Chem 2430 - 2021 Exam #1 Answers

1. $\langle 2|x^2|2\rangle = \frac{\hbar}{2m\omega}\langle 2|(a^\dagger + a)^2|2\rangle$

$= \frac{\hbar}{2m\omega}\langle 2|a^\dagger a + a a^\dagger|2\rangle = \frac{5\hbar}{2m\omega}$

$\langle i|x^3|i\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2}\langle 1|(a^\dagger + a)^3|i\rangle$

The allowed values of i are 0, 2, 4

$\langle 1|(a^\dagger + a)^3|0\rangle = \langle 1|a a^\dagger a^\dagger + a^\dagger a a^\dagger|0\rangle$

$= 2 + 1$

$\langle 1|(a^\dagger + a)^3|2\rangle = \langle 1|a^\dagger a a + a a^\dagger a + a a a^\dagger|2\rangle$

$= \sqrt{2} + \sqrt{2}\sqrt{2}\sqrt{2} + \sqrt{3}\sqrt{3}\sqrt{2} = 6\sqrt{2}$

$\langle 1|(a^\dagger + a)^3|4\rangle = \langle 1|a a a|4\rangle = \sqrt{4}\sqrt{3}\sqrt{2} = 2\sqrt{6}$

These numbers need to be combined with $\left(\frac{\hbar}{2m\omega}\right)^{3/2}$

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2. 2D rotor in xy plane

$x = r_0\cos\phi, \quad y = r_0\sin\phi$

$\langle m|\cos\phi|n\rangle \propto \int_0^{2\pi} e^{-im\phi}(e^{i\phi} + e^{-i\phi})e^{in\phi}\,d\phi$

$= \int_0^{2\pi} e^{-im\phi}e^{i\phi}e^{in\phi}\,d\phi + \int_0^{2\pi} e^{-im\phi}e^{-i\phi}e^{in\phi}\,d\phi$

Nonzero integrals result when $n = m \pm 1$.

The situation is the same when the operato

3. The potential is $\frac{-1}{1+x^2}$

A reasonable trial wavefunction is e^{-ax^2}

$$\frac{d^2}{dx^2} e^{-ax^2} = (-2a + 4a^2x^2)e^{-ax^2}$$

$$-\frac{1}{2}\frac{d^2}{dx^2}\psi = (a - 2a^2x^2)\, e^{-ax^2}$$

$$\int_{-\infty}^{\infty} e^{-2ax^2} dx = \sqrt{\frac{\pi}{2a}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-2ax^2} dx = \frac{\sqrt{\pi/2}}{4a^{3/2}}$$

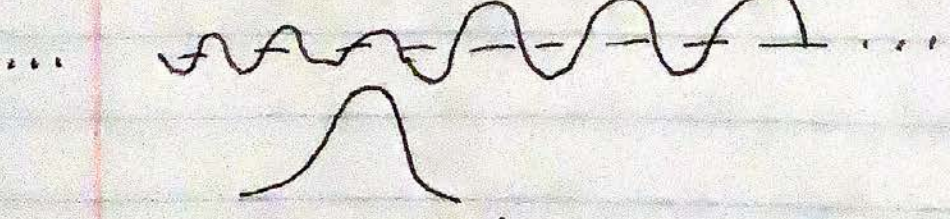
$$\int_{-\infty}^{\infty} \frac{e^{-2ax^2}}{1+x^2} dx = \pi e^{2a}\, \mathrm{erf}(\sqrt{2a})$$

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{a\sqrt{\frac{\pi}{2a}} - 2a^2\frac{\sqrt{\pi/2}}{4a^{3/2}} - \pi e^{2a}\,\mathrm{erf}(\sqrt{2a})}{\sqrt{\frac{\pi}{2a}}}$$

$$= a - a/2 - \sqrt{2a\pi}\, e^{2a}\,\mathrm{erf}(\sqrt{2a})$$

Now consider the potential $\frac{1}{1+x^2}$

Sketch the wavefunction in the case of a particle incident from the right with $E > 1$.



One would expect a high probability of transmission but also some probability of reflection.

4. $\psi = e^{i\phi} + e^{2i\phi}$

a) Normalize $\langle\psi|\psi\rangle = 4\pi$

$$\psi = \frac{1}{\sqrt{4\pi}}\left(e^{i\phi} + e^{2i\phi}\right)$$

b) This is not an eigenfunction of H and thus is not a stationary state

c) What is the uncertainty in ϕ?

We could do the integral for $\langle\phi\rangle$ but this is obviously π.

$$\langle\phi^2\rangle = \frac{1}{4\pi}\int_0^{2\pi}\left(e^{-i\phi}+e^{-2i\phi}\right)\phi^2\left(e^{i\phi}+e^{2i\phi}\right)d\phi$$

$$= \frac{1}{4\pi}\int_0^{2\pi}\phi^2\left(2 + e^{i\phi} + e^{-i\phi}\right)d\phi$$

$$= \frac{1}{4\pi}\left[\frac{2\phi^3}{3} + e^{i\phi}\left(-i\phi^2 + 2\phi + 2i\right) + e^{-i\phi}\left(i\phi^2 + 2\phi - 2i\right)\right]_0^{2\pi}$$

$$= \frac{1}{4\pi}\left[\frac{2\phi^3}{3} + 4\phi\right] = \frac{1}{4\pi}\left[\frac{16}{3}\pi^3 + 8\pi\right] = \frac{4}{3}\pi^2 + 2$$

$$\langle\phi^2\rangle - \langle\phi\rangle^2 = \frac{4}{3}\pi^2 + 2 - \pi^2 = \frac{\pi^2}{3} + 2$$

$$\sqrt{\langle\phi^2\rangle - \langle\phi\rangle^2} = \sqrt{\pi^2/3 + 2}$$

$$\langle L_z\rangle = \frac{\hbar}{i4\pi}\int_0^{2\pi}\left(e^{-i\phi}+e^{-2i\phi}\right)\left(ie^{i\phi} + 2ie^{2i\phi}\right)d\phi$$

$$= \frac{\hbar}{4\pi}\left[2\pi + 4\pi\right] = \frac{3}{2}\hbar$$

$$\langle L_z^2\rangle = \frac{\hbar^2}{4\pi i^2}\int_0^{2\pi}\left(e^{-i\phi}+e^{-2i\phi}\right)\left(i^2e^{i\phi} + 4i^2e^{2i\phi}\right)d\phi$$

$$= -\frac{\hbar^2}{4\pi}\left[-2\pi - 8\pi\right] = \frac{5}{2}\hbar^2$$

$$\langle L_z^2\rangle - \langle L_z\rangle^2 = \left(\frac{5}{2} - \frac{9}{4}\right)\hbar^2 = \frac{1}{4}\hbar^2$$

5. $V = \frac{1}{2}k(x^2 + y^2 + z^2)$

This obviously separates in Cartesian coord and $E = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega$.

Now consider spherical coordinates.

$$-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)e^{-ar^2} = ?$$

$$\frac{d}{dr}e^{-ar^2} = -2are^{-ar^2}, \quad \frac{d^2}{dr^2}e^{-ar^2} = (-2a + 4a^2r^2)e^{-ar^2}$$

$$-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)e^{-ar^2} + \frac{1}{2}kr^2e^{-ar^2} = Ee^{-ar^2}$$

$$\frac{1}{2}\left[2a - 4a^2r^2 + 4a\right] + \frac{1}{2}kr^2 = E$$

$$E = \frac{3a}{2}, \quad 2a^2 = \frac{1}{2}k \quad a = \sqrt{k}/2$$

Same ground state energy as when we used cartesian coordinates

To obtain the general solution, we could include the angular momentum operator and make use of a series expansion to find the general solution