

July 5
2012

qm-que-21001

To find α so that the trial wave function

$$\psi(x) = N \exp(-\frac{\alpha^2 x^2}{2})$$

may give best estimate for ground state energy of a particle in Dirac δ function potential.

$$V(x) = -g\delta(x) \quad g > 0$$

First fix the normalization

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

$$\text{or } \int_{-\infty}^{\infty} N^2 \exp(-\alpha^2 x^2) dx = 1 \Rightarrow N^2 = \frac{\alpha}{\sqrt{\pi}}$$

Next compute average of kinetic energy

$$\begin{aligned} \langle KE \rangle &= \int_{-\infty}^{\infty} \psi^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi(x) dx \\ &= -\frac{\hbar^2}{2m} N^2 \int_{-\infty}^{\infty} (-\alpha^2 + \alpha^4 x^2) e^{-\alpha^2 x^2} dx \\ &= \dots = \frac{\hbar^2}{4m\alpha^2} \end{aligned}$$

$$\begin{aligned} \langle PE \rangle &= \int_{-\infty}^{\infty} \psi^*(x) (-g\delta(x)) \psi(x) dx \\ &= -g |\psi(0)|^2 = -g N^2 = -\frac{g\alpha}{\sqrt{\pi}} \end{aligned}$$

$$\langle E \rangle_{\alpha} = \frac{\hbar^2 \alpha^2}{4m} - \frac{g\alpha}{\sqrt{\pi}}$$

minimize energy w.r.t. α

$$\frac{\partial E}{\partial \alpha} = 0 \Rightarrow \left(\alpha = \frac{2gm}{\hbar^2 \sqrt{\pi}} \right)$$

$$\therefore \alpha = \frac{2gm}{\hbar^2 \sqrt{\pi}}$$

Note: Useful integrals to remember

$$\int_{-\infty}^{\infty} \exp(-\lambda x^2) dx = \sqrt{\frac{\pi}{\lambda}}$$

Differentiate w.r.t. λ to get

$$-\int_{-\infty}^{\infty} x^2 \exp(-\lambda x^2) dx = -\frac{1}{2} \sqrt{\frac{\pi}{\lambda^3}}$$

$$\therefore \int_{-\infty}^{\infty} x^2 \exp(-\lambda x^2) dx = \frac{1}{2} \sqrt{\frac{\pi}{\lambda^3}}$$

Remark Corresponding energy value turns out to be

$$\begin{aligned} E &= \frac{\hbar^2 \alpha^2}{4m} - \frac{g\alpha}{\sqrt{\pi}} = \frac{\hbar^2}{4m} \left(\frac{4g^2 m^2}{\hbar^4 \pi} \right) - \frac{g}{\sqrt{\pi}} \left(\frac{2gm}{\hbar^2 \sqrt{\pi}} \right) \\ &= \frac{-g^2 m}{\pi \hbar^2} \end{aligned}$$

Which is greater than the exact value $-\frac{mg^2}{2\hbar^2}$, as it should be.