Delta function well F2016

Problem 4: 3D Attractive Potential (10 pts)

Consider a particle that moves subjected to a three dimensional attractive potential

$$V(x, y, z) = -\frac{\hbar^2}{2m}[\lambda_1\delta(x) + \lambda_2\delta(y) + \lambda_3\delta(z)],$$

where $\lambda_1, \lambda_2, \lambda_3 > 0$.

a) Find the energy and the wavefunction of the particle in this potential. (4 points)

b) Interpret the meaning of this state. Calculate the probability of finding the particle inside a rectangular volume centered at the origin, with size $\ell_i = 1/\lambda_i$, with $i = 1, 2, 3$ for the x, y, z directions respectively. (2 points)

c) Compute the spatial and momentum uncertainties $(\Delta\mathbf{x})^2$ and $(\Delta\mathbf{p})^2$ for the state of item a) and explicitly check Heisenberg's inequality. (4 points)

Hint:

$$\frac{d|x|}{dx} = \frac{x}{|x|} \equiv \text{sign}(x) \qquad \frac{d}{dx}\text{sign}(x) = 2\delta(x)$$

Problem 4 — 3D Attractive Potential

$\boxed{\text{Part (a)}}$

In general, the Schrödinger equation tells us

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = E\psi.$$

In our case, we have

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{\hbar^2}{2m}\left(\lambda_1\delta(x)+\lambda_2\delta(y)+\lambda_3\delta(z)\right)\right]\psi = E\psi$$

at $x=0$ and

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

everywhere else. We can assume a separable product solution,

$$\psi(x,y,z) = \psi(x)\psi(y)\psi(z).$$

We will also assume bound states, such that $E<0$. Then everywhere except $x=0$, we have

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x)\psi(y)\psi(z) = E\psi(x)\psi(y)\psi(z)$$

$$\psi(y)\psi(z)\frac{\partial^2\psi(x)}{\partial x^2} + \psi(x)\psi(z)\frac{\partial^2\psi(y)}{\partial y^2} + \psi(x)\psi(y)\frac{\partial^2\psi(z)}{\partial z^2} = -\frac{2mE}{\hbar^2}\psi(x)\psi(y)\psi(z)$$

Dividing by $\psi(x)\psi(y)\psi(z)$, we have

$$\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2} + \frac{1}{\psi(z)}\frac{\partial^2\psi(z)}{\partial z^2} = -\frac{2mE}{\hbar^2}.$$

We know E is independent of position, so since each term on the left is dependent upon a different variable, we know each term is also constant. Define

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = k_x^2$$

$$\frac{1}{\psi(y)}\frac{d^2\psi(y)}{dy^2} = k_y^2$$

$$\frac{1}{\psi(z)}\frac{d^2\psi(z)}{dz^2} = k_z^2,$$

such that

$$k_x^2 + k_y^2 + k_z^2 = -\frac{2mE}{\hbar^2}.$$

The form of all three of our equations is the same, so we can analyze one to determine the wavefunction for the others. We will look at the x equation. We have

$$\frac{d^2\psi(x)}{dx^2} = k_x^2\psi(x),$$

which gives us

$$\psi_-(x) = Ae^{k_x x} + Be^{-k_x x}, \quad x < 0$$

$$\psi_+(x) = De^{k_x x} + Fe^{-k_x x}, \quad x > 0.$$

As $x \to -\infty$, the B term blows up, so we must have $B = 0$. As $x \to \infty$, the D term blows up, so we must have $D = 0$.

Then we have

$$\psi_-(x) = Ae^{k_x x}, \; x < 0$$
$$\psi_+(x) = Fe^{-k_x x}, \; x > 0.$$

The wave-function must be continuous at $x = 0$, so

$$\psi_-(0) = \psi_+(0)$$
$$Ae^{(0)} = Fe^{(0)}$$
$$A = F$$

and so

$$\psi_-(x) = Ae^{k_x x}, \; x < 0$$
$$\psi_+(x) = Ae^{-k_x x}, \; x > 0.$$

Now we need to consider what happens at $x = 0$. Our Schrödinger equation is

$$\nabla^2 \psi + (\lambda_1 \delta(x) + \lambda_2 \delta(y) + \lambda_3 \delta(z))\psi = -\frac{2mE}{\hbar^2}\psi$$

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + \lambda_1 \delta(x) + \frac{1}{\psi(y)}\frac{d^2\psi(y)}{dy^2} + \lambda_2 \delta(y) + \frac{1}{\psi(z)}\frac{d^2\psi(z)}{dz^2} + \lambda_3 \delta(z) = -\frac{2mE}{\hbar^2}$$

Similarly to our previous equation, we let

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + \lambda_1 \delta(x) = l_x$$
$$\frac{1}{\psi(y)}\frac{d^2\psi(y)}{dy^2} + \lambda_2 \delta(y) = l_y$$
$$\frac{1}{\psi(z)}\frac{d^2\psi(z)}{dz^2} + \lambda_3 \delta(z) = l_z,$$

where l_x, l_y, and l_z are constants.

Looking at our x equation, we have

$$\frac{d^2\psi(x)}{dx^2} + \lambda_1 \delta(x)\psi(x) = \ell_x \psi(x).$$

Integrating about an ε-neighborhood, we have

$$\int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi(x)}{dx^2}dx + \int_{-\varepsilon}^{\varepsilon} \lambda_1 \delta(x)\psi(x)dx = \int_{-\varepsilon}^{\varepsilon} \ell_x \psi(x)dx$$

$$\left.\frac{d\psi(x)}{dx}\right|_{-\varepsilon}^{\varepsilon} + \lambda_1 \psi(0) = \int_{-\varepsilon}^{\varepsilon} \ell_x \psi(x)dx$$

Now let $\varepsilon \to 0$. Since the derivative is not continuous, we have

$$\left(\left.\frac{d\psi_+}{dx}\right|_{\varepsilon\to 0^+} - \left.\frac{d\psi_-}{dx}\right|_{\varepsilon\to 0^-}\right) + \lambda_1\psi(0) = 0,$$

with the right-hand side going to zero since $\psi(x)$ is continuous. Then we have

$$\left(-k_x A - k_x A\right) + \lambda_1 (A) = 0$$

$$-2k_x A = -\lambda_1 A$$

$$k_x = \frac{\lambda_1}{2}.$$

Then

$$\psi_-(x) = Ae^{\frac{\lambda_1 x}{2}}, \quad x < 0$$

$$\psi_+(x) = Ae^{-\frac{\lambda_1 x}{2}}, \quad x > 0.$$

or

$$\psi(x) = Ae^{-\frac{\lambda_1 |x|}{2}}.$$

Then similarly for our other variables,

$$\psi(y) = A' e^{-\frac{\lambda_2 |y|}{2}}$$

$$\psi(z) = A'' e^{-\frac{\lambda_3 |z|}{2}} .$$

We know that our overall wavefunction must be continuous at the origin, so

$$\psi(x=0) = \psi(y=0) = \psi(z=0)$$

$$A = A' = A''$$

Set these equal to R such that

$$A = A' = A'' = R^{1/3}.$$

Then our total wavefunction is

$$\psi(x,y,z) = R e^{-\frac{1}{2}(\lambda_1|x| + \lambda_2|y| + \lambda_3|z|)} .$$

We want to normalize this. So since the wavefunction is symmetric about the origin, we must have

$$2 \int_0^\infty \int_0^\infty \int_0^\infty |\psi_+(x,y,z)|^2 \, dx\,dy\,dz = 1$$

$$2R^2 \int_0^\infty \int_0^\infty \int_0^\infty e^{-\lambda_1 x} e^{-\lambda_2 y} e^{-\lambda_3 z} \, dx\,dy\,dz = 1$$

$$-2R^2 \left[\frac{1}{\lambda_1}(0-1) \cdot \frac{1}{\lambda_2}(0-1) \cdot \frac{1}{\lambda_3}(0-1) \right] = 1$$

$$\frac{2R^2}{\lambda_1 \lambda_2 \lambda_3} = 1$$

$$R = \sqrt{\frac{\lambda_1 \lambda_2 \lambda_3}{2}}$$

and thus,

$$\boxed{\psi(x,y,z) = \sqrt{\frac{\lambda_1 \lambda_2 \lambda_3}{2}}\, e^{-\frac{1}{2}(\lambda_1 |x| + \lambda_2 |y| + \lambda_3 |z|)}}.$$

Since

$$k_x = \frac{\lambda_1}{2}, \quad k_y = \frac{\lambda_2}{2}, \quad k_z = \frac{\lambda_3}{2}$$

we have

$$k_x^2 + k_y^2 + k_z^2 = \frac{1}{4}(\lambda_1^2 + \lambda_2^2 + \lambda_3^2).$$

But

$$k_x^2 + k_y^2 + k_z^2 = -\frac{2mE}{\hbar^2},$$

so

$$-\frac{2mE}{\hbar^2} = \frac{1}{4}(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)$$

$$\boxed{E = -\frac{\hbar^2}{8m}(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)}$$

Part (b)

We want to determine

$$P_{tot} = \int_{-\frac{1}{2\lambda_1}}^{\frac{1}{2\lambda_1}} \int_{-\frac{1}{2\lambda_2}}^{\frac{1}{2\lambda_2}} \int_{-\frac{1}{2\lambda_3}}^{\frac{1}{2\lambda_3}} |\psi(x,y,z)|^2 dx\,dy\,dz.$$

Since our rectangular volume and wavefunction are symmetric about $x=0$, we know

$$P_{tot} = 2P_+ = 2\int_0^{\frac{1}{2\lambda_1}} \int_0^{\frac{1}{2\lambda_2}} \int_0^{\frac{1}{2\lambda_3}} |\psi_+(x,y,z)|^2 dx\,dy\,dz$$

$$= \lambda_1\lambda_2\lambda_3 \int_0^{\frac{1}{2\lambda_1}} \int_0^{\frac{1}{2\lambda_2}} \int_0^{\frac{1}{2\lambda_3}} e^{-\lambda_1 x} e^{-\lambda_2 y} e^{-\lambda_3 z} dx\,dy\,dz$$

$$= -\lambda_1\lambda_2\lambda_3 \left[\frac{1}{\lambda_1}\left(\frac{1}{\sqrt{e}}-1\right) \cdot \frac{1}{\lambda_2}\left(\frac{1}{\sqrt{e}}-1\right) \cdot \frac{1}{\lambda_3}\left(\frac{1}{\sqrt{e}}-1\right) \right]$$

$$\boxed{P_{tot} = \left(1-\frac{1}{\sqrt{e}}\right)^3} \approx 6.09\%$$

This answer seems to make sense because as the volume grows larger, we approach $P_{tot} \to 1$, which is obviously what we require since the wavefunction extends from $-\infty$ to ∞ in all dimensions.

Part (c)

We want to determine

$$(\Delta\vec{x})^2 = \langle x^2 \rangle - \langle x \rangle^2$$

and

$$(\Delta\vec{p})^2 = \langle p^2 \rangle - \langle p \rangle^2.$$

We know, in general, that

$$\Delta\sigma_{r_i} \Delta p_j \geq \frac{\hbar}{2} \delta_{ij}.$$