Manifestation of restructuring of the electron shells in atoms in the course of ionization

M. Ya. Amus'ya, V. K. Ivanov, S. A. Sheĭnerman, S. I. Sheftel', and A. F. Ioffe

A. F. Ioffe Physicotechnical Institute, USSR Academy of Sciences
and Leningrad Institute of Nuclear Physics, USSR Academy of Sciences
(Submitted 13 February 1979; resubmitted 15 October 1979)
Zh. Eksp. Teor. Fiz. **78**, 910–923 (March 1980)

It is shown that in the study of the ionization of an atom in the region of the thresholds of the inner shells it is necessary to take into account, besides the correlations of the random-phase approximation with exchange (RPAE), which gave good account of itself for the outer shells, also the restructuring of the core of the atom when a slow electron is removed from it. A method is developed for simultaneously taking into account this restructuring in the static limit with the RPAE correlations. This is followed by calculations of the photoionization cross sections of the $4d^{10}$ shells of the atoms of xenon, cesium, and barium, of the $3d^{10}$ shell of xenon, of the $2p^6$ subshell of argon, and also of the generalized oscillator strengths of $2p^6$ Ar and $5s^2$ Xe. It is found that allowance for the restructuring changes greatly the cross section in the near-threshold region and leads to good agreement with experiment. A strong influence of the restructuring on the interaction between the shells is also demonstrated.

PACS numbers: 32.80.Fb, 32.70.Cs, 31.30. – i, 31.20. – d

1. INTRODUCTION

The use of the formalism of many-body theory and the random-phase approximation with exchange (RPAE) formulated with its aid has made it possible to obtain an quite satisfactory description of the ionization process for large number of outer and intermediate shells of a number of atoms (see Ref. 1 and the bibliography therein). It turned out that ionization should be regarded as a multielectron process, since all the electrons of the given subshell participate in it as a rule, and frequently also some electrons of several nearest subshells.

Recent definite experimental data, however, cannot be described within the framework of the RPAE method, particularly data on the ionization of the inner shells of a number of atoms.[2,3] In these cases, in the vicinity of the threshold, the ionization cross section obtained in the RPAE greatly exceeds, sometimes by two or more times, the experimental value. Since these deviations certainly exceed the experimental errors, it must be concluded that an approach outside the framework of the RPAE is necessary.

In a justification of the applicability of the RPAE to the atom, we have guided ourselves by the analogy with a uniform electron gas of high density.[4] The obvious difference—the essential inhomogeneity of the electron density of the atom—was accounted for by the fact that the single-electron wave functions employed were those obtained in the Hartree-Fock approximation. There is, however, one more difference between electrons in an atom and an electron gas: since the energy distance between shells is large, each shell, rather than their aggregate as a hole, can be regarded as an element of the electron gas. Therefore, because of the interaction between the electrons, the density of one "element" of the gas (atomic shell) can change when an electron is removed from another. This process—the restructuring of the atomic subshells upon ionization of the atom—is not taken into account within the framework of the RPAE. A development of a method for taking the restructuring into account is in fact the subject of the present paper.

The restructuring of the atomic shells in the course of ionization influences the wave functions of the emitted electron, changes the ionization energy and the interaction of the electron with the hole. Let us examine the conditions under which the influence of the restructuring is substantial. The time during which the atom is restructured as a result of an appearance of a hole in a state i will be estimated with the aid of the relation ($\hbar = m = e = 1$)

$$\tau \sim \frac{1}{\Delta E} = \frac{1}{-E_i - (E_{at} - E_{ion})}; \tag{1}$$

here ΔE is the restructuring energy, $E_i < 0$ is the energy of the i-th hole state in the Hartree-Fock approximation, E_{at} and E_{ion} are the total energies of the atom and ion. The knocked-out electron leaves the atom within a time

$$t \sim 1/v \sim \varepsilon^{-1/2}, \tag{2}$$

where ε is the energy of the outgoing electron and v is its velocity. The influence of the restructuring in the ionization process is appreciable if the electron leaves the atom quite slowly, i.e., at $t \gtrsim \tau$, which yields

$$\varepsilon \lesssim [E_{ion} - E_{at} - E_i]^2. \tag{3}$$

For example, when the p^6 subshell of argon is ionized, the restructuring according to the estimate (3) is significant at energies $\varepsilon \lesssim 0.8$ Ry. At higher energies there is not enough time for the restructuring to take place during the time of emission of the electron. Its influence decreases rapidly with increasing ε. This means that it is precisely in the near-threshold region that a difference is observed between the results of calculations by the RPAE method and experiment.[2,3,5]

It is quite complicated to take full account of the dynamics of the restructuring of the electron shells when the atom is ionized. It is therefore important to obtain approximate methods to make allowance for its influence. In the present paper we propose in fact a method that makes it possible to generalize the RPAE approximation and to take account of the bulk of the corrections

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necessitated by the restructuring. It is assumed here that the ionized electron moves in the field of a completely restructured core. This is taken into account by a suitable choice of the single-particle wave functions of the electron and hole, employed subsequently in the RPAE equations. The results obtained with the aid of the proposed method are in satisfactory agreement with the experimental data on the cross sections of photoionization and inelastic scattering of fast electrons on the inner shells.

In Sec. 2 we note the limitations of the RPAE method and discuss possibility of its generalization. In Sec. 3, using the diagram technique of many-body theory, we derive equations that make it possible to take into account the screening of the interaction between the hole and the outgoing electron. The result is a system of self-consistent equations of the Hartree-Fock type for the determination of the wave functions of the electron in the field of the restructured ion. The use of these functions in the RPAE equations makes it possible to take into account the many-electron correlations of the random-phase approximation as well as those connected with the restructuring of the atom.

In Secs. 4 and 5 we present the results of concrete calculations of the cross sections of the photoionization of the $4d^{10}$ shells of a number of atoms, the $3d^{10}$ shell of xenon, the sp^6 shell of argon, and of the generalized oscillator strengths of the $2p^6$ shell of argon and the $5s^2$ shell of xenon. It is shown that allowance for the restructuring changes substantially the magnitude of the cross section in the near-threshold region and leads to good agreement with experiment. Using as a concrete example the action of the $4d$ electrons on the electrons of the outer $5s$ and $5p$ shells of xenon and barium, we demonstrate the influence of the restructuring on the intershell interaction.

2. LIMITATIONS OF THE RANDOM-PHASE METHOD

When using the method of the many-body theory in an investigation of the structure of the electron shells of atoms, the usually chosen bases wave functions are those satisfying the system of equations of the single-configuration Hartree-Fock approximation ($\hbar = m = e = 1$):[6]

$$(\hat{H}_0 - E_k)\varphi_k(\mathbf{r}) \equiv \left(-\frac{\nabla^2}{2} - \frac{Z}{r} + \sum_{i\leqslant F}\int \varphi_i^*(\mathbf{r}_1)\frac{d\mathbf{r}_1}{|\mathbf{r}-\mathbf{r}_1|}\varphi_i(\mathbf{r}_1)\right)\varphi_k(\mathbf{r}) - \sum_{i\leqslant F}\delta_{s_i s_k}\int \varphi_i^*(\mathbf{r}_1)\frac{1}{|\mathbf{r}-\mathbf{r}_1|}\varphi_k(\mathbf{r}_1)\,d\mathbf{r}_1\varphi_i(\mathbf{r}) - E_k\varphi_k(\mathbf{r}) = 0; \quad (4)$$

here k and i correspond to different sets of the quantum numbers of the electron (hole): n, l, m, and s; $i \leqslant F$ denotes summation over only the occupied (hole) states in the atom. The eigensolutions (4) determine a set of wave functions $\varphi^{N+1}(r)$, where N is the number of electrons in the atom.[7] This notation emphasizes the fact that at $k > F$ Eq. (4) determines the wave functions of the $N+1$-st electron moving in the self-consistent field produced by all the N electrons of the atom.

The cross section of the single-electron ionization is expressed in terms of the matrix element of the transition of the electron from an initial state $n_i l_i$ to a final state $n_j l_j$:[6]

$$\sigma(\omega) \sim |\langle n_j l_j|\hat{D}|n_i l_i\rangle|^2, \quad (5)$$

where ω is the energy transferred to the atom. In the RPAE method there is substituted in (5) a matrix element with allowance for the correlation determined by the integral equation[1,7]

$$\langle \nu_2|D(\omega)|\nu_1\rangle = \langle \nu_2|d|\nu_1\rangle + \sum_{\substack{\nu_4>F\\ \nu_3\leqslant F}}\left(\frac{\langle \nu_4|D(\omega)|\nu_3\rangle\langle \nu_3\nu_2|U|\nu_4\nu_1\rangle}{\omega - E_{\nu_4} + E_{\nu_3} + i\delta} - \frac{\langle \nu_3|D(\omega)|\nu_4\rangle\langle \nu_4\nu_2|U|\nu_3\nu_1\rangle}{\omega + E_{\nu_4} - E_{\nu_3} - i\delta}\right). \quad (6)$$

Here E_ν is the Hartree-Fock energy of the state ν, $\langle \nu_2|d|\nu_1\rangle$ is the matrix element of the transition in the Hartree-Fock approximation,

$$\langle \nu_3\nu_2|U|\nu_4\nu_1\rangle = \langle \nu_3\nu_2|V|\nu_4\nu_1\rangle - \langle \nu_3\nu_2|V|\nu_1\nu_4\rangle, \quad (7)$$

and V is the Coulomb interelectron interaction.

In practical calculations it is more convenient to use a basis of wave functions $\varphi^N(\mathbf{r})$ that take into account the fact that the electron removed from the atom does not move in the field of a neutral atom with N electrons, but in the field of a positive ion. These wave functions, as shown in Ref. 7, already include a definite part of the multielectron correlations of the RPAE method.

Although the RPAE method did succeed in attaining for the first time good agreement between the calculation results and the experimental data in a large number of cases,[1,7] recently differences were also observed for the inner and some intermediate shells.[2,3] Thus, the calculated cross sections of the ionization of the inner shells have high and narrow peaks at the ionization threshold, something not observed in experiment. The maximum at the threshold is the result of the fact that the removed electron moves in the attracting Coulomb field of the hole. The discrepancy between theory and experiment means thus that the hole field taken into account in the RPAE is too strong. Indeed, in the course of formation of a vacancy in an inner or intermediate shell, the electron shells of the atom (particularly the outer ones) become restructured, a fact not accounted for in the RPAE. The outer electrons approach somewhat the nucleus, and as a result the screening of the hole becomes stronger and the interaction of the hole with the removed electron weakens, so that the cross section at the threshold decreases.

Let us note which principal processes not accounted for in the RPAE determine, from the point of view of many-body theory, the influence of the restructuring on the ionization of the atoms.

1) The screening of the interaction of the outgoing electron and hole. Instead of the pure Coulomb interaction of the electron and hole, take into account by the RPAE method, it is necessary to consider more complicated diagrams, of the type shown in Fig. 1a and 1b. Inclusion of these processes constitutes a refinement of the vertex part of the ionization matrix element $\langle \nu_2|d|\nu_1\rangle$ (Fig. 1a) and of the Coulomb interaction $\langle \nu_3\nu_2|U|\nu_4\nu_1\rangle$ in Eq. (6) (Fig. 1b).

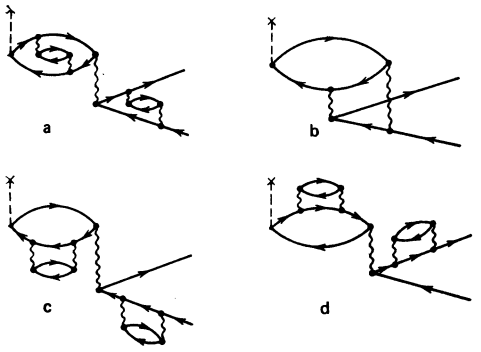

FIG. 1. Diagrams for the ionization amplitude with allowance for the restructuring effects. The lines with the arrows pointing right (left) correspond to propagation of an electron (hole) described by a wave function φ^{N+1} (φ^{N}), the wavy line corresponds to Coulomb interaction, and the dashed line with the cross corresponds to the external ionizing field.

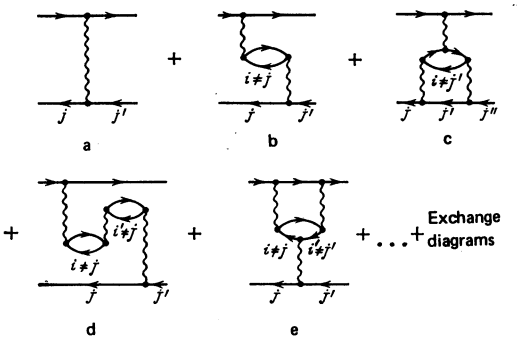

FIG. 2. Feynman diagrams describing the interaction of the electron and hole.

2) Corrections to the self-energy part of the Green's function of the hole or, in other words, corrections to the self-consistent field of the hole compared with the Hartree-Fock shield. An example of a diagram for the ionization amplitude with simplest corrections of this type is shown in Fig. 1c. In particular, the restructuring of the electron shells influences the position of the hole itself, i.e., leads to a change of the ionization potential, which was previously assumed, in accordance with the Koopman theorem,[8] to be equal to the single-particle energy of a hole in a neutral atom. The latter, however, does not coincide, as a result of the restructuring, with the true ionization potential, defined as the difference between the total energies of the atom and the ion.

3) Corrections to self-energy part of the outgoing electron (for example, diagram *d* on Fig. 1), which describe the influence of polarization of the atomic core on the wave function of the electron. We note that in most cases the polarizability of positive ions is small, at any rate much less than the corresponding value for neutral atoms. Therefore the polarization potential acting on the outgoing electron is also small. This is all the more true for ions of noble gases, concrete calculations for the neutral atoms of which have shown that the dynamic polarizability is small.[9] We shall therefore neglect hereafter the corrections similar to those shown in Fig. 1d.

3. SCREENING OF THE ELECTRON-HOLE INTERACTION IN THE STATIC APPROXIMATION

Let us examine the perturbation-theory terms that describe the interaction of an electron and a hole. Figure 2 shows diagrams that are irreducible in the particle-hole channel. We note that the term with $i=j$ makes no contribution in the loop in the sum over the intermediate hole states, since it is cancelled out by the corresponding exchange diagram. Diagram *a* of Fig. 2 describes the Coulomb interaction of the knocked-out electron with the hole (an interaction taking into account within the framework of the RPAE), while the remaining diagrams determine the corrections to this interaction, which are necessitated by the restructuring of the electron shells of the atom. The influence of the restructuring has a dynamic character and depends on the velocity of the removed electron, so that an exact calculation of the aggregate of diagrams of Fig. 2 is an exceedingly complicated problem.

In the present paper we confine ourselves to a simpler case—the static approximation, which is valid if (3) is satisfied. It is assumed in this approximation that the restructuring of the electron shell has already taken place by the instant of departure of the ionized electron, and the latter moves in a self-consistent field that is modified by the appearance of the hole. This assumption is written in the form of the condition

$$E_j=E_{j'}=E_{j''}=\dots, \tag{8}$$

i.e., we retain in the diagrams of Fig. 2 only terms diagonal in the hole state. We note that by virtue of the large energy spacing between the inner shells and subshells, and also by virtue of the fact that the largest are the overlap integrals for identical states, it is precisely these terms which make the principal contribution to the interaction of the electron and hole *j*. The irreducible diagrams of Fig. 2, in which the electron interacts two or more times with the remaining electrons of the atom (for example, diagram *e*, are similar under the condition (8) to the polarization diagrams of Fig. 1c. Therefore, since the polarization potential is small, these diagrams can be neglected, as mentioned in Sec. 2.

Thus, in our approximation we confine ourselves to account of diagrams that are diagonal in the hole state *j* and include in the irreducible part only single interaction with the departing electron. The sequence of precisely these diagrams corresponds to scattering of an electron by the additional potential produced by the hole *j*. We summed this sequence and obtain new equations for the wave function of the electron with allowance for the restructuring of the electron shells. In fact, an element of the diagram of Fig. 2 transforms in the manner shown in Fig. 3. The transformed element of diagram 3, which is equal to

$$\int V|\varphi_j(\mathbf{r}')|^2\,d\mathbf{r}'=\int V(|\mathbf{r}-\mathbf{r}'|)\rho_j(\mathbf{r}')\,d\mathbf{r}', \tag{9}$$

is the contribution of the hole *j* to the self-consistent potential. Analytic expressions for the transformed diagrams of Fig. 3 differ from the corresponding diagrams in Fig. 2 only by the factor $(-1)^m$, where *m* is the number of acts of interaction with the hole *j*. We

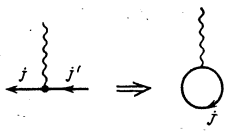

FIG. 3.

can therefore replace the summation of our chosen sequence by summation of a sequence of transformed diagrams with proper account taken of the signs.

In the solution of Eq. (4), to determine the Hartree-Fock wave function φ_k^{N+1} one takes automatically into account diagrams[10] that contain the elements (9), but only in (4) is summation carried out in these electron-hole and hole loops over all the states below the Fermi limit $\sum_{i\leqslant F}$, including $i=j$, and they enter in Eq. (4) with opposite sign, namely $(-1)^{n+1}$. Therefore summation of the sequence of transformed diagrams leads to cancellation of the same terms in the Hartree-Fock interaction of the electron with the atom. Consequently, by "subtracting" the contribution of the infinite sequence of the transformed diagrams from the electron wave function φ^{N+1} we redefine the electron wave function and by the same token take into account the influence of the restructuring in the static limit.

Figure 4 shows in graphic form the system of integral equations for the determination of the "restructured" wave function $\tilde{\varphi}_k$ of the electron. The thin line corresponds to the wave function φ^{N+1}, the double line to the reconstructed wave function $\tilde{\varphi}$ of the electron, and the thick line to the hole. With the aid of an iteraction procedure we can verify that the system of equations shown in Fig. 4 contains the sequence of diagrams of Fig. 2, transformed in accordance with Fig. 3. In analytic form, the system of equations shown graphically in Fig. 4 can be expressed in the form

$$\langle\tilde{k}|=\langle k|+\sum_n\langle n|\frac{1}{E_k-E_n}\Big[\sum_{\substack{i\leqslant F\\ i\neq j}}\langle\tilde{k}\tilde{l}|\hat{V}|n\tilde{i}-\tilde{i}n\rangle-\sum_{i\leqslant F}\langle\tilde{k}i|\hat{V}|ni-in\rangle\Big],\quad k>F; \tag{10a}$$

and

$$|\tilde{i}\rangle=\sum_n|n\rangle\frac{1}{E_i-E_n}\Big[\sum_{\substack{i\leqslant F\\ i\neq j}}\langle n\tilde{l}|\hat{V}|\tilde{i}\tilde{l}-\tilde{l}\tilde{i}\rangle-\sum_{i\leqslant F}\langle nl|\hat{V}|\tilde{i}l-l\tilde{i}\rangle\Big],\quad i\leqslant F. \tag{10b}$$

Here $\langle\tilde{k}|\equiv\varphi_k$, and $\langle k|\equiv\varphi_k^{N+1}$; (10b) is a system of self-

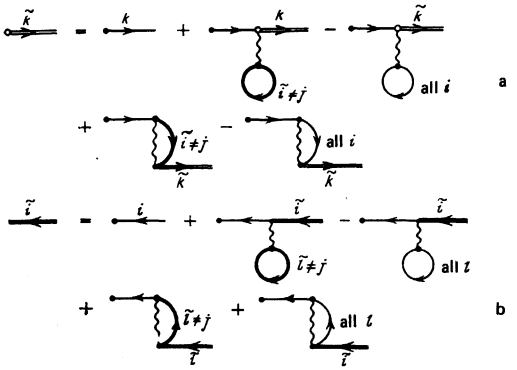

FIG. 4. Equations for the determination of the "restructured" wave function $\tilde{\varphi}_k$ of an ionized electron.

consistent equations for the determination of the wave functions $|\tilde{i}\rangle$ of the restructured ion with a hole in the state j, produced after ionization, while (10a) is the equation for the wave function $\tilde{\varphi}_k$ of the knocked-out electron in the field of this ion.

We proceed now to an integrodifferential form of these equations. We apply the operator $\hat{H}_0-E_i$ from the left to both halves of (10b), and the operator $\tilde{H}_0-E_k$ from the right to both halves to (10a). Using (4) and the boun-boundary conditions for the bound states, we obtain

$$\langle\tilde{k}|(\hat{H}_0-E_k)=-\sum_n\langle n|\Big(\sum_{\substack{i\leqslant F\\ i\neq j}}\langle\tilde{k}\tilde{l}|\hat{V}|n\tilde{i}-\tilde{i}n\rangle-\sum_{i\leqslant F}\langle\tilde{k}i|\hat{V}|ni-in\rangle\Big),\quad k>F; \tag{11a}$$

$$(\hat{H}_0-E_i)|\tilde{i}\rangle=-\sum_n|n\rangle\Big(\sum_{\substack{l\leqslant F\\ l\neq j}}\langle n\tilde{l}|\hat{V}|\tilde{i}\tilde{l}-\tilde{l}\tilde{i}\rangle-\sum_{l\leqslant F}\langle nl|\hat{V}|\tilde{i}l-l\tilde{i}\rangle\Big),\quad i\leqslant F. \tag{11b}$$

Changing the order of integration and using the completeness of the set of functions φ_n^{N+1} and the explicit form of the operator $\hat{H}_0$ from (4), we get ultimately

$$\Big(-\frac{\nabla^2}{2}-\frac{Z}{r}+\sum_{\substack{i\leqslant F\\ i\neq j}}\int\tilde{\Phi}_i^*(\mathbf{r}_1)\frac{1}{|\mathbf{r}-\mathbf{r}_1|}\tilde{\Phi}_i(\mathbf{r}_1)\,d\mathbf{r}_1\Big)\tilde{\Phi}_k(\mathbf{r})$$
$$-\sum_{\substack{i\leqslant F\\ i\neq j}}\delta_{s_i s_k}\int\tilde{\Phi}_i^*(\mathbf{r}_1)\frac{1}{|\mathbf{r}-\mathbf{r}_1|}\tilde{\Phi}_k(\mathbf{r}_1)\,d\mathbf{r}_1\tilde{\Phi}_i(\mathbf{r})-E_k\tilde{\Phi}_k(\mathbf{r})=0. \tag{12}$$

Since the structure of the equations for the electron and hole states is the same, they are combined into one, where k is taken to mean both types of the states. At $k\leqslant F$ we obtain the ordinary Hartree-Fock equations for the determination of the hole states of the single ion. To obtain the wave function of the outgoing electron ($k>F$), the determination of the ground state of the singly charged ion is the intermediate solution stage necessary to find the self-consistent field in which the electron moves.

Thus, the use of the electron wave function obtained by solving the system of equations (12) is equivalent to taking into account an infinite sequence of the diagrams of Fig. 2 in the static approximation, which described the direct and screened (as a result of the restructuring of the electron shells) interaction between the electron and the produced hole. The ionization amplitude calculated in the RPAE approximation with such electron functions will include a contribution from processes of type a on Fig. 1 and with even more complicated inserts between the electron and the hole determined by the diagrams shown in Fig. 2.

We note that the diagram a in Fig. 2 is taken into account within the framework of the RPAE method,[1,7] so that in the construction of the generalized RPAE variant on the basis of new electron functions [of solutions (12)] it is necessary to make sure that the same processes are not taken into account twice. This is done by excluding the corresponding terms when solving Eq. (6).

Calculations within the RPAE framework, as already noted, overestimate the results for the ionization cross sections in the near-threshold region. Estimates show that allowance for the succeeding terms of the aggregate of the diagrams of Fig. 2 (b, etc.) should decrease the value of the cross section in this region. In fact,

diagram b on Fig. 2 (for $j=j'$) reaches the maximum value at low energies E and E' of the electron, the sign of its contribution is the reverse of the sign of the contribution of diagram a. Allowance for diagram b, consequently, leads to a weakening of the field of the hole and to a decrease of the cross section at the threshold.

We examine now the corrections to the self-energy $\Sigma_{jj'}$, of the hole, i.e., to the potential of the ionization from the state j, determined in the Hartree-Fock approximation. Figure 1c shows one of the diagrams with the corresponding inset in the hole state in the lowest order of perturbation theory. Considering an infinite sequence of diagrams that contribute to the self-energy of the hole, we confine ourselves here, as above, to the static approximation, in which are retained only the matrix element diagonal in the hole state j. These elements, as a rule, make the principal contribution to Σ_{jj}, since the diagrams that are off-diagonal in the hole state j are small in most cases because of the large energy distance between the inner shells and subshells. Then this sequence of terms of the perturbation-theory series describes in fact the change of the self-consistent field acting on the restructured hole (cf. the preceding exposition for the restructured particle).

Allowance for the diagrams of type Fig. 1c in the static approximation lead to a satisfactory agreement between the calculated potential of the ionization and the experimental value.[9,11] The hole wave function itself changes little in this case. The reason is the small change of the self-consistent field acting on the hole (the main change of the field occurs in the region of the outer atomic shells). The last statements were verified by calculation. Taking this into account, we have used in the calculation the experimental values of their ionization potentials and the nonrestructed wave function obtained for the hole by solving (4).

4. INFLUENCE OF RESTRUCTURING IN THE PHOTOIONIZATION PROCESS

The method of taking restructuring into account, which was developed in the preceding sections, was used by us in calculations of the photoionization cross sections of the inner and intermediate shells of a number of atoms. The wave functions of the ground state of an ion with vacancy in an ionizable subshell was obtained by us from (4), the restructured wave functions of the knocked-out electron were obtained from (12), while the restructured wave functions of the hole was determined from the solution of Eqs. (4) for the ground state of the neutral atom. This was followed by calculation of the dipole matrix element[7] and by the solution of Eq. (6), from which we ultimately obtained the matrix elements of the photoionization with allowance for the restructuring and the correlations of the RPAE.

The proposed method was first used on the basis of qualitative purely physical considerations for an investigation of the photoionization of the $1s^2$ and $2p^6$ subshells of argon,[5] where the cross section, without allowance for the restructuring, has a sharp maximum at

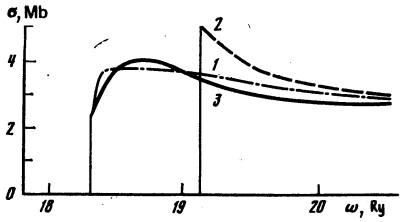

FIG. 5. Photoionization cross section of the $2p^6$ subshell of argon: 1—experiment,[2] 2—RPAE method, 3—RPAE with restructuring.

the ionization threshold. Figure 5 shows the experimental photoionization cross section[2] of $2p^6$Ar and the theoretical curves obtained in the RPAE approximation with and without allowance for the restructuring. Allowance for the latter led to a change in the position of the threshold, to elimination of the narrow maximum in its vicinity, and to a substantial improvement of the agreement with experiment. We note that here and hereafter the principal role and elimination of the sharp maximum at the threshold is played by the screened interaction of the electron and hole (i.e., the processes shown in Fig. 2). The corrections to the self-energy of the hole alter the ionization potential and, as it turned out, lead also to internal self-consistency of the calculation, for when they are taken into account the sum rule is satisfied and the cross sections obtained with the operators $\mathbf{r}$ and ∇ coincide.

To trace the variation of the relative role of the restructuring with increasing charge of the nucleus, we have calculated the photionization cross sections of the

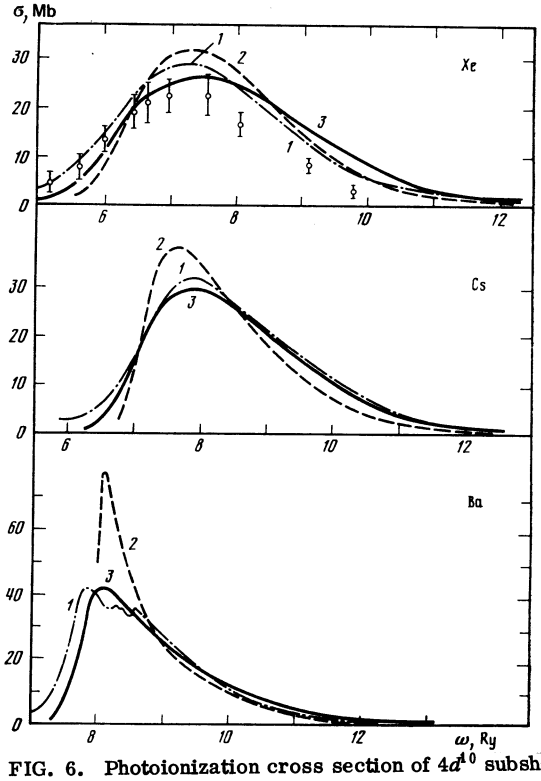

FIG. 6. Photoionization cross section of $4d^{10}$ subshells of xenon, cesium, and barium atoms: 1—experiment for xenon from Ref. 13, cesium from Ref. 14, and barium from Ref. 3. ○—experiment for $4d^{10}$ Xe from Ref. 15; 2—calculation by RPAE method, 3—RPAE with restructuring.

$4d^{10}$ subshells of the atoms xenon, cesium, and barium.[12] The results of the calculations are shown in Fig. 6. The general features of the influence of the restructuring are that the cross section at the threshold decreases, and the maxima become broader and shift towards larger energies. It is also seen from Fig. 6 that the relative role of the restructuring increases on going from xenon to barium. The reason is that the effective charge of the nucleus acting on the $4d$ subshell increases, and the cross section of the photionization at the threshold increases accordingly. Therefore the role of the restructuring is more visible in the total cross section, since it is more concentrated at the threshold.

The method described above for calculating the ionization cross sections was used in an investigation of the $3d$ shell of xenon.[16] Interest in this shell is due to the published prediction of the existence of a collective excitation level, which is the analog of the plasma oscillation of an electron gas. Solving in the statistical approximation equations of the RPAE types (without exchange), Kirzhnits *et al.*[17] have shown that there should exist two levels with energy $\omega_2 > \omega_1 = Z$ Ry and very small width $\Gamma_2 < \Gamma_1 \approx 2.2 \cdot 10^{-4}$ Ry. The oscillator strength of the first level turned out to be $0.1\,Z$. As applied to xenon, $\omega_1 = Z$ Ry corresponds to ionization of the $3d^{10}$ shell—approximately 1 Ry beyond the threshold. We have performed RPAE calculations in this energy region outside the framework of the statistical approximation and compared the results with the available experimental data.[18] We observed no maxima not connected with the ionization threshold of the $3d^{10}$ shell in the studied energy region, but the RPAE results in the vicinity of the threshold differed substantially from the experimental results. The reason is the neglect of the restructuring effects, whose influence turned out to be quite substantial, as is illustrated by Fig. 7. In Fig. 7, account is taken of the spin-orbit splitting of the thresholds of the $3d_{3/2}$ and $3d_{5/2}$ shells under the assumption that, at the same energy of the removed electron, the ratio of the cross sections of ionization with $j_{5/2}$ and $j_{3/2}$ is $(2j+1)/2j = 1.5$. Allowance for the restructuring has led to good agreement with experiment and confirmed the absence of specific maxima not connected with thresholds. Obviously, the statistical model is very crude when it comes to describing the photoionization of specific atoms.

We now examine the role of restructuring when an internal shell j acts on the ionization of an outer shell i. A necessary condition for the influence of the restructuring on the intershell interaction is the following time-dependent relation

$$\tau_{j\,\mathrm{rest}} \leqslant \tau_j, \tag{13}$$

where $\tau_{j\ \mathrm{rest}}$ is the time of restructuring of the ion with hole j [see formula (1)], τ_j is the "lifetime" of the intermediate state:

$$\tau_j \sim \frac{1}{\omega - \varepsilon - I_j}, \tag{14}$$

here ε is the energy of the electron in the intermediate state, I_j is the ionization potential of the shell j. Since the restructuring is significant at low energies ε [see the estimate (3)], we find that the influence of the restructuring of the inner shell j manifests itself in the ionization cross section of the outer shell only in the vicinity of the ionization threshold of the inner shell: $\omega \sim I_j$. It is larger the closer to the threshold and the sharper the maximum in the cross section for the ionization of the inner shell.

Concrete results were obtained for the photoionization of the $5p^6$ and $5s^2$ subshells of xenon, cesium, and barium with account taken of the influence of the $4d^{10}$ subshell in the vininity of the ionization potential I_{4d}. Figure 8 shows the photoionization cross section of the $5p^6$ subshell of barium, which was strongly influenced by the restructuring in the $4d^{10}$ subshell. This is directly connected with the considerable changes resulting from the restructuring and the cross section of the photoionization of the barium $4d^{10}$ subshell itself (Fig. 6). These changes are smaller for xenon, and consequently the influence of the restructuring in the $4d^{10}$ shell on the ionization of the $5p^6$ and $5s^2$ subshell is smaller. The influence of the restructuring on the angular distribution of the photoelectrons[19] turned out to be relatively weak.

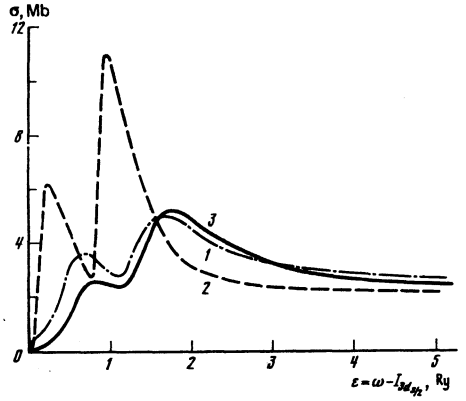

FIG. 7. Photoionization cross section of $3d^{10}$ subshell of xenon: 1—experiment from Ref. 19, 2—calculation by RPAE method, 3—RPAE with allowance for restructuring.

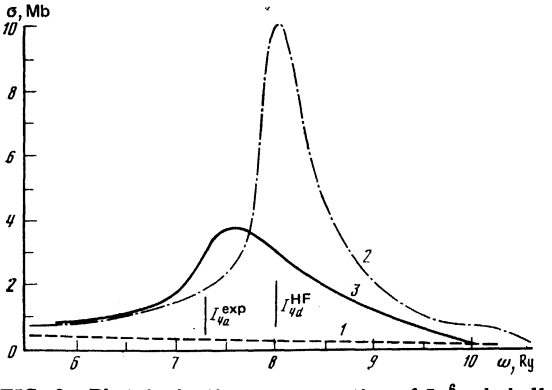

FIG. 8. Photoionization cross section of $5p^6$ subshell of barium in the vicinity of the threshold I_{4d}: 1—RPAE method, 2—RPAE with allowance for the influence of the $4d^{10}$ subshell, 3—RPAE with allowance for the restructured $4d^{10}$ subshell.

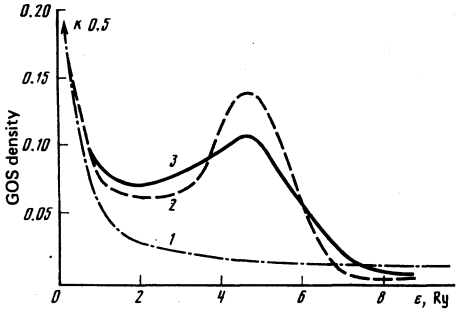

FIG. 9. Density of generalized oscillator strengths for $5s^2$ subshell of xenon: 1—calculation in the Hartree-Fock approximation, 2—RPAE method, 3—RPAE with restructuring in the $4d^{10}$ subshell.

5. INFLUENCE OF RESTRUCTURING ON THE DENSITY OF THE GENERALIZED OSCILLATOR STRENGTHS

To investigate the influence of restructuring of the electron shells on the ionization of the atom, with nonzero momentum transfer to the atom, we have calculated the densities of the generalized oscillator strengths (GOS) of the $2p^6$ subshell of argon and of the $5s^2$ subshell of xenon. (A preliminary calculation of the GOS for the $2p^6$ subshell of argon without allowance for the influence of the $2s^2$ subshell was published in Ref. 20.) We investigated the behavior of the monopole, dipole, and quadrupole components of the GOS density in the range of the outgoing electron energy ε from 0 to 20 Ry and in the range of momentum transferred to the atom q from 0 to 4 at.un.

In the case of the $2p^6$ subshell of argon, the character of the influence of the restructuring[20] turns out in general to be the same as in the case of photoionization: the maximum at the threshold decreases in magnitude, broadens, and shifts towards higher energies ε. With further increase of ε, this influence decreases. A similar picture is observed in the region of all the considered momentum transfers q. For $q = 1.3$ at. un. there are experimental data,[21] the agreement with which improves to a greater degree in calculations with restructuring of the core.[20] For the partial densities of the GOS, the calculations yielded the same results as for the total density of the GOS.[20]

To study the influence of the restructuring on the interaction between the shells, we have examined the GOS density of the $5s^2$ subshell (Fig. 9). The relaxation of the core alters substantially (no less than in the case of barium, see Fig. 8) the intershell interaction of the $5s$ and $5d$ electrons, and leads to a lowering of the GOS density of the $5s^2$ electrons in the vicinity of the threshold of the $4d^{10}$ subshell, compared with the density calculated within the framework of the RPAE.

6. CONCLUSION

The results of the calculations and the comparison with the experimental data show that the ionization of the inner shells is accompanied by restructuring or relaxation of the outer electrons, a restructuring most substantial in the near-threshold region of energies. The procedure proposed in the paper for taking the restructuring into account consisted of altering the RPAE method. The attained degree of agreement with experiment offers evidence that the static restructuring is the principal effect that must be taken into account, besides the RPAE correlation, in the description of the ionization of intermediate and inner shells.

The restructuring of the electron shells can manifest itself in the ionization process in the fact that the vacancy produced in the inner shell undergoes Auger decay within the time during which the photoelectron leaves the atom. As a result, the outgoing electron turns out to be in a different field, modified not only by the restructuring of the outer shells but also the Auger decay. The action of the field modified by the Auger effect on the outgoing electron, called post-collisional interaction in the literature,[22] leads to a substantial change in the ionization cross section directly at the threshold itself. Allowance for the joint influence of these two factors is a very urgent problem that awaits its solutions.

In conclusion, the authors are sincerely grateful to L. V. Chernysheva for compiling the program for the computer calculations, and to N. A. Cherepkov and M. Yu. Kuchiev for discussion of the results.

[1]M. Ya. Amusia and N. A. Cherepkov, Case Studies in Atom. Phys. 5, 47 (1975).
[2]R. D. Hudson and L. J. Kiefer, Atomic Data 2, 205 (1975).
[3]P. Rabe, K. Radler, and H.-W. Wolf, Vacuum Ultraviolet Radiation Physics, Pergamon-Vieweg, 1974, p. 247.
[4]D. Pines, Many-Body Problem, Benjamin, 1961.
[5]M. Ya. Amus'ya, V. K. Ivanov, and N. A. Cherepkov, Abstracts, 5th All-Union Conf. on the Physics of Electron and Atom Collisions, Uzhgorod, 1972, p. 131.
[6]I. I. Sobel'man, Vvedenie v teoriyu atomnykh spektrov (Introduction to the Theory of Atomic Spectra), Fizmatgiz, 1963 [Pergamon, 1973].
[7]M. Ya. Amus'ya and N. A. Cherepkov, Zh. Eksp. Teor. Fiz. 60, 160 (1971) [Sov. Phys. JETP 33, 90 (1971)].
[8]H. A. Bethe, Intermediate Quantum Mechanics, Benjamin, 1954 (Russ. transl., Mir, 1965, pp. 70–71).
[9]M. Ya. Amus'ya, N. A. Cherepkov, and S. G. Shapiro, Zh. Eksp. Teor. Fiz. 63, 889 (1972) [Sov. Phys. JETP 36, 468 (1972)].
[10]J. Goldstone, Proc. Roy. Soc. 239, 267 (1957).
[11]R. V. Vedrinskiĭ, V. V. Krivitskiĭ, and A. N. Pavlov, Izv. Vyssh. Ucheb. Zaved. Fizika 5, 58 (1976).
[12]M. Ya. Amusia, V. K. Ivanov, and L. V. Chernysheva, Phys. Lett. 59A, 191 (1976).
[13]R. Haense, G. Keitel, P. Schreiber, and G. Kunz, Phys. Rev. 188, 1375 (1969).
[14]H. Petersen, K. Radler, B. Sonntag, and R. Haensel, Preprint DESY-SR-74/14, Hamburg, 1974.
[15]J. P. West, P. R. Woodruff, K. Codling, and P. G. Houlgate, J. Phys. B: Atom. Molec. Phys. 9, 407 (1976).
[16]M. Ya. Amusia and V. K. Ivanov, Phys. Lett. 65A, 217 (1978).
[17]G. V. Gadiyak, D. A. Kirzhnits, and Yu. E. Lozovik, Zh. Eksp. Teor. Fiz. 69, 122 (1975) [Sov. Phys. JETP 42, 62 (1975)] D. A. Kirzhnits, Yu. E. Lozovik, and G. V. Shpatakovskaya, Usp. Fiz. Nauk 117, 3 (1975) [Sov. Phys. Usp. 18, 649 (1975)].
[18]R. D. Deslattes, Phys. Rev. Lett. 20, 483 (1968).
[19]M. Ya. Amusia and V. K. Ivanov, Phys. Lett. 59A, 194 (1976).
[20]M. Ya. Amus'ya, S. A. Sheinerman, and S. I. Sheftel', Zh. Tekh. Fiz. 47, 1432 (1977) [Sov. Phys. Tech. Phys. 22, 822

(1977)].
[21]V. V. Afrosimov, Yu. S. Gordeev, V. M. Lavrov, and S. G. Shchemlinin, Zh. Eksp. Teor. Fiz. 55, 1569 (1968) [Sov. Phys. JETP 28, 821 (1969)].
[22]G. C. M. King, F. H. Read, and R. C. Bradford, J. Phys. B: Atom. Molec. Phys. 8, 2210 (1975).

Translated by J. G. Adashko

Transitions between levels of multiply charged ions in a strong external field

G. L. Klimchitskaya

Leningrad State University
(Submitted 3 September 1979)
Zh. Eksp. Teor. Fiz. 78, 924–928 (March 1980)

A scheme is proposed for a fully relativistic calculation of the transition probabilities between levels of multiply charged ions in a strong homogeneous electric field. The probability of the magnetic dipole transitions between the state $2s1/2$–$1s1/2$ of a single-electron ion is calculated. It is shown that interactions with a strong field can lead to an appreciable increase of the probability of a transition that is weak in the absence of a field.

PACS numbers: 33.55. + c, 33.70. — w

Much attention is being paid in recent years to experimental and theoretical investigations of the spectra of multiply charged ions. These spectra were observed both in the study of the solar corona and in special laboratory setups. The principal laboratory methods for the investigation of ions with high degree of ionization, with the aid of which most data on the spectra and transition probabilities were obtained, are passage of an ion beam through a foil and the action of laser radiation on matter. In the latter case, the multiply charged ions are situated in a strong electric field (whose intensity can reach 10^9 V/cm, comparable with intraatomic fields). The theoretical investigation of the spectra of multiply charged ions in a strong electric field is therefore of considerable interest.

Labzovskiĭ and the author[1] have considered the influence of a homogeneous electric field on the energy levels in multiply charged ions. A relativistic calculation was made of the energy levels of two-electron ions in the configuration $1s2s + 1s2p$ with ion charge $10 \leqslant Z \leqslant 50$, situated in an external electric field that can be either weak or strong in comparison with the Coulomb interaction of the electrons. It was observed that in an external field new crossings of levels with different parity take place. As already shown,[2,3] these crossings can be used to check on the hypothesis that there are no weak neutral currents in atomic systems.

An external field, however, exerts a substantial influence not only on the energy levels, but also on the probability of the transitions between them. This change of the probabilities of the transitions by external electric field must be taken into account, in particular, when searching for situations that are most favorable for the observation of parity nonconservation effects. In the present study, which is a continuation of an investigation initiated in Ref. 1, we consider the influence of a homogeneous electric field on the transition probabilities in multiply charged single-electron ions. The transition probabilities are expressed in terms of the S-matrix element[4]

$$W_{AB}=2\pi|\langle B|M|A\rangle|^2,$$
$$\langle B|S|A\rangle=-2\pi i\langle B|M|A\rangle\delta(E_A^0-E_B^0). \tag{1}$$

To carry out a fully relativistic calculation, we shall use as the wave functions of the initial (A) and final (B) states the functions

$$\psi_{njm}=\sum_l a_l(nj)\psi_{njlm}, \tag{2}$$

where ψ_{njlm} are Dirac wave functions, and the coefficients $a_l(nj)$ are calculated in the course of diagonalization of the Hamiltonian that takes into account the interaction with the uniform electric field:

$$H(\mathbf{r})=h(\mathbf{r})+\alpha^{1/2}Fz. \tag{3}$$

Here $h(\mathbf{r})$ is the relativistic single-electron Dirac Hamiltonian for an electron in the field of a nucleus, z is the Cartesian coordinate of the electron in the field direction, F is the field intensity, and α is the fine-structure constant. We use a system of units in which $\hbar = c = m = 1$ (m is the electron mass).

In the calculation of the probability of the transition, in first-order perturbation theory in the interaction with the external field, account must be taken of the contribution from the diagrams a–c of Fig. 1. A wavy line denotes here the emitted photon, a dashed line the photon absorbed from the external field, and a double line the electron propagator.

The matrix elements of the S matrix are determined using the exact relativistic operator of interaction with the electromagnetic field.[5] Summation over the virtual states is carried out using the Coulomb Green's func-

 0038-5646/80/030465-03$02.40