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CHEM 1410 EXAM 1 SPRING 2001

(25 pts)

1. Which of the following is true?

a) ψ^2 is always positive. Not true if ψ is complex

[✓ b)] $\frac{h}{2a}$ is a possible value for the momentum of a particle in a box of length a.

$$\frac{\hbar}{i}\frac{d}{dx} e^{\frac{i\pi x}{a}} = \frac{\hbar \pi}{a} = \frac{h}{2a}$$

[✓ c)] $\hat{A} = x^2$ is a Hermitian operator

x^2 is an obsevable, so the operator must be Hermetian

[✓ d)] $e^{2i\phi}$ is an eigenfunction of the Hamiltonian for a particle-on-the-ring $\left(H = -\frac{\hbar^2}{2m}\frac{d^2}{d\phi^2}\right)$ and of the $\hat{L}_z$ angular momentum operator $\left(\frac{\hbar}{i}\frac{d}{d\phi}\right)$.

e) For the harmonic oscillator problem, the potential energy commutes with the total Hamiltonian.

Not true as the K.E. and P.E. terms do not commute

(18 pts)

2. For the H_2 molecule in the v = 0 vibrational level, estimate the spread in the H–H bond length (in Å).

$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$. $\langle x\rangle = 0$. From the homework,

$$\langle x^2\rangle = \frac{1}{2\alpha} = \frac{\hbar}{2\sqrt{\mu k}} = \frac{1.054\times10^{-34}}{2\sqrt{(.8142\times10^{-27})(510)}}$$

$$= .808\times10^{-22}$$

$$\sigma_x = \sqrt{\langle x^2\rangle} = 0.90\times10^{-11}\,\text{m} = .09\,\text{Å}$$

(16 pts)

3. For the particle in the one-dimensional box problem, consider the wavefunction 0.5 sin $\left(\frac{\pi x}{a}\right)$ + 0.5 sin $\left(\frac{2\pi x}{a}\right)$. (Note - This is not normalized.) What is the energy of this system?

$$E = \int_0^a \psi H \psi\, dx \Big/ \int_0^a \psi\psi\, dx$$

$$= \frac{\int_0^a \left[.5\sin\left(\frac{\pi x}{a}\right) + .5\sin\left(\frac{2\pi x}{a}\right)\right]\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right)\left[.5\sin\left(\frac{\pi x}{a}\right) + .5\sin\left(\frac{2\pi x}{a}\right)\right] dx}{\int_0^a \left[.5\sin\left(\frac{\pi x}{a}\right) + .5\sin\left(\frac{2\pi x}{a}\right)\right]^2 dx}$$

$$= \frac{0.25}{0.25}\int_0^a \left[\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{2\pi x}{a}\right)\right]\left[E_1\sin\left(\frac{\pi x}{a}\right) + E_2\sin\left(\frac{2\pi x}{a}\right)\right] dx \Big/ \left[\int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx + \int_0^a \sin^2\left(\frac{2\pi x}{a}\right) dx\right]$$

$$= a/2\,(E_1 + E_2) \Big/ \frac{a}{2}(2) = (E_1 + E_2)/2$$

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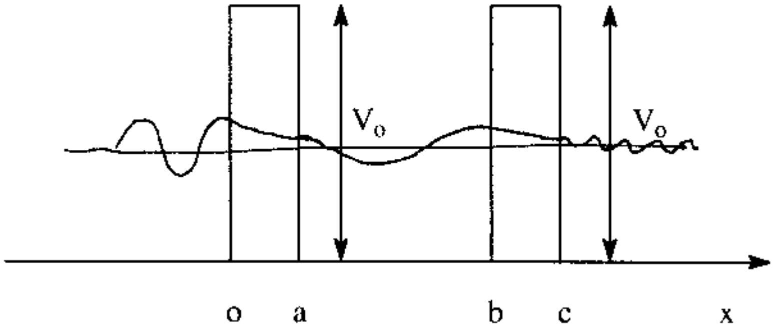
(18 pts)

4. Consider the situation where there are two repulsive barriers of height V_0, and there is a particle impinging from the left with $E < V_0$. Sketch the wavefunction for this system, on the adjacent figure. Be certain to include all regions.

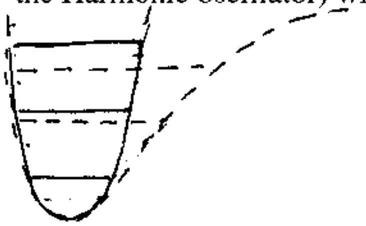


Do you think that the tunneling probability could depend sensitively on E ($E < V_0$)? Why or why not?

Yes - at some energies, the wavefunction will just "fit in".

(18 pts)

5. The energy levels of the Harmonic oscillator are evenly spaced. If a more realistic model of the potential energy curve of a diatomic molecule were adopted (*e.g.*, the Morse potential), would you expect the levels to be more closely spaced or spaced further apart (compared to the Harmonic oscillator) with increasing energy. Justify your answer.



They will be more closely spaced compared to the harmonic oscillator levels. This is because the attractive region ("box size") grows as the energy increases.

Recall the particle-in-the-box problem. The bigger the box, the more closely spaced are the energy levels.