

TPV

SoSe 2018

Blatt 13

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Exercise 25 *Hydrogen atom*

In the following we use the same notations as on Blatt 9 exercise 19. We consider the central potential

$$V(\hat{\mathbf{r}}) = -\frac{e^2}{4\pi\hat{r}}, \quad (1)$$

where $\hat{r} = \sqrt{\hat{x}^2 + \hat{y}^2 + \hat{z}^2}$.

a) We use the following form of the wave function

$$\hat{\psi} = \begin{pmatrix} \hat{\psi}_A \\ \hat{\psi}_B \end{pmatrix} = \begin{pmatrix} g(r)\mathcal{Y}_{j,l_A}^{j_3} \\ if(r)\mathcal{Y}_{j,l_B}^{j_3} \end{pmatrix}. \quad (2)$$

Here $\mathcal{Y}_{j,l}^{j_3}$ are the eigenfunctions of $\hat{\mathbf{J}}^2$, J_3 and $\hat{\mathbf{L}}^2$ and they fulfill

$$\frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{r}}}{\hat{r}} \mathcal{Y}_{j,l_A}^{j_3} = -\mathcal{Y}_{j,l_B}^{j_3}, \quad (3)$$

$$\frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{r}}}{\hat{r}} \mathcal{Y}_{j,l_B}^{j_3} = -\mathcal{Y}_{j,l_A}^{j_3}, \quad (4)$$

where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)^T$. Using Eqs. (3), (4) and

$$\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} = \frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{r}}}{\hat{r}^2} \left(-i\hbar\hat{r} \frac{\partial}{\partial r} + i\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{L}} \right), \quad (5)$$

show that

$$-c\hbar \left(\frac{df}{dr} + \frac{1-\kappa}{r} f \right) = (E - V - mc^2)g,$$

$$c\hbar \left(\frac{dg}{dr} + \frac{1+\kappa}{r} g \right) = (E - V + mc^2)f.$$

(1 Point)

b) Defining the functions $F(r) = rf(r)$, $G(r) = rg(r)$, the constants $c_1 = (mc^2 + E)/(\hbar c)$, $c_2 = (mc^2 - E)/(\hbar c)$, $\alpha = e^2/(4\pi\hbar c)$ and the rescaled radius $\rho = \sqrt{c_1 c_2} r$ show that

$$\left(\frac{d}{d\rho} - \frac{\kappa}{\rho} \right) F - \left(\sqrt{\frac{c_2}{c_1}} - \frac{\alpha}{\rho} \right) G = 0, \quad (6)$$

$$\left(\frac{d}{d\rho} + \frac{\kappa}{\rho} \right) G - \left(\sqrt{\frac{c_1}{c_2}} + \frac{\alpha}{\rho} \right) F = 0. \quad (7)$$

| n | $n' = n - \kappa \geq 0$ | $\kappa = \pm(j + \frac{1}{2})$ | notation |
|-----|----------------------------|---------------------------------|------------|
| 1 | 0 | -1 | $1s_{1/2}$ |
| 2 | 1 | -1 | $2s_{1/2}$ |
| 2 | 1 | 1 | $2p_{1/2}$ |
| 2 | 0 | -2 | $2p_{3/2}$ |
| 3 | 2 | -1 | $3s_{1/2}$ |
| 3 | 2 | 1 | $3p_{1/2}$ |
| 3 | 1 | -2 | $3p_{3/2}$ |
| 3 | 1 | 2 | $3d_{3/2}$ |
| 3 | 0 | -3 | $3d_{5/2}$ |

Table 1: Relations between relativistic quantum numbers n' , κ and the notations in spectroscopy

Write F and G as series of the form $F = e^{-\rho} \rho^s \sum_{m=0}^{\infty} f_m \rho^m$ and $G = e^{-\rho} \rho^s \sum_{m=0}^{\infty} g_m \rho^m$ with $f_0, g_0 \neq 0$. Show then that the recursion relations

$$(s + q - \kappa)f_q - f_{q-1} + \alpha g_q - \sqrt{\frac{c_2}{c_1}} g_{q-1} = 0, \quad (8)$$

$$(s + q + \kappa)g_q - g_{q-1} - \alpha f_q - \sqrt{\frac{c_1}{c_2}} f_{q-1} = 0, \quad \text{with } q \geq 1 \quad (9)$$

need to be fulfilled. Show that s solves the equation $s^2 = \kappa^2 - \alpha^2$. Why does only the positive root of $\kappa^2 - \alpha^2$ lead to a valid solution? (2 Points)

- c) We assume now that there is a n' such that $f_{n'+1} = g_{n'+1} = 0$ and $f_{n'} \neq 0 \neq g_{n'}$. Derive a relation between $g_{n'}$ and $f_{n'}$ and show that the energy eigenvalue is given by

$$E = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{\left(n' + \sqrt{\left(j + \frac{1}{2}\right)^2 - \alpha^2}\right)^2}}}. \quad (10)$$

Use Eq. (10) to derive which states in table 1 are degenerate.

Exercise 26 Thomson-Scattering

We want to calculate the cross section for the scattering of a photon with wave vector \mathbf{k} and polarization $\boldsymbol{\epsilon}$ and an electron bounded to an atom. Here we consider the energy of a photon $\hbar\omega$ to be much larger than the ionization energy E_I of the atom but sufficiently small such that the dipole approximation holds. In this exercise we neglect the center of mass motion of the atom. The atom is located in the origin of the coordinate system and the system of atom and photon is considered to be initially in the state $|\phi_i\rangle = |a, 1_{\boldsymbol{\lambda}}\rangle$. Here $|a\rangle$ is the ground state of the atom and $|1_{\boldsymbol{\lambda}}\rangle$ is the state of the electromagnetic field where $\boldsymbol{\lambda} = (\boldsymbol{\epsilon}, \mathbf{k})$. Use the Hamiltonian

$$\hat{H}_I = \hat{H}_I^{(1)} + \hat{H}_I^{(2)} \quad (11)$$

with

$$\hat{H}_I^{(1)} = -\frac{q}{mc} \hat{\mathbf{p}} \cdot \hat{\mathbf{A}}_{\perp}(0) \quad \text{und} \quad \hat{H}_I^{(2)} = \frac{q^2}{2mc^2} \hat{\mathbf{A}}_{\perp}^2(0), \quad (12)$$

where the vector potential is given by

$$\hat{\mathbf{A}}_{\perp}(0) = \sum_{\lambda} \sqrt{\frac{2\pi\hbar c^2}{\omega_{\lambda} V}} \left[\hat{a}_{\lambda} \boldsymbol{\epsilon}_{\lambda} + \hat{a}_{\lambda}^{\dagger} \boldsymbol{\epsilon}_{\lambda} \right]. \quad (13)$$

- a) Calculate up to second order in q/c the contributions of $\hat{H}_I^{(1)}$ and $\hat{H}_I^{(2)}$ to the matrix element \mathcal{T}_{fi} with

$$\mathcal{T}_{fi} = \langle \phi_f | \hat{H}_I | \phi_i \rangle + \lim_{\eta \rightarrow 0^+} \langle \phi_f | \hat{H}_I (E_i - \hat{H}_0 + i\eta)^{-1} \hat{H}_I | \phi_i \rangle + \dots \quad (14)$$

Here $|\phi_i\rangle$ is the initial state and $|\phi_f\rangle = |a, 1_{\lambda'}\rangle$ with $\boldsymbol{\lambda}' = (\boldsymbol{\epsilon}', \mathbf{k}') \neq \boldsymbol{\lambda}$ is the final state. For the calculation of the second order term of $\hat{H}_I^{(1)}$ introduce excited states $|b\rangle$ of the atom and express the result as sum over all possible excited states $|b\rangle$. Why this is a scattering process? (3 Points)

- b) Determine, which term, $\mathcal{T}_{fi}^{(1)} = \langle \phi_f | \hat{H}_I^{(1)} | \phi_i \rangle + \dots$ or $\mathcal{T}_{fi}^{(2)} = \langle \phi_f | \hat{H}_I^{(2)} | \phi_i \rangle + \dots$, contribute more to \mathcal{T}_{fi} . In order to do this argue first which terms contribute to $\mathcal{T}_{fi}^{(1)}$ and then approximate the remaining terms by using the condition $\hbar\omega \gg E_I$. Do this by expanding $\mathcal{T}_{fi}^{(1)}$ up to first order in $\frac{E_b - E_a}{\hbar\omega}$. Determine then the magnitude of the ratio between the two terms, $\mathcal{T}_{fi}^{(1)}$ and $\mathcal{T}_{fi}^{(2)}$, as a function of $E_I/\hbar\omega$ and argue with this, which term contributes more to \mathcal{T}_{fi} . (2 Points)

- c) The transition probability per time and solid angle Ω' is given by

$$\frac{\delta w_{fi}}{\delta \Omega'} = \frac{2\pi}{\hbar} |\mathcal{T}_{fi}(E_f = E_i; \Omega'; \phi_i)|^2 \rho(E_f = E_i; \Omega'), \quad (15)$$

where $\mathcal{T}_{fi}(E_f = E_i; \Omega'; \phi_i)$ is the previously calculated matrix element in highest order $\frac{E_I}{\hbar\omega}$, and $\rho(E_f = E_i; \Omega')$ is the density of states for the final state. The latter is given by

$$\rho(E_f = E_i; \Omega') = \frac{V}{8\pi^3} \frac{(\hbar\omega)^2}{\hbar^3 c^3}. \quad (16)$$

Derive the scattering cross section

$$\frac{d\sigma}{d\Omega'} = r_0^2 (\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}')^2, \quad (17)$$

using Eq. (15) and dividing by the photon flux c/V . Use the definition of classical electron radius $r_0 = q^2/(mc^2)$. Integrate Eq. (17) over the solid angle to get the total scattering cross section and compare it to the result for an elastically bound electron coupled to a classical electromagnetic field

$$\sigma_{\text{classical}} = \frac{8\pi}{3} r_0^2. \quad (18)$$

(2 Points)