}$$

Consider the real part of (*3.18.18*):

$$1-2\left[\cos(ka)+\frac{\lambda}{2ka}\sin(ka)\right]\cos\phi+\cos(2\phi) = 0 \tag{3.18.19}$$

Using the relation $\cos(2\phi) = 2\cos^2\phi - 1$, we arrive at

$$\cos\phi = \cos(ka)+\frac{\lambda}{2ka}\sin(ka) \tag{3.18.20}$$

Note that since $k = \sqrt{2mE/\hbar^2}$, (*3.18.20*) is a constraint on the possible energies E:

$$\left|\cos(ka)+\frac{\lambda}{2ka}\sin(ka)\right| \le 1 \tag{3.18.21}$$

We can represent this inequality schematically in the following manner. The function

$$f(k) = \cos(ka)+\frac{\lambda}{2ka}\sin(ka) \tag{3.18.22}$$

behaves for $k \to \infty$ as $\cos(ka)$ approximately. The schematic behavior of $f(k)$ is depicted in Fig. 3-10.

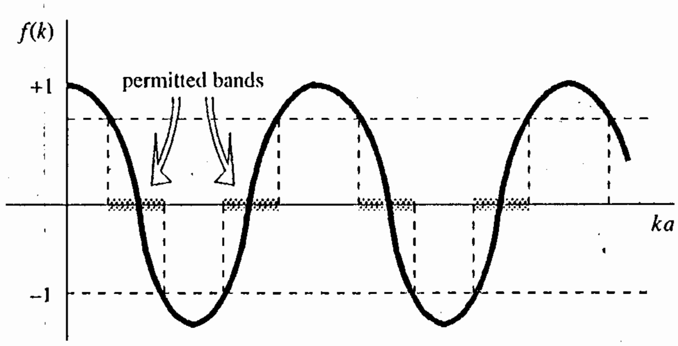

Fig. 3-10

We see that there are permitted bands of possible energies separated by domains where $|f(k)| \ge 1$, and therefore the corresponding energy E does not correspond to a possible state. For $E \to \infty$ the forbidden bands become very narrow, and the spectrum of the energy is almost continuous.

3.19. Consider a particle of mass m held in a three-dimensional potential written in the form

$$\tilde{V}(x, y, z) = V(x) + U(y) + W(z) \tag{3.19.1}$$

Derive the stationary Schrödinger equation for this case, and use a separation of variables in order to obtain three independent one-dimensional problems. Relate the energy of the three-dimensional state to the effective energies of the one-dimensional problem.

In our case the stationary Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}) + [V(x)+U(y)+W(z)]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{3.19.2}$$

where $\Psi(\mathbf{r})$ is the stationary three-dimensional state and E is the energy of the state. We assume that $\Psi(\mathbf{r})$ can be written in the form $\Psi(\mathbf{r}) = \phi(x)\chi(y)\psi(z)$, so substituting in (*3.19.2*) gives

$$-\frac{\hbar^2}{2m}\left[\left(\frac{d^2\phi(x)}{dx^2}\right)\chi(y)\psi(z) + \phi(x)\left(\frac{d^2\chi(y)}{dy^2}\right)\psi(z) + \phi(x)\chi(y)\left(\frac{d^2\psi(z)}{dz^2}\right)\right]$$
$$+ [V(x)+U(y)+W(z)]\,\phi(x)\chi(y)\psi(z) = E\phi(x)\chi(y)\psi(z) \tag{3.19.3}$$

Dividing (*3.19.4*) by $\Psi(\mathbf{r})$ and separating the x-dependent part, we get

$$-\frac{\hbar^2}{2m}\frac{1}{\phi(x)}\frac{d^2\phi(x)}{dx^2} + V(x) = E - \left[U(y) + W(z) - \frac{\hbar^2}{2m}\left(\frac{1}{\chi(y)}\frac{d^2\chi(y)}{dy^2} + \frac{1}{\psi(z)}\frac{d^2\psi(z)}{dz^2}\right)\right] \tag{3.19.4}$$

The left-hand side of (*3.19.4*) is a function of x only, while the right-hand side is a function of y and z, but does not depend on x. Therefore, both sides cannot depend on x; thus they equal a constant, which we will denote by E_x. We have

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) = E_x\phi(x) \tag{3.19.5}$$

We see that $\phi(x)$ is governed by the equation describing a particle of mass m held in the one-dimensional potential $V(x)$. Returning to (*3.19.4*), we can write

$$-\frac{\hbar^2}{2m}\frac{1}{\chi(y)}\frac{d^2\chi(y)}{dy^2} + U(y) = E - E_x - \left[W(z) - \frac{\hbar^2}{2m}\frac{1}{\psi(z)}\frac{d^2\psi(z)}{dz^2}\right] \tag{3.19.6}$$

In (*3.19.6*) the left-hand side depends only on y, while the right-hand side depends only on z. Again, both sides must equal a constant, which we will denote by E_y. We have

$$-\frac{\hbar^2}{2m}\frac{d^2\chi(y)}{dy^2} + U(y)\chi(y) = E_y\chi(y) \tag{3.19.7}$$

Thus, $\chi(y)$ is a stationary state of a fictitious particle held in the one-dimensional potential $U(y)$. Finally, we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} + W(z)\psi(z) = E_z\psi(z) \tag{3.19.8}$$

where we set $E_z = E - E_x - E_y$. Hence, the three-dimensional wave function $\Psi(\mathbf{r})$ is divided into three parts. Each part is governed by a one-dimensional Schrödinger equation. The energy of the three-dimensional state equals the sum of energies corresponding to the three one-dimensional problems, $E = E_x + E_y + E_z$.

Supplementary Problems

3.20. Solve Problems 3.11 and 3.12 for the case of particles with energy $0 < E < V_0$. *Ans.* $R = 1$ and $T = 0$.

3.21. Consider a particle held in a one-dimensional *complex* potential $V(x)(1 + i\xi)$ where $V(x)$ is a real function and ξ is a real parameter. Use the Schrödinger equation to show that the probability current $j = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$ and the probability density $\rho = \psi^*\psi$ satisfy the *corrected* continuity equation $\frac{\partial j}{\partial x} + \frac{\partial\rho}{\partial t} = \frac{2\xi V(x)\rho}{\hbar}$. (Hint: Compare with Problem 3.4.)

3.22. Consider a particle of mass m held in a one-dimensional infinite potential well:

$$V(x) = \begin{cases} V_0 & 0 \le x \le a \\ \infty & \text{otherwise} \end{cases} \tag{3.22.1}$$

Find the stationary states and the corresponding energies.

Ans. $E_n = \dfrac{\pi^2\hbar^2 n^2}{2ma^2} + V_0 \quad (n = 1, 2, 3, \ldots)$. The corresponding states are the same as in Problem 3.10.

3.23. Consider an electron of energy 1 eV that encounters a potential barrier of width 1 Å and of energy-height 2 eV. What is the probability of the electron crossing the barrier? Repeat the same calculation for a proton.

Ans. For an electron $T \cong 0.78$; for a proton $T \cong 4 \times 10^{-19}$.

3.24. (*a*) A particle of mass m and energy $E > 0$ encounters a potential well of width l and depth V_0:

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & 0 < x < l \\ 0 & l < x \end{cases} \tag{3.24.1}$$

Find the transmission coefficient. (Hint: Compare with Problem 3.14.) (*b*) For which values of l will the transmission be complete, if the particle is an electron of energy 1 eV and $V_0 = 4$ eV?

Ans. (*a*) $T = \dfrac{1}{1 + \dfrac{V_0^2}{4E(E+V_0)}\sin^2\left[\dfrac{\sqrt{2m(E+V_0)}\,l}{\hbar}\right]}$; (*b*) $l \cong 2.7n$ Å, where n is an integer.

3.25. An electron is held in a finite square potential well of width 1 Å. For which values of the well's depth V_0 are there exactly two possible bound stationary states for the electron?

Ans. $V_1 \le V_0 \le 4V_1$, where $V_1 = \dfrac{\pi^2\hbar^2}{2ma^2} = 37.6$ eV.

3.26. Consider the wave function $\psi(x) = \dfrac{N}{x^2 + \alpha^2}$. (*a*) Calculate the normalization constant N where α is a real constant. (*b*) Find the uncertainty $\Delta x\, \Delta p$ (be careful in calculating Δp!). *Ans.* (*a*) $N = \sqrt{\dfrac{2\alpha^3}{\pi}}$; (*b*) $\Delta x\, \Delta p = \dfrac{\hbar}{\sqrt{2}}$.

3.27. Consider a particle of energy $E > 0$ confined in the potential (Fig. 3-11)

$$V(x) = \begin{cases} \infty & x < -a \\ 0 & -a < x < -b \\ V_0 & -b < x < b \\ 0 & b < x < a \\ \infty & a < x \end{cases} \tag{3.27.1}$$

Show that for a stationary state with a nonvanishing probability of finding the particle to the right of the barrier (i.e., at $b < x < a$), there is also a nonvanishing probability of finding it to the left of the barrier (i.e., $-a < x < -b$). Note: For $E < V_0$ this is another example of the tunnel effect of Problem 3.15.

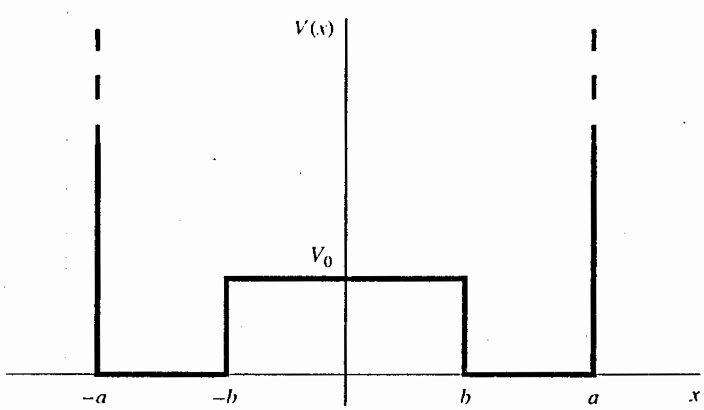

Fig. 3-11

3.28. Consider a particle of mass m confined in a one-dimensional infinite potential well:

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{otherwise} \end{cases} \tag{3.28.1}$$

Suppose that the particle is in the stationary state, $\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ of energy $E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2}$. Calculate (*a*) $\langle x\rangle$ and $\langle p\rangle$; (*b*) $\langle x^2\rangle$ and $\langle p^2\rangle$; (*c*) $\Delta x\,\Delta p$.

Ans. (*a*) $\langle x\rangle = \frac{L}{2}$, $\langle p\rangle = 0$; (*b*) $\langle x^2\rangle = L^2\left(\frac{1}{3} - \frac{1}{2\pi^2 n^2}\right)$, $\langle p^2\rangle = \frac{\pi^2\hbar^2 n^2}{L^2}$; (*c*) $\Delta x\,\Delta p = n\pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2\pi^2 n^2}}$.

3.29. Consider a particle of mass m held in the potential

$$V(x) = -V_0\left[\delta(x) + \delta(x - l)\right] \tag{3.29.1}$$

where l is a constant. Find the bound states of the particles. Show that the energies are given by the relation

$$e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\alpha}\right) \tag{3.29.2}$$

where $E = -\hbar^2\rho^2/2m$ and $\alpha = 2mV_0/\hbar^2$.