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RESONANCE PROCESSES IN THE PHOTOEFFECT

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It is shown that the polarizability of the atomic remainder leads to the appearance of resonance areas on the plots of the coefficient of photoelectric absorption of quanta by an outer electron at a quantum energy on the order of the excitation energy of the remainder.

WHEN an electromagnetic wave is incident on an optical electron of an atom, the behavior of the electron cannot be regarded rigorously without taking into account the influence of the field on the atomic remainder. In other words, the self-consistent-field approximation for the calculation of the wave functions of the external electron is not valid for the determination of the probability of radiative transitions. Bersuker[1,2] has shown that the influence of the core can be described in terms of the polarizability or a quantity reminescent of polarizability, which gives rise to an additional linear and coherent component of the electromagnetic field acting on the electron. It was shown in[3] that the influence exerted on the optical electron by the remainder exhibits dispersion. Several limiting assumptions imposed by Bersuker during the course of his derivation can be eliminated, and the result depends on the dynamic polarizability of the atomic remainder.

When the frequency of the incident radiation is close to the excitation-level energy of the remainder, the effect acquires a resonant character. Since the corresponding levels can lie at energies on the order of several dozen electron volts, the resonant polarization of the remainder should affect the probability of the photoelectric detachment of the external electron by the light wave. Roughly speaking, the remainder first absorbs a quantum with energy close to its excitation energy, and then transfers this energy to the optical electron, which is emitted from the atom. In fact, however, interference takes place between the two photoeffect mechanisms (direct and via excitation of the core), similar to the interference between potential and resonant scattering of neutrons in nuclear physics. In this paper we shall consider the resonant photoeffect.

The variables describing the state of the atomic system will be denoted by two indices, the first pertaining to the core and the second to the external electron. Accordingly we introduce the three amplitudes c_{00}, c_{n0}, and c_{0E}. The index n pertains to the excited state of the core, the energy of which is close to the energy of the incident quanta; E denotes the energy of the photoelectron. The matrix elements of the optical transitions are denoted respectively H_{0n} and H_{0E}, assuming that they pertain either to the core or to the external electron. They do not include the time dependence. The off-diagonal matrix element of the interaction between the core and the external electron will be denoted $V_{n0,0E}$. It is written out, for example, in[3], but its explicit form does not matter here. For the amplitudes c_{n0} and c_{0E} we have the equations

$$i\dot{c}_{0E} = V_{0E,\,n0}e^{-i(\omega_E-\omega_n)t}\,c_{n0} + H_{0E}e^{-i(\omega_E-\omega)t}\,c_{00}, \tag{1}$$

$$i\dot{c}_{n0} = \sum_{E'} V_{n0,\,0E'}e^{i(\omega_{E'}-\omega_n)t}\,c_{0E'} + H_{0n}e^{i(\omega-\omega_n)t}\,c_{00}. \tag{2}$$

Here ω_n and ω_E are the corresponding transition frequencies and ω is the frequency of the quantum.

The problem can be solved by perturbation theory with respect to c_{00}, putting $c_{00} = 1$. Then the system (1)–(2) has a rigorous solution. Let us get rid first of the explicit dependence on the time in the equations, putting

$$c_{0E} = e^{-i(\omega_E-\omega)t}\,c'_{0E}(t), \quad c_{n0} = e^{i(\omega-\omega_n)t}\,c'_{n0}(t).$$

Then the equations for the primed quantities are:

$$i\dot{c}'_{0E} + (\omega_E-\omega)\,c'_{0E} = V_{0E,\,n0}c'_{n0} + H_{0F}, \tag{3}$$

$$i\dot{c}'_{n0} + (\omega_n-\omega)\,c'_{n0} = \sum_{E'} V_{n0,\,0E'}c'_{0F'} + H_{0n}, \tag{4}$$

with initial conditions $c'_{0E}(0) = 0$ and $c'_{n0}(0) = 0$. According to (3), we represent c'_{0E} in the form of a quadrature

$$c'_{0E} = -i\int_0^t (H_{0E} + V_{0E,\,n0}c'_{n0}(t'))\,e^{-i(\omega_E-\omega)(t'-t)}\,dt'. \tag{5}$$

This expression must be substituted in (4) and summed over E′. To this end, it is convenient first to integrate the second term under the integral sign on the right by parts, with allowance for the initial condition

$$\int_0^t c'_{n0}(t')\,e^{-i(\omega_E-\omega)(t'-t)}\,dt' = \frac{ic'_{n0}(t)}{\omega_E-\omega} - i\int_0^t \frac{e^{-i(\omega_E-\omega)(t'-t)}\,\dot{c}'_{n0}(t')}{\omega_E-\omega}\,dt'$$

$$= i\int_0^t \frac{1-e^{-i(\omega_E-\omega)(t'-t)}}{\omega_E-\omega}\,\dot{c}'_{n0}(t')\,dt'.$$

It is then necessary to change the order of summation over E′ and integration with respect to t. We go over from the summation to the integration by introducing the differential of the number of states $\rho(E')\,dE'$. Since we shall henceforth need a solution that is valid at large values of the time, we employ the asymptotic formula

$$\int dE'\varphi(E')\,\frac{1-e^{-i(\omega_{E'}-\omega)t}}{\omega_{E'}-\omega} = -\pi i\varphi(\omega),$$

from which we get finally

$$\sum_{E'} V_{n0,\,0E'}\,c'_{0E'} = -\pi i(V_{n0,\,0\omega}\,H_{0\omega}\rho(\omega) + |V_{n0,\,0\omega}|^2\rho(\omega)\,c_{n0}'(t)). \tag{6}$$

Thus, c'_{n0} satisfies the ordinary differential equation

$$i\dot{c}_{n0}' + (\omega_n - \omega + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega)) c_{n0}' = -\pi i \rho(\omega) V_{n0,\,0\omega} H_{0\omega} + H_{0n}. \tag{7}$$

Its solution is

$$c_{n0}'(t) = (H_{n0} - \pi i \rho(\omega) V_{n0,\,0\omega} H_{0\omega}) \frac{\exp\{i(\omega_n - \omega + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega))t\} - 1}{i(\omega_n - \omega + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega))}.$$

The now known expression for $c'_{n0}(t)$ is then substituted in (6), from which we get the sought probability amplitude $c'_{0E}(t)$:

$$c_{0E}' = \left[H_{0E} - \frac{(\pi i \rho(\omega) V_{n0,\,0\omega} H_{0\omega} - H_{0n}) V_{0\omega,\,n0}}{\omega_n - \omega + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega)}\right] \frac{e^{i(\omega_E - \omega)t} - 1}{i(\omega_E - \omega)} - \frac{H_{0n} - \pi i \rho(\omega) V_{n0,\,0\omega} H_{0\omega}}{\omega_n - \omega + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega)} \times \frac{\exp\{i(\omega_n - \omega_E + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega))t\} - 1}{i(\omega_n - \omega_E + \pi i |V_{n0,\,0\omega}|^2 \rho(\omega))}. \tag{9}$$

It is necessary to take the square of the modulus of this quantity and to integrate over a certain interval of the continuous spectrum E. It can be shown that a nonzero contribution proportional to t is made only by the quantity in the square brackets. Indeed, the exponentially damped term must be set equal to zero, since it is connected with the choice of the initial conditions at t = 0. The damped exponential can always be discarded at sufficiently large t. The term containing $(\exp[i(\omega_E - \omega)t] - 1)/(\omega_E - \omega)$ is linear, and upon integration with respect to E it yields a contribution that does not depend on the time, so that it drops out upon further differentiation with respect to t. The same pertains to the number 1 in the second term of the expression (9). We are left with the usual resonant integration, which yields for the transition probability

$$W = 2\pi\rho(\omega) \frac{|H_{0\omega}(\omega_n - \omega) + V_{0\omega,n0} H_{0n}|^2}{(\omega_n - \omega)^2 + [\pi |V_{0\omega,\,n0}|^2 \rho(\omega)]^2}. \tag{10}$$

Neglecting the interaction between the core and the external electron, we obtain, obviously, the probability of the direct photoeffect

$$W_{\mathrm{ph}} = 2\pi\rho(\omega) |H_{0\omega}|^2.$$

Introducing the abbreviated notation

$$\frac{\omega_n - \omega}{2\pi |V_{n0,\,0\omega}|^2 \rho(\omega)} \equiv x, \qquad \left|\frac{H_{n0}}{H_{0\omega} \cdot 2\pi\rho(\omega) V_{n0,\,0\omega}}\right| \equiv \alpha,$$

we see that the form of the resonant curve is determined by the expression

$$f(x) = \frac{(x + \alpha)^2}{x^2 + {}^1/_4}. \tag{11}$$

This function has a minimum value equal to zero when $x = -\alpha$ and a maximum when $x = \alpha/4$. It is easy to show that $f(0) = f_{\max} - 1 = f_{\max} - f(\infty)$. From this we can obtain the exact position of the resonance from the absorption curve.

Let us estimate now the expected width of the resonant region. The matrix element $V_{n0,0\omega}$ will be chosen approximately equal to $V_{n0,0\omega} \sim e^2 x_{n0} x_{0\omega} / r_0^3$, where r_0 is on the order of the atomic radius. The cross section of the photoeffect far from the resonant region is expressed in the form

$$\sigma_{\mathrm{ph}} \cong \frac{e^2}{hc} \left(\frac{m\omega}{h}\right)^{3/2} r_0^3 x_{0\omega}^2.$$

From this we get the sought width of the region

$$\Delta\omega \sim \frac{e^2}{hc} \frac{c^2 x_{n0}^2 \sigma_{\mathrm{ph}}}{r_0^6 \omega}.$$

Assuming that the transition in the core is allowed, we put $x_{0n} \sim r_0 z^{-1/3}$, obtaining $\Delta\omega \sim 10^8 Z^{-2/3} \sigma_{\mathrm{ph}}$. We have assumed here $\omega \sim 10^{16}$. Choosing the quantum energy on the order of ten times the ionization energy, we estimate σ_{ph} for the M-shell of not too heavy elements at 10^{-19} cm², giving for $\Delta\omega$ approximately 1 eV. The parameter α is of the order of magnitude $r_0^3 \omega / c\sigma_{\mathrm{ph}}$. Under the same assumptions, it is approximately equal to unity. But if $\sigma_{\mathrm{ph}} \ll 10^{-19}$, then α becomes much larger, giving a strong excess of the peak over the smooth curve of the photoeffect.

All the foregoing uncovers a certain possibility of studying the levels of atomic cores. We note also that similar effects can be observed also in nuclear photoeffect.

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[3] A. S. Kompaneets, Opt. Spektrosk. **16**, 706 (1964).

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