Boğaziçi University
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Phys 311/407 Summer 2013

Problem Set #9 Solutions

Answer 1:

The energy of an electron in an infinite square well is given by:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{(\hbar c)^2 n^2 \pi^2}{2(mc^2)L^2}$$

where m is the electron mass, 0.511 MeV/c^2, and n is the state number:

$$E_n = \frac{(197 \text{ nm} \cdot \text{eV})^2 \pi^2}{2 \times (0.511 \times 10^6 \text{ eV})(0.05\, nm)^2} n^2 \approx 150\, n^2 \text{ eV}$$

a) The ground state energy is E_1:

$$E_1 \approx 150 \text{ eV}$$

b) The first excited state energy is E_2:

$$E_2 \approx 150 \times 2^2 = 600 \text{ eV}$$

Answer 2:

The energy of a particle in an infinite square well is

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

$n = 1$ for the ground state. Then, we write conservation of energy:

$$\begin{aligned} E_{initial} &= E_{final} \\ E_n &= E_1 + E_\gamma \\ E_\gamma &= E_n - E_1 = \frac{\hbar^2 \pi^2}{2mL^2}(n^2 - 1) \end{aligned}$$

Answer 3:

a) Let us define:

$$\begin{aligned} \psi_2(x,t) &\equiv \frac{1}{\sqrt{2}} \psi_2(x) \cdot e^{-iE_2 t/\hbar} \\ \psi_3(x,t) &\equiv \frac{1}{\sqrt{2}} \psi_3(x) \cdot e^{-iE_3 t/\hbar} \end{aligned} \tag{1}$$

Then the wave function given in this question can be written as:

$$\psi(x,t) = \psi_2(x,t) + \psi_3(x,t)$$

The time dependent Schrödinger Equation is:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right] \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t)$$

$V(x,t) = 0$ within the well.

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x,t) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_3(x,t) &= i\hbar\frac{\partial}{\partial t}\psi_2(x,t) + i\hbar\frac{\partial}{\partial t}\psi_3(x,t) \\ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x,t) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_3(x,t) &= i\hbar\left[\frac{-iE_2}{\hbar}\right]\psi_2(x,t) + i\hbar\left[\frac{-iE_3}{\hbar}\right]\psi_3(x,t) \end{aligned}$$

Using the definitions given in equation (1), we can rewrite this equation in terms of $\psi_{2,3}(x)$:

$$\frac{1}{\sqrt{2}}e^{-iE_2t/\hbar}\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x)-E_2\psi_2(x)\right\}+\frac{1}{\sqrt{2}}e^{-iE_3t/\hbar}\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_3(x)-E_3\psi_3(x)\right\}=0 \qquad (2)$$

Note that $\psi_2(x)$ and $\psi_3(x)$ are the solutions for time independent Schrödinger Equation for an infinite square well. Thus:

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x) &= E_2\psi_2(x)\\ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_3(x) &= E_3\psi_3(x)\end{aligned}$$

Thus, the terms inside the curly brackets in equation (2) are equal to zero, which yields:

$$\frac{1}{\sqrt{2}}e^{-iE_2t/\hbar}\{0\}+\frac{1}{\sqrt{2}}e^{-iE_3t/\hbar}\{0\}=0$$

$$0=0$$

Thus, the wave function satisfies the time dependent Schrödinger Equation.

b) The integrated probability over the allowed region should be 1:

$$\begin{aligned}1 &= \int_0^L \mathrm{d}x\,|\psi(x,t)|^2\\ &= \int_0^L \mathrm{d}x\,\psi^*(x,t)\,\psi(x,t)\\ &= \frac{1}{2}\int_0^L \mathrm{d}x\,\left(\psi_2(x)e^{iE_2t/\hbar}+\psi_3(x)e^{iE_3t/\hbar}\right)\cdot\left(\psi_2(x)e^{-iE_2t/\hbar}+\psi_3(x)e^{-iE_3t/\hbar}\right)\\ &= \frac{1}{2}\int_0^L \mathrm{d}x\,[\psi_2(x)]^2+[\psi_3(x)]^2+\psi_2(x)\psi_3(x)e^{i(E_2-E_3)t/\hbar}+\psi_2(x)\psi_3(x)e^{-i(E_2-E_3)t/\hbar}\\ &= \frac{1}{2}\left[\int_0^L \mathrm{d}x\,|\psi_2(x)|^2+\int_0^L \mathrm{d}x\,|\psi_3(x)|^2+2\cos\left[(E_2-E_3)t/\hbar\right]\int_0^L \mathrm{d}x\,\psi_2(x)\,\psi_3(x)\right] \qquad (3)\end{aligned}$$

The first two terms are unity due to being the definition of normalization equation for the time independent wave functions for each state:

$$\int_0^L \mathrm{d}x\,|\psi_2(x)|^2=1 \qquad \int_0^L \mathrm{d}x\,|\psi_3(x)|^2=1$$

The third term vanishes, because $\psi_2(x)$ and $\psi_3(x)$ are orthogonal to each other (shown in class):

$$\int_0^L \mathrm{d}x\,\psi_2(x)\,\psi_3(x)=0$$

Thus, we get

$$1=\frac{1}{2}(1+1+0)=1$$

Thus, the given wave function is normalized. That means that the particle is *always* between $0<x<L$ as one expects for an infinite square well.

c) The probability in question is:

$$P(t)|_{0<x<L/2}=\int_0^{\frac{L}{2}}\mathrm{d}x\;|\psi(x,t)|^2$$

We use equation (3) found in part b), with the proper integral limits: $x = 0 \to L/2$

$$P(t) = \frac{1}{2}\left[\int_0^{L/2} \mathrm{d}x\, |\psi_2(x)|^2 + \int_0^{L/2} \mathrm{d}x\, |\psi_3(x)|^2 + 2\cos\left[(E_3 - E_2)t/\hbar\right] \int_0^{L/2} \mathrm{d}x\, \psi_2(x)\, \psi_3(x)\right]$$

Since $\psi_2(x)$ and $\psi_3(x)$ are symmetric around $L/2$, the first and the second terms give $1/2$:

$$\begin{aligned}
P(t) &= \frac{1}{2} + \cos\left[(E_3 - E_2)t/\hbar\right] \int_0^{L/2} \mathrm{d}x\, \frac{2}{L} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{3\pi x}{L}\right) \\
&= \frac{1}{2} + \frac{2}{L} \cos\left[(E_3 - E_2)t/\hbar\right] \frac{1}{2} \int_0^{L/2} \mathrm{d}x\, \left(\cos\frac{\pi x}{L} - \sin\frac{5\pi x}{L}\right) \\
&= \frac{1}{2} + \frac{1}{L} \cos\left[(E_3 - E_2)t/\hbar\right] \left\{\int_0^{L/2} \mathrm{d}x\, \cos\frac{\pi x}{L} - \int_0^{L/2} \sin\frac{5\pi x}{L}\right\} \\
&= \frac{1}{2} + \frac{1}{L} \cos\left[(E_3 - E_2)t/\hbar\right] \left\{\frac{L}{\pi} - \frac{L}{5\pi}\right\}
\end{aligned}$$

$$\boxed{P(t) = \tfrac{1}{2} + \tfrac{4}{5\pi} \cos\left[(E_3 - E_2)t/\hbar\right]}$$

The probability of being at the left half of the well and right half of the well fluctuates: (left $\leftrightarrow$ right) with a frequency of $w = (E_3 - E_2)/\hbar$, which means that sometimes (with the given frequency) finding the particle at the left half of the well is larger than the right side, and vice versa...

$$\begin{aligned}
w = 2\pi f &= \frac{E_3 - E_2}{\hbar} \\
2\pi f &= \frac{1}{\hbar}\left(\frac{\hbar^2 \pi^2}{2mL^2}\right)(3^2 - 2^2)
\end{aligned}$$

$$\boxed{f = \frac{5\hbar\pi}{4mL^2}}$$

Answer 4:

$$
\begin{aligned}
E_{n_x n_y n_z} &= \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{n_x}{L}\right)^2 + \left(\frac{n_y}{L/\sqrt{3}}\right)^2 + \left(\frac{n_z}{L/2}\right)^2\right] \\
&= \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + 3n_y^2 + 4n_z^2)
\end{aligned}
$$

We do not have a golden rule to find the lowest energy states for an asymmetric 3D box. We have to find this by trial-and-error. However, we can reduce the number of trials by examining the relative contribution of each term.

Changing n_z –the dominant term– from 1 to 2, increases the unitless number in the parenthesis by $4(2^2 - 1^2) = 12$. The minimum increase in n_x to compensate this is $n_x = 1 \rightarrow 4$ which changes the first term by $4^2 - 1^2 = 15 > 12$. And similarly, $n_y = 1 \rightarrow 3$ gives $3(3^2 - 1^2) = 24 > 12$. Thus, we try all combinations of $n_x = \{1, 2, 3, 4\}$, $n_y = \{1, 2, 3\}$, $n_z = \{1, 2\}$ which should give the first $4 \times 3 \times 2 = 24$ lowest energy states, then we sort them out:

$$
\begin{aligned}
E_{111} &= \frac{\hbar^2\pi^2}{2mL^2} \cdot 8 \\
E_{211} &= \frac{\hbar^2\pi^2}{2mL^2} \cdot 11 \\
E_{311} &= \frac{\hbar^2\pi^2}{2mL^2} \cdot 16 \\
E_{121} &= \frac{\hbar^2\pi^2}{2mL^2} \cdot 17 \\
E_{112} &= E_{221} = \frac{\hbar^2\pi^2}{2mL^2} \cdot 20 \qquad \text{degenerate states}
\end{aligned}
$$

Luckily, the next degenerate state is within this first 24 states:

$$
E_{212} = E_{411} = \frac{\hbar^2\pi^2}{2mL^2} \cdot 23
$$