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Quantum Mechanics 2 - Problem Set 11

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Abgabe: The problem set will be discussed in the tutorials on **Thursday, 11.01.2018, 11:00** (German) and **Friday, 12.01.2018, 13:30** (English).

34. Coulomb and Exchange integrals for helium *5+1 Punkte*

The energy of excited states in helium can be shown to be, to leading order in perturbation theory, given by

$$E_{nl,\pm} = E_{100} + E_{nlm} + J_{nl} \pm K_{nl},$$

where the Coulomb- and exchange integrals for helium are given by

$$J_{nl} = \frac{e^2}{4\pi\epsilon_0} \langle u_{100}(\mathbf{r_1}) u_{nlm}(\mathbf{r_2})| \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} |u_{100}(\mathbf{r_1}) u_{nlm}(\mathbf{r_2})\rangle,$$

and

$$K_{nl} = \frac{e^2}{4\pi\epsilon_0} \langle u_{100}(\mathbf{r_1}) u_{nlm}(\mathbf{r_2})| \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} |u_{nlm}(\mathbf{r_1}) u_{100}(\mathbf{r_2})\rangle,$$

respectively. Here u_{nlm} is the hydrogen atom wave-function with $Z = 2$ and eigenenergy E_{nlm}.

(a) Calculate the Coulomb- and exchange integrals for $n = 2, l = 1$.

Hint: Express $1/|\mathbf{r_1} - \mathbf{r_2}|$ *as a sum over spherical harmonics and use orthogonality of these to perform the angular integrals.*

(b) Make a sketch of the energy levels $E_{nl,\pm}$ for $n = 2, l = 1$.

35. Emission from an atom *1+3+3+4+3 Punkte*

In this problem we will consider a single-electron (the extension to multi-electron atoms is straightforward but we will consider the single-electron case for simplicity) atom with Hamiltonian

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}),$$

subject to an external electromagnetic field with vector potential $\mathbf{A}(\mathbf{r}, t)$.

(a) Convince yourself that the Hamiltonian of the atom is given by $\hat{H}_0 + \hat{H}_{\text{para}} + \hat{H}_{\text{dia}}$ with $\hat{H}_{\text{para}} = \frac{e}{m}\mathbf{A}\cdot\hat{\mathbf{p}}$ denoting the paramagnetic term and $\hat{H}_{\text{dia}} = \frac{1}{2m}(e\mathbf{A})^2$ denoting the diamagnetic term.

(b) In Problem Set 9 we found that the Hamiltonian of the electromagnetic field can be written as

$$\hat{H}_{\text{rad}} = \sum_{\mathbf{k},\lambda=\pm} \hbar\omega_{\mathbf{k}} \left(a^{\dagger}_{\mathbf{k},\lambda} a_{\mathbf{k},\lambda} + \frac{1}{2} \right),$$

with $\omega_{\mathbf{k}} = c|\mathbf{k}|$ and where $a^{\dagger}_{\mathbf{k},\lambda}$ and $a_{\mathbf{k},\lambda}$ create and annihilate photons with wavevector $\mathbf{k}$ and polarization λ. These operators satisfy the usual commutation relations of ladder operators and act on a state with $n_{\mathbf{k}\lambda}$ photons as $a_{\mathbf{k}\lambda}|n_{\mathbf{k}\lambda}\rangle = \sqrt{n_{\mathbf{k}\lambda}}|n_{\mathbf{k}\lambda}-1\rangle$ and $a^{\dagger}_{\mathbf{k}\lambda}|n_{\mathbf{k}\lambda}\rangle = \sqrt{n_{\mathbf{k}\lambda}+1}|n_{\mathbf{k}\lambda}+1\rangle$. Moreover if the system is confined to a volume V, the vector potential can be expanded as

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k},\lambda=\pm} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}V}} \left(\hat{\mathbf{e}}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + \hat{\mathbf{e}}^{*}_{\mathbf{k}\lambda} a^{\dagger}_{\mathbf{k}\lambda} e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} \right).$$

The eigenstates of the combined system of atom and electromagnetic field can then be written as $|nlm\rangle \otimes |n_{\mathbf{k}\lambda}\rangle$, where the first part refers to the atomic part of the Hamiltonian and the last part to the radiation part of the Hamiltonian.

Treating the paramagnetic part of the Hamiltonian as a perturbation, show that the probability of a transition between a state $|i\rangle \otimes |n_{\mathbf{k}\lambda}\rangle$ and a state $|f\rangle \otimes |n_{\mathbf{k}\lambda}+1\rangle$ is given by

$$\Gamma_{if} = \frac{2\pi}{\hbar} \left| \langle f| \frac{e}{m} \sqrt{\frac{\hbar(n_{\mathbf{k}\lambda}+1)}{2\epsilon_0\omega_{\mathbf{k}}V}} e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\mathbf{e}}^{*}_{\mathbf{k}\lambda}\cdot\hat{\mathbf{p}}|i\rangle \right|^2 \delta(E_i - E_f - \hbar\omega_{\mathbf{k}}).$$

Hint: You may find it helpful to start from Fermi's golden rule which you may use without proof.

(c) The expression in part (b) is rather complicated. To simplify the matrix element, expand the exponential to zeroth order in $\mathbf{k}\cdot\mathbf{r}$ (this is valid for $Z\alpha \ll 1$ (why?)) and use the identity $\hat{\mathbf{p}} = \frac{im}{\hbar}[\hat{H}_0, \hat{\mathbf{r}}]$, to show that

$$\Gamma_{if} = \frac{\pi\omega_{\mathbf{k}}(n_{\mathbf{k}\lambda}+1)}{\epsilon_0 V} |\langle f|\hat{\mathbf{e}}_{\mathbf{k}\lambda}\cdot\mathbf{d}|i\rangle|^2 \delta(E_i - E_f - \hbar\omega_{\mathbf{k}}),$$

where $\mathbf{d} = -e\mathbf{r}$ is the dipole moment of an electron. This approximation is known as the dipole approximation.

(d) The probability calculated above only tells us about the scattering of photons with the particular momentum $\mathbf{k}$. To get the total probability of scattering photons with polarization λ into a solid angle $d\Omega$ we have to perform the sum $d\Gamma = \sum_{\mathbf{k}} \Gamma_{if}$. By converting the sum into an integral, assuming that $n_{\mathbf{k}\lambda} = n_\lambda(k)$ is isotropic in $\mathbf{k}$, and using the dipole approximation show that the total probability per unit solid angle is given by

$$\frac{d\Gamma}{d\Omega} = \frac{1}{4\pi\epsilon_0} \frac{\omega^3 (n_\lambda(\omega/c) + 1))}{2\pi\hbar c^3} |\langle f|\hat{\mathbf{e}}_{\mathbf{k}\lambda} \cdot \mathbf{d}|i\rangle|^2.$$

Here $\hbar\omega = E_i - E_f$.

(e) Show that the angular average of $|\langle f|\hat{\mathbf{e}}_{\mathbf{k}\lambda} \cdot \mathbf{d}|i\rangle|^2$ is given by $d_{if}^2/3$, with $d_{if}^2 = |\langle f|ex|i\rangle|^2 + |\langle f|ey|i\rangle|^2 + |\langle f|ez|i\rangle|^2$ and thus derive the total emission probability.

Hint: Choose coordinates such that $\mathbf{k}$ *points in the z-direction and* $\mathbf{d_{if}} = \langle f|\mathbf{d}|i\rangle = (d_{if}\sin\theta, 0, d_{if}\cos\theta)$. *Finally use the Coulomb gauge to derive a condition on* $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$.