Chemistry 3502/4502

Exam I

February 6, 2006

1) Circle the correct answer on multiple-choice problems.

2) There is *one* correct answer to every multiple-choice problem. There is no partial credit. On the short-answer problem, show your work in full.

3) A table of useful integrals and other formulae is provided at the end of the exam.

4) You should try to go through all the problems once quickly, saving harder ones for later.

5) There are 10 multiple-choice problems. Each is worth 8 points. The short-answer problem is worth 20 points.

6) There is no penalty for guessing.

7) Please write your name at the bottom of each page.

8) Please mark your exam with a pen, not a pencil. If you want to change an answer, cross your old answer out and circle the correct answer. Exams marked with pencil or correction fluid will not be eligible for regrade under any circumstances.

Score on Next Page after Grading

NAME: ____

1. Which of the following phenomena could be explained by classical physics and did *not* require a quantum hypothesis in order to make theory agree with experiment?

(a)	Blackbody spectra	(e)	Atomic line spectra
(b)	Diffraction of light	(f)	(b) and (e)
(c)	Low-temperature heat capacity in perfect crystals	(g)	(a), (b), and (d)
(d)	The photoelectric effect	(h)	(c) and (d)

2. If a normalized wave packet Ψ is given as $\Psi(x, y, z, t) = \sum_{n=1}^{\infty} c_n \psi_n(x, y, z) e^{-iE_n t/\hbar}$, what is the probability that an experiment will cause the system to collapse to the specific stationary state j?

(a)	Quantum mechanics does not allow you to know this probability	(e)	c_j
(b)	One	(f)	$\lvert c_j \rvert^2$
(c)	$< \psi_j \lvert H \rvert \psi_j >$	(g)	(b) and (d)
(d)	c_j^*	(h)	Only Schrödinger's cat knows

3. Which of the following statements about the de Broglie wavelength λ are *false*?

(a)	λ decreases as mass increases if velocity is constant	(e)	A particle that has zero velocity has an infinite de Broglie wavelength
(b)	$\lambda = h / p$	(f)	All of the above
(c)	λ increases as momentum increases	(g)	(a), (b) and (e)
(d)	λ is a constant, like Planck's constant	(h)	(c) and (d)

4. Which of the following statements about a well behaved wave function is *true*?

(a)	It must be continuous	(e)	Its square modulus has units of probability density
(b)	It may take on complex values	(f)	It must be an eigenfunction of the momentum operator
(c)	It must be quadratically integrable	(g)	(d) and (f)
(d)	It must be equal to its complex conjugate	(h)	(a), (b), (c), and (e)

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5. Which of the below equations will be true for any pair of orthonormal functions f and g that are eigenfunctions of the Hamiltonian H?

(a)	$fg = 0$	(e)	$< f \mid g > = 0$
(b)	$< \lvert f \rvert^2 >< \lvert g \rvert^2 > = 1$	(f)	(a) and (c)
(c)	$f^*g - g^*f = 0$	(g)	(b), (d) and (e)
(d)	$< f \mid H \mid g > = 0$	(h)	All of the above

6. Which of the below expectation values are or may be non-zero?

(a)	$< \sin x \mid x \mid \cos x >$	(e)	$< f \mid g > - < g \mid f >$
(b)	$< \sin^2 x \mid x \mid \cos^2 x >$	(f)	$<\boldsymbol{\mu}_{mn}>$ for a forbidden transition
(c)	$< f \mid [A,B] \mid g >$ where A and B commute	(g)	(a), (d) and (e)
(d)	$< \Psi \mid H \mid \Psi >$ where Ψ is a stationary state	(h)	(b), (c), and (f)

7. Which of the following did Bohr assume in order to derive a model consistent with the photoemission spectra of one-electron atoms?

(a)	The electron is a delocalized wave	(e)	The ionization potential is equal to the work function
(b)	The angular momentum of the electron is quantized	(f)	(a) and (b)
(c)	The one-electron atom is like a particle in a box	(g)	(b) and (d)
(d)	The Coulomb potential is quantized	(h)	None of the above

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8. Which of the following statements are *false* about the free particle?

(a)	Its Schrödinger equation is $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-E\right)\Psi(x)=0$	(e)	Valid wave functions include $\Psi(x)=Ae^{ikx}+Be^{-ikx}$ where $k=\frac{\sqrt{2mE}}{\hbar}$
(b)	It may be regarded as having a wave function that is the superposition of a left-moving particle and a right-moving particle	(f)	Valid wave functions include $\Psi(x)=N\cos kx$ where N is a normalization constant and k is defined in (e) above
(c)	Its energy levels are all non-negative	(g)	All of the above
(d)	Its energy levels are not quantized	(h)	None of the above

9. Given a particle of mass m in a box of length L having the wave function $\Psi(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$, what is the energy of the level corresponding to n = 4?

(a)	Since this wave function is not an eigenfunction of the Hamiltonian the question cannot be answered	(e)	$\frac{8\pi^2\hbar^2}{mL^2}$
(b)	16 times the energy of the ground state	(f)	(c) and (d)
(c)	$<\Psi \mid p_x^2 \mid \Psi>$	(g)	(b) and (e)
(d)	$8\hbar^2 / mL^2$	(h)	None of the above

10. On which of the below functions does the parity operator Π act in the fashion $\Pi[f(x)] = (-1)f(x)$?

(a)	x	(e)	Any eigenfunction of the Hamiltonian
(b)	x^2	(f)	(b) and (d)
(c)	e^{ix}	(g)	(a), (b), and (d)
(d)	$\cos x$	(h)	(b), (d), and (e)

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Short-answer (20 points)

Prove that, given a pair of normalized but *not* orthogonal functions ψ_1 and ψ_2, the function $\psi_3 = \psi_2 - S\psi_1$ is orthogonal to ψ_1 if S is the overlap integral of ψ_1 and ψ_2. Is ψ_3 normalized? (Use the back of the page if necessary).

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Some Potentially Useful Mathematical Formulae

Trigonometric Relations

$$\sin\alpha\sin\beta = \frac{1}{2}\left[\cos(\alpha-\beta)-\cos(\alpha+\beta)\right]$$

$$\cos\alpha\cos\beta = \frac{1}{2}\left[\cos(\alpha-\beta)+\cos(\alpha+\beta)\right]$$

$$\sin\alpha\cos\beta = \frac{1}{2}\left[\sin(\alpha-\beta)+\sin(\alpha+\beta)\right]$$

$$\sin(\alpha\pm\beta) = \sin\alpha\cos\beta \pm \sin\beta\cos\alpha$$

$$\cos(\alpha\pm\beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta$$

$$\frac{d}{dx}\sin x = \cos x$$

$$\frac{d}{dx}\cos x = -\sin x$$

Complex Relations

$$\sqrt{-1} = i = -\frac{1}{i}$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

Some Operators

$x \equiv$ multiply by x

$\mathbf{r} \equiv$ multiply by $\mathbf{r}$

$$p_x \equiv -i\hbar\frac{d}{dx}$$

$$H = T + V$$

$$\boldsymbol{\mu} \equiv e\mathbf{r}$$

Integrals

$$\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)dx = \frac{L}{2}\delta_{mn}$$

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

$$\int x^2\cos(ax)dx = \frac{2x\cos ax}{a^2} + \frac{a^2x^2-2}{a^3}\sin ax$$

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