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Physics 3 Test #1-repeated
Quantum Mechanics

1 Theoretical questions

(answer them in short and clear sentences including the necessary formulas when needed)

1. Enumerate the phenomena that lead to the development of quantum physics. (**1 point**)
   Solution:
   - *Black body radiation*
   - *(external) Photoelectric effect*
   - *Compton effect*
   - *Stability of atoms*
   - *Line spectrum of atoms*
   - *Frank-Hertz experiment*

2. What is the difference between the behavior of a classical particle and a wave? What is the wave-particle duality? (**1 point**)
   Solution:
   A classical particle has a well defined position and velocity (momentum), i.e. a well defined trajectory. A classical wave presents diffraction and interference phenomena. Wave particle duality - under suitable circumstances the quantum mechanical particle behaves like either a wave or a particle.
   Background info: the particle's behavior is described by a probability (density) wave whose absolute square gives the probabilities. When in a process the probabilities can be added to get the resultant probability (example: two electrons in two separate atoms, when the electronic wave functions do not interlap) then the particle behaves like a classical particle, and when the amplitudes of the waves must be added to get the resulting amplitude (example: 2 slits experiment) we got diffraction.

3. What is tunneling? Give the most important characteristics. (**1 point**)
   Solution:
   Tunneling is the phenomena when a particle, with a total energy less than the potential in a region of space still may pass through this region, although in classical mechanics this would be impossible. In 1D the transition probability decreases fast when either the width of the region or the height of the potential barrier increases.

4. What physical quantity do we call "potential" in quantum mechanics (**1 point**)
   Solution:
   The "potential" in quantum mechanics is called the potential energy in classical physics.

5. What do we call an atomic orbital? What is a molecular orbital? (**1 point**)
   Solution:
   An atomic orbital is the wave function of the electron inside the atom. The molecular orbital is the same for a molecule. (In chemistry the same term may be applied to the region of space where the electron is found with suitable high (e.g. 90%) probability.)
   Background info:

6. How can we determine the solution of the time-dependent Schrödinger equation from the solutions of the stationary equation? (**1 point**)
   Solution:
   The eigenfunctions of the time dependent Schrödinger equation are the products of the eigenfunctions of the corresponding stationary Schrödinger equation and the function $e^{-E/\hbar t}$. Therefore the solution of the time dependent equation may be written as a linear combination of such products.
   In 1D e.g.:
   $$\psi(x,t) = \sum_E \phi_E(x) e^{-E/\hbar t}$$

7. What are selection rules and what do they mean? (**1 point**)
   Solution:
   Selection rules constrain the possible transitions of a system. They can be formulated for electronic, vibrational or rotational transitions. Examples: for electronic transitions the total angular momentum difference between the initial and final states must be an integer multiple of $\hbar$. Transitions prohibited by a selection rule may still happen by allowing other kind of interactions taking place. Usually these transitions have a much smaller probability than the one prohibited by the selection rule.

8. Is it always true that the wave function of a system of electrons must be antisymmetric for the exchange of the coordinates of two electrons? Explain. (**1 point**)
   Solution:
   False. The total wave function (including the spin) of a system of electrons must always be antisymmetric to the exchange of the coordinates of two electrons. This wave function can be written as a product of two functions. One that depend on the spatial coordinates of the electrons the other one depends on their spin. So when the spin dependent part is antisymmetric the spatial coordinate dependent part must be symmetric.

9. What is hybridization? (**1 point**)
   Solution:
   Hybridization means the mixing of atomic orbitals to create orbitals which qualitatively describe the atomic bonding in molecules. Their name is derived from the corresponding atomic orbitals used. Example: an sp^3 orbital is the linear combination of one s and 3 p orbitals (like in CH_4)

10. What are the assumptions of the Bose-Einstein and of the Fermi-Dirac statistics? (**1 point**)
    Solution:

Both statistics are valid for indistinguishable particles. Fermi-Dirac statistics is valid for half-spin particles called fermions (like electrons) where no two particle may occupy the same quantum state, while Bose-Einstein statistics is valid for particles of integer spin (bosons), where any number of particles may be in the same quantum state.

2 Problems

Useful constants: $h = 6.63\,10^{-34}\,Js$, $e = 1.6\,10^{-19}\,C$, $m_e = 9.1\,10^{-31}\,kg$

11. What is the acceleration voltage in an electron gun, if the average wavelength of the emitted electrons is 3.1 nm? (**2 points**)

    Solution:

    $$p = \frac{h}{\lambda}, \quad E = \frac{p^2}{2m_e} = e\Delta U \quad \Rightarrow \Delta U = \frac{p^2}{2\,m_e\,e} = \frac{h^2}{2\,m_e\,e\,\lambda^2}$$

    $$\Delta U = \frac{(6.63\,10^{-34})^2}{2 \cdot 9.1\,10^{-31} \cdot 1.6\,10^{-19} \cdot (3.1\,10^{-9})^2} = 0.16V$$

12. An electron is confined in a 3D potential box with sides $10\mu m$, $20\mu m$ and $30\mu m$. Give the energy and degeneracy of the 3 lowest states. (**2 points**)

    Solution:

    The possible energy levels in one direction:

    $$E_n = \frac{h^2}{8\,m_e\,L^2}n^2$$

    therefore in 3D

    $$E_{n_1,n_2,n_3} = \frac{h^2}{8\,m_e}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right)$$

    $$= 6.02\,10^{-28}\left(\frac{n_1^2}{1} + \frac{n_2^2}{4} + \frac{n_3^2}{9}\right)[J]$$

    $$= 3.76\,10^{-9}\left(\frac{n_1^2}{1} + \frac{n_2^2}{4} + \frac{n_3^2}{9}\right)[eV]$$

    The 3 lowest lying energy states can be determined by trying out different combinations of the 3 numbers and selecting the 3 smallest values:

n_1	n_2	n_3	factor
1	1	1	1.36
1	1	2	1.47
1	2	1	1.61
2	1	1	2.36
2	2	1	2.61
1	2	2	1.72
1	1	3	1.58

From this table the indices for the 3 lowest levels are: (1,1,1), (1,1,2) and (1,2,1).

The corresponding energies and degeneracies:

Energy level	$E(\times 10^{-28}\ J)$	$E(\times 10^{-9}\ eV)$	degeneracy
E_{111}	8.20	5.11	1
E_{112}	8.87	5.53	1
E_{121}	12.7	7.94	1
E_{113}	13.6	8.46	1
E_{122}	14.7	9.19	1
E_{211}	26.3	16.39	1
E_{212}	28.3	17.7	1
E_{221}	30.8	19.2	1
E_{222}	32.8	20.47	1

13. An electron gun emits electrons with energies between 3.2 keV and 3.3 keV. What is the minimum uncertainty of the position of the electrons?(**2 points**)

Solution:

Because

$$U = \frac{p^2}{2\,m_e\,e}$$

$$p = \sqrt{2\,m_e\,e\,U},$$

and

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$

and

$$\Delta p = p_2 - p_1 = \sqrt{2\,m_e\,e\,U} - \sqrt{2\,m_e\,e\,U}$$
$$= 3.1036419\,10^{-23} - 3.0562553\,10^{-23} = 4.74\,10^{-25}\ kg\,m^2/s^2$$

$$\Delta x = \frac{\hbar}{2\,\Delta p} = 1.11\,10^{-10}\ m$$

Using $h/2$ instead of $\hbar/2$ would give $6.99\,10^{-10}$ m, while with h this would be $1.39\,10^{-9}$ m.

14. The Zeeman components of a 500 nm spectral line are 0.0116 nm apart when the magnetic field is 1.00 T. Find the e/m_e ratio for the electron from these data. (**2 points**)

Solution:

The magnitude of the energy shift from the given $\Delta\lambda$ value is

$$\Delta E_B = h\,\Delta\nu = h\left(\frac{c}{\lambda_2} - \frac{c}{\lambda_1}\right) = \frac{c\,h}{\lambda_1\,\lambda_2}(\lambda_1 - \lambda_2) = -\frac{c\,h\,\Delta\lambda}{\lambda_1\,\lambda_2}$$

Where $\lambda_{1,2} = \lambda \pm \Delta\lambda/2$. But $\Delta\lambda \ll \lambda$ therefore in the denominator $\lambda_1\,\lambda_2 \approx \lambda^2$.

$$|\Delta E_B| = \frac{h\,c\,\Delta\lambda}{\lambda^2} = \frac{6.63 \cdot 10^{-34} \cdot 3 \cdot 10^8 \cdot 0.0116 \cdot 10^{-9}}{(500 \cdot 10^{-9})^2} = 9.22\,10^{-24}\,J$$

For the Zeeman effect

$$\Delta E_B = \frac{e}{2m_e}\mathbf{L} \cdot \mathbf{B}$$

$$\frac{e}{m_e} = \frac{2\,|\Delta E_B|}{L \cdot B}$$

Substituting ΔE_B and taking L and B parallel, $B = 1\,T$ and $L = 1\,\hbar$

$$\frac{e}{m_e} = \frac{2 \cdot 9.22 \cdot 10^{-24}}{1.05 \cdot 10^{-34}} = 1.748\,10^{11}$$

The exact value is $1.76\,10^{1}1$

15. The un-normalized wave function of an electron is $\psi(x) = 12x^2 - 8x$ Calculate the kinetic energy of this electron. (**2 points**)

   Solution:

   The kinetic energy is determined from the formula:

$$< E_{kin} >= \frac{\int_{-\infty}^{\infty} \psi^*(x)\frac{\hat{p}^2}{2m_e}\psi(x)dx}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx}$$

   where the denominator contains the normalization factor. For our wave function both integrals are infinite, so this function is not a physical wave function in the whole space. After integration the numerator contains 3rd an 2nd powers of x, while the one in the denominator (the normalization factor) contains 5th and 4th power of x too. If we now set the limits of the integration to $\pm a$ and calculate the limit of this fraction as a tends to ∞ we may see that the denominator goes faster to infinity than the numerator does, i.e. the value of kinetic energy tends to 0.