2

The Schrödinger Wave Equation - Solutions

1. (a) Using Eq. (2.17) for the energies of a particle in an infinite well:

$$E = \frac{n^2h^2}{2mL^2}$$

Solving this for L:

$$L = \sqrt{\frac{n^2h^2}{8mE}}$$

Using the given energy $E_1 = 1.0\ eV = 1.6 \times 10^{-19}\ J$ and the mass of the electron from Appendix A, the lowest energy is found when the electron is in the ground state ($n = 1$):

$$L = \sqrt{\frac{1^2(6.63 \times 10^{-34}\ J \cdot s)^2}{8(9.11 \times 10^{-31}\ kg)(1.6 \times 10^{-19}\ J)}} = 6.14 \times 10^{-10}\ m$$

(b) Now that we have L, the energy for the next excited state ($n = 2$):

$$E_2 = \frac{n^2h^2}{2mL^2} = \frac{2^2(6.626 \times 10^{-34}\ J \cdot s)^2}{8(9.11 \times 10^{-31}\ kg)(6.14 \times 10^{-10}\ m)^2} = 2.14 \times 10^{-18}\ J$$

Converting the units, $E_2 = 2.14 \times 10^{-18}\ J/(1.6 \times 10^{-19} J/eV) = 4.00\ eV$. Finally, the energy needed to transition from the ground state (E_1) to the first excited state (E_2) is $\Delta E = E_2 - E_1 = 3.0\ eV$.

2. Using Eq. (2.20), the wave function for an infinite square well with center at $x = 0$ and odd n is:

$$\psi(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right)$$

Plugging in $n = 3$ and $L = 10\ nm$,

$$\psi(x) = \sqrt{\frac{2}{10\ nm}} \cos\left(\frac{3\pi x}{10\ nm}\right)$$

with boundaries $-5\ nm < x < 5\ nm$. This has numerical values:

x (nm)	$\psi(x)$
0	0.447
2	−0.139
4	−0.364
8	0
10	0

The last two are zero because they are outside of the infinite square well.

3. We need to calculate the energy levels for the 10 nm wide infinite well for $n = 3$ and $n = 2$:

$$\begin{aligned}
E_3 = \frac{3^2h^2}{8mL^2} &= \frac{9(6.63 \times 10^{-34}\ J \cdot s)^2}{8(9.11 \times 10^{-31}\ kg)(10 \times 10^{-9}\ m)^2} \\
&= 5.43 \times 10^{-21}\ J \cdot \frac{1\ eV}{1.6 \times 10^{-19}\ J} = 0.034\ eV \\
E_2 = \frac{2^2h^2}{8mL^2} &= \frac{4(6.63 \times 10^{-34}\ J \cdot s)^2}{8(9.11 \times 10^{-31}\ kg)(10 \times 10^{-9}\ m)^2} \\
&= 2.41 \times 10^{-21}\ J \cdot \frac{1\ eV}{1.6 \times 10^{-19} J} = 0.015\ eV \\
\Delta E &= 0.034\ eV - 0.015\ eV = 0.019\ eV
\end{aligned}$$

where ΔE is the energy of the emitted photon. Using Eq. (1.5) to calculate the wavelength of the light:

$$\lambda = \frac{hc}{E_{photon}} = \frac{1240\ eV \cdot nm}{0.019\ eV} = 65 \times 10^3\ nm = 65\ mm$$

4. Following Eq. (2.21), the average value of the momentum squared is:

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} p^2\ |\psi(x)|^2\ dx$$

Using $p^2 = 2mE$ and Eq. (2.17) for E,

$$p^2 = 2m\left(\frac{n^2h^2}{8mL^2}\right) = \frac{n^2h^2}{4L^2}$$

Plugging this into the integral and using Eq. (2.20) for $\psi(x)$:

$$\langle p^2 \rangle = \frac{n^2h^2}{4L^2} \int_{-L/2}^{L/2} \frac{2}{L} \cos^2\left(\frac{n\pi x}{L}\right)\ dx \qquad (n \text{ odd})$$

$$\langle p^2 \rangle = \frac{n^2h^2}{4L^2} \int_{-L/2}^{L/2} \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right)\ dx \qquad (n \text{ even})$$

The integral is normalized in both cases (see Example 2.2 for details) and is equal to unity. For both cases:

$$\langle p^2 \rangle = \frac{n^2 h^2}{4L^2}$$

5. Using Eq. (2.39), the energy of the ground state depends on θ:

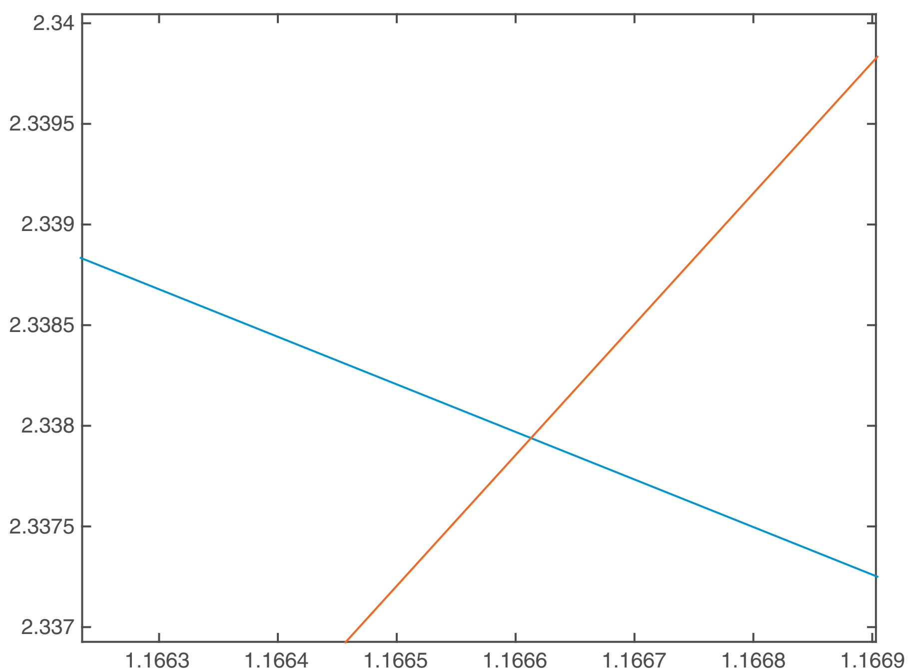
$$E = \frac{2\hbar^2 \theta^2}{mL^2}$$

where $m = 0.067 m_e$ is the effective mass of the electron in GaAs and $L = 10\ nm$ is the width of the finite well. To find θ, we need to find the graphical solution, as shown in Figure 2.6 but for the well depth of this problem, $V_0 = 0.2\ eV$. Plugging this into Eq. (2.36) and using $m_e c^2 = 511 \times 10^3\ eV$:

$$\theta_0^2 = \frac{mc^2 V_0 L^2}{2(\hbar c)^2} = \frac{(3.4 \times 10^4\ eV)(0.2\ eV)(10\ nm)^2}{2(197.3\ eV \cdot nm)^2} = 8.80$$

in units of radians^2. Following the example MATLAB Program 2.1, but with the new value of θ_0^2, the graphical value of θ where the two curves meet is found to be $\theta = 1.1666$. Finally, we use Eq. (2.39) above to get the lowest energy state of the electron:

$$E = \frac{2(\hbar c)^2 \theta^2}{(mc^2)L^2} = \frac{2(197.3\ eV \cdot nm)^2 (1.1666)^2}{(3.4 \times 10^4\ eV)(10\ nm)^2} = 0.0312\ eV$$



6. Inside the finite well, the wave function is given by Eq. (2.30), which depends on k. Since we know θ from the previous problem, we can find k from Eq. (2.34):

$$k = \frac{2\theta}{L} = \frac{2(1.1666)}{10\ nm} = 0.2333\ nm^{-1}$$

Now we can plot the part of the wave function inside the well using Eq. (2.30):

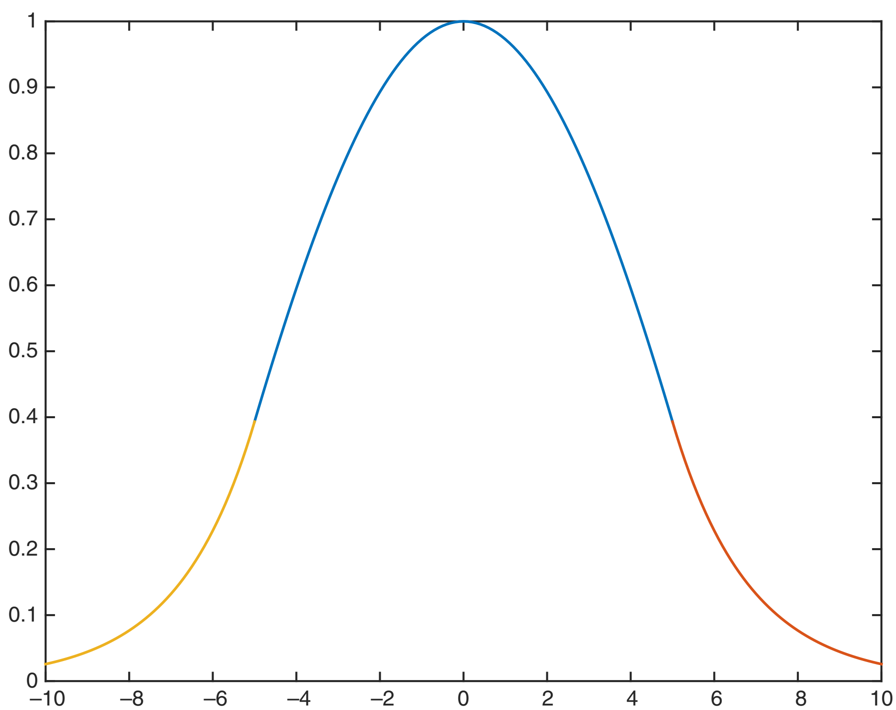
$$\psi(x) = (1.0)\cos(0.2333x)$$

where we have set the normalization constant $A = 1$ for now. (To determine the actual value of A requires a numerical integration, which is beyond the scope of this chapter.) Outside the well, the wave function is given by Eq. (2.31), which depends on κ. Dividing Eq. (2.33) by Eq. (2.32):

$$\kappa = k\ \tan(kL/2) = (0.2333)\tan(0.2333 \cdot 5) = 0.545$$

Note that the argument of the tangent is in radians. Now we can plot the part of the wave function outside the well using Eq. (2.31):

$$\psi(x) = Be^{-0.545x}$$



The value of B can be found by matching at the boundary using Eq. 2.32 with $A = 1$:

$$B = \frac{\cos(kL/2)}{e^{-\kappa L/2}} = \frac{\cos(1.1666)}{e^{-2.725}} = 6.000$$

Any plotting software can now be used to draw the wave function. For convenience here are commands for plotting this using MATLAB:

```
x = -5.0:0.1:5.0;
Inside = 1.0*cos(0.2333*x);
x1 = 5.0:0.1:10.0;
Outside1 = 6.0*exp(-0.545*x1);
x1 = -10.0:0.1:-5.0;
Outside1 = 6.0*exp(0.545*x1);
plot(x,Inside,x1,Outside1,x2,Outside2)
```

7. The harmonic oscillator wave functions are given by Eq. (2.45):

$$\psi_n(y) = A_n e^{-y^2/2} H_n(y)$$

where A_n is the normalization coefficient, y is a dimensionless variable and $H_n(y)$ are the Hermite Polynomials (see Table 2.1). The A_0 coefficient can be set to unity for this problem, since no oscillator parameters are given. The other A_n coefficients should be scaled appropriately. It is now a simple matter to use any plotting software to draw the wave functions. For convenience, here are commands for plotting using MATLAB:

```
y = -5.0:0.1:5.0;
psi0 = 1.0*exp(-0.5*y.*y);
A1 = 1.0/sqrt((2)*1);
H1 = 2*y;
psi1 = A1*psi0.*H1;
A2 = 1.0/sqrt((4)*2*1);
H2 = 2.0-4.0*y.*y;
psi2 = A2*psi0.*H2;
A3 = 1.0/sqrt((8)*3*2*1);
H3 = 12.0*y-8.0*y.*y.*y;
psi3 = A3*psi0.*H3;
plot(y,psi0,y,psi1,y,psi2,y,psi3)
```

Note that all punctuation (especially the period symbols) must be typed as shown. See Appendix C for more help on MATLAB usage.

8. The wave functions for an electron in an infinite well are shown in Figure 2.2. These may be compared with the wave functions for the finite well in Problems 5 and 6, or the plots shown in Figure 2.7, which are very similar.

The most noticeable difference is that the wave functions of the infinite well go immediately to zero at the boundaries, whereas the wave functions of the finite well "leak out" beyond the boundaries. However, the general shape of the wave functions in both cases is similar, looking like a cosine function centered on zero for the ground state (and the even excited states) and a sine function centered on zero for the first excited state (and the odd excited states. This similarity in general shape means that the wave functions of the infinite square well can be used as a crude approximation for the wave functions of the finite well, provided that the well width L is not too different between the two cases.

9. The same procedures as for Example 2.1 can be followed. The boundary conditions are now:

$$\psi(0) = 0$$
$$\psi(L) = 0$$

For the even solutions, we the boundary conditions give:

$$A\cos(0) = 0$$
$$A\cos(kL) = 0$$

and these equations can only be true if $A = 0$, meaning there are no even solutions. For the odd solutions, the boundary conditions give:

$$B\sin(0) = 0$$
$$B\sin(kL) = 0$$

where again k is a solution to the Schrödinger equation, $(\hbar k)^2 = 2mE$. These equations are satisfied when $kL = n\pi$, so we get:

$$\psi(x) = B\sin\left(\frac{n\pi x}{L}\right) = 0 \qquad (0 \leq x \leq L)$$

Using Eq. (2.12), the energy levels are given when k satisfies the boundary conditions:

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

which is exactly the same as Eq. (2.17). This makes sense, since we have merely moved the origin of the coordinate system, which should not effect the observables.

10. Outside the finite potential well, $V = V_0$, so the time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$$

Multiplying both sides by $-2m/\hbar^2$:

$$\frac{d^2\psi}{dx^2} - \frac{2mV_0}{\hbar^2}\psi = -\frac{2mE}{\hbar^2}\psi$$

Moving $2mE/\hbar^2$ to the LHS:

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\psi = 0$$

We make the following substitution:

$$k = \left(\frac{2m(E-V_0)}{\hbar^2}\right)^{\frac{1}{2}}$$

Since E is greater than V_0, k is now a real number and the Schrödinger equation becomes:

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

We can confirm by substitution that the general form of the solution to this equation is a linear combination of the functions, $A\cos(kx)$ and $B\sin(kx)$.

11. Starting from the Eqs. (2.34) and (2.26) and solving for θ

$$\theta = \frac{kL}{2} = \sqrt{\frac{2mE}{\hbar^2}}\frac{L}{2}$$

Using the definition of θ_0^2 from Eq. (2.36) and the equation above:

$$\frac{\theta_0^2}{\theta^2} = \frac{\frac{mV_0L^2}{2\hbar^2}}{\frac{mEL^2}{2\hbar^2}} = \frac{V_0}{E}$$

Taking the squared ratio of Eqs. (2.29) and (2.26):

$$\frac{\kappa^2}{k^2} = \frac{2mV_0 - E}{2mE} = \frac{V_0}{E} - 1 = \frac{\theta_0^2}{\theta^2} - 1$$

After taking the square root, we get the desired result of Eq. (2.41). Of course, Eq. (2.40) is a trivial rearrangement of the definition in Eq. (2.34).

12. Evaluating the second derivative:

$$\frac{d\psi}{dx} = -A\frac{m\omega x}{\hbar}e^{-m\omega x^2/2\hbar}$$
$$\frac{d^2\psi}{dx^2} = -A\frac{m\omega}{\hbar}e^{-m\omega x^2/2\hbar} + A\frac{m^2\omega^2x^2}{\hbar^2}e^{-m\omega x^2/2\hbar}$$

Substituting this into the LHS of Eq. (2.43) and canceling common factors:

$$\frac{-\hbar^2}{2m}\left(-\frac{m\omega}{\hbar}+\frac{m^2\omega^2x^2}{\hbar^2}\right)+\frac{1}{2}m\omega^2x^2=E$$

Carrying out the algebra:

$$E=\frac{\hbar\omega}{2}$$

which is the same as Eq. (2.44) when $n = 0$. Hence this is the ground state wave function that satisfies Schrödinger's equation.

13. The normalized wave function must satisfy Eq. (2.18):

$$\int_{-\infty}^{\infty}|\psi(x)|^2dx=1$$

$$\int_{-\infty}^{\infty}|Ae^{-m\omega x^2/2\hbar}|^2dx=\int_{-\infty}^{\infty}A^2e^{-m\omega x^2/\hbar}=1$$

Dividing both sides by A^2 and noticing the symmetry of the integral:

$$\frac{1}{A^2}=\int_{-\infty}^{\infty}e^{-m\omega x^2/\hbar}dx=2\int_0^{\infty}e^{-m\omega x^2/\hbar}dx$$

Now substitute $a = m\omega/\hbar$ and use the integral given in the problem:

$$\frac{1}{A^2}=\sqrt{\frac{\pi}{\frac{m\omega}{\hbar}}}=\sqrt{\frac{\pi\hbar}{m\omega}}$$

$$A=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$$

14. (a) The wave function is zero for $x < 0$ then starts to rise linearly for small x, then turns over and goes back to zero at large x due to the exponential. **(b)** Using the normalization condition, Eq. (2.18):

$$\int_0^{\infty}A^2x^2e^{-2ax}=1$$

Integrating this by parts twice and solving for A gives:

$$A^2=4a^3$$

(c) We want to find the maximum of the square of the wave function. Taking the derivative and setting it equal to zero:

$$\frac{d}{dx}|\psi(x)|^2=\frac{d}{dx}(4a^3x^2e^{-2ax})=8a^3xe^{-2ax}-8a^4x^2e^{-2ax}=0$$

Solving for x yields $x = 1/a$ for the maximum probability.
(d) The average value of the position is given by Eq. (2.21):

$$\langle x \rangle = \int_0^\infty 4a^3 x^3 e^{-2ax} dx$$

Integrating by parts three times yields $\langle x \rangle = 3/(2a)$.

15 (a) $V = 0$ in the region $0 \leq x \leq L$, so the Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

Now $V = V_0$ in the region $x \geq L$ so:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0 = E\psi$$

(b) Defining:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Then,

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad (0 \leq x \leq L)$$
$$\frac{d^2\psi}{dx^2} - k^2\psi = 0 \qquad (x \geq L)$$

Similar to the situation of the finite well discussed in the text, the above equations are satisfied by the general solutions:

$$\psi(x) = A\ cos(kx) \text{ and } \psi(x) = A\ sin(kx) \qquad (0 \leq x \leq L)$$
$$\psi(x) = Be^{-\kappa x} \qquad (x \geq L)$$

(c) The potential is infinite at $x = 0$, so the wave function must go to zero there. Examining the new boundary conditions at $x = 0$:

$$Even : \psi(0) = A\ cos(0) = 0$$
$$Odd : \psi(0) = A\ sin(0) = 0$$

The even solution requires $A = 0$, and hence there are no even solutions. We are left with: $\psi(x) = A\ sin(kx)$ for $0 \leq x \leq L$. Next, we examine the boundary conditions at $x = L$:

$$\psi(L) = A\ sin(kL) = Be^{-\kappa L}$$

Imposing the continuity of the first derivative:

$$\psi'(L) = Ak\ cos(kL) = -B\kappa e^{-\kappa L}$$

Dividing the above two equations gives:

$$\frac{\psi'(L)}{\psi(L)} = -cot(kL) = \frac{\kappa}{k}$$

Inserting κ as defined in part (b):

$$-cot(kL) = \sqrt{\frac{2mV_0}{\hbar^2 k^2} - \frac{2mE}{\hbar^2 k^2}}$$

Substitute k into the second term of the RHS:

$$-cot(kL) = \sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1}$$

Let $\theta = kL$:

$$-cot(\theta) = \sqrt{\frac{2mV_0 L^2}{\hbar^2 \theta^2} - 1}$$

We can transform this into a form similar to that of Eq. (2.35) if:

$${\theta_0}^2 = \frac{2mV_0 L^2}{\hbar^2}$$

The equation we need to solve is now:

$$-cot(\theta) = \sqrt{\frac{{\theta_0}^2}{\theta^2} - 1}$$

This can be solved graphically for the values of θ for which the LHS and RHS expressions intersect. Note that the value for ${\theta_0}^2$ derived above is slightly different from that of Eq. (2.34). This occurs because the definition for θ is also different, due to the boundary condition taking place at $x = L$ rather than at $x = L/2$ as in section 3.2.

16. Starting from Eq. (2.47):

$$\psi(x,t) = Ae^{ikx} \cdot e^{-i\omega t}$$

Taking the second derivative

$$\frac{d^2\psi}{dx^2} = -Ak^2 e^{ikx} e^{-i\omega t}$$

Taking the partial derivative

$$\frac{\partial \psi}{\partial t} = -i\omega A e^{ikx} e^{-i\omega t}$$

Plugging into the time-dependent Schrödinger equation, Eq. (2.53), gives:

$$\frac{\hbar^2 k^2}{2m}\psi(x,t) + V(x,t)\psi(x,t) = \hbar\omega\psi(x,t)$$

This equivalence is satisfied for a free particle ($V = 0$) when

$$\frac{\hbar^2 k^2}{2m} = \hbar\omega$$

Using de Broglie's relation $p = \hbar k$ from Eq. (1.27) and Einstein's relation $E = hf = \hbar\omega$ from Eq. (1.1), we see that the above is the same as the familiar formula $E = p^2/2m$. The traveling wave satisfies the time-dependent Schrödinger equation.

17. The wording of this problem could be confusing, since the infinite potential well represents a situation where the potential energy does not evolve with time. The goal here is to solve the time-dependent Schrödinger equation in the case of a static potential. The time-dependent solutions must then satisfy Eq. (2.53):

$$\Psi(x,t) = \psi(x)e^{-i\omega t}$$

where $\omega = E/\hbar$. From Eq. (2.20), the normalized even spatial wave functions of a particle in an infinite well are:

$$\psi(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)$$

The corresponding energies are given by Eq. (2.17):

$$E = \frac{n^2 h^2}{8mL^2}$$

where n is even for this problem. Calculating ω from the above:

$$\omega = \frac{E}{\hbar} = \frac{n^2 \pi h}{4mL^2}$$

for even n. The total wave function for even solutions is then:

$$\Psi(x,\ t) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) exp\left(-i\frac{n^2\pi h}{4mL^2}t\right)$$

for even n.