A UNIFIED DESCRIPTION OF THE RESONANCE LINE PROFILE IN THE ENERGY SPECTRA OF SCATTERED AND EMITTED ELECTRONS

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A unified description of the resonance line profiles in the energy spectra of scattered and emitted electrons is established on the basis of the diagonalization method of calculating the self-ionized states of atoms. Numerical calculations are carried out for the $(2s2p)^1P^{(-)}$ resonance in the helium atom. The interference between the resonance and direct transitions to the continuous spectrum leads to the strong dependence of the resonance line profile on the angle of emission. The results of these calculations explain the experimental data obtained from experiments with fast electron beams.

EXPERIMENTAL studies of resonance phenomena in electron and atomic collisions are undergoing rapid development. In particular, several papers have already appeared on the energy spectra of electrons emitted by atoms under fast particle bombardment.[1-4] studies in this area, which has not been extensively investigated, have revealed a number of properties which must be systematized and explained on a unified theoretical basis.

The aim of the present work was: a) to explain the main tendencies which determine the resonance line intensity and profile on the kinematic conditions of the experiment (energy of incident particles and angle of emission of electrons), and b) to investigate the connection between the resonance line profiles in the spectra of emitted electrons and the profiles of the corresponding resonance lines in the spectra of scattered fast particles.

1. We shall use the Born amplitude

$$T(\mathbf{k}',\mathbf{Q})=\left\langle \Psi_f(\mathbf{k}') \left| \sum_{i=1}^{Z} \exp(i\mathbf{Q}\mathbf{r}_i) \right| \Psi_i \right\rangle, \qquad (1)$$

which determines the probability of ionization of an atom by a fast particle subject to the condition that the emitted electron carries off a momentum $\mathbf{k}'$ and the fast particle loses the momentum $\mathbf{Q} = \mathbf{k}_0 - \mathbf{k}$:

$$\frac{d^3\sigma}{d\Omega_{\mathbf{k}}\, d\Omega_{\mathbf{k}'}\, dE}=\frac{4a_0^2}{Q^4}\frac{k}{k_0}|T(\mathbf{k}',\mathbf{Q})|^2; \qquad (2)$$

where $d\Omega_{\mathbf{k}}$ and $d\Omega_{\mathbf{k}'}$ are the solid angle elements in the direction of emission of the scattered particle and emitted electron, a_0 is the atomic unit of length, and E is the electron energy.

In the neighborhood of an isolated resonance, the amplitude (1) can be written as the sum of the amplitude of the direct process and the amplitude for the decay of the self-ionization state into the continuous spectrum[5]

$$T(\mathbf{k}',\mathbf{Q})=t(\mathbf{k}',\mathbf{Q})+t^{(L)}(\mathbf{k}',\mathbf{Q})\frac{q(Q)-i}{\varepsilon+i}, \qquad (3)$$

$$t(\mathbf{k}',\mathbf{Q})=\sum_{l=0}^{\infty} t^{(l)}(\mathbf{k}',\mathbf{Q}), \quad t^{(l)}(\mathbf{k}',\mathbf{Q})=(2l+1)R_l(Q)e^{i\delta_l}P_l(\mathbf{k}',\mathbf{Q}) \qquad (4)$$

for the sake of simplicity, we have written Eq. (3) for the case where the interaction between the electrons couples only one L-th partial wave to the continuous spectrum]. The quantity $\epsilon = 2(E - E_r)/\Gamma$ in Eq. (3), which shows the deviation from resonance, and the profile index $q(Q)$ are determined in the usual way and, in particular, precisely as was done in our previous paper,[6] which was concerned with the description of resonances in the spectra of energy losses of fast scattered electrons.

It is readily seen that, by substituting Eq. (3) in Eq. (2) and integrating over all directions of the momentum $\mathbf{k}'$, we obtain the Fano formula[5,7] for the loss spectrum:

$$\frac{d^2\sigma}{d\Omega_{\mathbf{k}}\, dE}=\left(\frac{d^2\sigma}{d\Omega_{\mathbf{k}}\, dE}\right)_{\text{backgr.}}+\left(\frac{d^2\sigma}{d\Omega_{\mathbf{k}}\, dE}\right)_{\text{res}}\frac{[\varepsilon+q(Q)]^2}{\varepsilon^2+1}, \qquad (5)$$

$$\left(\frac{d^2\sigma}{d\Omega_{\mathbf{k}}\, dE}\right)_{\text{backgr.}}=\frac{16\pi a_0^2}{k_0^2Q^4}\sum_{l\neq L}(2l+1)[R_l(Q)]^2,$$

$$\left(\frac{d^2\sigma}{d\Omega_{\mathbf{k}}\, dE}\right)_{\text{res}}=\frac{16\pi a_0^2}{k_0^2Q^4}(2L+1)[R_L(Q)]^2.$$

To describe the angular and energy distributions of the emitted electrons (assuming that the scattered particle is not registered), we must integrate Eq. (2) over all directions of $\mathbf{k}'$. The result can be conveniently written in the form

$$\frac{d^2\sigma}{d\Omega_{\mathbf{k}'}\, dE}=f(\mathbf{k}')+\frac{a(\mathbf{k}')\varepsilon+b(\mathbf{k}')}{\varepsilon^2+1}, \qquad (6)$$

where

$$f(\mathbf{k}')=\frac{4a_0^2k}{k_0}\int\frac{d\Omega_{\mathbf{k}}}{Q^4}|t(\mathbf{k}',\mathbf{Q})|^2,$$

$$a(\mathbf{k}')=\frac{8a_0^2k}{k_0}\int\frac{d\Omega_{\mathbf{k}}}{Q^4}\{\mathrm{Re}[t^*(\mathbf{k}',\mathbf{Q})t^{(L)}(\mathbf{k}',\mathbf{Q})(q(Q)-i)]\},$$

$$b(\mathbf{k}')=\frac{4a_0^2k}{k_0}\int\frac{d\Omega_{\mathbf{k}}}{Q^4}\{(q^2(Q)+1)|t^{(L)}(\mathbf{k}',\mathbf{Q})|^2$$
$$+2\,\mathrm{Im}[t^*(\mathbf{k}'\ \mathbf{Q})t^{(L)}(\mathbf{k}',\mathbf{Q})(q(Q)-i)]\}.$$

In this form, the first term describes the angular and energy distributions of electrons in the direct ejection process, the integral $b(\mathbf{k}')$ is proportional to the algebraic area under the resonance curve after subtraction of the probability for the direct transitions (this corresponds to the procedure used to isolate the contribution due to resonance as used in the experimental work),

and the integral $a(k')$ characterizes the asymmetry of the resonance. Of course, the expression given by Eq. (6) can be reduced to the Fano formula

$$\frac{d^2\sigma}{d\Omega_{k'}\,dE} = f_{\text{backgr.}}(k') + f_{\text{res}}(k')\,\frac{[\varepsilon + \tilde{q}(k')]^2}{\varepsilon^2 + 1}, \qquad (7)$$

if we substitute

$$f(k') = f_{\text{backgr.}}(k') + f_{\text{res}}(k'),$$
$$a(k') = 2\tilde{q}(k') f_{\text{res}}(k'), \qquad b(k') = [\tilde{q}^2(k') - 1] f_{\text{res}}(k'). \qquad (8)$$

However, in contrast to Eq. (5), this representation is purely formal since the parameters of Eq. (7) are complicated combinations of all the interfering amplitudes corresponding to the various excitation multipoles of the atom.

2. Interference between direct transitions and the resonance (through the self-ionization level) ionization of the atom leads to a number of properties in the behavior of the resonance parameters as functions of the emission angle. For example, if $b(k')$ is interpreted as the "yield" of the self-ionization state, it is clear that it can be substantially asymmetric relative to the angle of 90° to the direction of motion of the incident particles, whilst it is obvious that in the decay of the self-ionization state itself, this asymmetry is not observed. In the special case of the S resonance ($L = 0$), the resonance yield interpreted in this way turns out to depend on the angle of emission, whereas the self-ionization state itself decays isotropically.

To illustrate the scale of the changes which arise when interference between the resonance and direct transitions is taken into account, we have carried out a qualitative calculation on the excitation and decay of the self-ionization state $(2s2p)^1P^{(-)}$ during the interaction of helium atoms and fast electrons. All the approximations regarding the reaction mechanism and the atomic wave functions are the same as in[6].

The main results of the calculations are summarized in Figs. 1 and 2 for the equivalent representations given by Eqs. (6) and (7). We shall now list the most interesting properties exhibited by these results.

A. Interference between direct transitions and the resonance leads to a substantial change in the resonance line shape as a function of the angle of emission. The resonance profile index $\tilde{q}(k')$ is a complicated and generally nonmonotonic function of the emission angle. It cannot, therefore, be associated with any definite value of the profile index $q(Q)$ corresponding to the resonance in the spectrum of the scattered particles. In particular, the "optical limit" for $q(Q)$, which corresponds to the photoabsorption curve, cannot be used for this purpose. For the sake of greater clarity, Fig. 3 shows the calculated spectra of emitted electrons for two values of the angles, near a minimum and near a maximum of $\tilde{q}(k')$.

B. It was noted by a number of experimenters that, in the back hemisphere, the spectra of the emitted electrons are always more symmetric than in the front hemisphere. This is well explained by the shape of the curves for the parameters $\tilde{q}(k')$ and $a(k')$.

C. As the energy of the incident particles increases, the interference effects between the resonance and direct transitions are smoothed out: all the curves become more symmetric relative to 90°, and the function

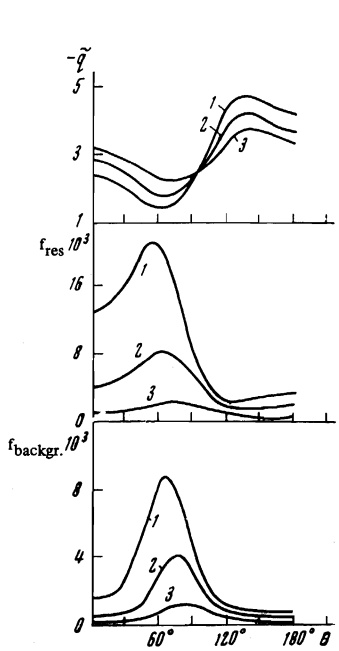

FIG. 1

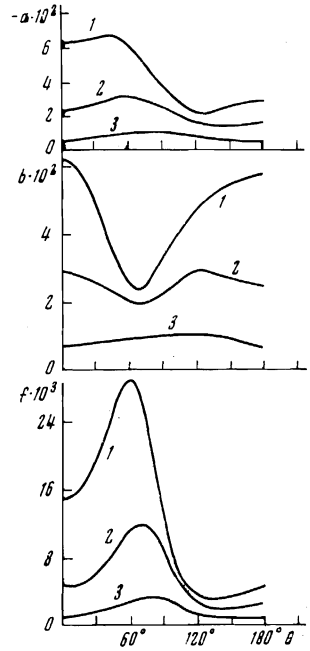

FIG. 2

FIG. 1. Parameters of the Fano formula for the $(2s2p)^1P^{(-)}$ resonance in the electron spectrum emitted by helium atoms for different incident-electron energies E_0: 1—400 eV; 2—1000 eV; 3—4000 eV. The values of f are given in units of a_0^2/at. un. sr.

FIG. 2. Parameters of the $(2s2p)^1P^{(-)}$ resonance in the spectrum of emitted electrons using Eq. (6) calculated for the same values of the incident-electron energies as in Fig. 1 (a, b, f are given in units of a_0^2/at. un. sr).

$\tilde{q}(k')$ becomes equal to a constant, which itself is equal to the optical limit for the q index. It is only in the limiting case $E_0 \gg 1$ keV that the same value of the index q characterizes the shape of the resonance lines in the spectra of the scattered and emitted electrons.

D. The change in $b(k')$ clearly reflects the behavior predicted earlier by the simpler calculation[6]: at low energies of the incident electrons, the Auger electrons are emitted preferentially in the direction of motion of the incident beam, and at very high energies they are emitted preferentially at right-angles to this direction ($\sim \sin^2\theta$); in the case of the $(2s2p)^1P^{(-)}$ resonance, the anisotropy coefficient passes through zero roughly at $E_0 = 1$ keV.

3. For a qualitative comparison of the calculations with experiment, we shall use the results of Mehlhorn,[1] who was the first to consider the change in the resonance--line profile as a function of the angle of emission. Mehlhorn measured the distribution of emitted electrons in a broad interval of energies near the $(2s2p)^1P^{(-)}$ resonance at an incident electron energy of 4 keV and detection angle of 54°. We have no knowledge of the energy resolution achieved in this work of the form of the instrumental curve which, in general, may affect the smearing of the resonance. We have therefore applied a Gaussian spread to our theoretical curve.

Figure 4 shows the Mehlhorn results together with our calculations for two values of the Gaussian parameter, namely, $\sigma = 0.2$ eV and $\sigma = 0.4$ eV. The discrep-

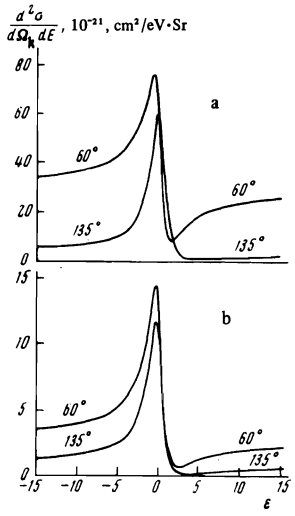

FIG. 3

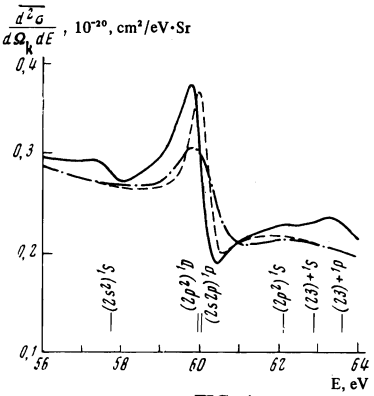

FIG. 4

FIG. 3. Profile of the $(2s2p)^1P^{(-)}$ resonance at different angles of emission and energies E_0: a—400 eV; b—4000 eV.

FIG. 4. Spectrum of electrons emitted by the helium atom at 54° for incident electron energy of 4 keV. Solid curve—experimental data of Mehlhorn [1], dashed curve—calculated for $\sigma = 0.2$ eV, dot-dash curve—ditto for $\sigma = 0.4$ eV; the self-ionization levels shown in the figure are classified in accordance with [13].

ancy between experiment and calculation at the excitation energy of 57.5 eV and at 62-64 eV is connected with the fact that we are taking into account only the $(2s2p)^1P^{(-)}$ resonance, whereas these energy intervals contain a number of other self-ionization states. On the whole, the agreement between theory and experiment as far as the shape of the resonance is concerned turns out to be quite satisfactory. We note that there is a shift of the entire resonance curve obtained by Mehlhorn relative to the calculated curve. The reasons for this shift are not clear. We note, however, that the mean value of the resonance energy reported by Mehlhorn is lower by 0.12 eV as compared with the photoabsorption experiments.

4. Summarizing, we note that our calculations are based on a simple method of solving the problem of the coupling between discrete and continuous spectra of the states of two-electron systems, which is based on the use of the diagonalization of the wave functions describing the self-ionization state.[8,9] This method was first tried in the case of the photoabsorption resonances,[8] and was subsequently applied to a number of problems in the theory of electron-atom collisions.[6,10-12] It has been found that the method is also convenient for the qualitative analysis of a broad class of phenomena, and is also a promising basis for quantitative descriptions. It seems to us that more fundamental methods, i.e., the strong coupling method and the method of coupled integral equations, would be difficult to use on such a large scale because of the volume of the necessary calculations. Our results show that the development of the diagonalization method, as applied to resonances in multielectron systems, is a very urgent task.

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