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# Höhere Quantenmechanik

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## Exercise sheet 5

(Submission date: Until 23.05.2022 12:00)

### Exercise 1: Photoelectric effect *(11 Points)*

The photoelectric effect describes the emission of electrons from a material subjected to electromagnetic radiation. Consider the interaction of a hydrogen atom in its ground state

$$\phi_0(\vec{r}) = \langle \vec{r}|0\rangle = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^3}} \tag{1}$$

with a classical monochromatic radiation field with polarization vector $\hat{\epsilon} = \hat{z}$. In the electric dipole approximation the transition rate $\Gamma_{0\to f}$ for the absorption process is proportional to

$$\Gamma_{0\to f} \propto \left|\left\langle 0 \left| \frac{\partial}{\partial z} \right| f \right\rangle\right|^2 \delta\left(E_f - E_0 - \hbar\omega\right). \tag{2}$$

where 0 is the initial state (the hydrogen ground state) and $f$ is a certain final state.

(i) We want to obtain the expression (2) for the transition rate by using first-order perturbation theory. The Hamiltonian of the system is

$$H(t) = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x},t)\right)^2 + U(r) \tag{3}$$

where $U(r)$ is the central potential of the nucleus of the hydrogen atom. In the kinetic part, we have used the so-called *minimal coupling* to account for the effect of the electromagnetic radiation, replacing $\vec{p} \mapsto \vec{p} - \frac{e}{c}\vec{A}(\vec{x},t)$, where $\vec{A}(\vec{x},t)$ denotes the vector potential. Expand the Hamiltonian to first-order in $\vec{A}(\vec{x},t)$ and bring it to the form $H = H_0 + V(t)$, where $H_0$ is the unperturbed Hamiltonian of the hydrogen atom. *(1 Point)*

(ii) We take the vector potential for a simple wave polarized along $\hat{z}$, i.e.

$$\vec{A}(\vec{x},t) = 2A_0\hat{z}\cos\left(\vec{k}\cdot\vec{x} - \omega t\right). \tag{4}$$

Here, $\vec{k} = \frac{\omega}{c}\hat{n}$ is the wave vector. We assume that $\vec{\nabla}\cdot\vec{A}(\vec{x},t) = 0$ (Coulomb gauge), which is a valid approximation if the wave length of the radiation is much larger than the size of the atom. Show that, under these assumptions, $V(t)$ can be written in the form $V(t) = Oe^{-i\omega t} + O^\dagger e^{i\omega t}$ (discussed in Section 4.3.2 of the notes of the course), where $O$ is a certain operator. What is $O$ here? *(2 Points)*

(iii) Show that the transition rate $\Gamma_{0\to f}$ for the absorption process has a form like the one of Eq. (2) for large times $T$. *(2 Points)*

(iv) For sufficiently large energies, the final state $|f\rangle$ of the electron can be approximated by a plane wave

$$\langle \vec{r}|f\rangle = \frac{e^{i\vec{p}_f\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}. \tag{5}$$

This means that the electron has been "extracted" from the material and has become a free particle with momentum $\vec{p}_f$. Compute an expression for the transition rate [you can use Eq. (2)]. How does the transition rate depend on the direction of the outgoing electron? *(6 Points)*

## Exercise 2: Pauli matrices and rotations *(9 Points)*

(i) Prove that the following equation holds for Pauli matrices

$$\sigma_j\sigma_k = \delta_{j,k}\mathbb{1} + i\varepsilon_{j,k,l}\sigma_l \tag{6}$$

where $\varepsilon_{j,k,l}$ is the Levi-Civita symbol. Note: repeated indices are implicitly meant to be summed over (Einstein notation). *(2 Points)*

(ii) Prove the general formula for rotations of Pauli matrices

$$U(\vec{n},\phi)\ \vec{\sigma}\ U^\dagger(\vec{n},\phi) = \vec{n}(\vec{n}\cdot\vec{\sigma}) - \vec{n}\times(\vec{n}\times\vec{\sigma})\cos(\phi) + (\vec{n}\times\vec{\sigma})\sin(\phi) \tag{7}$$

where $U(\vec{n},\phi) = e^{i\frac{\phi}{2}\vec{n}\cdot\vec{\sigma}}$ and $\vec{n}$ is a unit vector. *(7 Points)*

*Hints: using the property* (6) *two consecutive times may help you obtaining the double vector product. Remember also that, for three vectors* $\vec{a},\vec{b},\vec{c}$ *which commute among themselves, the property* $\vec{a}\times(\vec{b}\times\vec{c}) = \vec{b}(\vec{a}\cdot\vec{c}) - \vec{c}(\vec{a}\cdot\vec{b})$ *holds. In our case, this implies that*

$$\vec{n}\times(\vec{n}\times\vec{\sigma}) = \vec{n}(\vec{n}\cdot\vec{\sigma}) - \vec{\sigma} \tag{8}$$

*where we have used the fact that* $\vec{n}$ *is a unit vector.*