PC2232: Tutorial 6 solutions

Question 1: Harmonic oscillator ground state

Given that ψ satisfies

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi, \tag{1}$$

we can calculate some equations that will be useful later:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2m}{\hbar^2}E\psi+\frac{m^2\omega^2}{\hbar^2}x^2\psi, \tag{2}$$

$$\frac{\mathrm{d}^3\psi}{\mathrm{d}x^3} = -\frac{2m}{\hbar^2}E\frac{\mathrm{d}\psi}{\mathrm{d}x}+\frac{2m^2\omega^2}{\hbar^2}x\psi+\frac{m^2\omega^2}{\hbar^2}x^2\frac{\mathrm{d}\psi}{\mathrm{d}x} \tag{3}$$

(a) A new wavefunction ϕ is defined by

$$\phi=\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x}+m\omega x\psi. \tag{4}$$

Differentiating both sides of the equation gives

$$\frac{\mathrm{d}\phi}{\mathrm{d}x}=\hbar\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+m\omega\psi+m\omega x\frac{\mathrm{d}\psi}{\mathrm{d}x}. \tag{5}$$

Differentiating again gives

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}=\hbar\frac{\mathrm{d}^3\psi}{\mathrm{d}x^3}+m\omega\frac{\mathrm{d}\psi}{\mathrm{d}x}+m\omega\frac{\mathrm{d}\psi}{\mathrm{d}x}+m\omega x\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}. \tag{6}$$

Substituting (2) and (3) into (6), then rearranging the terms gives

$$\begin{aligned}
\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} &= -\frac{2m}{\hbar^2}E\left(\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x}+m\omega x\psi\right)+\frac{2m}{\hbar^2}\hbar\omega\left(\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x}+m\omega x\psi\right)\\
&\quad +\frac{2m}{\hbar^2}\frac{1}{2}m\omega^2x^2\left(\hbar\frac{\mathrm{d}\psi}{\mathrm{d}x}+m\omega x\psi\right)\\
&= -\frac{2m}{\hbar^2}E\phi+\frac{2m}{\hbar^2}\hbar\omega\phi+\frac{2m}{\hbar^2}\frac{1}{2}m\omega^2x^2\phi\\
-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}+\frac{1}{2}m\omega^2x^2\phi &= \underbrace{(E-\hbar\omega)}_{\text{energy of }\phi}\ \phi
\end{aligned} \tag{7}$$

Therefore ϕ satisfies Schrödinger's equation with an energy of $(E-\hbar\omega)$, which is lower than the energy of ψ by a value of $\hbar\omega$.

(b) Ground state ψ_0 has the lowest possible energy E_0. Therefore

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_0}{\mathrm{d}x^2}+\frac{1}{2}m\omega^2x^2\psi_0=E_0\psi_0, \tag{8}$$

Since E_0 is the lowest, a state $\phi = \left(\hbar\frac{\mathrm{d}}{\mathrm{d}x} + m\omega x\right)\phi$ where

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2x^2\phi = \underbrace{(E_0 - \hbar\omega)}_{\text{lower than } E_0}\phi \tag{9}$$

with a lower energy cannot exist. Therefore we conclude that $\phi = 0$:

$$\begin{aligned}
\phi = \hbar\frac{\mathrm{d}\psi_0}{\mathrm{d}x} + m\omega x\psi_0 &= 0 \\
\frac{\mathrm{d}\psi_0}{\psi_0} &= -\frac{m\omega}{\hbar}x\mathrm{d}x \\
\int\frac{\mathrm{d}\psi_0}{\psi_0} &= -\frac{m\omega}{\hbar}\int x\mathrm{d}x \\
\psi_0 &= C\mathrm{e}^{-m\omega x^2/2\hbar},
\end{aligned} \tag{10}$$

where C is an integration constant.

Question 2: Step potential

There are two distinct regions, as shown in the figure below:

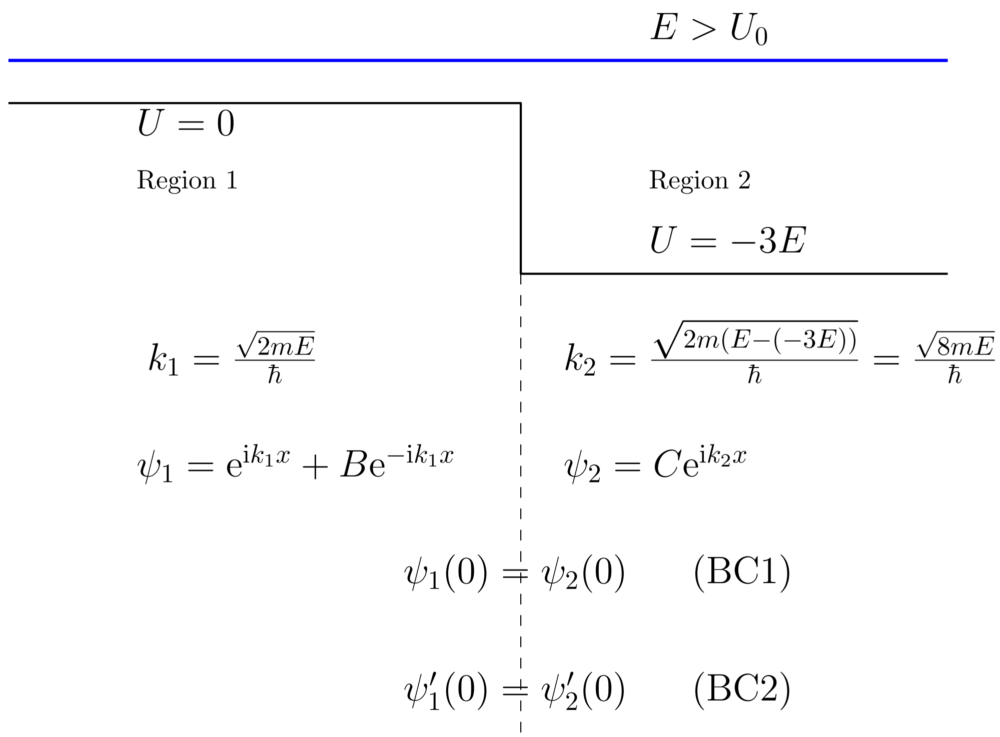

Figure 1: Step potential

(a) Classically, the particle would drop to a lower potential and have a gain in kinetic energy by a magnitude of $3E$.

(b) Based on Fig. 1, our wavefunction is

$$\psi(x) = \begin{cases} \mathrm{e}^{\mathrm{i}k_1 x} + B\mathrm{e}^{-\mathrm{i}k_1 x}, & x < 0, \\ C\mathrm{e}^{\mathrm{i}k_2 x}, & x > 0. \end{cases} \tag{11}$$

The values of k_1 and k_2 that satisfies Schrödinger's equation at their respective regions are

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad k_2 = \frac{\sqrt{2m\left[E - (-3E)\right]}}{\hbar} = \frac{\sqrt{8mE}}{\hbar}. \tag{12}$$

Applying boundary conditions: At BC1, $\psi_1(0) = \psi_2(0)$ leads to

$$1 + B = C. \tag{13}$$

BC2, $\psi_1'(0) = \psi_2'(0)$ gives

$$\begin{aligned} \mathrm{i}k_1 (1 - B) &= \mathrm{i}k_2 C \\ 1 - B &= \frac{k_1}{k_2} C = \frac{\sqrt{8mE}/\hbar}{\sqrt{2mE}/\hbar} C = 2C. \end{aligned} \tag{14}$$

Taking Eq. (13)+(14) gives

$$C = \frac{2}{3}, \tag{15}$$

and Eq. (13)-(14) gives

$$B = -\frac{1}{3}. \tag{16}$$

Therefore, the full solution is

$$\psi(x) = \begin{cases} \mathrm{e}^{\mathrm{i}\sqrt{2mE}x/\hbar} - \frac{1}{3}\mathrm{e}^{-\mathrm{i}\sqrt{2mE}x/\hbar}, & x < 0, \\ \frac{2}{3}\mathrm{e}^{\mathrm{i}\sqrt{8mE}x/\hbar}, & x > 0. \end{cases} \tag{17}$$

(c) The reflection probability is

$$R = \frac{|B|^2}{|A|^2} = \frac{(1/3)^2}{1} = \frac{1}{9}. \tag{18}$$

Question 3: Transmission resonance

There are three regions, as shown in Fig. 2

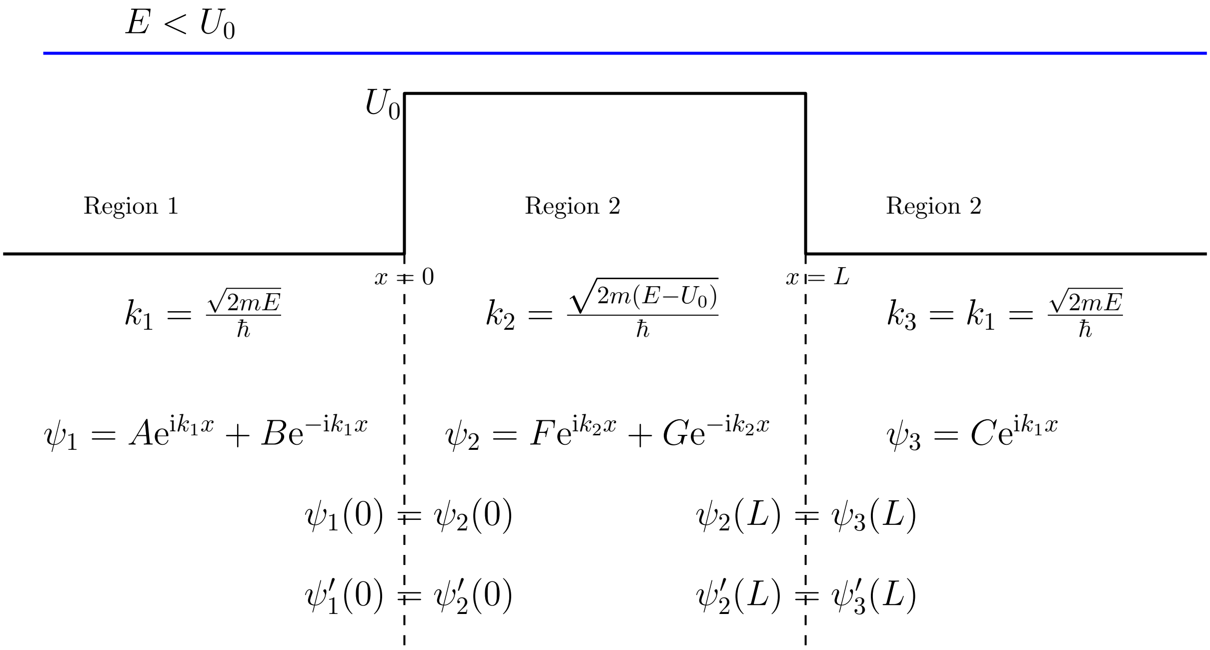

Figure 2: Tunneling through a barrier.

Since we are given $E - U_0 = \frac{\pi^2\hbar^2}{2mL^2}$, we get

$$k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar} = \frac{\pi}{L}. \tag{19}$$

The boundary conditions give

$$\begin{aligned}
\psi_1(0) = \psi_2(0) \quad &\rightarrow \quad A + B = F + G, && (20)\\
\psi_2(L) = \psi_3(L) \quad &\rightarrow \quad -(F + G) = C\mathrm{e}^{\mathrm{i}k_1 L}, && (21)\\
\psi_1'(0) = \psi_2'(0) \quad &\rightarrow \quad \mathrm{i}k_1(A - B) = \mathrm{i}k_2(F - G), && (22)\\
\psi_2'(L) = \psi_3'(L) \quad &\rightarrow \quad \mathrm{i}k_2(F\mathrm{e}^{\mathrm{i}\pi} - G\mathrm{e}^{-\mathrm{i}\pi}) = \mathrm{i}k_1 C\mathrm{e}^{\mathrm{i}k_1 L}. && (23)
\end{aligned}$$

Using Eqs. (20) and (21) to eliminate $(F + G)$ gives

$$A + B = -C\mathrm{e}^{\mathrm{i}k_1 x}. \tag{24}$$

Equation (23) gives

$$\begin{aligned}
k_2(F\mathrm{e}^{\mathrm{i}\pi} - G\mathrm{e}^{-\mathrm{i}\pi}) &= \mathrm{i}k_1 C\mathrm{e}^{\mathrm{i}k_1 L}\\
-\frac{\pi}{L}(F - G) &= k_1 C\mathrm{e}^{\mathrm{i}k_1 L} && (25)
\end{aligned}$$

Using Eqs. (22) and (25) to eliminate $(C - D)$ gives

$$A - B = -C\mathrm{e}^{\mathrm{i}k_1 L}. \tag{26}$$

Finally, taking (24)−(26) will lead to

$$B = 0. \tag{27}$$

Question 4: Two-dimensional well

Let

$$\psi(x, y) = F(x)G(y). \tag{28}$$

Substitute this into the 2D Schrödinger equation (in the region where $U = 0$) to get

$$\begin{aligned} G\frac{\mathrm{d}^2 F}{\mathrm{d}x^2} + F\frac{\mathrm{d}^2 G}{\mathrm{d}y^2} &= -\frac{2mE}{\hbar^2}FG \\ \frac{1}{F}\frac{\mathrm{d}^2 F}{\mathrm{d}x^2} + \frac{1}{G}\frac{\mathrm{d}^2 G}{\mathrm{d}y^2} &= -\frac{2mE}{\hbar^2}. \end{aligned} \tag{29}$$

For this equation to be true, each term on the left hand side must individually be constants:

$$\frac{1}{F}\frac{\mathrm{d}^2 F}{\mathrm{d}x^2} = C_x, \quad \frac{1}{G}\frac{\mathrm{d}^2 G}{\mathrm{d}y^2} = C_y. \tag{30}$$

Look at the general solution for the x equation first:

$$\frac{\mathrm{d}^2 F}{\mathrm{d}x^2} = C_x F, \quad \rightarrow \quad F = A_x \sin k_x x + B_x \cos k_x x. \tag{31}$$

We can see that

$$\frac{\mathrm{d}^2 F}{\mathrm{d}x^2} = -k^2 \left(A_x \sin k_x x + B_x \cos k_x x\right) = -k^2 F, \tag{32}$$

so that comparing Eq. (32) with (31), we conclude that

$$-k^2 = C_x. \tag{33}$$

For boundary conditions,

$$\begin{aligned} &F(0) = 0 = 0 + B_x, \quad \rightarrow \quad B_x = 0 \\ &F(L) = 0 = A_x \sin k_x L + \underbrace{B_x}_{=0} \cos k_x L, \quad \rightarrow k_x L = n\pi, \quad n = \text{integer}. \end{aligned} \tag{34}$$

Therefore,

$$k_x^2 = \frac{n^2\pi^2}{L^2}. \tag{35}$$

Do the similar calculation for y, and substitute the results into Eq. (30):

$$\begin{aligned} \frac{n_x^2\pi^2}{L^2} + \frac{n_y^2\pi^2}{L^2} &= \frac{2mE}{\hbar^2} \\ E &= \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2 + n_y^2\right). \end{aligned} \tag{36}$$

Normalization requires

$$1 = \int \mathrm{d}x\,\mathrm{d}y\,|\psi|^2 = \int \mathrm{d}x\,\mathrm{d}y A_x^2 A_y^2 \sin^2\frac{n_x\pi x}{L}\sin^2\frac{n_y\pi y}{L}. \tag{37}$$

This should give $A_xA_y = 2/L$. Therefore the final wavefunction should be

$$\psi(x,y) = F(x)G(y) = \frac{2}{L}\sin\frac{n_x\pi x}{L}\sin\frac{n_y\pi y}{L}. \tag{38}$$

The five lowest energy levels are

n_x	n_y	Energy, E	Degeneracy, d_n
1	1	$2K$	1
1	2	$5K$	2
2	1		
2	2	$8K$	1
3	1	$10K$	2
1	3		

where we have introduced the abbreviation

$$K = \frac{\pi^2\hbar^2}{2mL^2}. \tag{39}$$

Question 5: Tunneling

Given $E = 5.5$ eV $= 8.8 \times 10^{-19}$ J, $U_0 = 10.0$ eV $= 1.6 \times 10^{-18}$ J. Accordingly, for an electron,

$$\alpha = \frac{\sqrt{2m\left(U_0 - E\right)}}{\hbar} = 1.086 \times 10^{10}\ \mathrm{m}^{-1}. \tag{40}$$

The tunneling formula:

$$T \simeq \frac{16E}{U_0}\left(1-\frac{E}{U_0}\right)\mathrm{e}^{-2\alpha L}, \tag{41}$$

Tunneling probability is $T = 0.10\% = 0.001$, therefore

$$\begin{aligned} 0.001 &= 16\frac{5.5}{10}\left(1-\frac{5.5}{10}\right)\mathrm{e}^{-2\left(1.086\times10^{10}\right)L} \\ 2.525\times10^{-4} &= \mathrm{e}^{-\left(2.72\times10^{10}\right)L} \\ L &= 3.82\times10^{-10}\ \mathrm{m}. \end{aligned} \tag{42}$$