

Physics 3

Test
2012. March 20.

Useful constants: $h = 6.63 \cdot 10^{-34}$ Js, $e = 1.6 \cdot 10^{-19}$ C, $m_e = 9.1 \cdot 10^{-31}$ kg, $L_A = 6.022 \cdot 10^{23}$ 1/mol

Theoretical questions:

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

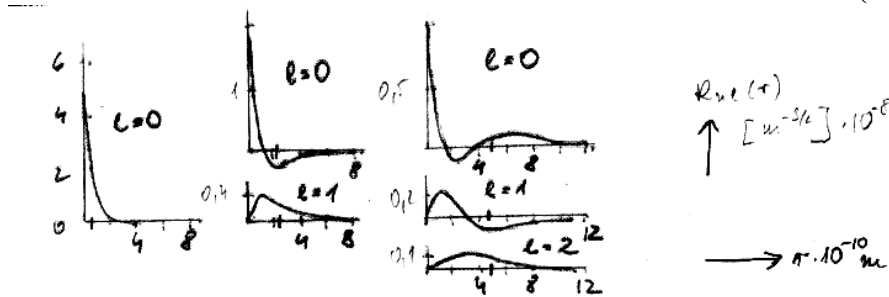
- “Observable electron interference patterns are formed only when there are many electrons present in a system at the same time and they interact with each other. A series of non-interacting single electrons does not create an interference pattern, no matter how many electrons are used”- Is this statement true or not? Explain! **(1 point)**
False. Interference patterns are formed, because every electron has a wave like state function. It doesn't matter how many electrons are simultaneously present, only the number of the electrons that matters

- We know all of the stationary $\phi_n(\mathbf{r})$ eigenfunctions and E_n eigenvalues of a Hamiltonian and we know the actual $\psi(\mathbf{r}) = \psi(\mathbf{r}, 0)$ function of a system at $t=0$. Write the formula for the time dependent $\psi(\mathbf{r}, t)$ wave function! **(1 point)**

$$\psi(\mathbf{r}) = \sum_n C_n \phi_n(\mathbf{r})$$

$$\psi(\mathbf{r}, t) = \sum_n C_n \phi_n(\mathbf{r}) \exp\left(-\frac{E_n}{\hbar}t\right)$$

- Sketch the radial part of the wave function of the hydrogen atom for $n=1$ and $n=2$! **(2 points)**



- Why is state $2s$ called a metastable state in a hydrogen atom? **(1 point)**

The transition $2s \rightarrow 1s$ is forbidden because in the first order (dipole) approximation only transitions between states whose angular momentum difference is $(\pm 1 \hbar)$ are allowed (the photon has a spin of 1) and states $2s$ and $1s$ have the same $l = 0$ angular momentum.

This transition may nevertheless occur, albeit with a far smaller probability, because higher order (non dipole) processes may also take place.

5. What is the meaning of the term “spin-orbit interaction”? **(2 points)**

In electronic states with non zero angular momentum there is a non zero \mathbf{B} ($\sim \mathbf{L}$) magnetic field in the coordinate system attached to the electron. This magnetic field interacts with the magnetic momentum that corresponds to (and proportional to) the electron spin \mathbf{S} . The interaction energy therefore $E_{SL} = \text{const } \mathbf{S} \cdot \mathbf{L}$.

Problems:

1. Consider the following hypothetical wave function for a particle confined in the region $-7 \leq x \leq 10$: $\psi(x) = A(70 + 3x - x^2)$ inside the region and 0 outside it

a) Sketch the wave function

Inverted parabola with peak $A \cdot 72.25$ at position 1.5

b) Normalize this wave function over the range the particle is confined in.

$$\int_{-7}^{10} |\psi(x)|^2 dx = 1 \Rightarrow A^2 \int_{-7}^{10} (70 + 3x - x^2)(70 + 3x - x^2) dx =$$

$$= A^2 \int_{-7}^{10} (4900 + 9x^2 + x^4 + 420x - 131x^2 - 6x^3) dx =$$

$$= A^2 [4900x + 3x^3 + 1/5 x^5 + 210x^2 - 131/3 x^3 - 6/4 x^4]_{-7}^{10} =$$

$$= A^2 * 51357.566666667 = 1 \Rightarrow A = 1 / 226.6221 = 4.41263 * 10^{-3}$$

$$\boxed{\psi(x) = 4.41263 \cdot 10^{-3} (70 + 3x - x^2)}$$

c) Determine the expectation value $\langle x \rangle$ using the normalized wave function.

$$\text{Expectation value of quantity } \langle O \rangle = \int_{-7}^{10} \psi^*(x) O \psi(x) dx$$

$$\langle x \rangle = 1.9471 * 10^{-5} \int_{-7}^{10} (4900x + 9x^3 + x^5 + 420x^2 - 131x^3 - 6x^4) dx$$

$$= 1.9471 * 10^{-5} [2450x^2 + 9/4 x^4 + 1/6 x^6 + 420/3 x^3 - 131/4 x^4 - 6/5 x^5]_{-7}^{10} =$$

$$= 1.7152$$

d) Again, using the normalized wave function, calculate the expectation value of the kinetic energy of the particle. **(4 points)**

$$\langle E_{kin} \rangle = \int_{-7}^{10} \psi^*(x) \left(\frac{-\hbar^2}{2m} \right) \frac{d^2 \psi(x)}{dx^2} dx = 1.9471 \cdot 10^{-5} \left(\frac{-\hbar^2}{2m} \right) \int_{-7}^{10} (70 + 3x - x^2) (-2) dx^2 =$$

$$1.9471 \cdot 10^{-5} \left(\frac{-\hbar^2}{2m} \right) \int_{-7}^{10} (-140 - 6x + 2x^2) dx$$

$$= 1.9471 \cdot 10^{-5} \left(\frac{-\hbar^2}{2m} \right) [-140x - 3x^2 + 2/3 x^3]_{-7}^{10} = 9.7377 \cdot 10^{-34} \text{ J} = 6.07 \cdot 10^{-15} \text{ eV}$$

2. Prove the following commutation relationships of operators A, B and C

$$[A + B; C] = [A, C] + [B, C]$$

$$[A, B C] = [A, B] C + B [A, C]$$

(1 point)

$$[a+b, c] = (a+b)c - c(a+b) = ac + bc - ca - cb = (ac - ca) + (bc - cb) = [a, c] + [b, c]$$

$$[a, bc] = a(bc) - (bc)a = a(bc) + b(ac) - b(ac) - (bc)a = (ab)c - (ba)c + b(ac) - b(ca) = [a, b]c + b[c, a]$$

3. What are the frequencies of the photons a rotating O₂ molecule can absorb in a transition between its 3rd and 4th energy state? (M_O = 31.9989 g/mol, d_O = 0.1208 nm)

(2 points)

This derivation is not required, knowing either of the resulting formulas (in gray) is enough

$$H = \frac{1}{2} \Theta \omega^2, \mathbf{L} = \Theta \boldsymbol{\omega} \Rightarrow H = \frac{L^2}{2\Theta}, [L, L_z] = 0 \Rightarrow L_z^2 \text{ has the same}$$

eigenfunctions than H, but the eigenvalues will differ. If the eigenvalue of L_z² is l² then the eigenvalue of L² is l(l+1).

$$L^2 = -\hbar^2 \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \text{ and } L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

$$\text{Using } L_z^2 \text{ instead of } L^2 \text{ in } H \Rightarrow H = \frac{L_z^2}{2\Theta}, L_z \psi = E \psi \Rightarrow -\frac{\hbar^2}{2\Theta} \frac{\partial^2 \psi}{\partial \phi^2} = E \psi$$

$$\psi(\phi) = A \exp\left(\pm i \sqrt{\frac{2\Theta E}{\hbar^2}} \phi\right)$$

ψ must be single valued: ψ(φ+2π) = ψ(φ) =>

$$E = \frac{\hbar^2}{2\Theta} n^2, \text{ where } n = 0, \pm 1, \pm 2, \dots$$

The exact result using L² instead of L_z then :

$$E = \frac{\hbar^2}{2\Theta} n(n+1), \text{ where } n = 0, \pm 1, \pm 2, \dots$$

For the O₂ molecule Θ = 2 m_O (d/2)², m_O = M_O / N_A = 31,9989 / 6.022 × 10²³ = 5.31 × 10⁻²³ kg, Θ = 3.88 × 10⁻⁴³ kgm²

$$E_1 = 1.43 \times 10^{-26} \text{ J} * n^2 = 8.95 \times 10^{-8} \text{ eV} * n^2$$

$$E_3 = 9E_1 = 8.06 \times 10^{-7} \text{ eV}, E_4 = 16E_1 = 1.43 \times 10^{-6} \text{ eV},$$

$$\Delta E_{3 \rightarrow 4} = -6.27 \times 10^{-7} \text{ eV} = 1.003 \times 10^{-25} \text{ J}$$

$$\nu = \Delta E_{3 \rightarrow 4} / h = 1.51 \times 10^8 \text{ Hz}$$

or with the correct n(n+1)

$$E_3 = 12E_1 = 1.07 \times 10^{-6} \text{ eV}, E_4 = 20E_1 = 1.79 \times 10^{-6} \text{ eV},$$

$$\Delta E_{3 \rightarrow 4} = -7.16 \times 10^{-7} \text{ eV} = 1.147 \times 10^{-25} \text{ J}$$

$$\nu = \Delta E_{3 \rightarrow 4} / h = 1.73 \times 10^8 \text{ Hz}$$

4. What are the four lowest lying state in a spherical harmonic oscillator in 3 dimensions? What will be the degeneracy of the levels?

The potential in this case is $V(\mathbf{r}) = \frac{1}{2} m \omega (x^2 + y^2 + z^2)$ **(1 point)**

in 1 dimension $E = \hbar \omega (n + \frac{1}{2})$,

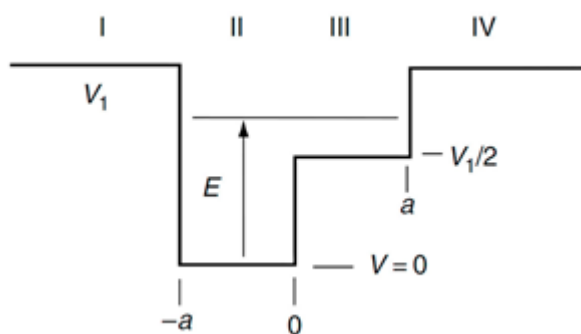
in 3D: $E = \hbar \omega (n_x + n_y + n_z + \frac{1}{2} + \frac{1}{2} + \frac{1}{2})$

n_x	n_y	n_z	E	Degeneracy
0	0	0	$3/2 \hbar \omega$	1
1	0	0	$5/2 \hbar \omega$	3
0	1	0		
0	0	1		
1	1	0	$7/2 \hbar \omega$	3
1	0	1		
0	1	1		

5. Consider a one-dimensional rectangular potential well structure such as shown here: Write the wave functions in regions I through IV and the equations (but do not try to solve these equations) describing the boundary conditions on these wave functions **(3 points)**

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Schrödinger equation:

$$-\frac{\hbar^2}{2m_e} \frac{d^2 \psi}{dx^2} + V \psi = E \psi$$

Because the potential is constant the solutions of Schrödinger easy to get:

$$\psi = C_+ \exp\left(i \frac{\sqrt{2m_e(E - V)}}{\hbar} x\right) + C_- \exp\left(-i \frac{\sqrt{2m_e(E - V)}}{\hbar} x\right)$$

Region I. $E < V_1$

$$\sqrt{2m_e(E - V_1)} = i \sqrt{2m_e(V_1 - E)},$$

$$\text{Let } q_1 = \frac{\sqrt{2m_e(V_1 - E)}}{\hbar}$$

$$\psi_I(x) = A e^{q_1 x}$$

and no $e^{-q_1 x}$ because otherwise ψ would increase with decreasing x

Region II. $E > V_{II} = 0$

$$\text{Let } k_2 = \frac{\sqrt{2m_e E}}{\hbar}$$

$$\psi_{II}(x) = B e^{i k_2 x} + C e^{-i k_2 x}$$

Region III. $E > V_{II} = V_1/2$

$$\text{Let } k_3 = \frac{\sqrt{2m_e(E - V_{II})}}{\hbar} = \frac{\sqrt{2m_e(E - V_1/2)}}{\hbar}$$

$$\psi_{III}(x) = D e^{i k_3 x} + E e^{-i k_3 x}$$

Region IV $E < V_{IV} = V_1$

similar to region I only now the member with the minus sign remains and q is the same

$$\psi_{IV}(x) = F e^{q_1 x}$$

The boundary conditions:

$\psi_I(-a) = \psi_{II}(-a)$ $\psi_I'(-a) = \psi_{II}'(-a)$	$A e^{-q_1 a} = B e^{-i k_2 a} + C e^{i k_2 a}$ $q_1 A e^{-q_1 a} = i k_2 (B e^{-i k_2 a} - C e^{i k_2 a})$
$\psi_{II}(0) = \psi_{III}(0)$ $\psi_{II}'(0) = \psi_{III}'(0)$	$B + C = D + E$ $k_2(B - C) = k_3(D - E)$
$\psi_{II}(a) = \psi_{IV}(a)$ $\psi_{II}'(a) = \psi_{IV}'(a)$	$F e^{-q_1 a} = D e^{-i k_3 a} + E e^{i k_3 a}$ $-q_1 F e^{-q_1 a} = i k_2 (D e^{-i k_2 a} - E e^{i k_2 a})$

6. Draw the formulas and sketch the curves for statistics Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein! **(1 point)**

$$f_{MB}(E) \sim \exp(-(E-\mu)/k_B T)$$

$$f_{BE}(E) = 1/(\exp(E-\mu)/k_B T - 1)$$

$$f_{FD}(E) = 1/(\exp(E - \mu)/k_B T + 1)$$

T(K)

distribution function: $\frac{1}{e^{\frac{E-\mu}{kT}} + \epsilon}$

$\langle N(E) \rangle$

2.0

1.5

1.0

0.5

0.0

- Bose-Einstein, $\epsilon = -1$
- Maxwell-Boltzmann, $\epsilon = 0$
- Fermi-Dirac, $\epsilon = +1$