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Chemistry 3502/4502

Exam II

February 27, 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

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1. What is the eigenvalue of L_z for Ψ if the eigenvalue of L^2 for Ψ is $25\hbar^2$ and the eigenvalue of L_x for Ψ is $-4\hbar$?

(a) The Heisenberg uncertainty principle dictates that Ψ cannot be an eigenfunction for L_z

(b) $16\hbar^2$

(c) $4i\hbar^2$

(d) $\pm 4\hbar$

(e) $\pm 3\hbar$

(f) 0

(g) π

(h) None of the above

2. For a spin-free hydrogenic wave function, which of the below relationships between quantum numbers is/are always true?

(a) $n > l > m_l$

(b) $n = l > m_l$

(c) $n > l + m_l$

(d) $n > l \geq m_l$

(e) $n = l + m_l$

(f) (b) and (c)

(g) (b) and (e)

(h) None of the above

3. What is the ground-state ionization potential for a one-electron atom having atomic number Z?

(a) Z^2 a.u.

(b) The negative of the energy of the electron in the 1s orbital

(c) $(1/2)Z^2$ a.u.

(d) $2Z^2$ a.u.

(e) 1 a.u.

(f) The energy required to infinitely separate the nucleus and electron

(g) (b), and (d)

(h) (b), (c), and (f)

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4. Which of the following statements is/are *false* for a given set of QMHO wave functions corresponding to the same harmonic potential V?

(a) The ground state energy is zero, i.e., the bottom of the potential

(b) The number of nodes is equal to $n+1$, where n is the energy level

(c) $\langle T \rangle_n = \langle V \rangle_n = \langle E \rangle_n$

(d) The wave functions have zero amplitude beyond the classical turning points

(e) The wave functions are not eigenfunctions of the parity operator

(f) The selection rule for spectroscopic transitions is $n \rightarrow n \pm 2$

(g) (c), (e), and (f)

(h) All of the above

5. An electron of spin β is in a 5f orbital. Which of the below sets of quantum numbers (n, l, m_l, m_s) might describe such an electron?

(a) (5, 4, 4, –1/2)

(b) (5, 2, 2, –1/2)

(c) (5, 3, 0, –1/2)

(d) (5, 3, 0, –7/2)

(e) (5, 3, 2, –1/2)

(f) (c) and (e)

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

(h) None of the above

6. For the diatomic molecule CD, where C has atomic mass 12 and D has atomic mass 2, what is the reduced mass?

(a) 7 / 12

(b) 12 / 7

(c) 1 / 7

(d) 2 / 7

(e) 10

(f) It depends on the vibrational state

(g) Cannot be determined from information given

(h) None of the above

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7. Which of the following statements about angular momentum operators and their eigenvalues and eigenfunctions is/are *true*?

(a) $L_+ = -(L_-)^*$

(b) $\langle L^2 \rangle = \langle L_z \rangle^2$ whenever $m_l = l$

(c) For each value of l there are $2l$ possible values of m_l

(d) The *real* spherical harmonics are not all eigenfunctions of L_z

(e) $[L_x, L_y] = 2\hbar L_z$

(f) $\langle Y_{l,0}|T|Y_{l,0}\rangle > \langle Y_{l',0}|T|Y_{l',0}\rangle$ if $l < l'$

(g) (b) and (f)

(h) All of the above

8. Which of the following wave functions has a degeneracy of 2?

(a) Particle in a box, level $n = 8$

(b) Rigid rotator, $l = 4$

(c) Quantum mechanical harmonic oscillator, level $n = 25$

(d) Spin-free hydrogenic wave function, $n = 6$, $l = 1$

(e) Spin-free hydrogenic wave function, $n = 4$

(f) Relativistic free electron at rest

(g) (b) and (f)

(h) (a) through (f) are all singly degenerate

9. For a diatomic rigid rotator having reduced mass 3 and bond length 2 a.u., which of the following statements is/are *true*?

(a) The ground-state energy is $2B$

(b) The energy separation between the first and second excited states is $(1/6)$ a.u.

(c) The rotational constant B is $(1/2)$ a.u.

(d) Transition from the ground state to the state $J = 1$ is forbidden

(e) The moment of intertia is 6 a.u.

(f) (a) and (b)

(g) (e) and (f)

(h) None of the above

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10. Which of the below statements about electron spin is/are *false*?

(a) The spin quantum number comes from including relativity in the electronic Schrödinger equation

(b) Spin couples with orbital angular momentum according to $\mathbf{J} = \mathbf{L} - \mathbf{S}$

(c) For a single electron, the only eigenvalues of S_z are $\pm(1/2)\hbar$

(d) Stern and Gerlach discovered electron spin by studying the magnetic moments of Ag atoms

(e) Spin-orbit coupling is proportional to the 4th power of the atomic number

(f) (a) and (c)

(g) (a), (c), and (d)

(h) All of the above

Short answer. Show that by proper choice of a, the function e^{-ar^2} is an eigenfunction of the operator

$$\left[\frac{d^2}{dr^2} - qr^2\right]$$

where q is a constant. What is the name of the general class of functions represented by e^{-ar^2}? How many nodes does this function have over r?

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Some Potentially Useful Mathematical Formulae

Trigonometric Relations

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

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

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

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

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

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

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

Integrals

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

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

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

$$\int_0^\infty r^n e^{-2r}dr = \frac{n!}{2^{n+1}}$$

Some Operators

$x \equiv$ multiply by x

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

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

$$H = T + V$$

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

$$\mathbf{L} \equiv \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ -i\hbar\frac{\partial}{\partial x} & -i\hbar\frac{\partial}{\partial y} & -i\hbar\frac{\partial}{\partial z} \end{vmatrix}$$

$L_+ = L_x + iL_y$ and $L_- = L_x - iL_y$

Complex Relations

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

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

Spherical Polar Volume Element

$$r^2 dr \sin\theta d\theta d\phi$$

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