1. Which of the wave functions in Fig. 5.15 cannot have physical significance in the interval shown? Why not?

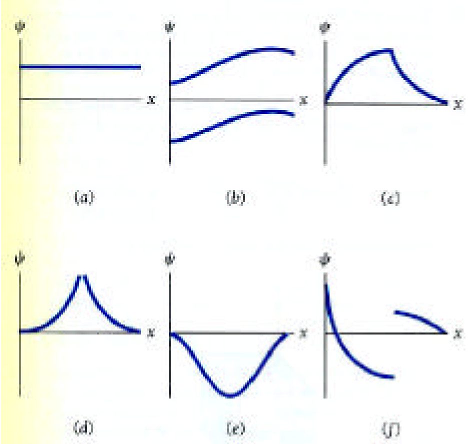

Figure 5.15

【Sol】

Figure (b) is double valued, and is not a function at all, and cannot have physical significance. Figure (c) has discontinuous derivative in the shown interval. Figure (d) is finite everywhere in the shown interval. Figure (f) is discontinuous in the shown interval.

3. Which of the following wave functions cannot be solutions of Schrödinger's equation for all values of x? Why not? (a) $y = A \sec x$; (b) $y = A \tan x$; (c) $y = A \exp(x^2)$; (d) $y = A \exp(-x^2)$.

【Sol】

The functions (a) and (b) are both infinite when $\cos x = 0$, at $x = \pm\pi/2, \pm 3\pi/2, \ldots \pm(2n+1)\pi/2$ for any integer n, neither $y = A \sec x$ or $y = A \tan x$ could be a solution of Schrödinger's equation for all values of x. The function (c) diverges as $x \to \pm\infty$, and cannot be a solution of Schrödinger's equation for all values of x.

5. The wave function of a certain particle is $\psi = A\cos^2 x$ for $-\pi/2 < x < \pi/2$. (a) Find the value of A. (b) Find the probability that the particle be found between $x = 0$ and $x = \pi/4$.

【Sol】

Both parts involve the integral $\int \cos^4 x\,dx$, evaluated between different limits for the two parts. Of the many ways to find this integral, including consulting tables and using symbolic-manipulation programs, a direct algebraic reduction gives

$$\cos^4 x = (\cos^2 x)^2 = \left[\tfrac{1}{2}(1+\cos 2x)\right]^2 = \tfrac{1}{4}\left[1 + 2\cos 2x + \cos^2(2x)\right]$$

$$= \tfrac{1}{4}\left[1 + 2\cos 2x + \tfrac{1}{2}(1+\cos 4x)\right] = \tfrac{3}{8} + \tfrac{1}{2}\cos 2x + \tfrac{1}{8}\cos 4x,$$

where the identity $\cos^2\theta = \tfrac{1}{2}(1+\cos 2\theta)$ has been used twice.

(a) The needed normalization condition is

$$\int_{-\pi/2}^{+\pi/2} \psi^* \psi\,dx = A^2 \int_{-\pi/2}^{+\pi/2} \cos^4 x\,dx$$

$$= A^2\left[\tfrac{3}{8}\int_{-\pi/2}^{+\pi/2} dx + \tfrac{1}{2}\int_{-\pi/2}^{+\pi/2} \cos 2x\,dx + \tfrac{1}{8}\int_{-\pi/2}^{+\pi/2} \cos 4x\,dx\right] = 1$$

The integrals

$$\int_{-\pi/2}^{+\pi/2} \cos 2x\,dx = \tfrac{1}{2}\sin 2x\Big|_{-\pi/2}^{+\pi/2} \quad \text{and} \quad \int_{-\pi/2}^{+\pi/2} \cos 4x\,dx = \tfrac{1}{4}\sin 4x\Big|_{-\pi/2}^{+\pi/2}$$

are seen to be vanish, and the normalization condition reduces to

$$1 = A^2\left(\frac{3}{8}\right)\pi, \quad \text{or} \quad A = \sqrt{\frac{8}{3\pi}}.$$

(b) Evaluating the same integral between the different limits,

$$\int_0^{\pi/4} \cos^4 x\,dx = \left[\tfrac{3}{8}x + \tfrac{1}{4}\sin 2x + \tfrac{1}{32}\sin 4x\right]_0^{\pi/4} = \frac{3\pi}{32} + \frac{1}{4},$$

The probability of the particle being found between $x = 0$ and $x = \pi/4$ is the product of this integral and A^2, or

$$A^2\left(\tfrac{3\pi}{32} + \tfrac{1}{4}\right) = \tfrac{8}{3\pi}\left(\tfrac{3\pi}{32} + \tfrac{1}{4}\right) = 0.46$$

7. As mentioned in Sec. 5.1, in order to give physically meaningful results in calculations a wave function and its partial derivatives must be finite, continuous, and single-valued, and in addition must be normalizable. Equation (5.9) gives the wave function of a particle moving freely (that is, with no forces acting on it) in the $+x$ direction as

$$\Psi = Ae^{-(i/\hbar)(Et - pc)}$$

where E is the particle's total energy and p is its momentum. Does this wave function meet all the above requirements? If not, could a linear superposition of such wave functions meet these requirements? What is the significance of such a superposition of wave functions?

【Sol】

The given wave function satisfies the continuity condition, and is differentiable to all orders with respect to both t and x, but is not normalizable; specifically, $\Psi^*\Psi = A^*A$ is constant in both space and time, and if the particle is to move freely, there can be no limit to its range, and so the integral of $\Psi^*\Psi$ over an infinite region cannot be finite if $A \neq 0$.

A linear superposition of such waves could give a normalizable wave function, corresponding to a real particle. Such a superposition would necessarily have a non- zero Δp, and hence a finite Δx; at the expense of normalizing the wave function, the wave function is composed of different momentum states, and is localized.

9. Show that the expectation values $<px>$ and $<xp>$) are related by

$$<px> - <xp> = \quad /i$$

This result is described by saying that p and x do not **commute,** and it is intimately related to the uncertainty principle.

【Sol】

It's crucial to realize that the expectation value $<px>$ is found from the combined operator $\hat{p}\hat{x}$, which, when operating on the wave function $\Psi(x, t)$, corresponds to "multiply by x, differentiate with respect to x and multiply by $/i$," whereas the operator $\hat{x}\hat{p}$ corresponds to "differentiate with respect to x, multiply by $/i$ and multiply by x." Using these operators,

$$(\hat{p}\hat{x})\Psi = \hat{p}(\hat{x}\Psi) = \frac{\hbar}{i}\frac{\partial}{\partial x}(x\Psi) = \frac{\hbar}{i}\left[\Psi + x\frac{\partial}{\partial x}\Psi\right],$$

where the product rule for partial differentiation has been used. Also,

$$(\hat{x}\hat{p})\Psi = \hat{x}(\hat{p}\Psi) = x\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right) = \frac{\hbar}{i}\left[x\frac{\partial}{\partial x}\Psi\right].$$

Thus $$(\hat{p}\hat{x} - \hat{x}\hat{p})\Psi = \frac{\hbar}{i}\Psi$$

and $$< px - xp >= \int_{-\infty}^{\infty} \Psi^* \frac{\hbar}{i}\Psi dx = \frac{\hbar}{i}\int_{-\infty}^{\infty} \Psi^* \Psi dx = \frac{\hbar}{i}$$

for $\Psi(x, t)$ normalized.

11. Obtain Schrödinger' s steady-state equation from Eq.(3.5) with the help of de Broglie' s relationship $l = h/mv$ by letting $y = y$ and finding ¶²y/¶x^2.

【Sol】

Using $\lambda\nu = v_p$ in Equation (3.5), and using y instead of y,

$$y = A\cos\left(2p\left(t - \frac{x}{v_p}\right)\right) = A\cos\left(2pnt - 2p\frac{x}{l}\right).$$

Differentiating twice with respect to x using the chain rule for partial differentiation (similar to Example 5.1),

$$\frac{\partial y}{\partial x} = -A\sin\left(2pnt - 2p\frac{x}{l}\right)\left(-\frac{2p}{l}\right) = \frac{2p}{l}A\sin\left(2pnt - 2p\frac{x}{l}\right),$$

$$\frac{\partial^2 y}{\partial x^2} = \frac{2p}{l}A\cos\left(2pnt - 2p\frac{x}{l}\right)\left(-\frac{2p}{l}\right) = \left(\frac{2p}{l}\right)^2 A\cos\left(2pnt - 2p\frac{x}{l}\right) = -\left(\frac{2p}{l}\right)^2 y$$

The kinetic energy of a nonrelativistic particle is

$$KE = E - U = \frac{p^2}{2m} = \left(\frac{h}{l}\right)^2 \frac{1}{2m}, \qquad \text{so that} \qquad \frac{1}{l^2} = \frac{2m}{h^2}(E-U)$$

Substituting the above expression relating $\frac{\partial^2 y}{\partial x^2}$ and $\frac{1}{l^2}y$

$$\frac{\partial^2 y}{\partial x^2} = -\left(\frac{2p}{l}\right)^2 y = -\frac{8p^2 m}{h^2}(E-U)y = -\frac{2m}{\hbar^2}(E-U)y, \qquad \text{which is Equation (5.32)}$$

13. One of the possible wave functions of a particle in the potential well of Fig. 5.17 is sketched there. Explain why the wavelength and amplitude of &P vary as they do.

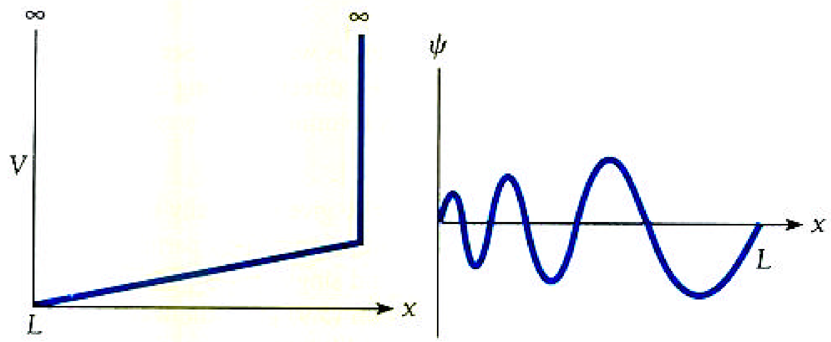

Figure 5.17

【Sol】

The wave function must vanish at $x = 0$, where $V \rightarrow \infty$. As the potential energy increases with x, the particle's kinetic energy must decrease, and so the wavelength increases. The amplitude increases as the wavelength increases because a larger wavelength means a smaller momentum (indicated as well by the lower kinetic energy), and the particle is more likely to be found where the momentum has a lower magnitude. The wave function vanishes again where the potential $V \rightarrow \infty$; this condition would determine the allowed energies.

15. An important property of the eigenfunctions of a system is that they are **orthogonal** to one another, which means that

$$\int_{-\infty}^{+\infty} y_n y_m \, dV = 0 \qquad n \neq m$$

Verify this relationship for the eigenfunctions of a particle in a one-dimensional box given by Eq. (5.46).

【Sol】

The necessary integrals are of the form

$$\int_{-\infty}^{+\infty} y_n y_m \, dx = \frac{2}{L}\int_0^L \sin\frac{npx}{L}\sin\frac{mpx}{L}dx$$

for integers n, m, with $n \neq m$ and $n \neq -m$. (A more general orthogonality relation would involve the integral of $y_n^* y_m$, but as the eigenfunctions in this problem are real, the distinction need not be made.)

To do the integrals directly, a convenient identity to use is

$$\sin a \sin b = \tfrac{1}{2}[\cos(a-b) - \cos(a+b)],$$

as may be verified by expanding the cosines of the sum and difference of a and b. To show orthogonality, the stipulation $n \neq m$ means that $a \neq b$ and $a \neq -b$ and the integrals are of the form

$$\int_{-\infty}^{+\infty}\psi_n\psi_m\,dx = \frac{1}{L}\int_0^L\left[\cos\frac{(n-m)\pi x}{L} - \cos\frac{(n+m)\pi x}{L}\right]dx$$

$$= \left[\frac{L}{(n-m)\pi}\sin\frac{(n-m)\pi x}{L} - \frac{L}{(n+m)\pi}\sin\frac{(n+m)\pi x}{L}\right]_o^L = 0,$$

where sin(n - m)π = sin(n - m)π = sin 0 = 0 has been used.

17. As shown in the text, the expectation value $\langle x\rangle$ of a particle trapped in a box L wide is $L/2$, which means that its average position is the middle of the box. Find the expectation value $\langle x^2\rangle$.

【Sol】

Using Equation (5.46), the expectation value $\langle x^2\rangle$ is

$$\langle x^2\rangle_n = \frac{2}{L}\int_0^L x^2\sin^2\left(\frac{n\pi x}{L}\right)dx.$$

See the end of this chapter for an alternate analytic technique for evaluating this integral using *Leibniz's Rule*. From either a table or repeated integration by parts, the indefinite integral is

$$\int x^2\sin^2\frac{n\pi x}{L}dx = \left(\frac{L}{n\pi}\right)^3\int u^3\sin u\,du = \left(\frac{L}{n\pi}\right)^3\left[\frac{u^3}{6} - \frac{u^2}{4}\sin 2u - \frac{u}{4}\cos 2u + \frac{1}{8}\sin 2u\right].$$

where the substitution $u = (n\pi/L)x$ has been made.

This form makes evaluation of the definite integral a bit simpler; when $x = 0$ $u = 0$, and when $x = L$ $u = n\pi$. Each of the terms in the integral vanish at $u = 0$, and the terms with sin $2u$ vanish at $u = n\pi$, $\cos 2u = \cos 2n\pi = 1$, and so the result is

$$< x^2 >_n = \frac{2}{L}\left(\frac{L}{np}\right)^3\left[\frac{(np)^3}{6} - \frac{np}{4}\right] = L^2\left[\frac{1}{3} - \frac{1}{2n^2p^2}\right].$$

As a check, note that

$$\lim_{n\to\infty} < x^2 >_n = \frac{L^2}{3},$$

which is the expectation value of $<x^2>$ in the classical limit, for which the probability distribution is independent of position in the box.

19. Find the probability that a particle in a box L wide can be found between $x = 0$ and $x = L/n$ when it is in the nth state.

【Sol】

This is a special case of the probability that such a particle is between x_1 and x_2, as found in Example 5.4. With $x_1 = 0$ and $x_2 = L$,

$$P_{0L} = \left[\frac{x}{L} - \frac{1}{2np}\sin\frac{2npx}{L}\right]_0^L = \frac{1}{n}.$$

21. A particle is in a cubic box with infinitely hard walls whose edges are L long (Fig. 5. 18). The wave functions of the particle are given by

$$\psi = A \sin\frac{n_x \pi x}{L} \sin\frac{n_z \pi y}{L} \sin\frac{n_z \pi z}{L} \qquad \begin{aligned} n_x &= 1, 2, 3, \ldots \\ n_y &= 1, 2, 3, \ldots \\ n_z &= 1, 2, 3, \ldots \end{aligned}$$

Find the value of the normalization constant A.

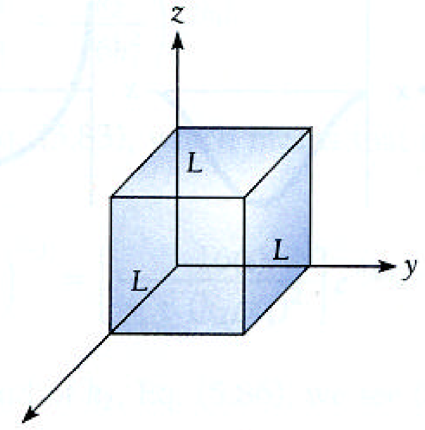

Figure 5.18 A cubic box.

【Sol】

The normalization constant, assuming A to be real, is given by

$$\int \psi^* \psi \, dV = 1 = \int \psi^* \psi \, dx\, dy\, dz$$

$$= A^2 \left(\int_0^L \sin^2 \frac{n_x \pi x}{L} dx \right) \left(\int_0^L \sin^2 \frac{n_y \pi y}{L} dy \right) \left(\int_0^L \sin^2 \frac{n_z \pi z}{L} dz \right).$$

Each integral above is equal to $L/2$ (from calculations identical to Equation (5.43)). The result is

$$A^2 \left(\frac{L}{2} \right)^3 = 1 \quad \text{or} \quad A = \left(\frac{2}{L} \right)^{3/2}$$

23. (a) Find the possible energies of the particle in the box of Exercise 21 by substituting its wave function *y* in Schrödinger's equation and solving for *E*. (Hint: inside the box *U* = 0.)
(b) Compare the ground-state energy of a particle in a one-dimensional box of length *L* with that of a particle in the three-dimensional box.

【Sol】

(a) For the wave function of Problem 5-21, Equation (5.33) must be used to find the energy. Before substitution into Equation (5.33), it is convenient and useful to note that for this wave function

$$\frac{\partial^2 y}{\partial x^2} = -\frac{n_x^2 p^2}{L^2} y, \quad \frac{\partial^2 y}{\partial y^2} = -\frac{n_y^2 p^2}{L^2} y, \quad \frac{\partial^2 y}{\partial z^2} = -\frac{n_z^2 p^2}{L^2} y.$$

Then, substitution into Equation (5.33) gives

$$-\frac{p^2}{L^2}(n_x^2 + n_y^2 + n_z^2) y + \frac{2m}{\hbar^2} E y = 0,$$

and so the energies are

$$E_{n_x, n_y, n_z} = \frac{p^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2).$$

(b) The lowest energy occurs when $n_x = n_y = n_z = 1$. None of the integers n_x, n_y, or n_z can be zero, as that would mean *y* = 0 identically. The minimum energy is then

$$E_{min} = \frac{3p^2 \hbar^2}{2mL^2},$$

which is three times the ground-state energy of a particle in a one-dimensional box of length *L*.

25. A beam of electrons is incident on a barrier 6.00 eV high and 0.200 nm wide. Use Eq. (5.60) to find the energy they should have if 1.00 percent of them are to get through the barrier.

【Sol】

Solving equation (5.60) for k_2,

$$k_2 = \frac{1}{2L}\ln\frac{1}{T} = \frac{1}{2(0.200\times10^{-9}\ \mathrm{m})}\ln(100) = 1.15\times10^{10}\ \mathrm{m}^{-1}$$

Equation (5.86), from the appendix, may be solved for the energy E, but a more direct expression is

$$E = U - KE = U - \frac{p^2}{2m} = U - \frac{(\hbar k_2)^2}{2m}$$

$$= 6.00\ \mathrm{eV} - \frac{\left((1.05\times10^{-34}\,\mathrm{J\cdot s})(1.15\times10^{10}\,\mathrm{m}^{-1})\right)^2}{2(9.1\times10^{-31}\,\mathrm{kg})(1.6\times10^{-19}\,\mathrm{J/eV})} = 0.95\ \mathrm{eV}$$

27. What bearing would you think the uncertainty principle has on the existence of the zero-point energy of a harmonic oscillator?

【Sol】

If a particle in a harmonic-oscillator potential had zero energy, the particle would have to be at rest at the position of the potential minimum. The uncertainty principle dictates that such a particle would have an infinite uncertainty in momentum, and hence an infinite uncertainty in energy. This contradiction implies that the zero-point energy of a harmonic oscillator cannot be zero.

29. Show that for the n = 0 state of a harmonic oscillator whose classical amplitude of motion is A, y = 1 at x = A, where y is the quantity defined by Eq. (5.67).

【Sol】

When the classical amplitude of motion is A, the energy of the oscillator is

$$\frac{1}{2}kA^2 = \frac{1}{2}hn, \quad \text{so} \quad A = \sqrt{\frac{hn}{k}}.$$

Using this for x in Equation (5.67) gives

$$y = \sqrt{\frac{2pmn}{\hbar}}\sqrt{\frac{hn}{k}} = 2p\sqrt{\frac{mn^2}{k}} = 1,$$

where Equation (5.64) has been used to relate n, m and k.

31. Find the expectation values <x> and <x^2> for the first two states of a harmonic oscillator.

【Sol】

The expectation values will be of the forms

$$\int_{-\infty}^{\infty} xy^*y\,dx \quad \text{and} \quad \int_{-\infty}^{\infty} x^2y^*y\,dx$$

It is far more convenient to use the dimensionless variable y as defined in Equation (5.67). The necessary integrals will be proportional to

$$\int_{-\infty}^{\infty} ye^{-y^2}dy, \quad \int_{-\infty}^{\infty} y^2e^{-y^2}dy, \quad \int_{-\infty}^{\infty} y^3e^{-y^2}dy, \quad \int_{-\infty}^{\infty} y^4e^{-y^2}dy,$$

The first and third integrals are seen to be zero (see Example 5.7). The other two integrals may be found from tables, from symbolic-manipulation programs, or by any of the methods outlined at the end of this chapter or in Special Integrals for Harmonic Oscillators, preceding the solutions for Section 5.8 problems in this manual. The integrals are

$$\int_{-\infty}^{\infty} y^2 e^{-y^2} dy = \frac{1}{2}\sqrt{p}, \qquad \int_{-\infty}^{\infty} y^4 e^{-y^2} dy = \frac{3}{4}\sqrt{p}.$$

An immediate result is that $\langle x \rangle = 0$ for the first two states of any harmonic oscillator, and in fact $\langle x \rangle = 0$ for any state of a harmonic oscillator (if $x = 0$ is the minimum of potential energy). A generalization of the above to any case where the potential energy is a symmetric function of x, which gives rise to wave functions that are either symmetric or antisymmetric, leads to $\langle x \rangle = 0$. To find $\langle x^2 \rangle$ for the first two states, the necessary integrals are

$$\int_{-\infty}^{\infty} x^2 y_o^* y_0 dx = \left(\frac{2mn}{\hbar}\right)^{1/2}\left(\frac{\hbar}{2pmn}\right)^{3/2}\int_{-\infty}^{\infty} y^2 e^{-y^2} dy$$

$$= \frac{\hbar}{2p^{3/2}mn}\frac{\sqrt{p}}{2} = \frac{(1/2)hn}{4p^2mn^2} = \frac{E_0}{k};$$

$$\int_{-\infty}^{\infty} x^2 y_1^* y_1 dx = \left(\frac{2mn}{\hbar}\right)^{1/2}\left(\frac{\hbar}{2pmn}\right)^{3/2}\int_{-\infty}^{\infty} 2y^4 e^{-y^2} dy$$

$$= \frac{\hbar}{2p^{3/2}mn} 2\frac{3\sqrt{p}}{2} = \frac{(3/2)hn}{4p^2mn^2} = \frac{E_1}{k}.$$

In both of the above integrals,

$$dx = \frac{dx}{dy}dy = \sqrt{\frac{\hbar}{2pmn}}dy$$

has been used, as well as Table 5.2 and Equation (5.64).

33. A pendulum with a 1.00-g bob has a massless string 250 mm long. The period of the pendulum is 1.00 s. (a) What is its zero-point energy? Would you expect the zero-point oscillations to be detectable? (b) The pendulum swings with a very small amplitude such that its bob rises a maximum of 1.00 mm above its equilibrium position. What is the corresponding quantum number?

【Sol】

(a) The zero-point energy would be

$$E_0 = \frac{1}{2}hn = \frac{h}{2T} = \frac{4.14\times10^{-15}\ \text{eV}\cdot\text{s}}{2(1.00\ \text{s})} = 2.07\times10^{-15}\ \text{eV},$$

which is not detectable.

(b) The total energy is $E = mgH$ (here, H is the maximum pendulum height, given as an uppercase letter to distinguish from Planck's constant), and solving Equation (5.70) for n,

$$n = \frac{E}{hn} - \frac{1}{2} = \frac{mgH}{h/T} = \frac{(1.00\times10^{-3}\ \text{kg})(9.80\ \text{m/s}^2)(1.00\ \text{s})}{6.63\times10^{-34}\ \text{J}\cdot\text{s}} - \frac{1}{2} = 1.48\times10^{28}.$$

37. Consider a beam of particles of kinetic energy E incident on a potential step at $x = 0$ that is U high, where $E > U$ (Fig. 5.19). (a) Explain why the solution $De^{-ik'x}$ (in the notation of appendix) has no physical meaning in this situation, so that $D = 0$. (b) Show that the transmission probability here is $T = CC^*v'/AA^*v_1 = 4k_1^2/(k_1 + k')^2$. (c) A 1.00-mA beam of electrons moving at $2.00\text{x}10^6$ m/s enters a region with a sharply defined boundary in which the electron speeds are reduced to $1.00\text{x}10^6$ m/s by a difference in potential. Find the transmitted and reflected currents.

【Sol】

(a) In the notation of the Appendix, the wave function in the two regions has the form

$$y_I = Ae^{ik_1x} + Be^{-ik_1x}, \quad y_{II} = Ce^{ik'x} + De^{-ik'x},$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar}}, \quad k' = \sqrt{\frac{2m(E-U)}{\hbar}}.$$

The terms corresponding to $\exp(ik_1x)$ and $\exp(ik'x)$ represent particles traveling to the left; this is possible in region I, due to reflection at the step at $x = 0$, but not in region II (the reasoning is the same as that which lead to setting $G = 0$ in Equation (5.82)). Therefore, the $\exp(-ik'x)$ term is not physically meaningful, and $D = 0$.

(b) The boundary condition at x= 0 are then

$$A+B=C, \quad ik_1A-ik_1B=ik'C \quad \text{or} \quad A-B=\frac{k'}{k_1}C.$$

Adding to eliminate B, $2A=\left(1+\frac{k'}{k_1}\right)C$, so

$$\frac{C}{A}=\frac{2k_1}{k_1+k'}, \quad \text{and} \quad \frac{CC^*}{AA^*}=\frac{4k_1^2}{(k_1+k')^2}.$$

(c) The particle speeds are different in the two regions, so Equation (5.83) becomes

$$T=\frac{|y_{II}|^2v'}{|y_I|^2v_1}=\frac{CC^*}{AA^*}\frac{k'}{k_1}=\frac{4k_1k'}{(k_1+k')^2}=\frac{4(k_1/k')}{((k_1/k')+1)^2}.$$

For the given situation, k_1/k' = v_1/v' = 2.00, so T = (4x2)/(2+1)2 = 8/9. The transmitted current is (T)(1.00 mA) = 0.889 mA, and the reflected current is 0.111mA.

As a check on the last result, note that the ratio of the reflected current to the incident current is, in the notation of the Appendix,

$$R=\frac{|y_{I-}|^2v_1}{|y_{I+}|^2v_1}=\frac{BB^*}{AA^*}$$

Eliminating C from the equations obtained in part (b) from the continuity condition as x = 0,

$$A\left(1-\frac{k'}{k_1}\right)=B\left(1+\frac{k'}{k_1}\right), \quad \text{so} \quad R=\left(\frac{(k_1/k')-1}{(k_1/k')+1}\right)=\frac{1}{9}=1-T$$