Chemistry 1410
Exam #1

Some potentially useful integrals and relations are:

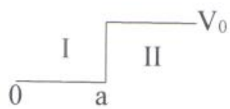
$$\sin(ax)\sin(bx) = \frac{1}{2}\left[\cos(a-b)x - \cos(a+b)x\right]$$

$$\int x\cos^2(ax)\,dx = \frac{x^2}{4} + \frac{x\sin(2ax)}{4a} + \frac{\cos(2ax)}{8a^2}$$

$$\int x\sin^2(ax)\,dx = \frac{x^2}{4} - \frac{x\sin(2ax)}{4a} - \frac{\cos(2ax)}{8a^2}$$

1. (28 points) True or False (Circle your choice)
   (a) All quantum mechanical systems exhibit tunneling. T F
   (b) The operators $\hat{p}_x$ and $\hat{p}_x^2$ commute. T F
   (c) A 3D box of dimensions $0 \le x \le a, 0 \le y \le b, 0 \le z \le \frac{b}{2}$ will display doubly degenerate enegy levels. T F
   (d) The wavefunction of a quantum mechanical system can be determined experimentally. T F

2. (24 points) Consider a particle of mass m impinging from the left on the step potential shown below.



(9) For the case that $E < V_0$, write the wavefunction for regions I and II.

$\psi_I = A e^{ikx} + B e^{-ikx}$

$\psi_{II} = C e^{-\kappa x}$

$k = \sqrt{2mE/\hbar^2}$

$\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$

(9) Show that the probability of reflection is 100%.

$\psi_I(a) = \psi_{II}(a) \Rightarrow A e^{ika} + B e^{-ika} = C e^{-\kappa a}$

$\psi_I'(a) = \psi_{II}'(a) \quad ik(A e^{ika} - B e^{-ika}) = -C\kappa e^{-\kappa a}$

$-\frac{C\kappa}{C} = \frac{ik(A e^{ika} - B e^{-ika})}{A e^{ika} + B e^{-ika}}$

$\frac{B}{A} = \frac{(ik - \kappa) e^{ika}}{(-ik - \kappa) e^{-ika}} \rightarrow \left|\frac{B}{A}\right|^2 = \frac{k^2 + \kappa^2}{k^2 + \kappa^2} = 1 \leftarrow$ 100% probability of reflection

If reflection is 100%, does this mean there is no tunneling? Explain your answer.

$c \neq 0$. So there is tunneling

The particle tunnels into the classically forbidden region, but then is reflected back to the left, resulting in 100% reflection.

3. (24 points) Consider a particle in a 1D box $(0 \le x \le a)$ with infinite potential outside the box.

$$\psi = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right) = \varphi_1 + \varphi_2$$

(a) What is the average value of x?

$$\langle x \rangle = \frac{\int (\varphi_1+\varphi_2) x (\varphi_1+\varphi_2) dx}{2} = \frac{\int \varphi_1 x \varphi_1 dx + \int \varphi_2 x \varphi_2 dx + 2\int \varphi_1 x \varphi_2 dx}{2}$$

$$= \int \varphi_1 x \varphi_2 dx = \frac{2}{a}\int_0^a \left(\sin\frac{\pi x}{a}\right) x \left(\sin\frac{2\pi x}{a}\right) dx$$

(b) What is the average energy?

$$\langle E \rangle = \frac{\frac{h^2}{8ma^2} + \frac{4h^2}{8ma^2}}{2} = \frac{5}{16}\frac{h^2}{ma^2}$$

(c) What is the average momentum?

$$\langle p_x \rangle = \frac{\frac{\hbar}{i}\int (\varphi_1+\varphi_2) \frac{\partial}{\partial x} (\varphi_1+\varphi_2)\, dx}{2} = 0$$

We know this is zero because measurements of an observable must give a real result.

(d) What is the value of σ_x?

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

Note: you cannot simply use the equations on pages 100-101 of the text.

$$\langle x^2\rangle = \underline{\int \varphi_1^2 x^2 dx + \int \varphi_2^2 x^2 dx + \int \varphi_1 x^2 \varphi_2 dx}$$

$$= \frac{1}{2}\left[\int_0^a \varphi_1^2 x^2 dx + \int_0^a \varphi_2^2 x^2 dx\right]$$

which can be evaluated using equations on page 101

(e) What value(s) of the energy can you get in an individual measurement?

$$+\frac{h^2}{8ma^2} \text{ or } \frac{4h^2}{8ma^2}$$

(f) What value(s) of the position can you get for an individual measurement?

any value between 0 and a.

4. (24 points) (a) What is the zero-point energy of the ground state of a particle in a two-dimensional square box of sides of length a?

$$\frac{h^2}{8ma^2} + \frac{h^2}{8ma^2} = \frac{h^2}{4ma^2}$$

(b) What is the probability of being in the region $\frac{a}{3} \le x \le \frac{2}{3}a$ and $\frac{a}{3} \le y \le \frac{2}{3}a$? Show your work.

$$\frac{4}{a^2}\int_{a/3}^{2a/3} \sin^2\frac{\pi x}{a}\,dx \int_{a/3}^{2a/3} \sin^2\frac{\pi y}{a}\,dy$$

$$= \frac{4}{a^2}\left[\int_{a/3}^{2a/3} \sin^2\frac{\pi x}{a}\,dx\right]^2$$