

Modern Physics II - HW2 Solution - Winter 2016

1. a) A quantum mechanical particle is confined to a one-dimensional infinitely-deep square-potential well (of length L). Assume the particle is in its second excited state. Calculate the probabilities of finding this particle within $\pm 1/1000 L$ segments (of L) that are centered around the positions $x = 1/6 L$ and $x = 1/3 L$ (2 points).

Using the same procedure as in HW1 problem 2(a) beginning with the normalized wave function for our trapped particle and technique for calculating the probability of it being within some specified range:

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad \text{and} \quad P_{n_{ab}} = \int_a^b \Psi_n^*(x) \Psi_n(x) dx$$

The general calculation of probability over some interval for the second excited state ($n=3$):

$$\begin{aligned} P_{3_{ab}} &= \frac{2}{L} \int_a^b \sin^2\left(\frac{3\pi x}{L}\right) dx \\ &= \frac{2}{L} \int_a^b \frac{1}{2} \left(1 - \cos\left(\frac{6\pi x}{L}\right)\right) dx, \text{ trig identity } \sin^2(\alpha x) = \frac{1}{2}(1 - \cos(2\alpha x)) \\ &= \frac{1}{L} \left[x - \frac{L}{6\pi} \sin\left(\frac{6\pi x}{L}\right) \right]_a^b \end{aligned}$$

Now plugging in the intervals in question:

$$\begin{aligned} P_{3_{\frac{L}{6} \pm \frac{L}{1000}}} &= \frac{1}{L} \left[x - \frac{L}{6\pi} \sin\left(\frac{6\pi x}{L}\right) \right]_{\frac{L}{6} - \frac{L}{1000}}^{\frac{L}{6} + \frac{L}{1000}} \\ &= \frac{2}{1000} - \frac{1}{6\pi} \sin\left(\pi + \frac{6\pi}{1000}\right) + \frac{1}{6\pi} \sin\left(\pi - \frac{6\pi}{1000}\right) \\ &\approx 0.40\% \end{aligned}$$

$$\begin{aligned} P_{3_{\frac{L}{3} \pm \frac{L}{1000}}} &= \frac{1}{L} \left[x - \frac{L}{6\pi} \sin\left(\frac{6\pi x}{L}\right) \right]_{\frac{L}{3} - \frac{L}{1000}}^{\frac{L}{3} + \frac{L}{1000}} \\ &= \frac{2}{1000} - \frac{1}{6\pi} \sin\left(2\pi + \frac{6\pi}{1000}\right) + \frac{1}{6\pi} \sin\left(2\pi - \frac{6\pi}{1000}\right) \\ &\approx 0.000012\% \end{aligned}$$

Understandably the probability of the particle being in the region around $L/3$ is tiny since this is centered on a null.

b) Now assume that this particle is in its ground state. Calculate an approximate value for finding this particle within a $1/100 L$ segment that is centered on $x = 5/8 L$ on the basis of the local probability density. Give a numerical measure of the goodness of your approximation by comparing your approximate result with the exact result (2 points).

Same deal as before except we want to do an approximation, since the region is fairly small and the probability density isn't changing particularly fast we can use a small angle approximation to linearize the term.

$$\begin{aligned}
 P_{lab} &= \frac{2}{L} \int_a^b \sin^2\left(\frac{\pi x}{L}\right) dx \\
 &\approx \frac{2}{L} \int_a^b \sin^2\left(\frac{\pi(a+b)}{2L}\right) dx \\
 &\approx \frac{2}{L} \sin^2\left(\frac{\pi(a+b)}{2L}\right) x \Big|_a^b \\
 &\approx \frac{2}{L} \sin^2\left(\frac{\pi m_{\text{point}}}{L}\right) \Delta x, \quad m_{\text{point}} \text{ being the middle of the integration range}
 \end{aligned}$$

Evaluating for our condition we have:

$$\begin{aligned}
 P_{\frac{5L}{8} \pm \frac{L}{200}} &\approx \frac{2}{L} \sin^2\left(\frac{5\pi}{8}\right) x \Big|_{\frac{5L}{8} - \frac{L}{200}}^{\frac{5L}{8} + \frac{L}{200}} \\
 &\approx 2 \sin^2\left(\frac{5\pi}{8}\right) \frac{1}{100} \\
 &\approx 1.70711\%
 \end{aligned}$$

Comparing to the exact solution:

$$\begin{aligned}
 P_{\frac{5L}{8} \pm \frac{L}{200}} &= \frac{1}{L} \left[x - \frac{L}{2\pi} \sin\left(\frac{2\pi x}{L}\right) \right] \Big|_{\frac{5L}{8} - \frac{L}{200}}^{\frac{5L}{8} + \frac{L}{200}} \\
 &= \frac{1}{100} - \frac{1}{2\pi} \sin\left(\frac{5\pi}{4} + \frac{2\pi}{200}\right) + \frac{1}{2\pi} \sin\left(\frac{5\pi}{4} - \frac{2\pi}{200}\right) \\
 &\approx 1.70699\%
 \end{aligned}$$

Which appears to have a good agreement between the approximation and exact solution, comparing directly we have:

$$\frac{\left| P_{\frac{5L}{8} \pm \frac{L}{200}}^{\text{exact}} - P_{\frac{5L}{8} \pm \frac{L}{200}}^{\text{approx}} \right|}{P_{\frac{5L}{8} \pm \frac{L}{200}}^{\text{exact}}} \cdot 100\% \approx 0.0068\%$$

For most circumstances this would be considered a perfectly acceptable amount of error.

Would using your approximation still be justifiable if the segments were either $1/10 L$ or $3/8 L$ wide? (1 point)

Intuitively $1/10 L$ should still be reasonably ok but $3/8 L$ would likely have a large disagreement since the small angle approximation is only ok for less than a radian (unless large errors are ok). Since this is the square of sine we should expect error to accumulate faster, such that after a radian we would have a fairly significant error. For the ground state we should be covering about 0.3 radians in $1/10 L$ and about 1.2 radians in $3/8 L$. In order to confirm this suspicion we should check the approximate values for these widths:

$$P_{1\text{approx}_{\frac{5L}{8} \pm \frac{L}{20}}} \approx 17.071\% \qquad P_{1\text{exact}_{\frac{5L}{8} \pm \frac{L}{20}}} \approx 16.955\%$$

$$P_{1\text{approx}_{\frac{5L}{8} \pm \frac{3L}{16}}} \approx 64.017\% \qquad P_{1\text{exact}_{\frac{5L}{8} \pm \frac{3L}{16}}} \approx 58.295\%$$

This indicates that $1/10 L$ is still a reasonable approximation using small angle on the ground state, but not so good for $3/8 L$.

2. A wav-icle (wave-particle-duality thingy) is confined to be in a very small but finite region of one dimensional space. (Interpret the confinement as the existence of walls that this thingy is never able to penetrate or overcome, while it is able to move in its allotted region of space freely.) Last week you calculated the expectation value of position (x) and its spread (Δx) for the first excited state of that thingy.

(a) To complement your considerations, calculate now the expectation value for the momentum (p) and its spread (Δp) for the same state. (2 points)

Same deal as before, particle in ideal box. Starting with the same excited state as last week ($n=2$) we just need to apply the momentum operator instead of the position operator.

$$\begin{aligned} \langle p \rangle_2 &= \int_{-\infty}^{\infty} \Psi_2^*(x) \hat{p} \Psi_2(x) dx \\ &= \frac{2}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \frac{\hbar}{i} \frac{\partial}{\partial x} \sin\left(\frac{2\pi x}{L}\right) dx \\ &= \frac{2}{L} \frac{\hbar}{i} \frac{2\pi}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi x}{L}\right) dx \\ &= \frac{\hbar}{i} \frac{4\pi}{L^2} \int_0^L \frac{1}{2} \sin\left(\frac{4\pi x}{L}\right) dx \\ &= 0 \end{aligned}$$

Zero due to integration of integral number of rotations of a sine function. Makes sense though, it seems likely that the particle would have an equal probability of going to the left and the right so the average

momentum would be equal to zero. To find the spread we need to first find the expectation of the momentum operator squared:

$$\begin{aligned}
 \langle p^2 \rangle_2 &= \int_{-\infty}^{\infty} \Psi_2^*(x) \hat{p}^2 \Psi_2(x) dx \\
 &= \frac{2}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) \frac{\hbar^2}{i^2} \frac{\partial^2}{\partial x^2} \sin\left(\frac{2\pi x}{L}\right) dx \\
 &= \frac{2\hbar^2}{L} \left(\frac{2\pi}{L}\right)^2 \int_0^L \sin^2\left(\frac{2\pi x}{L}\right) dx \\
 &= \frac{8\pi^2 \hbar^2}{L^3} \int_0^L \frac{1}{2} \left[1 - \cos\left(\frac{4\pi x}{L}\right)\right] dx \\
 &= \frac{4\pi^2 \hbar^2}{L^3} \left[x - \frac{L}{4\pi} \sin\left(\frac{4\pi x}{L}\right) \right]_0^L \\
 &= \frac{4\pi^2 \hbar^2}{L^2}
 \end{aligned}$$

Now to calculate the spread:

$$\begin{aligned}
 \Delta p_2 &= \sqrt{\langle p^2 \rangle_2 - \langle p \rangle_2^2} \\
 &= \sqrt{\frac{4\pi^2 \hbar^2}{L^2} - 0} \\
 &= \frac{2\pi \hbar}{L}
 \end{aligned}$$

Calculate the product of the two spreads ($\Delta x \Delta p$) (1 point) and relate it to Heisenberg's uncertainty principle (1 point). (Relating means in this context: does your product obey or violate (in both a numerical and conceptual sense) Heisenberg's principle?)

Taking the position spread from the last homework and using it with our result in the uncertainty principle:

$$\Delta x_2 \Delta p_2 \geq \frac{\hbar}{2}$$

$$\sqrt{\frac{L^2}{3} - \frac{L^2}{8\pi^2} - \frac{L^2}{4}} \frac{2\pi\hbar}{L} \approx 0.2658L \frac{2\pi\hbar}{L} \\ \approx 1.67\hbar$$

$$1.67\hbar > \frac{\hbar}{2}$$

In both senses it obeys the uncertainty principle. Numerically this is obvious but conceptually as well because as L shrinks we become more certain about the location of the particle by reasoning if the box is smaller and we know the particle is in the box that we know the location of the particle with a higher resolution. This comes at a cost though because the spread in the momentum increases as we shrink the box (things with shorter wavelengths have more energy). So by inspection these inverse relationships cancel so we are left with a constant amount of uncertainty that is greater than $\hbar / 2$ for all values of L in this energy state.

(b) While the thingy remains in this state, will the expectation values of the square of momentum, kinetic energy, and total energy all be sharp? 1 point

Yes. To show it we need to ensure the operators on our function produce an eigenvalue, but by inspection it should be fairly obvious they will. The condition to meet for sharpness is:

$$\hat{A}\Psi = \lambda\Psi$$

, where \hat{A} is our operator, Ψ the function, and λ the eigenvalue.

Assuming Ψ is an eigenfunction to the operator in question it will produce an eigenvalue. Alternatively you could run the spread calculation and ensure it is zero, but a single eigenvalue is sufficient and easier to show.

Now for the function in question:

$$\Psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

So any second derivative with respect to position will produce a constant times the original function, which is what we are looking for. The square of the momentum operator is:

$$\begin{aligned}\hat{p}^2 &= \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) = -\hbar^2 \frac{\partial^2}{\partial x^2} \\ \hat{p}^2 \Psi_2 &= -\hbar^2 \frac{\partial^2}{\partial x^2} \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) \\ &= \hbar^2 \sqrt{\frac{2}{L}} \left(\frac{2\pi}{L}\right)^2 \sin\left(\frac{2\pi x}{L}\right) \\ &= \frac{4\pi^2 \hbar^2}{L^2} \Psi_2\end{aligned}$$

This meets our condition for sharpness. Kinetic energy operator is obviously sharp following this because it is defined as:

$$\hat{K} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Which is just the momentum operator squared over twice the mass, by similarity to the momentum operator squared this is also sharp. To handle total energy we will use its relation to kinetic energy and the definition of the system to avoid the ambiguousness of the trivial solution because this function does not depend on time (energy operator is a time derivative). We know that:

$$E = K + U$$

, the total energy is equal to the sum of the kinetic energy and the potential energy.

But we also originally defined the bottom of our well to be at zero potential therefore potential energy is always zero. Since the kinetic energy is sharp, then the total energy is also sharp since the addition of zero does not change this.