THE UNIVERSITY OF QUEENSLAND
SCHOOL OF MATHEMATICS AND PHYSICS
PHYS2041 – Quantum Physics

Tutorial 4 Solutions

Problem 4.1

(a) We look at the Time-Independent Schrödinger equation (TISE) inside the well, i.e., for $V(x) = 0$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}E\psi(x). \tag{1}$$

Now if $E = 0$ then

$$\frac{d}{dx}\left(\frac{d\psi(x)}{dx}\right) = 0 \tag{2}$$

The solution to this differential equation is (simply perform an indefinite integral of the RHS twice),

$$\psi(x) = Ax + B \tag{3}$$

Now we look at boundary conditions

$$\psi(0) = B = 0 \tag{4}$$
$$\psi(a) = Aa = 0, \text{so } A = 0 \tag{5}$$

where the last line holds since $a \neq 0$. Hence $\psi(x) = 0$, for all x. Clearly this cannot be normalised.

(b) Once again we proceed by looking at the TISE (Eq.(1))

If $E < 0$, then this becomes

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \equiv k^2\psi \tag{6}$$

where $k = \sqrt{-2mE/\hbar^2}$ and is a *positive* real number. This ODE has a general solution of

$$\psi(x) = Ae^{kx} + Be^{-kx} \tag{7}$$

If you're unsure about why, try checking this by substituting the solution back into the TDSE, or use the method of characteristics and the roots of the characteristic equation.

Now we impose boundary conditions:

$$\psi(0) = A + B = 0 \tag{8}$$
$$\psi(a) = Ae^{ka} + Be^{-ka} = 0 \tag{9}$$

The top line could have been satisfied, for example, for $A = B = 0$, but this would give $\psi(x) = 0$ everywhere (for all x), which is un-normalisable. The other possibility is $A = -B$. Substituting this into the bottom line implies

$$A\left(e^{ka} - e^{-ka}\right) = 0. \tag{10}$$

Now, the only way that this doesn't give $A = 0$ (and hence also $B = 0$) is if $(e^{ka} - e^{-ka}) = 0$ which means $e^{2ka} = 1$, which in turn implies $ka = 0$, but neither k nor a is zero here, so indeed $A = B = 0$ and hence $\psi(x) = 0$ for all x.

We conclude that if $E \leq 0$, the wave function cannot be normalized and satisfy the boundary conditions.

Problem 4.2

(a) We know the energies of the infinite square well of length a are $E_n = n^2\pi^2\hbar^2/2ma^2$. The energy difference between the first excited state (with $n = 2$) and the ground state (with $n = 1$) is

$$\Delta E = \left(2^2 - 1^1\right)\frac{\pi^2\hbar^2}{2ma^2} = \frac{3\pi^2\hbar^2}{2ma^2}. \tag{11}$$

For a single ^{87}Rb atom (which has mass $m = 86.909$ atomic mass units (amu), see `https://en.wikipedia.org/wiki/Isotopes_of_rubidium#Rubidium-87`) in a well of length $a = 10\mu$m the energy difference is

$$\Delta E = \frac{3\pi^2}{2}\frac{(1.05\times10^{-34}\text{Js})^2}{(86.9\text{amu})(1.66\times10^{-27}\text{kg/amu})(1.0\times10^{-5}\text{m})^2} \simeq 1.1\times10^{-32}\text{J}. \tag{12}$$

In electron volts the energy is

$$\Delta E = (1.1\times10^{-30}\text{J})/(1.60\times10^{-19}\text{J/eV}) \simeq 7.1\times10^{-14}\text{eV}, \tag{13}$$

and in the equivalent temperature units (divide by Boltzmann's constant k_B),

$$\Delta E/k_B = (1.1\times10^{-30}\text{J})/(1.38\times10^{-23}\text{J/K}) \simeq 8.3\times10^{-10}\text{K}. \tag{14}$$

(b) [Tutors, please explain this better than I have time at the moment to write a detailed answer. Refer to Lecture notes.]

Energy measurement outcomes: $E_0 = \hbar\omega/2$ and $E_1 = 3\hbar\omega/2$.

The respective probabilities: first check if the overal wavefunction is normalized, and if yes (which is the case here), the probabilities are given by the mod-squared of the respective expansion coefficients, i.e., $|c_0|^2 = |1/\sqrt{3}|^2 = 1/3$ and $|c_1|^2 = |\sqrt{2}/\sqrt{3}|^2 = 2/3$. (Sanity check: the sum of the probabilities should be equal to 1, and this is indeed the case here.)

Problem 4.3 **[FOR ASSIGNMENT 2; max 10 points]**

(a) Before we begin it will be useful here (and essential for the next part of the question) to re-write the wavefunction as a superposition of energy eigenstates/stationary states. This could be done by calculating the coefficients $\Psi(x,0) = \sum_n c_n \psi_n(x)$ which are given by the integral $c_n = \int \psi_n^* \Psi(x,0) dx$, however (in principle) there are infinitely many of these, and besides, its nice to avoid doing integrals where possible.

Instead, it is simpler to make use of the double angle trigonometric identity $\sin(2\theta) = 2\cos(\theta)\sin(\theta)$. We get

$$\begin{aligned}
\Psi(x,0) &= \sqrt{\frac{8}{5a}}\left(1+\cos\left(\frac{\pi x}{a}\right)\right)\sin\left(\frac{\pi x}{a}\right) &(15)\\
&= \sqrt{\frac{8}{5a}}\left(\sin\left(\frac{\pi x}{a}\right)+\cos\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi x}{a}\right)\right) &(16)\\
&= \sqrt{\frac{8}{5a}}\left(\sin\left(\frac{\pi x}{a}\right)+\frac{1}{2}\sin\left(\frac{2\pi x}{a}\right)\right) &(17)\\
&= \sqrt{\frac{8}{5a}}\left(\sqrt{\frac{a}{2}}\psi_1+\frac{1}{2}\sqrt{\frac{a}{2}}\psi_2\right) &(18)\\
&= \sqrt{\frac{4}{5}}\psi_1+\sqrt{\frac{1}{5}}\psi_2, &(19)
\end{aligned}$$

so it turns out the initial state is simply a superposition of the ground and first excited states of the infinite square well (recall $\psi_n = \sqrt{2/a}\sin(n\pi x/a)$).

The probability density is

$$\begin{aligned}
|\Psi(x,0)|^2 &= \frac{4}{5}|\psi_1|^2+\frac{1}{5}|\psi_2|^2+\frac{2}{5}\left(\psi_1^*\psi_2+\psi_1\psi_2^*\right) &(20)\\
&= \frac{4}{5}(\psi_1)^2+\frac{1}{5}(\psi_2)^2+\frac{4}{5}\psi_1\psi_2, &(21)
\end{aligned}$$

where the second line follows because the eigenstates of the infinite square well are real. The probability that the particle is found in the left half of the well is

$$P(\text{left}) = \int_0^{a/2} |\Psi(x,0)^2| dx = \frac{4}{5}\int_0^{a/2}(\psi_1)^2 dx + \frac{1}{5}\int_0^{a/2}(\psi_2)^2 dx + \frac{4}{5}\int_0^{a/2}\psi_1\psi_2 dx. \qquad (22)$$

Because the integrals are *not* over the entire domain, we cannot use the orthonormality of the eigenstates $\int \psi_m^* \psi_n dx = \delta_{mn}$ to simplify our answer. However, we do know that ψ_n are normalised and symmetric about the centre of the well (see Figure 1). This means that we can immediately identify

$$\int_0^{a/2} (\psi_1)^2 dx = \int_0^{a/2} (\psi_2)^2 dx = \frac{1}{2}. \tag{23}$$

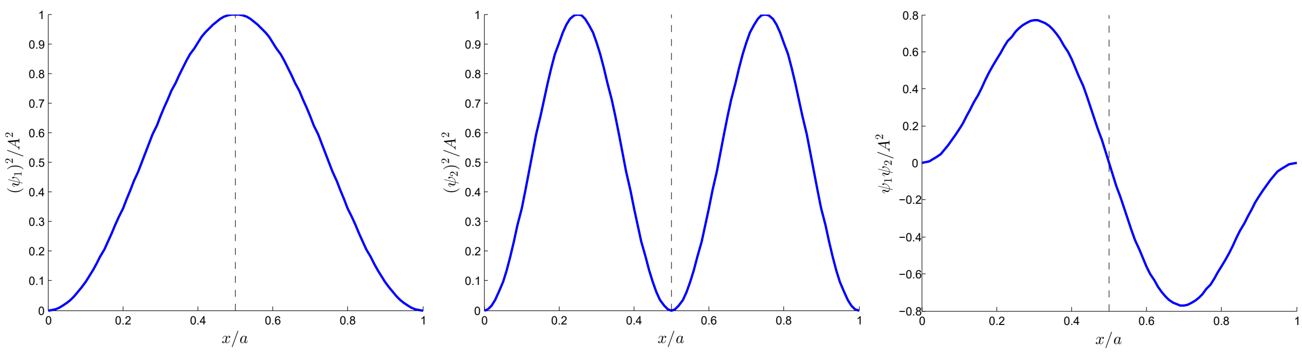

Figure 1: Plots of $(\psi_1)^2$ (left), $(\psi_2)^2$ (centre) and $\psi_1\psi_2$ (right), with $A = \sqrt{2/a}$. Usefully, they are all symmetric about the centre of the well at $x = a/2$ (black dashed line). Since the eigenstates are normalised (total area is one), clearly the area under the left half of $(\psi_1)^2$ and $(\psi_2)^2$ must be a half. Unfortunately this is *not* the case for the interference term $\psi_1\psi_2$.

Unfortunately we must still do the remaining integral by hand,

$$\int_0^{a/2} \psi_1\psi_2 dx = \frac{2}{a}\int_0^{a/2} \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right) dx \tag{24}$$

$$= \frac{1}{a}\int_0^{a/2} \cos\left(\frac{\pi x}{a}\right) dx - \frac{1}{a}\int_0^{a/2} \cos\left(\frac{3\pi x}{a}\right) dx \tag{25}$$

$$= \frac{1}{a}\left(\frac{a}{\pi} + \frac{a}{3\pi}\right) = \frac{4}{3\pi}, \tag{26}$$

where in the second line we used the trigonometric identity $2\sin(\theta)\sin(\phi) = \cos(\theta-\phi) - \cos(\theta+\phi)$.

Putting this all together gives the probability

$$P(\text{left}) = \frac{4}{5}\times\frac{1}{2} + \frac{1}{5}\times\frac{1}{2} + \frac{4}{5}\times\frac{4}{3\pi} = \frac{1}{2} + \frac{16}{15\pi} \approx 0.84. \tag{27}$$

(b) Since we know the particle is a superposition of the ground and first excited states, the possible outcomes are $E_1 = \pi^2\hbar^2/2ma^2$ or $E_2 = 4\pi^2\hbar^2/2ma^2$. The probabilities of each outcome are the magnitude of the coefficients $|c_n|^2$, so $P_1 = 4/5$ and $P_2 = 1/5$.

(c) By writing the initial state as a superposition of energy eigenstates $\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$, and remembering that the eigenstates are real and orthonormal (i.e. $\int_{-\infty}^{\infty} \psi_m \psi_n dx = \delta_{mn}$) we can show

$$\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\psi_n(x)\Psi(x,0)dx = \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\psi_n(x)\sum_{m=1}^{\infty}c_m\psi_m(x)dx \tag{28}$$

$$= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}c_m\int_{-\infty}^{\infty}\psi_n(x)\psi_m(x)dx \tag{29}$$

$$= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}c_m\delta_{mn} \tag{30}$$

$$= \sum_{n=1}^{\infty}c_n \tag{31}$$

The last line follows because the Kronecker delta in the sum δ_{mn} is 0 unless $m = n$, so only this single term in the m sum survives.

The quantity is equal to the sum of the expansion coefficients. For the initial state we have been given this is simply

$$\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\psi_n(x)\Psi(x,0)dx = \sqrt{\frac{4}{5}} + \sqrt{\frac{1}{5}} = \frac{3}{\sqrt{5}}. \tag{32}$$

Note that this is *not* the sum of the square magnitude of the coefficients $\sum_n |c_n|^2$ which must equal one by normalisation.

<u>Problem 4.4</u> [FOR ASSIGNMENT 2; max 10 points]

(a) Figure 2 shows a plot of $\Psi(x,0)$ in terms of a and A. To determine A, we can normalise $\Psi(x,0)$. Note that $\Psi(x,0)$ is symmetric about $\frac{a}{2}$.

$$1 = \int_{-\infty}^{\infty}|\Psi(x,0)|^2\ dx \tag{33}$$

$$= 2\int_0^{\frac{a}{2}} A^2x^2\ dx \tag{34}$$

$$= 2A^2\left[\frac{x^3}{3}\right]_0^{\frac{a}{2}} \tag{35}$$

$$\frac{1}{A^2} = \frac{a^3}{12} \tag{36}$$

$$A = \sqrt{\frac{12}{a^3}} \tag{37}$$

(b) The expansion coefficients, c_n, are given by

$$c_n = \int_{-\infty}^{\infty}\psi_n^*(x)\Psi(x,0)\ dx. \tag{38}$$

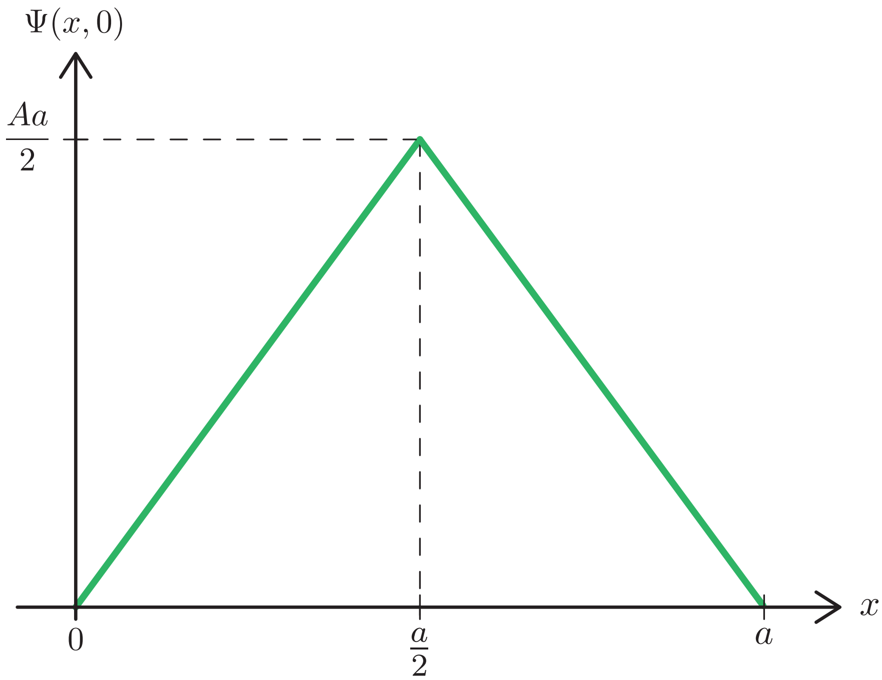

Figure 2: Sketch of $\Psi(x,0)$.

The eigenstates are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right). \tag{39}$$

So we have

$$\begin{aligned} c_n &= \sqrt{\frac{2}{a}}\sqrt{\frac{12}{a^3}}\left(\int_0^{\frac{a}{2}} \sin\left(\frac{n\pi x}{a}\right) x \, dx + \int_{\frac{a}{2}}^{a} \sin\left(\frac{n\pi x}{a}\right)(a-x)\, dx\right) \quad (40) \\ &= \frac{\sqrt{24}}{a^2}\left(\int_0^{\frac{a}{2}} \sin\left(\frac{n\pi x}{a}\right) x \, dx + a\int_{\frac{a}{2}}^{a} \sin\left(\frac{n\pi x}{a}\right)\, dx - \int_{\frac{a}{2}}^{a} \sin\left(\frac{n\pi x}{a}\right) x \, dx\right). \quad (41) \end{aligned}$$

First, do

$$\begin{aligned} \int \sin\left(\frac{n\pi x}{a}\right) x\, dx &= -\frac{a}{n\pi x}\cos\left(\frac{n\pi x}{a}\right) x + \frac{a}{n\pi}\int \cos\left(\frac{n\pi x}{a}\right)\, dx \quad (42) \\ &= -\frac{a}{n\pi}\cos\left(\frac{n\pi x}{a}\right) x + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi x}{a}\right) + C. \quad (43) \end{aligned}$$

Which means

$$\begin{aligned} \int_0^{\frac{a}{2}} \sin\left(\frac{n\pi x}{a}\right) x\, dx &= \left[-\frac{a}{n\pi}\cos\left(\frac{n\pi x}{a}\right) x + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi x}{a}\right)\right]_0^{\frac{a}{2}} \quad (44) \\ &= -\frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right) + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{2}\right) \quad (45) \end{aligned}$$

and

$$\int_{\frac{a}{2}}^{a} \sin\left(\frac{n\pi x}{a}\right) x\ dx = \left[-\frac{a}{n\pi}\cos\left(\frac{n\pi x}{a}\right) x + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi x}{a}\right)\right]_{\frac{a}{2}}^{a} \tag{46}$$

$$= -\frac{a^2}{n\pi}\cos(n\pi) + \left(\frac{a}{n\pi}\right)^2 \sin(n\pi) \tag{47}$$

$$- \left(-\frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right) + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{2}\right)\right) \tag{48}$$

$$= \frac{a^2}{n\pi}\left(\frac{1}{2}\cos\left(\frac{n\pi}{2}\right) - \cos(n\pi)\right) - \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{2}\right). \tag{49}$$

Also

$$a\int_{\frac{a}{2}}^{a} \sin\left(\frac{n\pi x}{a}\right)\ dx = -\frac{a^2}{n\pi}\left[\cos\left(\frac{n\pi x}{a}\right)\right]_{\frac{a}{2}}^{a} \tag{50}$$

$$= -\frac{a^2}{n\pi}\left(\cos(n\pi) - \cos\left(\frac{n\pi}{2}\right)\right). \tag{51}$$

Now, (9) becomes

$$c_n = \frac{\sqrt{24}}{a^2}\Bigg(-\frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right) + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{2}\right) - \frac{a^2}{n\pi}\left(\cos(n\pi) - \cos\left(\frac{n\pi}{2}\right)\right) \tag{52}$$

$$- \frac{a^2}{n\pi}\left(\frac{1}{2}\cos\left(\frac{n\pi}{2}\right) - \cos(n\pi)\right) + \left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{2}\right)\Bigg) \tag{53}$$

$$= \frac{\sqrt{24}}{a^2}\left(2\left(\frac{a}{n\pi}\right)^2 \sin\left(\frac{n\pi}{2}\right)\right) \tag{54}$$

$$= \frac{4\sqrt{6}}{(n\pi)^2}\sin\left(\frac{n\pi}{2}\right). \tag{55}$$

This can be written

$$c_n = \begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{4\sqrt{6}}{(n\pi)^2} & \text{if } n = 1, 5, 9, ... \\ -\frac{4\sqrt{6}}{(n\pi)^2} & \text{if } n = 3, 7, 11, ... \end{cases} \tag{56}$$

(c) When an energy measurement is performed, the wavefunction will collapse into an energy eigenstate with probability $|c_n|^2$. The energy eigenstate with the largest c_n corresponds to $n = 1$. Therefore, the most likely result of an energy measurement is $E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$.

Problem 4.5*

If $\psi(x)$ satisfies the Schrödinger equation, then changing variables $x \to -x$ should work too,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{d(-x)^2} + V(-x)\psi(-x) = E\psi(-x). \tag{57}$$

We are given that V is even, so we know $V(x) = V(-x)$ and its straight forward to show $d^2/d(-x)^2 = d^2/dx^2$ using the chain rule. Putting these together,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(x)\psi(-x) = E\psi(-x). \tag{58}$$

This means that $\psi(-x)$ also satisfies the Schrödinger equation for an even external potential.

To construct an even superposition of $\psi(x)$ and $\psi(-x)$ we require $\psi_+(x) = \psi_+(-x)$. So we can use $\psi_+(x) = \psi(x) + \psi(-x)$. The odd superposition means we have $\psi_-(-x) = -\psi_-(x)$, so we can use $\psi_-(x) = \psi(x) - \psi(-x)$. Adding these odd and even expressions gives $\psi(x) = \frac{1}{2}\left(\psi_+(x) + \psi_-(x)\right)$, so any solution can be expressed as a linear combination of odd and even solutions.