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THEORETICAL OPTICS: EXERCISE SHEET 12

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Hydrogen atom in an electric field - Two-level system - Rabi oscillations

Beyond Bohr's model and within a fully quantum mechanical treatment, the energy levels of hydrogen atom are characterized by two additional quantum numbers l and m, apart from the quantum number n. These quantum numbers are associated with the eigen-values of the operators $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$. Here $\hat{\boldsymbol{L}}$ denotes the angular momentum operator $\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$, with $\hat{\boldsymbol{r}}$ the position operator and $\hat{\boldsymbol{p}}$ the momentum operator. Since $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$ commute with the Hamiltonian, their eigen-functions constitute also eigen-functions of the Hamiltonian. Nonetheless, the energy levels of the hydrogen atom depend only on n, i.e. $E_{n,l,m} = -13.6/n^2\text{eV}$. The eigen-functions of the above operators are the spherical harmonics $Y_{l,m}(\theta,\varphi)$ satisfying $\hat{\boldsymbol{L}}^2 Y_{l,m}(\theta,\varphi) = l(l+1)\hbar^2 Y_{l,m}(\theta,\varphi)$ and $\hat{L}_z Y_{l,m}(\theta,\varphi) = m\hbar Y_{l,m}(\theta,\varphi)$. The complete wave-function of an atomic orbital $|n,l,m\rangle$ has the following form $\Psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)Y_{l,m}(\theta,\varphi)$, where $R_{n,l}(r)$ corresponds to the radial part of the wave-function. Finally, for a specific n the values of l and m are constrained in the following way $l = 0, 1, 2, \ldots, n-1$ and $m = 0, \pm 1, \pm 2, \ldots, \pm l$.

Here we focus on a two-level subsystem of the hydrogen atom levels: the lowest energy level $|1s\rangle \equiv |1,0,0\rangle$ along with one excited $|2p_z\rangle \equiv |2,1,0\rangle$, which are the most relevant when a weak electric field $\boldsymbol{\mathcal{E}}(t) = \mathcal{E}(t)\hat{\boldsymbol{z}}$ is applied. The corresponding wave-functions read:

$$\Psi_{1s}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \qquad \text{and} \qquad \Psi_{2p_z}(r,\theta,\varphi) = \frac{1}{4\sqrt{2\pi} a_0^{3/2}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta\,, \tag{1}$$

which are normalized $\iiint |\Psi_{n,l,m}|^2 r^2 \sin\theta dr d\theta d\varphi = 1$, with $r \in [0,\infty)$, $\theta \in [0,\pi]$, $\varphi \in [0,2\pi)$ and a_0 defines the Bohr radius. In the absence of the electric field these two levels are orthogonal, but when the field is switched on, they mix. The finite electric field shifts the potential energy of the system by $V_{el}(\hat{\boldsymbol{r}},t) = -\hat{\boldsymbol{d}} \cdot \boldsymbol{\mathcal{E}}(t)$, with $\hat{\boldsymbol{d}}$ the electron's electric dipole moment operator $\hat{\boldsymbol{d}} = -e\hat{\boldsymbol{r}}$ and e corresponds to the absolute value of the electron's charge. The Hamiltonian of this two-level system is described by the following 2×2 matrix

$$\widehat{\mathcal{H}}(t) = \begin{pmatrix} E_{1s} & -\langle 1s|\, \hat{d}_z\, |2p_z\rangle\, \mathcal{E}(t) \\ -\langle 2p_z|\, \hat{d}_z\, |1s\rangle\, \mathcal{E}(t) & E_{2p_z} \end{pmatrix}, \tag{2}$$

where E_{1s} and E_{2p_z} denote the energies of the atomic levels.

a. Calculate the matrix elements of the electric dipole moment operator and retrieve $\widehat{\mathcal{H}}(t)$. (4 points)

b. Diagonalize the Hamiltonian of Eq. (2) and retrieve the eigen-values and eigen-states, in the case of a static external electric field $\boldsymbol{\mathcal{E}}(t) = \mathcal{E}\hat{\boldsymbol{z}}$. (4 points)

c. Assume that at $t = 0$ the system's wave-function coincides with $|1s\rangle$. Determine the evolution of the system for $t > 0$ when a static electric field is applied as in **b.**. Calculate the probabilities to find the system in $|1s\rangle$ and $|2p_z\rangle$, at a time instant t. (5 points)

d. Express the Hamiltonian of **a.** using the 2×2 unit matrix $\hat{I}$ and the Pauli matrices

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{and} \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3}$$

(2 points)

e. Consider that the electric field has the following time-dependence $\mathcal{E}(t) = \mathcal{E}\cos\omega t$. Here $\omega = (E_{2p_z} - E_{1s})/\hbar + \Delta$, where $\Delta << (E_{2p_z} - E_{1s})/\hbar$ defines the detuning from the resonance. Separate the Hamiltonian into two parts $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_0 + \widehat{V}(t)$, where $\widehat{\mathcal{H}}_0 = -\hbar\omega\hat{\sigma}_z/2$. The dipole coupling to the electric field is contained in the second term. Starting from Schrödinger's time-dependent equation

$$i\hbar\frac{\partial\left|\Psi(t)\right\rangle}{\partial t} = \left[\widehat{\mathcal{H}}_0 + \widehat{V}(t)\right]\left|\Psi(t)\right\rangle \tag{4}$$

for an arbitrary state-vector $\left|\Psi(t)\right\rangle = c_{1s}(t)\left|1s\right\rangle + c_{2p_z}(t)\left|2p_z\right\rangle$, transfer to the *rotating frame* by effecting the transformation $\left|\Psi(t)\right\rangle = e^{-i\widehat{\mathcal{H}}_0 t/\hbar}\left|\Psi(t)\right\rangle'$. Retrieve the Hamiltonian $\widehat{\mathcal{H}}'(t)$ in the rotating frame, which satisfies

$$i\hbar\frac{\partial\left|\Psi(t)\right\rangle'}{\partial t} = \widehat{\mathcal{H}}'(t)\left|\Psi(t)\right\rangle' . \tag{5}$$

(6 points)

f. Apply the *rotating wave approximation* to **e.**, according to which, any fast oscillating term with frequency 2ω appearing in $\widehat{\mathcal{H}}'(t)$ can be neglected, rendering the latter time-independent. (3 points)

g. Diagonalize the approximate time-independent Hamiltonian obtained in **f.**. Retrieve the probabilities $|c_{1s}(t)|^2$ and $|c_{2p_z}(t)|^2$ of finding the electron in state $\left|1s\right\rangle$ or $\left|2p_z\right\rangle$ at a time instant t. Show that the latter probabilities oscillate in time and determine the frequency of the oscillations, which is called *Rabi frequency*. (6 points)