Chem 332: First Exam (80 pts. possible) KEY Wednesday, February 6, 2013

Please budget your time carefully and show all work for partial credit. Read each problem carefully!

$h = 6.62608 \times 10^{-34}$ J s	1 Å = 1×10^{-10} m = 0.1 nm	$\int_0^\infty x^n e^{-ax}\,dx = \frac{n!}{a^{n+1}}$
$N_A = 6.02214 \times 10^{23}$ mol^{-1}	1 amu = 1.66054×10^{-27} kg	
$c = 2.99792 \times 10^8$ m/s	$m_e = 9.10939 \times 10^{-31}$ kg	
$k_B = 1.38065 \times 10^{-23}$ J K^{-1}	$e^{\pm i\theta} = \cos\theta \pm i\sin\theta$	$\int_0^\infty x^2 e^{-ax^2}\,dx = \frac{1}{4a}\left(\frac{\pi}{a}\right)^{1/2}$

(1) (10 pts) Consider the photoelectric effect on zinc metal, which has a work function Φ of 5.816×10^{-19} J (i.e., a threshold frequency $\nu_0 = 8.777 \times 10^{14}$ s^{-1}). Use conservation of energy to calculate the maximum kinetic energy (in J) of an emitted electron when light of wavelength 140.0 nm strikes the surface of a sample of zinc metal.

Conservation of energy: $K.E.\ e^-\text{'s} = h\nu - \Phi$

$$= \frac{hc}{\lambda} - \Phi$$

$$K.E. = \frac{(6.62608 \times 10^{-34})(2.99792 \times 10^{8})}{140.0 \times 10^{-9}} - 5.816 \times 10^{-19}$$

$$= 8.373 \times 10^{-19}\ \text{J}$$

(2) (10 pts) Name four qualities that an acceptable quantum mechanical wavefunction must possess. Then in one sentence or less say why these qualities are required.

4 must be:

1) normalizable (square integrable)
2) finite everywhere
3) continuous
4) piecewise continuous 1st derivative's
5) single-valued
6) not zero everywhere

All of these are required so that $|\psi|^2$ is a proper probability distribution function.

(3) (10 pts) Calculate the expectation value of x^2 in the state described by $\psi = e^{-bx}$, where b is a constant. In this system x ranges from 0 to ∞.

$$\langle x^2 \rangle = \frac{\int_0^\infty e^{-bx}\, x^2\, e^{-bx}\, dx}{\int e^{-bx}\, e^{-bx}\, dx} = \frac{\int_0^\infty x^2 e^{-2bx}\, dx}{\int_0^\infty e^{-2bx}\, dx}$$

$$= \frac{\frac{2!}{(2b)^3}}{\frac{0!}{(2b)^1}} = \frac{2}{(2b)^2} = \frac{1}{2b^2}$$

(Sorry about previous error on the key)

(4) (25 pts) Using what you know about the momentum operator along the x direction, $\hat{p}_x$,

(a) show that the function $e^{\frac{ip_k}{\hbar}x}$ is an eigenfunction of $\hat{p}_x$ with eigenvalue p_k.

$$\hat{p}_x e^{ip_k x/\hbar} = \frac{\hbar}{i}\frac{d}{dx} e^{ip_k x/\hbar} = \left(\frac{\hbar}{i}\right)\left(\frac{ip_k}{\hbar}\right) e^{ip_k x/\hbar}$$

$$= p_k e^{ip_k x/\hbar}$$

$\therefore$ eigenfunction w/ eigenvalue p_k

(b) Now consider the case of a metal surface being struck by 195 nm light. The wavefunction of the fastest ejected electron is approximately described by the following superposition of normalized momentum eigenfunctions

$$\Psi(x) = \frac{1}{3}N_1 e^{\frac{ip_1}{\hbar}x} + \frac{1}{3}N_2 e^{\frac{ip_2}{\hbar}x} + \frac{\sqrt{7}}{3}N_3 e^{\frac{ip_3}{\hbar}x}$$

where $p_1 = 0.87$, $p_2 = 1.55$, $p_3 = 1.14$ (all in 10^{-24} kg m/s), and N_1, N_2, and N_3 are normalization constants. What are the possible outcomes and their associated probabilities for a measurement of the momentum of this electron? What is the <u>average</u> momentum of this electron in the state Ψ (in kg m/s) ?

<u>Outcome</u>	<u>prob</u>
$p_1 = 0.87$	$1/9$
$p_2 = 1.55$	$1/9$
$p_3 = 1.14$	$7/9$

$$\langle p_x \rangle = \frac{1}{9}(0.87) + \frac{1}{9}(1.55) + \frac{7}{9}(1.14) = 1.156 \times 10^{-24} \text{ kg m/s}$$

(c) Based on the average momentum calculated in (b), what is this electron's de Broglie wavelength (in nm) ?

$$\lambda = \frac{h}{p} = \frac{6.62608 \times 10^{-34}}{1.156 \times 10^{-24}}$$

$$= 5.73 \times 10^{-10} \text{ m} = 0.57 \text{ nm}$$

(5) (15 pts)

(a) Determine whether the operators $\hat{x}$ and $\hat{L}_z = -i\hbar\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)$ commute. In other words, please evaluate the commutator $\left[\hat{x}, \hat{L}_z\right]$.

$$[x, L_z]f = xL_z f - L_z x f$$

$$= -i\hbar\left[x^2\frac{\partial f}{\partial y} - xy\frac{\partial f}{\partial x} - x\frac{\partial}{\partial y}xf + y\frac{\partial}{\partial x}xf\right]$$

$$= -i\hbar\left[x^2\frac{\partial f}{\partial y} - xy\frac{\partial f}{\partial x} - x^2\frac{\partial f}{\partial y} + yx\frac{\partial f}{\partial x} + yf\right]$$

$$= -i\hbar y f$$

(b) Based on your result in (a), what can you briefly say (if anything) about your ability to simultaneously and precisely measure the position x and the z-component of $\vec{L}$? Be specific.

x and L_z do not commute, so the Heisenberg Uncertainty Principle applies and we are limited to how accurately we can simultaneously measure x and L_z.

(6) (10 pts) Show that the operator defined as the linear combination $\hat{B} + i\hat{C}$ is not hermitian if $\hat{B}$ and $\hat{C}$ are hermitian operators.

if $B + i\hat{C}$ was hermitian;

$$\int \psi^*(B+iC)\phi\, d\tau = \int [(B+iC)\psi]^*\phi\, d\tau$$

$$\int \psi^* B\phi\, d\tau + i\int \psi^* C\phi\, d\tau = \int B^*\psi^*\phi\, d\tau - i\int C^*\psi^*\phi\, d\tau$$

since B and C are hermitian;

$$\int B^*\psi^*\phi\, d\tau + i\int C^*\psi^*\phi\, d\tau \neq \int B^*\psi^*\phi\, d\tau - i\int C^*\psi^*\phi\, d\tau$$