PC2232: Tutorial 5 solutions

Question 1: Spin probabilities

(a) Since

$$\begin{pmatrix} 1 & 0 \end{pmatrix} \Psi = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_z(+\frac{1}{2}) \\ \psi_z(-\frac{1}{2}) \end{pmatrix} = \psi_z\left(+\frac{1}{2}\right). \tag{1}$$

Therefore

$$\left|\begin{pmatrix} 1 & 0 \end{pmatrix} \Psi\right|^2 = \left|\psi_z\left(+\frac{1}{2}\right)\right|^2. \tag{2}$$

And similarly for $\psi_z(-\frac{1}{2})$.

(b) The total probability must be equal to 1. Therefore this equation must be satisfied

$$\begin{aligned} |\Psi_z|^2 = 1 = \left|\psi_z\left(+\frac{1}{2}\right)\right|^2 + \left|\psi_z\left(-\frac{1}{2}\right)\right|^2 &= \psi_z^*\left(+\frac{1}{2}\right)\psi_z\left(+\frac{1}{2}\right) + \psi_z^*\left(-\frac{1}{2}\right)\psi_z\left(-\frac{1}{2}\right) \\ 1 &= \frac{3}{5} + c^*c \\ c^*c &= \frac{2}{5}. \end{aligned} \tag{3}$$

Therefore a possible value of c could be

$$c = \sqrt{\frac{2}{5}}. \tag{4}$$

(Actually, note that $c = \sqrt{\frac{2}{5}}e^{i\theta}$ for any value of θ is also possible).

(c) Using $c = \sqrt{\frac{2}{5}}$,

$$\Psi_y = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{3}{5}} \\ \sqrt{\frac{2}{5}} \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}-i\sqrt{2}}{\sqrt{10}} \\ \frac{\sqrt{3}+i\sqrt{2}}{\sqrt{10}} \end{pmatrix} \tag{5}$$

Therefore, in the y-axis, the probability of measuring $s_y = +1/2$ is

$$\left|\psi_y\left(+\frac{1}{2}\right)\right|^2 = \frac{(\sqrt{3}+i\sqrt{2})(\sqrt{3}-i\sqrt{2})}{10} = \frac{5}{10} = \frac{1}{2}. \tag{6}$$

The probability of measuring $s_y = -\frac{1}{2}$ is

$$\left|\psi_y\left(-\frac{1}{2}\right)\right|^2 = 1 - \left|\psi_y\left(+\frac{1}{2}\right)\right|^2 = \frac{1}{2}. \tag{7}$$

Question 2: Separation of variables

Given the wavefunction

$$\Psi(\vec{r},t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\psi(\vec{r}), \tag{8}$$

we calculate the time derivative to be

$$\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[\frac{\partial}{\partial t}\mathrm{e}^{-\mathrm{i}Et/\hbar}\right]\psi(\vec{r}) = -\frac{\mathrm{i}E}{\hbar}\mathrm{e}^{-\mathrm{i}Et/\hbar}\psi(\vec{r}). \tag{9}$$

Substituting into the time-dependent Schrödinger equation results in

$$\mathrm{i}\hbar\left(-\frac{\mathrm{i}E}{\hbar}\right)\mathrm{e}^{-\mathrm{i}Et/\hbar}\psi(\vec{r}) = \mathrm{e}^{-\mathrm{i}Et/\hbar}\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right]\psi(\vec{r}). \tag{10}$$

Cancelling the exponential factors on both sides, we have

$$E\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})\right]\psi(\vec{r}) \tag{11}$$

If $\psi(\vec{r}) = \psi(x)$, we have

$$\vec{\nabla}^2\psi(x) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x) = \frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}. \tag{12}$$

Therefore the Schrödinger equation reduces to

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2m}{\hbar}(E - U_0)\psi. \tag{13}$$

Question 3: Ininite well

We can split our calculation into three regions:

$$\psi(x) = \begin{cases} \psi_1, & x < 0, \qquad \text{(Region 1)} \\ \psi_2, & 0 < x < L, \quad \text{(Region 2)} \\ \psi_3, & x > L \qquad \text{(Region 3).} \end{cases} \tag{14}$$

In Regions 1 and 3, the potential is infinite. The particle cannot exist there. Therefore $\psi_1 = \psi_3 = 0$.

In Region 2, the potential is zero. Therefore the Schrödinger equation reduces to

$$\frac{\mathrm{d}^2\psi_2}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi_2. \tag{15}$$

This is a second-order differential equation with a general solution

$$\psi_2(x) = A\sin(kx) + B\cos(kx). \tag{16}$$

Boundary condition states that $\psi(0) = 0$, therefore

$$\psi_2(0) = A\sin(0) + B\cos(0) \tag{17}$$

$$0 = B. \tag{18}$$

Therefore the solution is

$$\psi_2(x) = A\sin(kx). \tag{19}$$

The second boundary condition states that $\psi(L) = 0$. Therefore

$$\psi_2(L) = 0 = A\sin(kL) \quad \rightarrow kL = n\pi, \tag{20}$$

where n is an integer.

Therefore the wavefunction is

$$\psi(x) = \begin{cases} 0 & x < 0, \\ A\sin\left(\frac{n\pi x}{L}\right), & 0 < x < L \\ 0 & x > L. \end{cases} \tag{21}$$

Next we determine the normalization constant A. The wavefunction must satisfy

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}x \ |\psi|^2 &= 1 \\ \int_0^L \mathrm{d}x \ A^2 \sin^2\left(\frac{n\pi x}{L}\right) &= 1 \\ \frac{A^2 L^2}{2} &= 1 \\ A &= \sqrt{\frac{2}{L}}. \end{aligned} \tag{22}$$

Therefore the solution is

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L. \tag{23}$$

Question 4: Finite well

We have three regions, hence we seperate the wavefunction into three parts:

$$\psi(x) = \begin{cases} \psi_1(x), & x < 0 \\ \psi_2(x), & 0 < x < L \\ \psi_3(x), & x > L. \end{cases} \tag{24}$$

(a) For $E < U_0$, therefore $E - U_0$ is a negative number. Therefore the Schrödinger equation in region 1 is

$$\frac{\mathrm{d}^2\psi_1}{\mathrm{d}x^2} = \underbrace{-\frac{2m}{\hbar^2}(E - U_0)}_{\text{positive}}\psi. \tag{25}$$

The general solution to this second-order equation is

$$\psi_1(x) = A\mathrm{e}^{k_1 x} + B\mathrm{e}^{-k_1 x} \tag{26}$$

Eq. (26) will satisfy (25) if

$$k_1 = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}. \tag{27}$$

In region 2, $U = 0$, therefore

$$\frac{\mathrm{d}^2\psi_1}{\mathrm{d}x^2} = -\frac{2m}{\hbar^2}E\psi. \tag{28}$$

In Eq. (28), the coefficient of ψ on the right-hand-side is always negative (energy is positive), therefore the general solution is

$$\psi_2(x) = F\mathrm{e}^{\mathrm{i}k_2 x} + G\mathrm{e}^{-\mathrm{i}k_2 x} \tag{29}$$

Eq. (29) will satisfy (28) if

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}} \tag{30}$$

Region 3 is similar to region 1, therefore

$$\psi_3(x) = C\mathrm{e}^{k_3 x} + D\mathrm{e}^{-k_3 x}, \quad k_3 = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}. \tag{31}$$

The full general solution is

$$\psi(x) = \begin{cases} Ae^{k_1 x} + Be^{-k_1 x}, & x < 0, \\ Fe^{ik_2 x} + Ge^{-ik_2 x}, & 0 < x < L, \\ Ce^{k_3 x} + De^{-k_3 x}, & x > L. \end{cases} \tag{32}$$

(b) For $E > U_0$, then $E - U_0 > 0$. In region 1, the Schrödinger equation becomes

$$\frac{d^2\psi_1}{dx^2} = \underbrace{-\frac{2m}{\hbar^2}(E - U_0)}_{\text{negative}}\psi. \tag{33}$$

Therefore the general solution is

$$\psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}. \tag{34}$$

For Regions 2 and 3 are the same, the coefficient on the right hand sides are negative. Therefore the general solution is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x}, & x < 0, \\ Fe^{ik_2 x} + Ge^{-ik_2 x}, & 0 < x < L, \\ Ce^{ik_3 x} + De^{-ik_3 x}, & x > L. \end{cases} \tag{35}$$

For $E < U_0$, there are exponentially decaying terms in Regions 1 and 3, with an oscillating wavefunction in Region 2. Therefore there is a higher probability of finding the particle stuck in Region 2.

For $E > U_0$, we have an oscillating solution more or less uniformly across all three regions (no exponentally decaying terms).

Question 5: Schrödinger equation $\leftrightarrow$ Conservation of energy

Substituting

$$\psi(x) = A \sin kx \tag{36}$$

into the Schrödinger equation, we have

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U\psi = & -\frac{\hbar^2}{2m}(-k^2)A\sin kx + UA\sin kx = EA\sin kx \\ \frac{\hbar^2 k^2}{2m} + U = E & \end{aligned} \tag{37}$$

Since $\hbar k = p$,

$$\frac{p^2}{2m} + U = E. \tag{38}$$

Question 6: (Optional)

Using the main general result

$$E_n = \frac{n^2 h^2}{8mL^2}, \tag{39}$$

the energies of the various cases are:

$$E_a = \frac{h^2}{8m_1(3\text{ nm})^2}. \tag{40}$$

$$E_b = \frac{4h^2}{8m_1(3\text{ nm})^2}. \tag{41}$$

$$E_c = \frac{h^2}{8(2m_1)(1.5\text{ nm})^2}. \tag{42}$$

$$E_d = \text{slightly smaller than } E_a. \tag{43}$$

$$E_e = \text{slightly smaller than } E_b. \tag{44}$$

$$E_f = 0. \tag{45}$$

Comparing the values, the ranking is

$$E_b > E_a > E_c > E_a > E_d > E_f. \tag{46}$$