Introduction to Quantum Mechanics: Problem Set 3

1 Derive the expressions for T and R on page 16 of lecture 18.

Solution: We'll solve this problem from scratch, but you can start from the expressions given in Lecture Note 18.

We assume the particle approaches the barrier from the left, so the wavefunction on the left of the barrier will be a superposition of incident and reflected waves whereas the wavefunction on the right of the barrier will only contain the transmitted wave. Note that $E > V_0$, so we expect an oscillatory solution inside the barrier region, not a decaying solution as you would expect for $E < V_0$.

The time-independent Schrödinger equation is

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

$$\frac{d^2\psi(x)}{dx} = \frac{-2mE}{\hbar^2}\psi(x) \qquad \text{outside the barrier region}$$

$$\frac{d^2\psi(x)}{dx} = \frac{-2m(E-V_0)}{\hbar^2}\psi(x) \qquad \text{inside the barrier region}$$

We define $k_1 \equiv \frac{\sqrt{2mE}}{\hbar}$ and $k_2 \equiv \frac{\sqrt{2m(E-V_0)}}{\hbar}$ so that we can rewrite the equations as

$$\frac{d^2\psi(x)}{dx} = -k_1^2\psi(x) \qquad \text{outside the barrier region } (x < 0 \text{ and } x > a)$$

$$\frac{d^2\psi(x)}{dx} = -k_2^2\psi(x) \qquad \text{inside the barrier region } (0 < x < a)$$

These are two second-order ordinary differential equations whose solutions in the three regions $\{x < 0, 0 < x < a, x > a\}$ can be written

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad x < 0$$

$$\psi(x) = Fe^{ik_2x} + Ge^{-ik_2x} \qquad 0 < x < a$$

$$\psi(x) = Ce^{ik_1x} \qquad x > a$$

Notice that for $x > a$ we only make use of the solution that propagates from left to right (positive k_1x), since the only way probability can get into this region is if it was transmitted through the barrier from the left side.

Since the potential is everywhere finite both the wavefunction and its first derivative must be continuous over the steps in the potential at $x = 0$ and $x = a$. This gives us four continuity conditions to satisfy:

At $x = 0$ the condition on continuity of $\psi(x)$ is

$$\begin{aligned} Ae^{ik_1 0} + Be^{-ik_1 0} &= Fe^{ik_2 0} + Ge^{-ik_2 0} \\ A + B &= F + G \end{aligned} \tag{a}$$

and the continuity of $\frac{d\psi(x)}{dx}$ gives

$$\begin{aligned} Aik_1e^{ik_1 0} - Bik_1e^{-ik_1 0} &= Fik_2e^{ik_2 0} - Gik_2e^{-ik_2 0} \\ Ak_1 - Bk_1 &= Fk_2 - Gk_2 \end{aligned} \tag{b}$$

Similarly at $x = a$, continuity in $\psi(x)$ requires

$$Fe^{ik_2 a} + Ge^{-ik_2 a} = Ce^{ik_1 a} \tag{c}$$

and continuity of $\frac{d\psi(x)}{dx}$ requires

$$\begin{aligned} Fik_2e^{ik_2 a} - Gik_2e^{-ik_2 a} &= Cik_1e^{ik_1 a} \\ Fk_2e^{ik_2 a} - Gk_2e^{-ik_2 a} &= Ck_1e^{ik_1 a} \end{aligned} \tag{d}$$

We now have four linear equations for five unknown constants (A, B, C, F, G), so the system is degenerate with an infinite number of linearly dependent solutions (which we expect since we haven't specified normalization). We can use the four equations to eliminate any three of the variables and get a relation in the other two. We want to find the reflection coefficient $R = \frac{|B|^2}{|A|^2}$ and the transmission coefficient $T = \frac{|C|^2}{|A|^2}$, so we'll reduce the equation system to an equation relating B and A and to another relating C and A.

Reflection coefficient We want to eliminate F, G, and C from the equation system. Let's start by combining (a) and (b) to solve for G:

$$\begin{aligned} Ak_1 - Bk_1 &= Fk_2 - Gk_2 \\ Ak_1 - Bk_1 &= (A + B - G)k_2 - Gk_2 \\ Ak_1 - Bk_1 - Ak_2 - Bk_2 &= -2Gk_2 \\ G = A\left(\frac{k_2 - k_1}{2k_2}\right) &+ B\left(\frac{k_2 + k_1}{2k_2}\right) \end{aligned}$$

And we can use this result to solve (a) for F

$$F = A + B - \left[A\left(\frac{k_2 - k_1}{k_2}\right) + B\left(\frac{k_2 + k_1}{k_2}\right)\right]$$

$$F = \frac{1}{2k_2}\left[2Ak_2 - A(k_2 - k_1) + 2Bk_2 - B(k_1 + k_2)\right]$$

$$F = \frac{1}{2k_2}\left[A(k_2 + k_1) + B(k_2 - k_1)\right]$$

$$F = A\left(\frac{k_2 + k_1}{2k_2}\right) + B\left(\frac{k_2 - k_1}{2k_2}\right)$$

So we've eliminated two variables. We can eliminate C by plugging (c) into (d).

$$Fk_2e^{ik_2a} - Gk_2e^{-ik_2a} = k_1\left(Fe^{ik_2a} + Ge^{-ik_2a}\right)$$

$$Fe^{ik_2a}(k_2 - k_1) - Ge^{-ik_2a}(k_2 + k_1) = 0$$

And now we can plug in the solutions for F and G and we'll have an equation in A and B only.

$$\left[A\left(\frac{k_2 + k_1}{2k_2}\right) + B\left(\frac{k_2 - k_1}{2k_2}\right)\right]e^{ik_2a}(k_2 - k_1) -$$

$$\left[A\left(\frac{k_2 - k_1}{2k_2}\right) + B\left(\frac{k_2 + k_1}{2k_2}\right)\right]e^{-ik_2a}(k_2 + k_1) = 0$$

We can now isolate the A and B terms on the two sides of the equation.

$$A\left[e^{ik_2a}\left(\frac{(k_2 + k_1)(k_2 - k_1)}{2k_2}\right) - e^{-ik_2a}\left(\frac{(k_2 - k_1)(k_2 + k_1)}{2k_2}\right)\right] =$$

$$-B\left[e^{ik_2a}\left(\frac{(k_2 - k_1)(k_2 - k_1)}{2k_2}\right) - e^{-ik_2a}\left(\frac{(k_2 + k_1)(k_2 + k_1)}{2k_2}\right)\right]$$

Applying $\sin\phi = (e^{i\phi} - e^{-i\phi})/2i$ and multiplying both sides by $2k_2$ we obtain

$$A(k_2^2 - k_1^2)(2i\sin k_2a) \quad = -B\left[(k_2 - k_1)^2e^{ik_2a} - e^{-ik_2a}(k_2 + k_1)^2\right]$$

Now we take the magnitude squared of each side and arrive at

$$|A|^2(k_2^2 - k_1^2)^2(4\sin^2 k_2a) = |B|^2\left|(k_2 - k_1)^2e^{ik_2a} - e^{-ik_2a}(k_2 + k_1)^2\right|^2$$

Now if we have two complex numbers $A_1e^{i\phi}$ and $A_2e^{-i\phi}$ (with ϕ, A_1

and A_2 real), then

$$\begin{aligned}\left|A_1e^{i\phi} - A_2e^{-i\phi}\right|^2 &= \left(A_1e^{i\phi} - A_2e^{-i\phi}\right)\left(A_1e^{-i\phi} - A_2e^{i\phi}\right) \\ &= A_1^2 - A_1A_2e^{2i\phi} - A_1A_2e^{-2i\phi} + A_2^2 \\ &= A_1^2 - A_1A_2\left(e^{2i\phi} + e^{-2i\phi}\right) + A_2^2 \\ &= A_1^2 + A_2^2 - 2A_1A_2\cos 2\phi \\ &= A_1^2 + A_2^2 - 2A_1A_2(1 - 2\sin^2\phi)\end{aligned}$$

Applying this result to the right side of the equation, we obtain

$$\begin{aligned}&|A|^2(k_2^2 - k_1^2)^2(4\sin^2 k_2a) = \\ &\quad |B|^2\left((k_2 - k_1)^4 + (k_2 + k_1)^4 - 2(k_2 - k_1)^2(k_2 + k_1)^2(1 - 2\sin^2 k_2a)\right) \\ &\quad = |B|^2\left((k_2 - k_1)^4 + (k_2 + k_1)^4 - 2(k_2^2 - k_1^2)^2 + 4(k_2^2 - k_1^2)^2\sin^2 k_2a\right)\end{aligned}$$

Now we need to break up these expressions in k_1 and k_2. Using the binomial theorem, we get $(k_2 + k_1)^4 = k_2^4 + 4k_2^3k_1 + 6k_2^2k_1^2 + 4k_2k_1^3 + k_1^4$ and $(k_2 + k_1)^4 = k_2^4 - 4k_2^3k_1 + 6k_2^2k_1^2 - 4k_2k_1^3 + k_1^4$ so $(k_2 - k_1)^4 + (k_2 + k_1)^4 = 2k_2^4 + 12k_2^2k_1^2 + 2k_1^4$. Also, $(k_2^2 - k_1^2)^2 = k_2^4 - 2k_1^2k_2^2 + k_1^2$, so $(k_2 - k_1)^4 + (k_2 + k_1)^4 - 2(k_2^2 - k_1^2)^2 = 16k_1^2k_2^2$. The expression therefore simplifies to

$$\begin{aligned}|A|^2(k_2^2 - k_1^2)^2(4\sin^2 k_2a) &= |B|^2\left(16k_1^2k_2^2 + 4(k_2^2 - k_1^2)^2\sin^2 k_2a\right) \\ |A|^2(k_2^2 - k_1^2)^2\sin^2 k_2a &= |B|^2\left(4k_1^2k_2^2 + (k_2^2 - k_1^2)^2\sin^2 k_2a\right)\end{aligned}$$

So

$$\begin{aligned}R = \frac{|B|^2}{|A|^2} &= \left[\frac{\left(4k_1^2k_2^2 + (k_2^2 - k_1^2)^2\sin^2 k_2a\right)}{(k_2^2 - k_1^2)^2\sin^2 k_2a}\right]^{-1} \\ &= \left[1 + \frac{4k_1^2k_2^2}{(k_2^2 - k_1^2)^2\sin^2 k_2a}\right]^{-1}\end{aligned}$$

Now we can substitute in the original definitions $k_1 = \frac{\sqrt{2mE}}{\hbar^2}$ and $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar^2}$

$$
\begin{aligned}
R &= \left[1 + \frac{4k_1^2 k_2^2}{(k_2^2 - k_1^2)^2 \sin^2 k_2 a}\right]^{-1} \\
&= \left[1 + \frac{4\frac{2mE}{\hbar^2}\frac{2m(E-V_0)}{\hbar^2}}{(\frac{2m(E-V_0)}{\hbar^2} - \frac{2mE}{\hbar^2})^2 \sin^2 k_2 a}\right]^{-1} \\
&= \left[1 + \frac{4E(E-V_0)}{(-V_0)^2 \sin^2 k_2 a}\right]^{-1} \\
&= \left[1 + \frac{4E(E-V_0)}{V_0^2 \sin^2 k_2 a}\right]^{-1}
\end{aligned}
$$

Which is the desired result.

Transmission Coefficient: Now we have to calculate T. The easy way to do this is to argue that on physical grounds we need to have an equal amount of probability approaching the barrier as leaving it. From the left the probability flow towards the barrier is $|A|^2 k_1$ and away from the barrier is $|B|^2 k_1$. On the right of the barrier the probability flow away from the barrier is $|C|^2 k_1$. Probability flow into the barrier equals probability flow out, so

$$
|A|^2 k_1 = |B|^2 k_1 + |C|^2 k_1
$$

Dividing both sides by $|A|^2 k_1$ we have

$$
\begin{aligned}
\frac{|B|^2}{|A|^2} + \frac{|C|^2}{|B|^2} &= 1 \\
R + T &= 1
\end{aligned}
$$

Plugging the derived expression for R into $T = 1 - R$,

$$\begin{aligned}
T &= 1 - \left[1 + \frac{4E(E-V_0)}{V_0^2 \sin^2 k_2 a}\right]^{-1} \\
&= 1 - \left[\frac{V_0^2 \sin^2 k_2 a + 4E(E-V_0)}{V_0^2 \sin^2 k_2 a}\right]^{-1} \\
&= 1 - \left[\frac{V_0^2 \sin^2 k_2 a}{V_0^2 \sin^2 k_2 a + 4E(E-V_0)}\right] \\
&= \left[\frac{V_0^2 \sin^2 k_2 a + 4E(E-V_0) - V_0^2 \sin^2 k_2 a}{V_0^2 \sin^2 k_2 a + 4E(E-V_0)}\right] \\
&= \left[\frac{4E(E-V_0)}{V_0^2 \sin^2 k_2 a + 4E(E-V_0)}\right] \\
&= \left[\frac{V_0^2 \sin^2 k_2 a + 4E(E-V_0)}{4E(E-V_0)}\right]^{-1} \\
&= \left[1 + \frac{V_0^2 \sin^2 k_2 a}{4E(E-V_0)}\right]^{-1}
\end{aligned}$$

As required.

The hard way is to prove the result is to go through the derivation for R, but solving the equation system to eliminate F, G and B instead.

We can add (c) to (d)$\div k_2$ to eliminate G

$$\begin{aligned}
2Fe^{ik_2a} &= Ce^{ik_1a}\left(1 + \frac{k_1}{k_2}\right) \\
F &= Ce^{i(k_1-k_2)a}\left(\frac{k_2+k_1}{2k_2}\right)
\end{aligned}$$

Similarly, we can take the difference of (c) and (d)$\div k_2$ to obtain

$$\begin{aligned}
2Ge^{-ik_2a} &= Ce^{ik_1a}\left(1 - \frac{k_1}{k_2}\right) \\
G &= Ce^{i(k_1+k_2)a}\left(\frac{k_2-k_1}{2k2}\right)
\end{aligned}$$

We can use (a) to eliminate B from (b)

$$\begin{aligned}
Ak_1 - (F+G-A)k_1 &= Fk_2 - Gk_2 \\
2Ak_1 - F(k_2+k_1) + G(k_2-k_1) &= 0
\end{aligned}$$

And substitute the solutions just obtained for G and F in terms of C

$$2Ak_1 - Ce^{i(k_1-k_2)a}\left(\frac{k_2+k_1}{2k_2}\right)(k_2+k_1) + Ce^{i(k_1+k_2)a}\left(\frac{k_2-k_1}{2k_2}\right)(k_2-k_1) = 0$$

$$2Ak_1 = Ce^{ik_1a}\left[e^{-ik_2a}\left(\frac{(k_2+k_1)^2}{2k_2}\right) - e^{ik_2a}\left(\frac{(k_2-k_1)^2}{2k_2}\right)\right]$$

Taking the magnitude squared of this we get

$$4|A|^2k_1^2 = |C|^2\left|e^{-ik_2a}\left(\frac{(k_2+k_1)^2}{2k_2}\right) - e^{ik_2a}\left(\frac{(k_2-k_1)^2}{2k_2}\right)\right|^2$$

$$= |C|^2\left[\left(\frac{(k_1^2+k_2^2)^2}{2k_2}\right)^2 + \left(\frac{(k_1-k_2)^2}{2k_2}\right)^2 - 2\left(1-2\sin^2 k_2a\right)\left(\frac{(k_1^2+k_2^2)^2(k_1^2-k_2^2)^2}{(2k_2)^2}\right)\right]$$

Using our binomial expansions in k_1 and k_2 we get

$$16|A|^2k_1^2k_2^2 = |C|^2\left[16k_1^2k_2^2 + 4\sin^2 k_2a(k_1^2-k_2^2)^2\right]$$

$$4|A|^2k_1^2k_2^2 = |C|^2\left[4k_1^2k_2^2 + \sin^2 k_2a(k_1^2-k_2^2)^2\right]$$

So that

$$T = \frac{|C|^2}{|A|^2} = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 + \sin^2 k_2a(k_1^2-k_2^2)^2}$$

Substituting in $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-V_0}}{\hbar}$ gives

$$T = \frac{4\frac{2mE}{\hbar^2}\frac{2m(E-V_0)}{\hbar^2}}{4(\frac{2mE}{\hbar^2}\frac{2m(E-V_0)}{\hbar^2}) + \sin^2 k_2a(\frac{2mE}{\hbar^2} - \frac{2m(E-V_0)}{\hbar^2})^2}$$

$$T = \frac{4E(E-V_0)}{4E(E-V_0) + \sin^2 k_2a\left(E-(E-V_0)\right)^2}$$

$$T = \left[\frac{4E(E-V_0) + V_0^2\sin^2 k_2a}{4E(E-V_0)}\right]^{-1}$$

$$T = \left[1 + \frac{V_0^2\sin^2 k_2a}{4E(E-V_0)}\right]^{-1}$$

As required.

2 A particle in an infinite square well is in the ground state of the system. The well has walls at $x = a$ and $x = -a$ if we move the walls instantaneously to $x = 2a$ and $x = -2a$, what is the probability of finding the particle in the ground state of the new system?

Solution: Initially the particle is in the ground state of the smaller well. The expression for the states of this well are given in the textbook on page 158. Notice that they are different than those given in the notes since the well runs from $-a$ to a rather than from 0 to a. Notably the ground state of the well is a cosine rather than a sine function.

$$\begin{aligned}
\psi_0(x) &= \sqrt{\frac{1}{a}} \cos \frac{\pi x}{2a} && -a < x < a \\
&= 0 && \text{elsewhere}
\end{aligned}$$

After the walls of the well have moved the eigenfunctions of the new well are

$$\begin{aligned}
\phi_n(x) &= \sqrt{\frac{1}{2a}} \cos \frac{\pi n x}{4a} && -a < x < a \\
&= 0 && \text{elsewhere}
\end{aligned}$$

$\psi_0(x)$ could be expanded in the eigenfunctions of the new well as

$$\psi_0(x) = \sum_n A_n \phi_n(x)$$

where

$$A_n = \int_{-2a}^{2a} \psi_0(x) \phi_n(x) \mathrm{d}x$$

The probability of finding the particle in state $\psi_0(x)$ to be in the n^{th} eigenstate is $|A_n|^2$. In particular, the probability of finding the particle to be in the ground state is $|A_1|^2$, and

$$\begin{aligned}
A_1 &= \sqrt{\frac{1}{2a}} \int_{-2a}^{2a} \psi_0(x) \cos \frac{\pi x}{4a} \mathrm{d}x \\
&= \sqrt{\frac{1}{2a}} \sqrt{\frac{1}{a}} \int_{-a}^{a} \cos \frac{\pi x}{2a} \cos \frac{\pi x}{4a} \mathrm{d}x
\end{aligned}$$

Where we've reduced the range of integration since $\psi_0(x)$ is zero except over $\{-a, a\}$.

We can apply the trig identity $\cos a \cos b = \frac{1}{2} \left(\cos\left(a+b\right) + \cos\left(a-b\right) \right)$

to obtain

$$\begin{aligned}
A_1 &= \frac{1}{2\sqrt{2}a}\int_{-a}^{a}\left(\cos\frac{3\pi x}{4a}+\cos\frac{3\pi x}{4a}\right)\mathrm{d}x \\
&= \frac{1}{2\sqrt{2}a}\left[\frac{4a}{3\pi}\sin\frac{3\pi x}{4a}+\frac{4a}{\pi}\sin\frac{\pi x}{4a}\right]_{x=-a}^{x=a} \\
&= \frac{\sqrt{2}}{\pi}\left[\frac{1}{3}\left(\sin\frac{3\pi}{4}-\sin\frac{-3\pi}{4}\right)+\left(\sin\frac{\pi}{4}-\sin\frac{-\pi}{4}\right)\right] \\
&= \frac{\sqrt{2}}{\pi}\left[\frac{\sqrt{2}}{3}+\sqrt{2}\right] \\
&= \frac{8}{3\pi}
\end{aligned}$$

So $|A_1|^2 = 64/(9\pi^2) \approx 0.72$.

There is a 72% probability of finding the particle in the ground state of the well after the walls are moved.

4 A particle is in an infinite square with walls at $x = 0$, $x = a$. Calculate:

(a) $\langle \mathbf{x}_n \rangle$, $\langle \mathbf{p}_n \rangle$, $\langle \mathbf{x}_n^2 \rangle$, and $\langle \mathbf{p}_n^2 \rangle$.

(b) Calculate $\Delta x_n \Delta p_n$ $\left(\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}\right)$

(c) Estimate the ground state energy using the result above. Compare to the result we obtained

Solution:

(a) These are just a bunch of integrals that need to be crunched through. The n subscript implies that we are looking for the expectation values for the energy eigenstates given in the notes, namely:

$$\phi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{\pi n x}{a}$$

Notice that the functions are different than in the previous problem because the well runs from 0 to a rather than from $-a$ to a.

The expectation value for an operator $\mathbf{A}$ in the state $\psi(x)$ is defined to be

$$\langle \mathbf{A} \rangle = \int \psi^*(x)\mathbf{A}\psi(x)\mathrm{d}x$$

The operators we need are $\mathbf{x} = x$, $\mathbf{p} = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}$, $\mathbf{x^2} = x^2$ and $\mathbf{p}^2 = -\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}^2x}$. These can all be found in chapter 3 of the text. So let's rock some integrals!

$$
\begin{aligned}
\langle \mathbf{x}_n \rangle &= \frac{2}{a}\int_0^a \sin\frac{\pi n x}{a} x \sin\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{2}{a}\int_0^a x\sin^2\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{2}{a}\int_0^a \frac{x}{2}\left(1-\cos\frac{2\pi n x}{a}\right)\mathrm{d}x \\
&= \frac{1}{a}\int_0^a x\mathrm{d}x - \frac{1}{a}\int_0^a x\cos\frac{2\pi n x}{a}\mathrm{d}x \\
&= \frac{1}{a}\frac{x^2}{2}\bigg|_0^a - \frac{1}{a}\left(\frac{xa}{2\pi n}\sin\frac{2\pi n x}{a}\bigg|_0^a - \frac{a}{2\pi n}\int_0^a \sin\frac{2\pi n x}{a}\mathrm{d}x\right) \\
&= \frac{a}{2} - \left(0 - \frac{1}{2\pi n}\frac{a}{2\pi n}\cos\frac{2\pi n x}{a}\bigg|_0^a\right) \\
&= \frac{a}{2} + \frac{a}{(2\pi n)^2}\left(\cos 2\pi n - 1\right)
\end{aligned}
$$

(I integrated by parts to get the fifth line)

But n is an integer, so $\cos 2\pi n = 1$, the second term vanishes and we're left with $\langle \mathbf{x}_n \rangle = a/2$. The average position of a particle in the well is the centre of the well. Not too surprising. Onwards!

$$
\begin{aligned}
\langle \mathbf{p}_n \rangle &= \frac{2}{a}\int_0^a \sin\frac{\pi n x}{a}\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\sin\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{-2i\hbar}{a}\int_0^a \sin\frac{\pi n x}{a}\left(\frac{\pi n}{a}\cos\frac{\pi n x}{a}\right)\mathrm{d}x \\
&= \frac{-2i\hbar\pi n}{a^2}\int_0^a \sin\frac{\pi n x}{a}\cos\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{-2i\hbar\pi n}{a^2}\int_0^a \frac{1}{2}\sin\frac{2\pi n x}{a}\mathrm{d}x \\
&= \frac{-i\hbar\pi n}{a^2}\left[-\frac{a}{2\pi n}\cos\frac{2\pi n x}{a}\right]_0^a \\
&= \frac{i\hbar}{2a}\left[\cos 2\pi n - 1\right]
\end{aligned}
$$

Again $\cos 2\pi n = 1$, so $\langle \mathbf{p}_n \rangle = 0$. This completely makes sense. If the particle is trapped in the well then by definition it isn't moving anywhere so its average momentum must be zero.

$$
\begin{aligned}
\left\langle \mathbf{x}_n^2 \right\rangle &= \frac{2}{a}\int_0^a \sin\frac{\pi n x}{a} x^2 \sin\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{2}{a}\int_0^a x^2 \sin^2\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{1}{a}\int_0^a x^2 \left(1-\cos\frac{2\pi n x}{a}\right)\mathrm{d}x \\
&= \frac{1}{a}\int_0^a x^2\mathrm{d}x - \frac{1}{a}\int_0^a x^2\cos\frac{2\pi n x}{a}\mathrm{d}x \\
&= \frac{1}{a}\frac{x^3}{3}\bigg|_0^a - \frac{1}{a}\left(\frac{x^2 a}{2\pi n}\sin\frac{2\pi n x}{a}\bigg|_0^a - \frac{a}{2\pi n}\int_0^a (2x)\sin\frac{2\pi n x}{a}\mathrm{d}x\right) \\
&= \frac{a^2}{3} - \left(0 - \frac{1}{\pi n}\int_0^a x\sin\frac{2\pi n x}{a}\mathrm{d}x\right) \\
&= \frac{a^2}{3} + \frac{1}{\pi n}\left(\frac{-xa}{2\pi n}\cos\frac{2\pi n x}{a}\bigg|_0^a - \frac{-a}{2\pi n}\int_0^a \cos\frac{2\pi n x}{a}\mathrm{d}x\right) \\
&= \frac{a^2}{3} + \frac{1}{\pi n}\left(\left(\frac{-a^2}{2\pi n}\cos\frac{2\pi n}{a} - 0\right) + \frac{a^2}{(2\pi n)^2}\sin\frac{2\pi n x}{a}\bigg|_0^a\right) \\
&= \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2} \\
&= a^2\left(\frac{1}{3} - \frac{1}{2\pi^2 n^2}\right)
\end{aligned}
$$

And finally...

$$
\begin{aligned}
\left\langle \mathbf{p}_n^2 \right\rangle &= \frac{2}{a}\int_0^a \sin\frac{\pi n x}{a}\left(-\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}^2 x}\right)\sin\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{-2\hbar^2}{a}\int_0^a \sin\frac{\pi n x}{a}\left(-\frac{\pi^2 n^2}{a^2}\sin\frac{\pi n x}{a}\right)\mathrm{d}x \\
&= \frac{2\hbar^2\pi^2 n^2}{a^3}\int_0^a \sin^2\frac{\pi n x}{a}\mathrm{d}x \\
&= \frac{\hbar^2\pi^2 n^2}{a^3}\int_0^a \left(1-\cos\frac{2\pi n x}{a}\right)\mathrm{d}x \\
&= \frac{\hbar^2\pi^2 n^2}{a^3}\left(\int_0^a \mathrm{d}x - \int_0^a \cos\frac{2\pi n x}{a}\mathrm{d}x\right) \\
&= \frac{\hbar^2\pi^2 n^2}{a^3}\left(a - \frac{a}{2\pi n}\sin\frac{2\pi n x}{a}\bigg|_0^a\right) \\
&= \frac{\hbar^2\pi^2 n^2}{a^3}(a-0) \\
&= \frac{\hbar^2\pi^2 n^2}{a^2}
\end{aligned}
$$

Both these expressions have the right units. The only scale given in the problem is the length scale given by the width of the well a. All momenta should therefore be proportional to $\hbar/a$.

(b) Let's find the uncertainties:

$$\begin{aligned}
\Delta x &= \sqrt{\langle \mathbf{x}_n^2 \rangle - \langle \mathbf{x}_n \rangle^2} \\
&= \sqrt{a^2 \left(\frac{1}{3} - \frac{1}{2\pi^2 n^2} \right) - \frac{a^2}{4}} \\
&= a\sqrt{\frac{1}{12} - \frac{1}{2\pi^2 n^2}}
\end{aligned}$$

And

$$\begin{aligned}
\Delta p &= \sqrt{\langle \mathbf{p}_n^2 \rangle - \langle \mathbf{p}_n \rangle^2} \\
&= \sqrt{\frac{\hbar^2 \pi^2 n^2}{a^2} - 0} \\
&= \frac{\hbar \pi n}{a}
\end{aligned}$$

So

$$\begin{aligned}
\Delta x \Delta p &= \hbar \pi n \sqrt{\frac{1}{12} - \frac{1}{2\pi^2 n^2}} \\
&= \hbar \sqrt{\frac{\pi^2 n^2}{12} - \frac{1}{2}}
\end{aligned}$$

By Heisenberg's principle the uncertainty product $\Delta x \Delta p$ must always be greater than or equal to $\hbar/2$. It's apparent that the minimum uncertainty product is minimal when $n = 1$ and then $\Delta x \Delta p \approx 0.57$, so the result seems reasonable.

(c) For trapped particles there is a relation between the momentum uncertainty and the expectation value of the energy.

$$\begin{aligned}
\langle E \rangle &= \left\langle \frac{p^2}{2m} \right\rangle \\
\langle E \rangle &= \frac{\langle p^2 \rangle}{2m} \\
\langle E \rangle &= \frac{\Delta p^2 + \langle p \rangle^2}{2m} \\
\langle E \rangle &= \frac{\Delta p^2}{2m}
\end{aligned}$$

From the result of part (b), we have $\Delta p = 0.57\hbar/\Delta x$ in the ground state. The width of the in the ground state is $\Delta x \approx 0.18a$.

$$\langle E \rangle \approx \frac{0.57^2 \hbar^2}{2m\Delta\left(0.18^2 x^2\right)}$$
$$\langle E \rangle \approx 5.0 \frac{\hbar^2}{2ma^2}$$

The exact solution is

$$E_n \approx \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$
$$E_1 \approx 4.9 \frac{\hbar^2}{ma^2}$$

So our approximation is good.

This question is somewhat vague, so any reasonable use of the uncertainty principle to estimate energy is good for full marks.