Homework 10

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1. (4 pts) A particle is confined between rigid walls it cannot penetrate separated by a distance $L = 0.189$ nm. The particle is in the second excited state. Evaluate the probability to find the particle in an interval of width 1.00 pm at $x = 0.188$ nm.

Solution:

This is an infinite square well problem:

Because potential is infinite, the probability of the particle being in region I or III is zero. Therefore, the wave equation is:

Piecewise regions & potentials:

$$\begin{aligned} I:&\quad x<0 &\quad u=\infty\\ II:&\quad 0\le x\le L &\quad u=0\\ III:&\quad x>L &\quad u=\infty \end{aligned}$$

$$-\frac{\hbar}{2m}\frac{\partial^2\psi_{II}(x)}{\partial x^2} = E\psi_{II}(x) \to \psi'' + k^2\psi = 0 \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$r^2 + k^2 = 0 \implies r = i \pm k$$

Therefore the general solution is:

$$\psi_{II}(x) = A\sin(kx) + B\cos(kx)$$

(a) Continuity condition:

$$\begin{aligned} \psi_{II}(0) = \psi_I(0) &\to B\xcancel{\cos(0)}^{1} = 0\\ &\implies B = 0\\ \psi_{II}(L) = \psi_{III}(L) &\to A\sin(kx) = 0\\ &\implies A = 0 \text{ or } kL = n\pi \end{aligned}$$

(b) Normalization Condition:
Because $|\psi_n(x)|^2$ is the PDF of the position of the particle:

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\psi_n(x)|^2\, dx \to \int_0^L \psi_n(x)\, dx\\ &= \int_0^L |A|^2 \sin^2\left(\frac{n\pi x}{L}\right)\, dx\\ &= A^2\frac{L}{2} \implies A = \sqrt{\frac{2}{L}} \end{aligned}$$

Therefore, our final wave equation is: $\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$. To evaluate the given probability:

$$\int_{0.188\text{nm}-\frac{1}{2}\text{pm}}^{0.188\text{nm}+\frac{1}{2}\text{pm}} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\, dx = 0.0357\%$$

2. Consider a Gaussian wavefunction: $\psi(x) = A\exp\{-a(x-\mu)^2\}$, where $a > 0$.

   (a) (4 pts) Find the normalization factor A in terms of μ and a. (You can look up integration of Gaussian's an quote the results)

Solution: (Polar Transformation)

$$\psi = \int_{-\infty}^{\infty} \exp(-a(x-\mu)^2)\ dx \to \int_{-\infty}^{\infty} \exp(-a(u)^2)\ dx \tag{1}$$

Transformation (1) has a jacobian of one, which should make sense since $x - \mu$ does not scale the function. Now, we can temporarily square ψ to convert to polar coordinates.

$$\psi^2 = \int_{-\infty}^{\infty} \exp(-a(u^2+v^2))\ dx \to \int_0^{2\pi}\int_0^{\infty} \rho\exp(-a\rho^2)\ d\rho\ d\theta$$

Finally, a substitution of $a\rho^2 = w$ allows the integral to be solved to completion:

$$\begin{aligned}\psi^2 &= \frac{\cancel{2}\pi}{\cancel{2}a}\int_0^{\infty} e^{-w}\ dx \\ &= \frac{\pi}{a}\left(-e^{-w}\big|_0^{\infty}\right) \\ &= \sqrt{\frac{\pi}{a}}\end{aligned}$$

(This is the scale factor, so the inverse of this is the normalization factor A). Plotting the normalized wavefunction again shows that μ has no effect on the scale of the function, so it is normalized for all μ.

   (b) (4 pts) What is the probability that $x < \mu$?

Solution:
μ represents the location of the center of the wave function for all μ. Because the wave function is a (symmetrical) gaussian, this also is where the peak of the PDF occurs. Therefore, for $x < \mu$, the particle would be to the left of the center of the PDF. Therefore the probability is 50%

(c) (4 pts) For $a = 0.05$ m^{-2} and $\mu = 1.3$m, find the average position of the particle.

Solution:
The average position is defined as $\int_{-\infty}^{\infty} x|\psi(x)|^2 \, dx$.

$$\sqrt{\frac{\pi}{a}}^{-2} \int_{-\infty}^{\infty} x \exp^2(-a(x-\mu)^2) \, dx \to \frac{a}{\pi} \int_{-\infty}^{\infty} x \exp(-2a(x-\mu)^2) \, dx$$

(1) make the substitution: $x - \mu \to u$, $dx = du$

$$\begin{aligned} &\frac{a}{\pi} \int_{-\infty}^{\infty} (u+\mu) \exp(-2au^2) \, du \\ \to \frac{a}{\pi} &\left(\int_{-\infty}^{\infty} u \exp(-2au^2) \, du + \int_{-\infty}^{\infty} \mu \exp(-2au^2) \, du \right) \end{aligned}$$

(2) The first integral can be solved with a single substitution

$$\int_{-\infty}^{\infty} u \exp(-2au^2) \, du = \left(-\exp(-2au^2) \cdot \frac{1}{4a} \right)\Bigg|_{-\infty}^{\infty} = 0$$

(3) The second integral is a gaussian, and can be solved like in part (a).

$$\begin{aligned} \int_{-\infty}^{\infty} \mu \exp(-2au^2) \, du &= \left(\mu^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(-2a(x^2+y^2)) \, dy \, dx \right)^{\frac{1}{2}} \\ &= \left(\mu^2 \int_{0}^{2\pi} \int_{0}^{\infty} \rho \exp(-2a\rho^2) \, d\rho \, d\theta \right)^{\frac{1}{2}} \\ &= \left(\mu^2 \frac{2\pi}{2a} \int_{0}^{\infty} e^{-w} \, dw \right)^{\frac{1}{2}} \\ &= \mu \sqrt{\frac{\pi}{a}} \end{aligned}$$

(4) Substituting these into (1):

$$\frac{a}{\pi} \left(0 + \mu \sqrt{\frac{\pi}{a}} \right) = \frac{\mu a}{\pi} \sqrt{\frac{\pi}{a}} = 0.164 \text{ m}$$

(d) (7 pts) Standard deviation is defined as: $\sigma = \sqrt{[x^2]_{\text{ave}} - (x_{\text{ave}})^2}$, where $[x^2]_{\text{ave}}$ is the average of x^2 and x_{ave} is the average position. Find the standard deviation of the Gaussian wavefunction for arbitrary a, μ.

Solution:
x_{ave} was found in part (c). x^2_{ave} can be found as:

$$\begin{aligned}
\frac{a}{\pi}\int_{-\infty}^{\infty} x^2 \exp(-2a(x-\mu)^2)\;dx &= -2\frac{d}{da}\int_{-\infty}^{\infty} \exp(-2a(x-\mu)^2)\;dx \quad \text{(part a.)} \\
&= -2\frac{d}{da}\sqrt{\frac{\pi}{a}} \\
&= \frac{4}{a}\sqrt{\frac{\pi}{a}}
\end{aligned}$$

Therefore, the standard deviation σ is:

$$\sqrt{\frac{4}{a}\sqrt{\frac{\pi}{a}} - \left(\frac{\mu a}{\pi}\sqrt{\frac{\pi}{a}}\right)^2}$$