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Department of Physics

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74310 QUANTUM MECHANICS 1

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09.00 – 15.00

Allowed aids: Acceptable calculator
Rottmann: Matematisk formelsamling

Three pages with expressions and formulae are enclosed.

Examination results will be available on June 22, 1999.

Problem 1

a) A particle with mass m is in the Coulomb potential

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}.$$

What is the time-dependent Schrödinger equation for the particle?
What is meant by a quantum-mechanical stationary state?

At time $t = 0$ the wave function of the particle is

$$\Psi(\vec{r}, 0) = (3\pi a_0^3)^{-\frac{1}{2}} e^{-r/a_0} + (48\pi a_0^5)^{-\frac{1}{2}} r e^{-r/(2a_0)} \cos\vartheta, \tag{1}$$

where a_0 is the Bohr radius.

Is this wave function a stationary state?
What is the wave function at a later time t?

b) An energy measurement is performed when the particle is in the state (1). What are the possible results, and what are their probabilities?

c) The particle is then in the ground state in the Coulomb potential, with energy E_1^0. A weak constant electric field $\mathcal{E}$ in the z direction, corresponding to the potential

$$H' = -e\mathcal{E}\,z,$$

is applied. Here e is the charge of the particle. Assume that for a weak field the resulting ground-state energy may be expanded as a powers of the field strength:

$$E_1(\mathcal{E}) = E_1^0 + A\mathcal{E} + B\mathcal{E}^2 + \ldots \tag{2}$$

This is the Stark effect.

Use stationary perturbation theory to compute A, and to predict the sign of B.

d) What are the possible results one may obtain if one (for a general state) measures the square $\vec{L}^2$ and the component L_z of the angular momentum?

Let then the particle in the Coulomb potential at $t = 0$ have the following wave function

$$\chi(\vec{r}) = \frac{1}{\sqrt{\pi a_0^3(1+\alpha^2)}} \left(1 + \alpha\frac{z}{a_0}\right)\, e^{-r/a_0}, \tag{3}$$

with a mean energy

$$\langle\chi|H_0|\chi\rangle = -\frac{\hbar^2}{2ma_0^2(1+\alpha^2)}.$$

(This result is given for later use, proof is not required.) Here α is a real parameter, and H_0 is the Hamiltonian of the particle.

What are the possible measurement results for $\vec{L}^2$ and L_z for a particle in the special state (3)?

e) Show that the ground-state energy E_1 for a particle with Hamiltonian operator H never exceeds the Rayleigh-Ritz estimate

$$E_{RR} = \langle f|H|f\rangle = \int f^*(\vec{r})\; H\; f(\vec{r})\; d^3\vec{r},$$

for any function $f(\vec{r})$ that is normalized:

$$\langle f|f\rangle = \int |f(\vec{r})|^2\; d^3\vec{r} = 1.$$

f) Use the function $\chi(\vec{r})$, equation (3), as a trial function to obtain a Rayleigh-Ritz estimate for the Stark effect in the ground state in Coulomb potential, i.e. for the Hamiltonian operator

$$H = H_0 - e\mathcal{E}\,z.$$

It is the coefficient B in power series (2) that is to be determined.

Since $\chi(\vec{r})$ with parameter $\alpha = 0$ is the ground-state wave function with $\mathcal{E} = 0$, α is necessarily small when the electric field is weak. You may therefore simplify the calculation by expanding to second order in α.

g) The electron has spin 1/2. The total angular momentum of an electron is $\vec{J} = \vec{L} + \vec{S}$, where $\vec{L} = \vec{r} \times \vec{p}$ is the orbital angular momentum and $\vec{S}$ is the spin. Denote the quantum numbers for $\vec{L}^2$, L_z, $\vec{S}^2$, S_z, $\vec{J}^2$ and J_z by l, $m_l = m$, $s = 1/2$, m_s, j and m_j, respectively.

Assume now that $l = 1$. Which values are then possible for j and m_j?
Show that the state

$$|\psi\rangle = \sqrt{\tfrac{2}{3}}\;\left|l = 1, s = \tfrac{1}{2}, m_l = 1, m_s = -\tfrac{1}{2}\right\rangle - \sqrt{\tfrac{1}{3}}\;\left|l = 1, s = \tfrac{1}{2}, m_l = 0, m_s = \tfrac{1}{2}\right\rangle$$

is an eigenstate for $\vec{J}^2$ and J_z, and find the eigenvalues. Use, e.g., the relations

$$\vec{J}^2 = \vec{L}^{\,2} + \vec{S}^{\,2} + 2\vec{L}\cdot\vec{S} = \vec{L}^{\,2} + \vec{S}^{\,2} + L_+S_- + L_-S_+ + 2L_zS_z\ ,$$

where $L_\pm = L_x \pm \mathrm{i}L_y$, $S_\pm = S_x \pm \mathrm{i}S_y$, and

$$L_\pm\,|l, s, m_l, m_s\rangle = \hbar\,\sqrt{l(l+1) - m_l(m_l \pm 1)}\;\;|l, s, m_l \pm 1, m_s\rangle\ ,$$
$$S_\pm\,|l, s, m_l, m_s\rangle = \hbar\,\sqrt{s(s+1) - m_s(m_s \pm 1)}\;\;|l, s, m_l, m_s \pm 1\rangle\ .$$

In this state $|\psi\rangle$, what is the probability that $m_s = 1/2$?

Use the attached tables of Clebsch–Gordan-coefficients, and express the state with $l = 1$, $s = 1/2$, $m_l = 0$ and $m_s = 1/2$ as a linear combination of states with different j.

In this last state, what is the probability that $j = 1/2$?

h) Relativistic corrections (spin-orbit coupling) and corrections due to quantization of the electromagnetic field make the energy levels of the hydrogen atom dependent on the main quantum number n, the orbital angular momentum l and in addition on the quantum number j of $\vec{J}^2 = (\vec{L} + \vec{S})^2$. These corrections lift the degeneracy between energy levels with the same main quantum number n but with different values of l. We will neglect here all effects having to do with the electron spin, except for the energy splitting between the energy levels $2s$ og $2p$. Let ΔE denote the energy difference, so that $\Delta E = E_{2s} - E_{2p}$.

What spontaneous transitions between the states $2s$, $2p$ and $1s$ can take place by electric dipole radiation if $\Delta E > 0$, or if $\Delta E < 0$?

i) Assume here that the $2s$ level lies above the $2p$ level, and that the energy difference (known as the Lamb shift) is

$$\Delta E_L = \hbar\omega_L = 4,38\ 10^{-6}\ \text{eV}.$$

A transition from the $2s$ level to the $2p$ level may be induced by an oscillating homogeneous electric field, given by the potential

$$U(z,t) = -e\mathcal{E}\, z\sin(\omega t),$$

where $\mathcal{E}$ and ω are constants.

Use first order time dependent perturbation theory to compute the probability for an induced transition from $2s$ at $t = 0$ to $2p$ at $t = T$. Neglect the electron spin, and assume that the final state has $m_l = m = 0$.

How large must $\mathcal{E}$ be in order that the transition probabilty is $1\,\%$ during one second, when $\omega = \omega_L$?

Is there reason to believe that the first order approximation is good in this case?

Expressions and formulae

Parts of this may be useful.

Energy eigenvalues and eigenfunctions in the Coulomb potential

$$E_n^0 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{1}{n^2} = -\frac{\hbar^2}{2ma_0^2}\frac{1}{n^2}.$$

n	l	ψ_{nlm}	
1	0	$\psi_{100} = (\pi a^3)^{-\frac{1}{2}}\, e^{-r/a}$	$1s$
2	0	$\psi_{200} = (32\pi a^3)^{-\frac{1}{2}}\,(2 - r/a)\, e^{-r/(2a)}$	$2s$
	1	$\psi_{210} = (32\pi a^5)^{-\frac{1}{2}}\, r\, e^{-r/(2a)}\, \cos\vartheta$	$2p$
		$\psi_{211} = (64\pi a^5)^{-\frac{1}{2}}\, r\, e^{-r/(2a)}\, \sin\vartheta\, e^{i\varphi}$	
		$\psi_{21-1} = (64\pi a^5)^{-\frac{1}{2}}\, r\, e^{-r/(2a)}\, \sin\vartheta\, e^{-i\varphi}$	

Physical constants

The speed of light	$c = 2.9979 \cdot 10^8$ m/s
Planck's constant	$h = 2\pi\hbar = 6.6262 \cdot 10^{-34}$ Js
The electron charge e	$\lvert e\rvert = 1.6022 \cdot 10^{-19}$ C
The electron mass	$m_e = 9.1096 \cdot 10^{-31}$ kg
The fine structure constant	$\alpha = e^2/(4\pi\varepsilon_0\hbar c) = 1/137.05$
The Bohr radius	$a_0 = 4\pi\varepsilon_0\hbar^2/(m_e e^2)$

Time independent perturbation theory

For $H = H^0 + \lambda H_1$ we have

$$E_n = E_n^0 + \langle n|\lambda H_1|n\rangle + \sum_{m(\neq n)} \frac{|\langle m|\lambda H_1|n\rangle|^2}{E_n^0 - E_m^0} + \mathcal{O}(\lambda^3).$$

Integrals

$$\int_0^\infty e^{-x^2}\, dx = \tfrac{1}{2}\sqrt{\pi}$$

$$\int_0^\infty t^n\, e^{-t}\, dt = n!$$

The Laplace operator in spherical coordinates

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{\partial^2}{\partial \vartheta^2} + \cot\vartheta \frac{\partial}{\partial \vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial \varphi^2}\right]$$

Orbital angular momentum

In spherical coordinates: $\vec{L}^2 = -\hbar^2 \left[\frac{\partial^2}{\partial \vartheta^2} + \cot\vartheta \frac{\partial}{\partial \vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial \varphi^2}\right]$

Eigenvalues:
$$\begin{aligned} \vec{L}^2\, Y_{lm}(\vartheta,\varphi) &= l(l+1)\hbar^2\, Y_{lm}(\vartheta,\varphi) \\ L_z\, Y_{lm}(\vartheta,\varphi) &= m\hbar\;\, Y_{lm}(\vartheta,\varphi) \end{aligned}$$

Time dependent perturbation theory

In first order time dependent perturbation theory the probability amplitude for a transition from a state ψ_i at time $t = 0$ to a state ψ_f at $t = T$, induced by a time dependent perturbing potential $V(\vec{r}, t)$, is

$$a_{i\to f} = \frac{1}{\mathrm{i}\hbar}\int_0^T \mathrm{d}t\, V_{fi}(t)\, \mathrm{e}^{\mathrm{i}\omega_{fi}t}\ .$$

ψ_i and ψ_f are eigenstates of the unperturbed Hamiltonian operator with energies E_i and E_f, respectively. Furthermore, $\omega_{fi} = (E_f - E_i)/\hbar$, and

$$V_{fi}(t) = \int \mathrm{d}^3\vec{r}\ \psi_f^*(\vec{r})\, V(\vec{r}, t)\, \psi_i(\vec{r})\ .$$

In the electric dipole approximation the probability per time for spontaneous emission of electromagnetic radiation within an infinitesimal solid angle $\mathrm{d}\Omega$ and with a polarisation vector $\vec{\epsilon}$, with $|\vec{\epsilon}| = 1$, is

$$\mathrm{d}\lambda = \frac{\alpha\omega^3}{2\pi c^2}\left|\vec{\epsilon}\cdot\vec{d}\right|^2 \mathrm{d}\Omega.$$

Here $\omega = (E_i - E_f)/\hbar$, α is the fine structure constant, and

$$\vec{d} = \int \mathrm{d}^3\vec{r}\ \psi_f^*\, \vec{r}\, \psi_i\ .$$