Atomic Optical Susceptibility.// The stationary Schrödinger equation of a single electron in an atom is

$$\mathcal{H}_0\psi_n(\mathbf{r}) = \hbar\epsilon_n\psi_n(\mathbf{r}). \tag{1}$$

where $\hbar\epsilon_n$ and ψ_n are the energy eigenvalues and the corresponding eigenfunctions, respectively. For simplicity, we discuss the example of the hydrogen atom which has only a single electron. The Hamiltonian $\mathcal{H}_0$ is then given by the sum of the kinetic energy operator and the Coulomb potential in the form

$$\mathcal{H}_0 = -\frac{\hbar^2\nabla^2}{2m_0} - \frac{e^2}{\mathbf{r}}. \tag{2}$$

An optical field couples to the dipole moment of the atom and introduces time-dependent changes of the wave function

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[\mathcal{H}_0 + \mathcal{H}_1(t)\right]\psi(\mathbf{r},t) \tag{3}$$

with

$$\mathcal{H}_1(t) = -ex\mathcal{E}n(t) = -d\mathcal{E}(t) \tag{4}$$

Here, d is the operator for the electric dipole moment and we assumed that the homogeneous electromagnetic field is polarized in x-direction. Expand- ing the time-dependent wave functions into the stationary eigenfunctions of Eq. (1)

$$\psi(\mathbf{r},t) = \sum_m a_m(t)e^{-i\epsilon_m t}\psi m(\mathbf{r}) \tag{5}$$

inserting into Eq. (3), multiplying from the left by $\psi_m^*\ n(\mathbf{r})$ and integrating over space, we find for the coefficients an the equation

$$i\hbar\frac{da_n}{dt} = -\mathcal{E}(t)\sum_m e^{-i\epsilon_m nt}\left\langle n\left|d\right|m\right\rangle a_m, \tag{6}$$

where

$$\epsilon_m n = \epsilon_m - \epsilon_n \tag{7}$$

is the frequency difference and

$$\left\langle n\left|d\right|m\right\rangle = \int d^3r\psi_n^*(\mathbf{r})d\psi_m(\mathbf{r})\,dx \equiv d_n m \tag{8}$$

is the electric dipole matrix element. We assume that the electron was initially at $t \to -\infty$ in the state $|l\rangle$, i.e.,

$$a_n(t \to -\infty) + \delta_n, l. \tag{9}$$

Now we solve Eq. (6) iteratively taking the field as perturbation. For this purpose, we introduce the smallness parameter Δ and expand

$$a_n = a_n^{(0)} + \Delta a_n^{(1)} + \ldots \tag{10}$$

and

$$\mathcal{E}(t) \to \Delta\mathcal{E}(t). \tag{11}$$

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