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Chemistry 3502/4502

Exam I

September 19, 2003

1) This is a multiple choice exam. Circle the correct answer.

2) There is *one* correct answer to every problem. There is no partial credit.

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 first, saving harder ones for later.

5) There are 20 problems. Each is worth 5 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. Do not use correction fluid 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: ____________

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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)	Orbital motion of planets
(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)	None of the above

2. Which of the following statements about the integral $< g \mid A \mid g >$ where A is a Hermitian operator are *true*?

(a)	It must be zero if g is an arbitrary eigenfunction of A	(e)	It is zero if $[H,A] = 0$
(b)	It must be a real number	(f)	(a) and (b)
(c)	It is equal to $A< g \mid g >$	(g)	(a) and (c)
(d)	It is equal to zero if A has even parity	(h)	None of the above

3. 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)	$\lvert c_j \rvert^2$
(b)	One	(f)	c_j
(c)	$< \psi_j \mid H \mid \psi_j >$	(g)	(b) and (d)
(d)	c_j^*	(h)	Ask Schrödinger's cat

4. Which of the following statements about the de Broglie wavelength λ are *true*?

(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 decreases as momentum increases	(g)	(a), (b) and (e)
(d)	λ increases as kinetic energy decreases	(h)	(c) and (d)

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5. Which of the following is the time-dependent Schrödinger equation in one dimension?

(a) $-\frac{\hbar}{i}\frac{\partial^2\Psi(x,t)}{\partial t^2}=\left[-\frac{\hbar^2}{2m}\frac{\partial}{\partial x}+V(x)\right]\Psi(x,t)$

(b) $H\Psi = E\Psi$

(c) $-\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\Psi(x,t)$

(d) $\frac{\partial^2\Psi(x,t)}{\partial x^2}=\frac{1}{c^2}\frac{\partial^2\Psi(x,t)}{\partial t^2}$

(e) $\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t}=\left[\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\Psi(x,t)$

(f) $H\Psi(x,t) = (T + V)\Psi(x,t)$

(g) $\Psi(x,y,z,t)=\sum_{n=1}^{\infty}c_n\psi_n(x,y,z)e^{-iE_nt/\hbar}$

(h) None of the above

6. If H is the Hamiltonian, $H\phi_1 = a\phi_1$, $H\phi_2 = b\phi_2$, $H\phi_3 = b\phi_3$, $H\phi_4 = c\phi_4$, $a \neq b \neq c$, and B is some other operator for which $[B,H] = 0$, which of the following integrals must be zero?

(a) $< \phi_1 | \phi_4 >$

(b) $< \phi_1 | B | \phi_4 >$

(c) $< \phi_1 | H | \phi_3 >$

(d) $< \phi_2 + \phi_3 | B | \phi_2 - \phi_3 >$

(e) $< \phi_2 | \phi_4 >$

(f) (a), (c), and (e)

(g) (a), (b), and (c)

(h) (a), (b), (c), and (e)

7. Which of the below equations can be *false* for an arbitrary pair of orthonormal functions f and g?

(a) $|f|^2|g|^2 < 1$

(b) $< f | H | g > = 0$

(c) $< f | g > \neq < f | g >^*$

(d) $fg = 0$

(e) $f^*g - g^*f = 0$

(f) (a) and (c)

(g) (b), (d) and (e)

(h) All of the above

8. In what units may Planck's constant, h, be expressed?

(a) kcal mol^{-1} s

(b) Units of action

(c) Units of angular momentum

(d) (Energy) times (time)

(e) J s

(f) eV s

(g) (b), (c), (d), and (e)

(h) All of the above

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9. Which of the following statements about a Hermitian operator *A* are *true*?

(a) It has no degenerate eigenvalues
(b) It always commutes with the Hamiltonian operator
(c) $< f | A | g > = < g | A \ | f >$
(d) Its eigenfunctions are real-valued
(e) It is quadratically integrable
(f) It has either a finite or infinite number of all real eigenvalues
(g) (b), (c) and (e)
(h) None of the above

10. Which of the following statements about tunneling are *true*?

(a) Tunneling is more efficient near the top of the barrier than further down
(b) Tunneling is responsible for the radioactive emission of α particles
(c) Tunneling is more efficient for lighter particles
(d) Tunneling has no classical analog
(e) Tunneling is more efficient the narrower the barrier
(f) (c) and (d)
(g) All of the above
(h) None of the above

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

(a) $< \sin x \,|\, x \,|\, \cos x >$
(b) $< \sin^2 x \,|\, x \,|\, \cos^2 x >$
(c) $<$ f | $[A, B]$ | g $>$ where A and B commute
(d) $< \Psi_m \,|\, \mathrm{H} \,|\, \Psi_n >$ where Ψ_m and Ψ_n are non-degenerate stationary states
(e) $< f \,|\, g > - < g \,|\, f >^*$
(f) $<\boldsymbol{\mu}_{mn}>$ for a forbidden transition
(g) (a), (d) and (e)
(h) (b), (c), and (f)

12. 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
(b) The ionization potential is equal to the work function
(c) The one-electron atom is like a particle in a box
(d) The Coulomb potential is quantized
(e) The angular momentum of the electron is quantized
(f) (a) and (b)
(g) (b) and (d)
(h) None of the above

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13. Which of the following statements about the Heisenberg uncertainty principle are true?

(a) When two operators do not commute, we can simultaneously know the expectation values of those operators to perfect accuracy

(b) Two eigenfunctions of a Hermitian operator cannot be perfectly degenerate

(c) $\sigma_A \sigma_B \geq \frac{1}{2}\langle [A,B] \rangle^2$

(d) $\sigma_A^2 \sigma_B^2 \geq -\frac{1}{4}\langle [A,B] \rangle^2$

(e) When two operators are Hermitian, we cannot simultaneously know the expectation values of those operators to perfect accuracy

(f) (c) and (d)

(g) (b) and (e)

(h) (a), (c) and (d)

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

(a) It must be continuous

(b) It may take on complex values

(c) It must be quadratically integrable

(d) It must be equal to its complex conjugate

(e) Its square modulus has units of probability density

(f) It must be an eigenfunction of the momentum operator

(g) (d) and (f)

(h) (a), (b), (c), and (e)

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

(a) Its Schrödinger equation is $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - E\right)\Psi(x) = 0$

(b) It may be regarded as having a wave function that is the superposition of a left-moving particle and a right-moving particle

(c) Its energy levels are all non-negative

(d) Its energy levels are quantized

(e) Valid wave functions include $\Psi(x) = Ae^{ikx} + Be^{-ikx}$ where $k = \frac{\sqrt{2mE}}{\hbar}$

(f) Valid wave functions include $\Psi(x) = N\cos kx$ where N is a normalization constant and k is defined in (e) above

(g) All of the above

(h) None of the above

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16. 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 = 8?

(a) Since this wave function is not an eigenfunction of the Hamiltonian the question cannot be answered

(b) $< \Psi \mid p_x^2 \mid \Psi >$

(c) 64 times the energy of the ground state

(d) $\dfrac{32\pi^2\hbar^2}{mL^2}$

(e) $8\hbar^2 / mL^2$

(f) (c) and (d)

(g) (b) and (e)

(h) None of the above

17. What is the variance in the position operator x for the particle-in-a-box wave function above?

(a) $\dfrac{L^2}{12} - \dfrac{L^2}{2n^2\pi^2}$

(b) $<x^2> + (<x>)^2$

(c) It depends on the particle mass m

(d) $8h^2 / mL^2$

(e) Zero

(f) (c) and (e)

(g) (b) and (d)

(h) (b), (c), and (e)

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

(a) x

(b) x^3

(c) e^{ix}

(d) $\sin x$

(e) Any eigenfunction of the Hamiltonian

(f) (b) and (d)

(g) (a), (b), and (d)

(h) (b), (d), and (e)

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19. Which of the following statements about spectroscopic transitions between different particle-in-a-box energy levels are *true*?

(a) Transitions are only allowed between levels of the same parity

(b) Transition energies are not quantized

(c) Forbidden absorptions correspond to allowed emissions

(d) Spectroscopic transitions are accompanied by changes in $<x>$

(e) Spectroscopic transitions are accompanied by changes in kinetic energy

(f) (c) and (d)

(g) (b) and (e)

(h) (a), (c), and (d)

20. What is the commutator of $-x$ and p_x (in that order)?

(a) $[p_x,x]$

(b) $[x,p_x]$

(c) $h / 4\pi$

(d) $ih / 2\pi$

(e) $-[p_x,x]$

(f) Zero

(g) (b), (d), and (e)

(h) (b), (c), (d), and (e)

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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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