

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

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

where  $\hbar \epsilon_n$  and  $\psi_n$  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

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

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

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

with

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

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

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

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

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

where

$$\epsilon_m n = \epsilon_m - \epsilon_n \quad (7)$$

is the frequency difference and

$$\langle n | d | m \rangle = \int d^3r \psi_n^*(\mathbf{r}) d \psi_m(\mathbf{r}) \equiv d_{nm} \quad (8)$$

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

$$a_n(t \rightarrow -\infty) = \delta_{n,l}. \quad (9)$$

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

$$a_n = a_n^{(0)} + \Delta a_n^{(1)} + \dots \quad (10)$$

and

$$\mathcal{E}(t) \rightarrow \Delta \mathcal{E}(t). \quad (11)$$

## REFERENCES

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