

C

1. 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 | (e) 10  |
| (b) 12 / 7 | (f) It depends on the vibrational state         |
| (c) 1 / 7  | (g) Cannot be determined from information given |
| (d) 2 / 7  | (h) None of the above                           |

2. 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         | (e) The wave functions are not eigenfunctions of the parity operator            |
| (b) The number of nodes is equal to $n+1$ , where $n$ is the energy level      | (f) The selection rule for spectroscopic transitions is $n \rightarrow n \pm 2$ |
| (c) $\langle T \rangle_n = \langle V \rangle_n = \langle E \rangle_n$          | (g) (c), (e), and (f)   |
| (d) The wave functions have zero amplitude beyond the classical turning points | (h) All of the above  |

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

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|---|---|
| (a) $L_+ = -(L_-)^*$  | (e) $[L_x, L_y] = 2\hbar L_z$   |
| (b) $\langle L^2 \rangle = \langle L_z \rangle^2$ whenever $m_l = l$        | (f) $\langle Y_{l,0}   T   Y_{l,0} \rangle > \langle Y_{l',0}   T   Y_{l',0} \rangle$ if $l < l'$ |
| (c) For each value of $l$ there are $2l$ possible values of $m_l$           | (g) (b) and (f)   |
| (d) The <i>real</i> spherical harmonics are not all eigenfunctions of $L_z$ | (h) All of the above  |

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

- |  |                       |
|--|-----------------------|
| (a) The Heisenberg uncertainty principle dictates that $\Psi$ cannot be an eigenfunction for $L_z$ | (e) $\pm 3\hbar$      |
| (b) $16\hbar^2$  | (f) 0                 |
| (c) $4i\hbar^2$  | (g) $\pi$             |
| (d) $\pm 4\hbar$   | (h) None of the above |

5. 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 $2B$   | (e) The moment of inertia is 6 a.u. |
| (b) The energy separation between the first and second excited states is $(1/6)$ a.u. | (f) (a) and (b)                     |
| (c) The rotational constant $B$ is $(1/2)$ a.u.                                       | (g) (e) and (f)                     |
| (d) Transition from the ground state to the state $J = 1$ is forbidden                | (h) None of the above               |

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

- |                      |                       |
|----------------------|-----------------------|
| (a) $n = l > m_l$    | (e) $n = l + m_l$     |
| (b) $n > l \geq m_l$ | (f) (b) and (c)       |
| (c) $n > l + m_l$    | (g) (b) and (e)       |
| (d) $n > l > m_l$    | (h) None of the above |

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7. Which of the below statements about electron spin is/are *false*?
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|---|---|
| (a) The spin quantum number comes from including relativity in the electronic Schrödinger equation                          | (e) Spin-orbit coupling is proportional to the 4th power of the atomic number |
| <input type="checkbox"/> (b) Spin couples with orbital angular momentum according to $\mathbf{J} = \mathbf{L} - \mathbf{S}$ | (f) (a) and (c)   |
| (c) For a single electron, the only eigenvalues of $S_z$ are $\pm(1/2)\hbar$  | (g) (a), (c), and (d)   |
| (d) Stern and Gerlach discovered electron spin by studying the magnetic moments of Ag atoms                                 | (h) All of the above  |
8. An electron of spin  $\beta$  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, $-1/2$ ) | (e) (5, 3, 2, $-1/2$ )                   |
| (b) (5, 2, 2, $-1/2$ ) | <input type="checkbox"/> (f) (c) and (e) |
| (c) (5, 3, 0, $-1/2$ ) | (g) (b), (c), (d) and (e)                |
| (d) (5, 3, 0, $-7/2$ ) | (h) None of the above                    |
9. What is the ground-state ionization potential for a one-electron atom having atomic number  $Z$ ?
- |  |  |
|--|--|
| (a) $Z^2$ a.u.   | (e) 1 a.u.   |
| (b) The negative of the energy of the electron in the 2s orbital | (f) The energy required to promote the electron to the first excited state |
| <input type="checkbox"/> (c) $(1/2)Z^2$ a.u.                     | (g) (b), and (d)   |
| (d) $2Z^2$ a.u.  | (h) (b), (c), and (f)  |

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10. Which of the following wave functions has a degeneracy of 2?
- |  |   |
|--|---|
| (a) Particle in a box, level $n = 8$                       | (e) Spin-free hydrogenic wave function, $n = 4$ |
| (b) Rigid rotator, $l = 4$                                 | (f) Relativistic free electron at rest          |
| (c) Quantum mechanical harmonic oscillator, level $n = 25$ | (g) (b) and (f)                                 |
| (d) Spin-free hydrogenic wave function, $n = 6, l = 1$     | (h) (a) through (f) are all singly degenerate   |

**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  $r$ ?

To show that  $e^{-ar^2}$  is an eigenfunction with proper choice of  $a$  we require

$$\left[ \frac{d^2}{dr^2} - qr^2 \right] e^{-ar^2} = ze^{-ar^2}$$

Evaluating the l.h.s. we have

$$\begin{aligned} \left[ \frac{d^2}{dr^2} - qr^2 \right] e^{-ar^2} &= -2ae^{-ar^2} + 4a^2r^2e^{-ar^2} - qr^2e^{-ar^2} \\ &= -\left[ 2a + (q - 4a^2)r^2 \right] e^{-ar^2} \end{aligned}$$

and for the prefactor on the r.h.s. to be a constant (so as to satisfy the eigenvalue condition) it must be true that  $a$  is  $\sqrt{q}/2$  in which case the eigenvalue will be  $-2a$ , which is simply  $-\sqrt{q}$ .

The general class of functions here are “gaussian” functions. A gaussian has no nodes over  $r$ .

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