Simplified version of the random-phase-approximation-with-exchange method*

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By comparing the random-phase-approximation-with-exchange (RPAE) method of Amusia et al. for the calculation of photoionization cross sections from closed-shell atoms with the reaction-matrix method, we obtain a simplified version of the RPAE by which we calculate the dipole-transition amplitude much as in the reaction-matrix method, yet with ground-state correlation effects included simultaneously. Calculation of photoionization cross sections for the $3p \to \epsilon d$ transition of Ar and $4d \to \epsilon f$ transition of Xe by this method yields a substantial improvement on the calculation by the reaction-matrix method and good agreement with RPAE and with experiment.

I. INTRODUCTION

The photoionization spectra of the noble gases in the far ultraviolet have been studied in the last ten years experimentally and theoretically and have served as critical tests of theoretical procedures. For He and Ne, single-electron photoionization is reproduced fairly well by the independent-particle approximation.[1] For Ar, Kr, and Xe, on the other hand, qualitative discrepancies appeared between experiment and the result of independent particle approximations. Moreover, these discrepancies were only reduced but not eliminated by calculations that improved only the continuum final-state wave functions.[2] A good qualitative and quantitative fit of these spectra was first achieved by Amusia et al.[3] through RPAE calculations (random-phase approximation with exchange) which introduce a simultaneous improvement on the wave functions of the ground state and the continuum states. Similar results have been obtained by Wendin.[4]

This paper presents a simplified version of the RPAE method (SRPAE), which allows one to calculate the photoionization cross section in a way similar to the more familiar configuration-interaction procedures, specifically to the reaction-matrix method of Ref. 1, yet including an improvement of the ground-state wave function. In Sec. II, after a brief review of the reaction-matrix method and the RPAE method, we discuss the similarities and differences of the two approaches. It is then shown how to develop a SRPAE method by making approximations on the RPAE equations. The method utilizes an approximate property of interaction-matrix elements, which has been previously applied by Wendin.[4] The formulas thus obtained have a structure similar to those of the reaction-matrix method, but with extra terms resulting from improving the ground-state wave function simultaneously. In Sec. III, we use SRPAE method to recalculate the photoionization cross section for the $3p \to \epsilon d$ transition of Ar and the $4d \to \epsilon f$ transition of Xe. In fact, this calculation is done using the same residual interaction-matrix elements as were used by Starace[2] in his calculation by the reaction-matrix method. The substantial improvement of the cross sections calculated by this method, demonstrated by the curves in Figs. 1 and 2, manifests the importance of ground-state correlation effect. The result is also compared with the RPAE calculations of Amusia et al.[3] and with experiment.

II. SIMPLIFIED VERSION OF RPAE METHOD

The reaction-matrix method[5,6] represents the final-state wave function of the photoelectron-plus-ion system as

$$\psi_E = \sum_i \left(u_{iE} B_i(E) \right.$$
$$\left. + \sum_j P \int d\epsilon \, \frac{u_{i\epsilon} K_{i\epsilon, jE}(E)}{E - \epsilon} B_j(E) \right) . \quad (1)$$

In this equation, $u_{i\epsilon}$ is a Slater-determinant basis function of the many-electron system in an independent electron approximation, with ϵ the total energy of the system, i the channel index represented by an appropriate set of discrete quantum numbers; P indicates principal-part integration over the continuum states and summation over the discrete states. The coefficients B in Eq. (1) are determined by boundary conditions.[5,6] The matrix elements $K_{i\epsilon, jE}(E)$ are obtained by solving

$$K_{i\epsilon, jE}(E) = V_{i\epsilon, jE} + \sum_l \int d\epsilon' \, V_{i\epsilon, l\epsilon'}$$
$$\times [P/(E - \epsilon')] K_{l\epsilon', jE}(E), \quad (2)$$

with

$$V_{i\epsilon, jE} = (u_{i\epsilon}| V_{\text{res}}| u_{jE}) , \tag{3}$$

where

$$V_{\text{res}} = -\sum_i \left(\frac{Z}{r_i} + V_{\text{HS}}(r_i)\right) + \sum_{i < j} \frac{1}{r_{ij}} \tag{4}$$

is the residual interaction that was disregarded in generating the basis-set wave functions with model potential $V_{\text{HS}}(r)$; the summation in (4) extends over all the electrons in the atom with nuclear charge Z.

If we assume that the core electrons remain unrelaxed during the photoionization process, the single-particle wave functions of the core electrons remain the same for the initial- and final-state wave function of the system. Under this approximation, Eq. (1) constitutes essentially an improvement of the photoelectron wave function. If we use an "unimproved" ground-state wave function, i.e., a Slater determinant ψ_G of single-particle wave functions in the ground-state configuration, then the dipole amplitude $D^{(i)}(E)$ for transition to the channel i is given by

$$D^{(i)}(E) = \sum_i \left(d_{i_E} B_i(E) \right.$$

$$\left. + \sum_j P \int d\epsilon \, \frac{d_{i\epsilon} K_{i\epsilon, jE}(E)}{E - \epsilon} \, B_j(E) \right) , \tag{5}$$

where $d_{iE} = (\psi_G |\sum_j z_j| u_{iE})$, with j summed over all the electrons.

In this method, one usually generates the basis function by solving a Schrödinger equation with the model potential $V_{\text{HS}}(r)$ tabulated by Herman and Skillman.[7] These basis functions are then used to evaluate the residual interaction-matrix elements $V_{i\epsilon, jE}$ in Eq. (3) and the dipole amplitudes d_{iE}. After Eq. (2) is solved one can find the dipole amplitude $D^{(i)}(E)$ by doing the principal-part integration in Eq. (5).

The formulation of the RPA can be found in a number of references[8] and is not discussed here. In order to illustrate the close similarity between the equations of RPA and of the reaction-matrix method, we start from the formulas of Ref. 3 and use the name RPAE instead of RPA.[9] Matrix elements analogous (but not identical) to the K-matrix elements of Eq. (2) are called $(n_1 l_1, n_3 l_3 \| \Gamma_i(\omega) \| n_2 l_2, n_4 l_4)$ by Amusia et al. The matrix elements satisfy the system of equations

$$(n_1 l_1, n_3 l_3 \| \Gamma_i(\omega) \| n_2 l_2, n_4 l_4) = (n_1 l_1, n_3 l_3 \| U_i \| n_2 l_2, n_4 l_4)$$

$$+ \left(\sum_{\substack{n_5 \leq F \\ n_6 > F}} - \sum_{\substack{n_5 > F \\ n_6 \leq F}}\right) \frac{(n_1 l_1, n_6 l_6 \| U_i \| n_2 l_2, n_5 l_5)(n_5 l_5, n_3 l_3 \| \Gamma_i(\omega) \| n_6 l_6, n_4 l_4)}{(2l+1)[\omega - E_{n_6} + E_{n_5} + i\delta(1 - 2n_{n_5})]} , \tag{6}$$

which coincides with Eq. (18) of Ref. 3, except for correction of several misprints. In Eq. (6), $(n_1 l_1, n_3 l_3 \| U_i \| n_2 l_2, n_4 l_4)$ represents certain terms of the matrix element of the Hamiltonian between states in which two electrons have quantum numbers: $(n_1 l_1, n_3 l_3)$ and $(n_2 l_2, n_4 l_4)$, respectively; these terms include primarily the effects of 2^l pole interaction between these electrons. Also, δ is an infinitesimal real positive number, the summation is carried over all the intermediate single-particle states that are present $(n_5 \leq F)$ or absent $(n_6 > F)$ in the ground-state configuration of an atom with closed-shell structure. The summation is understood to extend over all hole states and all discrete particle states and to include integration over all continuum particle states. The Fermi step function n_{n_5} is defined as

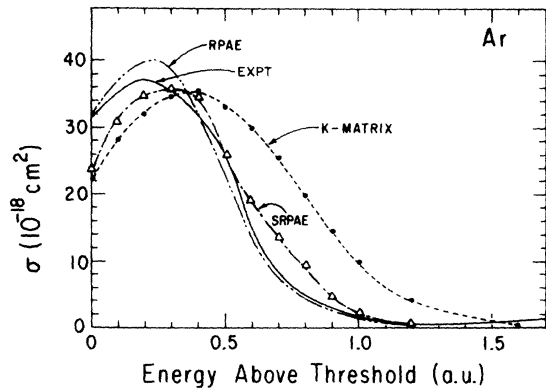$$n_{n_5} = 1 , \quad n_5 \leq F; \quad n_{n_5} = 0 , \quad n_5 > F , \tag{7}$$

FIG. 1. Photoionization cross sections of Ar.
(—·—△—·—·): SRPAE results of the present calculation;
(—·—●—·—): K-matrix results of Starace (Ref. 2);
(——··——··——): RPAE results of Amusia et al. (Ref. 3);
(——————): experimental results of Samson (Ref. 14).

and the matrix elements $(n_1l_1, n_3l_3 \| U_I \| n_2l_2, n_4l_4)$ are defined as in Eq. (19) of Ref. 3.

$$(n_1l_1 \| d \| n_2l_2) + \left(\sum_{\substack{n_3 \leq F \\ n_4 > F}} - \sum_{\substack{n_3 > F \\ n_4 \leq F}} \right) \frac{1}{3} \frac{\begin{pmatrix} l_3 & 1 & l_4 \\ 0 & 0 & 0 \end{pmatrix}}{\begin{pmatrix} l_1 & 1 & l_2 \\ 0 & 0 & 0 \end{pmatrix}} \left(\frac{(2l_3+1)(2l_4+1)}{(2l_1+1)(2l_2+1)} \right)^{1/2} \frac{(n_4l_4 \| d \| n_3l_3)(n_3l_3, n_1l_1 \| \Gamma_1(\omega) \| n_4l_4, n_2l_2)}{\omega - E_{n_4} + E_{n_3} + i\delta(1 - 2_{n_4})} ,$$

$$(8)$$

which is identical to Eq. (21) of Ref. 3, except for correction of several misprints. The radial dipole integral is defined as

$$(n_1l_1 \| d \| n_2l_2) \equiv \int_0^\infty P_{n_1l_1}(r)rP_{n_2l_2}(r)\,dr ,$$

with $P_{n_il_i}(r)$ the radial wave function of the electron.

In the RPAE method, a Hartree-Fock basis was used to evaluate the dipole integral and the interaction-matrix elements $(n_1l_1, n_3l_3 \| U_1 \| n_2l_2, n_4l_4)$. After Eq. (6) is solved for the $\Gamma_1(\omega)$ matrix elements, one finds the radial dipole amplitude by doing the integration in Eq. (8). In the numerical calculations, a proper choice of the Hartree-Fock basis functions is required. This is explained by Amusia et al. in Ref. 3 and is not discussed here. It is to be noted here that Eq. (6) holds for arbitrary choice of the initial potential, irrespective of the fact that a Hartree-Fock basis affords a better first approximation. Thus Eq. (6) can still be used when one starts from a central field approximation, like the Hermann-Skillman's tabulated potential, with appropriate modification in the definition of the matrix elements of U_1. As we have said, the reaction-matrix method provides a way to calculate the dipole transition amplitude $D^{(i)}(E)$ in Eq. (5), in which the final-state

FIG. 2. Photoionization cross sections of Xe.
(—·—△—·—): SRPAE results of the present calculation;
(—··—··—): K-matrix results of Starace (Ref. 2);
(————): experimental results of Haensel (Ref. 15).

wave function is improved, whereas RPAE provides a method to calculate the dipole amplitude in Eq. (8) in which the final-state and the ground-state wave function are improved simultaneously. Roughly speaking, the difference in the equation of the two formulations should be due to the improvement of the ground-state wave function. Indeed Eqs. (6) and (8) are seen to include terms which have no analog in Eqs. (2) and (5).

In order to clarify the notations we specialize the general formulas (2), (5), (6), and (8) to the single-channel $3p \rightarrow Ed$ transition of Ar. For this dipole transition, we set $l = 1$ in Eq. (6). The factor $(2l+1)$ in the denominator of Eq. (6) can be eliminated by defining $\overline{\Gamma}_l(\omega) = \Gamma_l(\omega)/(2l+1)$ and $\overline{U}_l = U_l/(2l+1)$. Specializing the hole state in Eq. (3) to $3p$ hole and the particle states to ϵd states, including nd with $n \geq 3$, Eq. (8) takes the form

$$(Ed \| d \| 3p)$$

$$+ \int d\epsilon \frac{(\epsilon d \| d \| 3p)(3pEd \| \overline{\Gamma}_1(\omega) \| \epsilon d3p)}{\omega - \epsilon + E_{3p} - i\delta}$$

$$- \int d\epsilon \frac{(3p \| d \| \epsilon d)(\epsilon dEd \| \overline{\Gamma}_1(\omega) \| 3p3p)}{\omega + \epsilon - E_{3p} + i\delta} , \quad (9)$$

where E is the energy of the photoelectron, E_{3p} is the energy of a $3p$ electron. The integral is understood to include a summation over all the discrete nd states.

Since we use a standing-wave representation for the wave function in the continuum, we have $(\epsilon d \| d \| 3p) = (3p \| d \| \epsilon d) \equiv d_\epsilon$. To simplify the notation, we write

$$(3pEd \| \overline{\Gamma}_1(\omega) \| \epsilon d3p) = \Gamma_{\epsilon, E}$$

and

$$(\epsilon dEd \| \overline{\Gamma}_1(\omega) \| 3p3p) = G_{\epsilon, E} .$$

If we express the photon energy ω in terms of the energy of the photoelectron E, we can rewrite Eq. (9) as

$$d_E + \int d\epsilon \frac{d_\epsilon \Gamma_{\epsilon, E}}{E - \epsilon - i\delta} - \int d\epsilon \frac{d_\epsilon G_{\epsilon, E}}{E + \epsilon + 2I_{3p}} , \quad (10)$$

where I_{3p} replaces E_{3p}. The small imaginary number $i\delta$ drops out in the denominator of the last
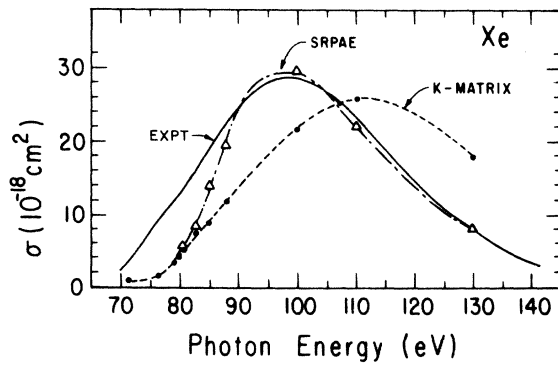
term of Eq. (10) because this denominator never approaches zero.

$$\Gamma_{\epsilon, E} = (3pEd \| \overline{U}_1 \| \epsilon d3p) + \int d\epsilon' \; \frac{(3p\epsilon'd \| \overline{U}_1 \| \epsilon d3p)\Gamma_{\epsilon', E}}{E - \epsilon' - i\delta} - \int d\epsilon' \frac{(3p3p \| \overline{U}_1 \| \epsilon d\epsilon'd)G_{\epsilon', E}}{E + \epsilon' + 2I_{3p}} \; , \tag{11}$$

$$G_{\epsilon, E} = (\epsilon dEd \| \overline{U}_1 \| 3p3p) + \int d\epsilon' \frac{(\epsilon d\epsilon'd \| \overline{U}_1 \| 3p3p)\Gamma_{\epsilon', E}}{E - \epsilon' - i\delta} - \int d\epsilon' \frac{(\epsilon d3p \| \overline{U}_1 \| 3p\epsilon'd)G_{\epsilon', E}}{E + \epsilon' + 2I_{3p}} \; , \tag{12}$$

where

$$(n_1 l_1, n_3 l_3 \| \overline{U}_1 \| n_2 l_2, n_4 l_4) = \tfrac{2}{3}(n_1 l_1, n_3 l_3 \| V_1 \| n_2 l_2, n_4 l_4) + \sum_{l'} (-1)^{l'} \begin{Bmatrix} l_1 & 1 & l_2 \\ l_3 & l' & l_4 \end{Bmatrix} (n_1 l_1, n_3 l_3 \| V_{l'} \| n_4 l_4, n_2 l_2) \; . \tag{13}$$

The matrix element

$$(n_1 l_1, n_3 l_3 \| V_l \| n_2 l_2, n_4 l_4)$$

is defined in Eq. (16) of Ref. 3.

In the reaction-matrix method, the dipole transition amplitude is written

$$\left\{ d_E + P \int \left[d_\epsilon K_{\epsilon, E}/(E - \epsilon) \right] d\epsilon \right\} / (1 - i\pi K_{E, E}) \; , \tag{14}$$

where $1/(1 - i\pi K_{E, E})$ is the normalization factor B of Eqs. (1) and (5). The K-matrix elements satisfy

$$K_{\epsilon, E} = V_{\epsilon, E} + P \int \left[V_{\epsilon, \epsilon'} K_{\epsilon', E}/(E - \epsilon') \right] d\epsilon' \; , \tag{15}$$

where

$$V_{\epsilon, E} = (3p^5 \epsilon d \, ^1P^0 | V_{\text{res}} | 3p^5 Ed \, ^1P^0) \; , \tag{16}$$

with V_{res} given by Eq. (4).

Comparing Eqs. (10) and (14), we see they are very similar, except for the last term of Eq. (10), which does not appear in (14). Similarly Eq. (11) differs from Eq. (15) primarily through the occurrence of its last term. This term involves the interaction-matrix element $(3p3p \| \overline{U}_1 \| \epsilon d\epsilon'd)$ corresponding to virtual excitation of two ground-state particles from $3p$ to $(\epsilon d, \epsilon'd)$, whereas the other terms depend on interactions that replace one excitation by another one. The inclusion of virtual excitations of pairs of $3p$ electrons in the RPAE equations means that these equations take ground-state correlations into account while the reaction-matrix method of Ref. 2 does not. The matrix $G_{\epsilon, E}$ has the main role of representing the effect of these ground-state correlations. Indeed, if we set $G_{\epsilon', E} = 0$ in Eqs. (10) and (11), then Eq. (10) reduces to Eq. (14) and Eq. (11) reduces to Eq. (15), with $\Gamma_{\epsilon, E}$ and $K_{\epsilon, E}$ related by

$$\Gamma_{\epsilon, E} = [K_{\epsilon, E}/(1 - i\pi K_{E, E})] \; . \tag{17}$$

This equivalence is proved by using the identity

$$\lim(x - i\alpha)^{-1} = Px^{-1} + i\pi\delta(x), \quad \text{as } \alpha \to 0^+ \; .$$

The integral equations satisfied by $\Gamma_{\epsilon, E}$ and $G_{\epsilon, E}$ are obtained by rewriting Eq. (6) as

In the comparison of the two methods, we have disregarded comparatively minor differences between the matrix elements $V_{\epsilon', \epsilon}$ of the reaction-matrix method and the corresponding elements of $\overline{U}_1$.

This comparison of RPAE and reaction matrix equations has suggested to us a procedure for incorporating the main effects of ground-state correlations in the reaction-matrix method. This procedure rests on the fact that the matrix element $(3p3p \| \overline{U}_1 \| \epsilon d\epsilon'd)$ for virtual excitation of a pair of ground-state electrons differs from the matrix element $(3p\epsilon'd \| \overline{U}_1 \| \epsilon d3p)$ for replacement of a single excitation by an amount that is small in the situations where pair excitations are important. The difference lies entirely in the $\sum_{l'}$ terms of Eq. (13), whereas the first term is dominant and identical for the two processes. If we set

$$(3p\epsilon'd \| \overline{U}_1 \| \epsilon d3p) \cong (3p3p \| \overline{U}_1 \| \epsilon d\epsilon'd) \tag{18}$$

in Eqs. (11) and (12), these equations become symmetric in $\Gamma_{\epsilon, E}$ and $G_{\epsilon, E}$, and are solved by setting

$$\Gamma_{\epsilon, E} = G_{\epsilon, E} \; , \tag{19}$$

where $\Gamma_{\epsilon, E}$ satisfies

$$\Gamma_{\epsilon, E} = (3pEd \| \overline{U}_1 \| \epsilon d3p)$$

$$+ \int d\epsilon' \left[(E - \epsilon' - i\delta)^{-1} - (E + \epsilon' + 2I_{3p})^{-1} \right]$$

$$\times (3p\epsilon'd \| \overline{U}_1 \| \epsilon d3p)\Gamma_{\epsilon', E} \; . \tag{20}$$

To estimate the inaccuracy of Eq. (18), we note that the first term of Eq. (13) is proportional to the $\mathcal{G}^1$ integral of Fano and Cooper[10] which is a generalization of Slater's G^1 integral to off-diagonal matrix elements. The coefficient in front of the $\mathcal{G}^1$ integral is the largest among all the terms in Eq. (13). The term with $\mathcal{G}^1$ represents the exchange interaction between the excited electron and *all the electrons* that remain in the ground-state shell $3p^5$. As the numerical calculation of Starace[2] shows, the $\mathcal{G}^1$ integral contributes more

than 85% of the magnitude of all the residual inter-
action-matrix elements of Ar and more than 80%
for those of Xe.

On the basis of the similarity between Eqs. (20)
and (15), we propose that for a single channel
problem, the ground-state correlation effect be
included in an *ad hoc* way by solving

$$\overline{K}_{\epsilon,\,E} = V_{\epsilon,\,E} + P \int \left[V_{\epsilon,\,\epsilon'} \overline{K}_{\epsilon',\,E} / (E - \epsilon') \right] d\epsilon'$$

$$- \int \left[V_{\epsilon,\,\epsilon'} \overline{K}_{\epsilon',\,E} / (E + \epsilon + 2 I_{3p}) \right] d\epsilon' \qquad (21)$$

instead of Eq. (15). The dipole transition ampli-
tude is then obtained by calculating

$$\left(d_E + P \int \left[d_\epsilon \overline{K}_{\epsilon,\,E} / (E - \epsilon) \right] d\epsilon \right.$$

$$\left. - \int \left[d_\epsilon \overline{K}_{\epsilon,\,E} / (E + \epsilon + 2 I_{3p}) \right] d\epsilon \right)$$

$$\times (1 - i\pi \overline{K}_{E,\,E})^{-1} \qquad (22)$$

instead of Eq. (14). We call our proposed method
SRPAE because Eqs. (21) and (22) are obtained by
approximating the RPAE equations. The calcula-
tion is to be done entirely by the procedure of the
reaction-matrix method. The advantage of this
approach is that one can obtain a much better nu-
merical result, as will be shown in Sec. III, with-
out spending as much computation time as in the
RPAE method. The importance of the ground-
state correlation effect can be evaluated by com-
paring the results calculated by SRPAE and by the
reaction-matrix method.

The main Eqs. (21) and (22) of SRPAE rest on
the approximate Eq. (18), whose range of validity
is discussed in the paragraph following Eq. (20).
Equations (21) and (22) are similar to Wendin's
Eqs. (3.7)–(3.9) of Ref. 4, except for a minor dif-
ference in the definition $V_{\epsilon,\,\epsilon'}$. By analyzing the po-
larization propagator diagrammatically, Wendin
argues that the interaction-matrix elements for the
final state and the ground state are exactly the
same,[11] that is, that Eq. (18) holds rigorously. We
have assumed Eq. (18) to hold only when the $\mathcal{G}^1$ in-
tegral dominates. In any actual calculations, the
magnitude of the residual interaction-matrix ele-
ments for the final state and for the ground state
depends on the choice of basis set. Whether or
not Eq. (18) holds probably depend on the basis
set also.

III. RESULTS AND CONCLUSIONS

The numerical procedure to calculate the photo-
ionization cross section by the SRPAE method is
basically the same as that used in the reaction-
matrix method, except for replacing Eqs. (14) and

(15), respectively, by Eqs. (22) and (21). One
starts by generating the single-particle wave func-
tion from the Schrödinger equation using Herman-
Skillman potential. These wave functions are used
to evaluate the dipole-matrix elements d_ϵ and the
residual interaction-matrix elements $V_{\epsilon,\,\epsilon'}$. Then
one solves the integral Eq. (21). The dipole ampli-
tude is obtained by doing the integrations in
Eq. (22).

The methods for evaluating the residual interac-
tion-matrix elements $V_{\epsilon,\,\epsilon'}$ and for solving the in-
tegral Eq. (21), which involves the principal-part
integration, have been discussed by Altick and
Moore[12] and by Starace.[2] In this paper, we intend-
ed to use the matrix elements $V_{\epsilon,\,\epsilon'}$ and dipole am-
plitudes d_ϵ calculated by Starace[2] for the $3p \rightarrow Ed$
transition of Ar and $4d \rightarrow Ef$ transition of Xe. In
fact, it was found feasible and most expedient to
introduce a further numerical approximation[13] for
$V_{\epsilon,\,\epsilon'}$, namely, by factorizing it in the form

$$V_{\epsilon,\,\epsilon'} = g(\epsilon) g(\epsilon') . \qquad (23)$$

No general arguments supporting the validity of
this assumption seem to have been advanced,
but the numerical values of $V_{\epsilon,\,\epsilon'}$ calculated by
Starace, are approximated by Eq. (23) to within
5%. It should be noted that the approximation (23)
appears to be valid under the same circumstances
as (18), that is, when the $\mathcal{G}^1$ integral of Ref. 10 is
dominant. In fact the quasifactorability of $\mathcal{G}^1$ and
its physical origin were discussed on p. 486 of this
reference.

The main effect of the factorization (23), also
noted in Ref. 13, is that it permits an analytical
solution of the reaction-matrix equation. Substi-
tuting (23) into Eq. (21) we find

$$\overline{K}_{\epsilon,\,E} = V_{\epsilon,\,E} \left/ \left(1 - P \int \frac{V_{\epsilon,\,\epsilon}}{E - \epsilon} d\epsilon + \int \frac{V_{\epsilon,\,\epsilon}}{E + \epsilon + 2 I_{3p}} d\epsilon \right) \right.$$

$$(24)$$

for the $\overline{K}$ matrix elements. The corresponding
K-matrix element in the factorable approximation
has the same form, except for the absence of the
last term in the denominator of Eq. (24).

The photoionization cross section calculated by
the SRPAE method using Eqs. (24) and (22) are
shown on Fig. 1 for the $3p \rightarrow Ed$ transition of Ar,
and on Fig. 2 for the $4d \rightarrow Ef$ transition of Xe.
The results of the calculations by Starace[2] using
the reaction-matrix method are also given. By
comparing with the experimental results of Sam-
son[14] for Ar and of Haensel *et al.*[15] for Xe, we
find that the cross sections calculated by the
SRPAE method are much better than those ob-
tained by Starace without any ground-state corre-
lation. The improvement is substantial, especial-

ly on the higher-energy side. Note that the re-
sults shown on the figures for both calculations
include the transition $3p \to Ed$ of Ar and $4d \to Ef$ of
Xe only, whereas the experiments measure the
total cross sections. The agreement with experi-
ment of the calculation by SRPAE method in Ar is
not as good as for Xe. This is probably due to the
limitations of RPAE itself, which assumes in es-
sence a high density of electrons in the shell to be
ionized; this density is higher for the $4d^{10}$ shell
of Xe than for the $3p^6$ shell of Ar.

A comparison of the SRPAE results with the full
RPAE calculation by Amusia *et al.* is possible.
We plot in Fig. 1 the result of the RPAE calcula-
tion for Ar, but not on Fig. 2 for Xe, because in
the latter case the RPAE results of Amusia *et al.*
agree with our SRPAE results to within 5–10%
over the energy range considered. For Ar, the
results of the two calculations deviate from ex-
periment by approximately the same amount, but
lie on opposite sides of the experimental curve.
This probably results from differences in the in-
teraction-matrix elements used in the two calcu-
lations.

We conclude that the SRPAE method provides a
simple and effective way to calculate the photo-
ionization cross section with simultaneous im-
provement of the ground-state and final-state wave
functions. Even though this method probably can-
not give better results than the complete RPAE
calculation, the simplicity of its numerical pro-
cedure should be emphasized; the SRPAE appears
to provide a simple way to calculate the dipole
transition amplitudes rather accurately when the
independent-particle approximation fails. The
SRPAE should be applicable as long as the 9^1 in-
tegral dominates the matrix elements of the resid-
ual interaction. Generalization of this method to
two or more channels is possible,[6] but one has to
check the validity of the approximation first.

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[9]RPA is ordinarily used in high-density media and em-
ploys a Hartree zeroth approximation. RPAE, as used
by Amusia *et al.* presupposes a Hartree-Fock zeroth
approximation and is a generalization of RPA.
[10]Reference 1, Sec. 6.1.
[11]In Ref. 4, Wendin also considers a modification of his
Eqs. (3.8) and (3.9) that reduces the ground-state
interaction matrix element by a factor of $(N-2)/(N-1)$,
where N is the number of electrons in a closed shell.
[12]P. L. Altick and E. N. Moore, Phys. Rev. 147, 59
(1966).
[13]Reference 1, Sec. 6.3.
[14]J. A. R. Samson, Advan. At. Mol. Phys. 2, 178 (1966).
[15]R. Haensel, G. Keitel, P. Schreiber, and C. Kunz,
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