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Relativistic random phase approximation applied to atoms of the He isoelectronic sequence*

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A relativistic version of the random phase approximation (RPA) is used to study allowed and forbidden radiative transitions in atoms. The theory is applied to the He isoelectronic sequence to test its utility. Precise numerical solutions to the relativistic RPA equations are obtained describing the transitions $1\,^1S_0 \rightarrow 2\,^3S_1$ ($M1$), $1\,^1S_0 \rightarrow 2\,^{1,3}P_1$ ($E1$), and $1\,^1S_0 \rightarrow 2\,^3P_2$ ($M2$). The resulting excitation energies and transition probabilities are in good agreement with accurate nonrelativistic calculations for low-Z elements. For intermediate- and high-Z elements where relativistic effects are more important, the results are expected to be very accurate also. Extensive comparison shows good agreement of the calculated forbidden transition rates with available beam-foil measurements and the calculated transition energies with several lines from solar corona for high-Z ($Z \sim 25$) elements.

I. INTRODUCTION

The need for reliable data concerning highly ionized atoms has increased in recent years because of studies of the solar corona, solar flares, and thermonuclear plasmas.[1] Theoretically determined data, moreover, can now be subjected to scrutiny in the laboratory using beam-foil spectroscopy.[2]

For atomic transitions in highly stripped ions relativistic effects become more and more important as the nuclear charge Z of the species increases. It seems desirable therefore to develop a theory of atomic transitions for high-Z atoms which includes relativistic effects nonperturbatively. Relativistic theories which do not account for correlations, however, are likely to be unreliable. The traditional configuration-interaction method used to treat correlations in the nonrelativistic theory appears to present computational difficulties in the relativistic case. Therefore in view of its successes and simplicity in nonrelativistic theory we have introduced a relativistic version of the random phase approximation (RPA) to treat those correlation effects important in the calculation of radiative transitions in closed-shell atoms.[3]

The RPA was originally developed to study extended systems such as electron gases or nuclear matter.[4] It has been applied to a wide class of atomic and molecular processes, especially for the computation of transition probabilities and photoionization cross sections.[5] The RPA leads to a treatment of correlations in which the computational advantages of an independent-particle theory are retained. From a physical point of view correlation effects in the initial and final states are treated simultaneously, leading to oscillator strengths which satisfy the Thomas-Reiche-Kuhn sum rule and which have identical values in the length and velocity forms.

Our purpose is to develop a relativistic RPA in which all of the correlations included in the nonrelativistic version are retained. In the nonrelativistic theory the RPA provides a generalization of the Hartree-Fock (HF) equations; the differences between the RPA and HF theory are due to certain correlation effects. Here we start with the Dirac-Hartree-Fock (DHF) equations to avoid perturbative treatment of relativity. A valuable consequence of the relativistic approach is that forbidden transitions are obtained with the same ease as allowed transitions.

The nonrelativistic RPA takes three equivalent forms[6] as applied by different workers, namely, time-dependent Hartree-Fock (TDHF) theory,[5a,7] the linearized-equations-of-motion method,[5b] and the Green's-function method.[8] The last two approaches usually involve some further approximation in the solution of the resulting RPA equations, since a truncated basis set is required. The Green's-function method can be analyzed in terms of diagrams, so that a comparison with many-body perturbation theory is possible.[9] For our purposes, it is easiest to study the relativistic RPA directly from the TDHF equations.[7]

The formulation of the theory is presented in Sec. II. In our treatment of relativity we adopt as fundamental the Dirac-Breit Hamiltonian consisting of a sum of Dirac one-electron terms and the electron-electron Coulomb interactions. We treat the Breit interaction as a perturbation and neglect the electron self-energy and vacuum polarization, together with higher-order quantum-electrodynamic effects.[10] Specific applications of the theory to the helium isoelectronic sequence are given in Sec. III. A discussion of the numerical methods used to solve the relativistic RPA equations is given in Sec. IV, and in Sec. V we describe the modifications of the theory required to introduce the Breit interaction. Results for the transitions ${}^1S_0 \rightarrow {}^{1,3}P_1(E1)$, ${}^1S_0 \rightarrow {}^3S_1(M1)$, and ${}^1S_0 \rightarrow {}^3P_2(M2)$ are presented in Sec. VI. Our allowed and forbidden transition rates compare favorably with the accurate Hylleraas-type calculations at low Z. Our results at high Z are expected to be very accurate, since correlation decreases with Z. Furthermore, the relativistic RPA can be readily extended to more complicated systems where accurate variational calculations are not available.

II. FORMULATION

Our practical calculations are based on the TDHF equations which are a variant of the RPA often used in atomic structure calculations. We assume an N-electron closed-shell atom[11] with its ground state described by a single determinant of the N DHF orbitals $u_i(\vec{r})$. The perturbations $w_{i\pm}(\vec{r})$ induced in the orbitals $u_i(\vec{r})$ by an external field $A_+e^{-i\omega t}+A_-e^{i\omega t}$ of frequency ω satisfy the RPA equations;

$$(h_0+V-\epsilon_i\mp\omega)w_{i\pm}=(A_\pm-V_\pm^{(1)})u_i\,,\quad i=1,2,\ldots,N\,, \tag{1}$$

where

$$h_0=\vec{\alpha}\cdot\vec{p}+\beta m-e^2Z/r\,,$$

$$Vw_i=\sum_{j=1}^{N}e^2\int\frac{d^3r'}{|\vec{r}-\vec{r}'|}[(u_j^*u_j)'w_i-(u_j^*w_i)'u_j]\,,$$

$$V_\pm^{(1)}u_i=\sum_{j=1}^{N}e^2\int\frac{d^3r'}{|\vec{r}-\vec{r}'|}[(u_j^*w_{j\pm})'u_i+(w_{j\mp}^*u_j)'u_i-(w_{j\mp}^*u_i)'u_j-(u_j^*u_i)'w_{j\pm}]\,.$$

$A_\pm(r)$ is the amplitude of external perturbation of frequency ±ω, and ϵ_i is the orbital eigenvalue of ith DHF equation. Natural units are used in Eq. (1) and throughout the paper.

The system of homogeneous equations which follow from Eqs. (1) with $A_\pm=0$ define an eigenvalue problem. The eigenvalues ω_k represent the atomic excitation energies; the corresponding eigenfunctions $w_{ik\pm}(\vec{r})$ are conveniently normalized by

$$\sum_{i=1}^{N}(\langle w_{ik+}|w_{ik+}\rangle-\langle w_{ik-}|w_{ik-}\rangle)=1. \tag{2}$$

The eigenfunctions of Eqs. (1) describe atomic states with definite values of angular momentum J, M and parity $\pi=\pm1$. Such an excited state may decay to the ground state by single-photon emission. If we let $\lambda=1$ (0) designate an electric (magnetic) multipole field, then the multipolarity J, M, λ of the emitted photon is related to the parity π of the excited state by $\pi=(-1)^{J-\lambda+1}$. We designate the vector potential of the multipole field by $\vec{a}_{JM}^{(\lambda)}$, and we have

$$\begin{aligned}\vec{a}_{JM}^{(1)}&=\left(j'_J(\omega r)+\frac{j_J(\omega r)}{\omega r}\right)\vec{Y}_{JM}^{(1)}(\hat{r})\\&\quad+\frac{[J(J+1)]^{1/2}j_J(\omega r)}{\omega r}\vec{Y}_{JM}^{(-1)}(\hat{r})\,,\\\vec{a}_{JM}^{(0)}&=j_J(\omega r)\vec{Y}_{JM}^{(0)}(\hat{r})\,,\end{aligned} \tag{3}$$

where $j_L(x)$ is a spherical Bessel function and $\vec{Y}_{JM}^{(\lambda)}(\hat{r})$ is a vector spherical harmonic.

The transition rate from the excited state k to the ground state 0 by emission of a photon with quantum numbers ω_k, J, M, λ is given by

$$A_{k\rightarrow0}=8\pi\alpha\omega_k|M_k|^2\,,$$

where

$$M_k=\sum_{i=1}^{N}(\langle u_i|\vec{a}_{JM}^{(\lambda)*}\cdot\vec{\alpha}|w_{ik+}\rangle+\langle u_i|\vec{\alpha}\cdot\vec{a}_{JM}^{(\lambda)}|w_{ik-}\rangle)\,. \tag{4}$$

Similar formulas can be developed within the framework of the RPA to treat transitions from one excited state k to another excited state k'.[12]

In the present paper we determine some of the low-lying states of a two-electron ion by solving the homogeneous RPA equations (1); we determine the transition rates from these states to the atomic ground state by evaluating the transition matrix element M_k in Eq. (4).

For electric multipole transitions there are equivalent ways of writing the matrix element M_k corresponding to the velocity and length forms of the nonrelativistic dipole matrix element.[13] The expression for $\vec{a}_{JM}^{(1)}$ given in Eq. (3) reduces to the velocity form in the nonrelativistic limit. The relativistic length form is obtained by replacing $\vec{\alpha}\cdot\vec{a}_{JM}^{(1)}$ by $b_{JM}+\vec{\alpha}\cdot\vec{c}_{JM}$, where

$$b_{JM}(\vec{r})=i\left(\frac{J+1}{J}\right)^{1/2}\left(j_J(\omega r)-\frac{\omega r j_{J+1}(\omega r)}{J+1}\right)Y_{JM}(\hat{r})\,,$$

$$\vec{c}_{JM}=\frac{\omega r j_J(\omega r)}{[J(J+1)]^{1/2}}\hat{r}Y_{JM}(\hat{r})\,.$$

The equivalence of the two forms in the relativistic RPA follows directly from Eqs. (1) and the identity $\vec{\alpha}\cdot\vec{a}_{JM}^{(1)}=[h_0, b_{JM}]/\omega+\vec{\alpha}\cdot\vec{c}_{JM}$; the equivalence of the two forms in the nonrelativistic RPA is well known.

III. REDUCTION OF THE RPA EQUATION FOR TWO-ELECTRON IONS

We describe the DHF orbitals $u(\vec{r})$ using the following quantum numbers: n is the principal quantum number, $\kappa = \mp(j+\frac{1}{2})$ for $j = l \pm \frac{1}{2}$, where j and l are angular momentum quantum numbers, and the angular momentum projection quantum number m $(-j \leq m \leq j)$. The orbital $u_{n\kappa m}(\vec{r})$ is written in terms of two radial functions, a large component $G_{n\kappa}(r)$ and a small component $F_{n\kappa}(r)$. Introducing the spherical spinor $\Omega_{\kappa m}(\hat{r})$ to describe the angular dependence of u, we may write

$$u_{n\kappa m}(\vec{r}) = \frac{1}{r}\begin{pmatrix} iG_{n\kappa}(r)\Omega_{\kappa m}(\hat{r}) \\ F_{n\kappa}(r)\Omega_{-\kappa m}(\hat{r}) \end{pmatrix}. \qquad (5)$$

For He there are just two orbitals with $n=1$, $\kappa = -1$, and $m = \pm\frac{1}{2}$ for the $(1s_{1/2})^2$ ground-state configuration. The DHF equations reduce to a pair of coupled radial differential equations for the large-component and small-component radial functions. Let us define the differential operator

$$\mathcal{L}_\kappa = \begin{pmatrix} m - \dfrac{e^2Z(r)}{r} & \left(\dfrac{d}{dr} - \dfrac{\kappa}{r}\right) \\ -\left(\dfrac{d}{dr} + \dfrac{\kappa}{r}\right) & -m - \dfrac{e^2Z(r)}{r} \end{pmatrix}, \qquad (6)$$

where $Z(r) = Z - Y(r)$ and where

$$Y(r) = \int_0^r dr'\,(G_0^2 + F_0^2)' + r\int_r^\infty \frac{dr'}{r'}\,(G_0^2+F_0^2)'\,.$$

We use the subscript 0 to designate the ground state. With the aid of $\mathcal{L}_\kappa$ we may rewrite the radial DHF equations as

$$(\mathcal{L}_{-1} - \epsilon_0)\mathfrak{F}_0 = 0\,, \qquad (7)$$

with

$$\mathfrak{F}_0 = \begin{pmatrix} G_0(r) \\ F_0(r) \end{pmatrix}$$

We solve Eqs. (7) for ϵ_0, $\mathfrak{F}_0(r)$, and $Z(r)$ using numerical self-consistent-field techniques. Once we have obtained the ground-state function $\mathfrak{F}_0$ we are in a position to solve the RPA equations (1) for the excited states.

To illustrate the method used to reduce the RPA equations to radial equations, we consider the special case $J=1$, $\pi=-1$; an electric dipole ($E1$) excitation. The orbitals used to describe an $E1$ excited state must have angular quantum numbers $\kappa=1$ or $\kappa=-2$ corresponding to excitations $s_{1/2}\rightarrow p_{1/2}$ $(\kappa=1)$ or $s_{1/2}\rightarrow p_{3/2}$ $(\kappa=-2)$. The perturbations $w_\pm$ of Eq. (1) are given as linear combinations of $p_{1/2}$ and $p_{3/2}$ excited orbitals chosen to give a final $J=1$ state.

In the general case we designate the orbitals with definite angular momenta (the $s_{1/2}\rightarrow p_{1/2}$ excitations above, for example) by

$$w_{\kappa m\pm}(r) = \frac{1}{r}\begin{pmatrix} iS_{\kappa\pm}(r)\Omega_{\kappa m}(\hat{r}) \\ T_{\kappa\pm}(r)\Omega_{-\kappa m}(\hat{r}) \end{pmatrix}. \qquad (8)$$

The excitation $w_{i\pm}$ of the ith electron (angular momentum κ, m) is then made up as a combination of the orbitals (8) given by

$$w_{i\pm}(r) = \sum_{\kappa' m'} \pm iI_J(\kappa', m', \kappa, m)\,w_{\kappa' m' \pm}(r)\,, \qquad (9)$$

where

$$I_J(\kappa', m', \kappa, m) = \langle\kappa' m'\,|\,Y_{J0}\,|\,\kappa m\rangle\,.$$

With the ansatz (9) the RPA equations reduce to a set of coupled radial equations for the functions $S_\kappa(r)$ and $T_\kappa(r)$ The states described by Eqs. (11) all have parity $\pi = (-1)^J$; they decay to the ground state by electric multipole radiation. To describe states of parity $\pi = (-1)^{J-1}$ which decay by magnetic multipole radiation we simply perform the replacement

$$I_J(\kappa', m', \kappa, m) \rightarrow I_J(\kappa', m', -\kappa, m)$$

in Eq. (9); this replacement preserves the angular momentum but reverses the parity of the excitation.

We designate the pair of radial functions $S_{\kappa\pm}(r)$ and $T_{\kappa\pm}(r)$ by

$$\mathcal{S}_{\kappa\pm}(r) = \begin{pmatrix} S_{\kappa\pm}(r) \\ T_{\kappa\pm}(r) \end{pmatrix},$$

and we let

$$Y_L(\kappa, \pm, r) = r\int_0^\infty dr' \frac{r_<^L}{r_>^{L+1}}(S_{\kappa\pm}G_0 + T_{\kappa\pm}F_0)'\,.$$

We then find upon substituting Eq. (9) into the RPA equations (1) a set of radial equations which take the simple form

$$(\mathcal{L}_\kappa - \epsilon_0 \mp \omega)\mathcal{S}_{\kappa\pm} = O_{\kappa\pm}\mathfrak{F}_0\,. \qquad (10)$$

For EJ excitations Eqs. (10) are a set of coupled equations for $\kappa = J$ and $\kappa = -J-1$. We now describe the exchange terms occurring on the right-hand side of Eq. (10).

EJ-excitation exchange terms:

$$\begin{aligned} O_{J,\pm} = -\frac{e^2}{(2J+1)^2}\bigg(&-\frac{Y_J(J,\pm,r)}{r} \\ &+(2J+2)\frac{Y_J(-J-1,\pm,r)}{r} \\ &+(2J+1)\frac{Y_J(J,\mp,r)}{r}\bigg), \\ O_{-J-1,\pm} = -\frac{e^2}{(2J+1)^2}\bigg(&2J\,\frac{Y_J(J,\pm,r)}{r} \\ &+\frac{Y_J(-J-1,\pm,r)}{r} \\ &+(2J+1)\frac{Y_J(-J-1,\mp,r)}{r}\bigg). \end{aligned} \tag{11}$$

MJ-excitation exchange terms: For MJ excitations Eqs. (10) are a set of equations for $\kappa=-J$ and $\kappa=J+1$. The exchange terms are

$$\begin{aligned} O_{-J,\pm} = \frac{e^2}{2J-1}\bigg(&\frac{Y_{J-1}(-J,\pm,r)}{r} \\ &+\frac{Y_{J-1}(-J,\mp,r)}{r}\bigg), \\ O_{J+1,\pm} = \frac{e^2}{2J+3}\bigg(&\frac{Y_{J+1}(J+1,\pm,r)}{r} \\ &+\frac{Y_{J+1}(J+1,\mp,r)}{r}\bigg). \end{aligned} \tag{12}$$

The system of equations (10) for electric multipole excitations are intermediate coupling equations. The resulting states reduce in the nonrelativistic limit to singlet and triplet states with $L=J$ The eigenvalues ω of Eqs. (10) for EJ states appear in closely spaced pairs, separated by the singlet-triplet fine structure. The system (10) for MJ excitations decouples into a set of equations for $\kappa=-J$ and a set for $\kappa=J+1$, as is seen from the exchange integrals (12). The eigenfunctions of the MJ excitations are nonvanishing for $\kappa=-J$ or for $\kappa=J+1$, but not for both. States formed from $\kappa=-J$ reduce in the nonrelativistic limit to triplet states with $L=J-1$; those formed from $\kappa=J+1$ reduce to triplets with $L=J+1$.

The ansatz (9) can be used for a general closed-shell atom to reduce the RPA equations (1) to coupled radial equations. The resulting radial equations in the general case are more complicated than those given in Eqs. (10)-(12) and will not be written here.

IV. NUMERICAL SOLUTIONS TO THE RADIAL RPA EQUATIONS

In this sections we describe the procedures used to solve the radial RPA equations (10) and (11) for electric excitations. The simpler equations (10) and (12) for magnetic excitations are treated by parallel methods.

An approximate solution to Eqs. (10), corresponding to nth excited state with a given J (configuration $1s$, nJ), is obtained in terms of the DHF orbitals $\mathcal{F}_{n\kappa}(r)$ with $\kappa=J,-J-1$. These orbitals $\mathcal{F}_{n\kappa}$ satisfy DHF equations in the ion potential $-e^2Z(r)/r$,

$$(\mathcal{L}_\kappa-\epsilon_{n\kappa})\mathcal{F}_{n\kappa}=0\,. \tag{13}$$

The approximate solutions to the RPA equations (10) are given in terms of $\mathcal{F}_{n\kappa}$ by $\mathcal{S}_{\kappa+}^{(0)}(r)=a_\kappa\mathcal{F}_{n\kappa}$ and $\mathcal{S}_{\kappa-}^{(0)}(r)=0$. The coefficients a_κ and the approximate excitation energy ω are yet to be found. With this zeroth approximation in mind we rewrite Eqs. (10) as

$$\begin{aligned} (\mathcal{L}_\kappa-\epsilon_{n\kappa})\mathcal{S}_{\kappa+} &= O_{\kappa+}\mathcal{F}_0-(\omega_{n\kappa}-\omega)\mathcal{S}_{\kappa+}\,, \\ (\mathcal{L}_\kappa-2\epsilon_0+\epsilon_{n\kappa})\mathcal{S}_{\kappa-} &= O_{\kappa-}\mathcal{F}_0+(\omega_{n\kappa}-\omega)\mathcal{S}_{\kappa-}\,, \end{aligned} \tag{14}$$

with $\omega_{n\kappa}=\epsilon_{n\kappa}-\epsilon_0$. Equations (14) are to be solved iteratively using the zeroth approximation described above to evaluate the right-hand side at the first stage. To determine the parameters a_κ and ω in the zeroth approximation we make use of the integrability condition for the upper equations in the system (14), viz.,

$$\int dr\,\mathcal{F}_{n\kappa}(r)[O_{\kappa+}\mathcal{F}_0(r)-(\omega_{n\kappa}-\omega)\mathcal{S}_{\kappa+}(r)]=0\,. \tag{15}$$

Using the zeroth approximation to evaluate Eqs. (15) we obtain a linear eigenvalue equation $Ma=\omega a$ for the vector $a=(a_J, a_{-J-1})$ and for the frequency ω. The resulting zeroth-approximation excitation functions $\mathcal{S}_{\kappa+}^{(0)}(r)$ represent an intermediate coupling Hartree-Fock state. The first and higher approximations to Eqs. (14) take us beyond the Hartree-Fock theory.

We obtain our first approximation by solving Eqs. (14). This first approximation is then used to construct a new right-hand side to Eqs. (14). The first approximation for ω is obtained again with the aid of the integrability condition (15). The iteration procedure is continued in this way until a suitable convergence is obtained. In practice five iterations usually gave an energy accurate to seven or eight significant figures.

Green's functions[14] were determined for the operators $\mathcal{L}_\kappa-\epsilon_{n\kappa}$ and $\mathcal{L}_\kappa-2\epsilon_0+\epsilon_{n\kappa}$, and these numerical Green's functions were used to construct solutions to Eqs. (14) at each stage of the iteration procedure.

V. BREIT INTERACTION

As mentioned in Sec. I we include the Breit interaction in the present calculation as a perturbation. For the case of two electrons the Breit interaction has the form[15]

TABLE I. $1\,{}^1S_0 \rightarrow 2\,{}^1P_1$ ($E1$). RPA excitation energies (in a.u.) including the Breit correction and the RPA oscillator strengths, compared with other values.

Z	ω_{RPA}	ω_{other}	f_{RPA}	f_{other}
2	0.797	0.780 [a]	0.2518	0.2762 [b]
3	2.305	2.286	0.4438	0.4566
4	4.564	4.545	0.5443	0.5516
5	7.574	7.555	0.6042	0.6089
6	11.336	11.316	0.6435	0.6471
7	15.849	15.828	0.6712	0.6742
8	21.115	21.094	0.6915	0.6944
9	27.134	27.112	0.7070	0.7101
10	33.908	33.884	0.7190	0.7226
12	49.723	49.694 [c]	0.7361	0.740 [d]
14	68.573	68.536	0.7464	0.750
16	90.471	90.423	0.7514	0.759
18	115.434	115.372	0.7516	0.764
20	143.483	143.401	0.7470	0.784 [e]
30	330.921	330.644	0.6661	0.808
40	600.275	599.557	0.5764	
50	957.718	956.209	0.5175	
60	1412.225	1412.231 [f]	0.4737	
70	1976.740	1976.757	0.4341	
80	2670.139	2670.172	0.3937	
90	3520.882	3520.921	0.3504	
100	4574.409	4574.434	0.3029	

[a] Accad *et al.*, Ref. 16.
[b] Schiff *et al.*, Ref. 19.
[c] Scofield, Ref. 17.
[d] Dalgarno, Ref. 20.
[e] Dalgarno and Parkinson, Ref. 21.
[f] Ivanov *et al.*, Ref. 18.

$$B = -(e^2/2r_{12})(\vec{\alpha}_1 \cdot \vec{\alpha}_2 + \vec{\alpha}_1 \cdot \hat{r}_{12}\vec{\alpha}_2 \cdot \hat{r}_{12})\,. \tag{16}$$

The angular dependence of the DHF orbitals $u(\vec{r})$ and of the perturbations $w_\pm(\vec{r})$ is not changed by B, since B is a rotational scalar. If we let $\mathcal{F}_1(r)$ represent the modification of $\mathcal{F}_0(r)$ due to the Breit interaction and let ϵ_1 be the modification of ϵ_0, we find that the DHF equation for the modified orbital is

$$(\mathcal{L}_{-1} - \epsilon_0)\mathcal{F}_1 = \epsilon_1\mathcal{F}_1(r) - B(r)\,. \tag{17}$$

In a similar way we let $\mathcal{X}_{\kappa\pm}(r)$ represent the change in $\mathcal{S}_{\kappa\pm}(r)$ and let ω_1 be the first-order excitation energy. We find a set of perturbed radial RPA equations which describe the modifications of Eqs. (10):

$$(\mathcal{L}_\kappa - \epsilon_0 \mp \omega)\mathcal{X}_{\kappa\pm} = O_{\kappa\pm}(\mathcal{X})\mathcal{F}_0 + (\epsilon_1 \pm \omega_1)\mathcal{S}_{\kappa\pm} + O_{\kappa\pm}(\mathcal{S})\mathcal{F}_1 + B_{\kappa\pm}\,. \tag{18}$$

The Breit corrections $B(r)$ and $B_{\kappa\pm}(r)$ are somewhat complicated; they are written out in the Appendix. In solving Eqs. (18) the numerical techniques described in Sec. IV were employed.

The decay rates follow again from the matrix element of Eq. (4), but now the first-order corrections to both u_i and $w_{i\pm}$ are used to give the first-order correction to M_k. It is in this way that the equality of the velocity and length forms of M_k for electric excitations is maintained to first order in the Breit interaction.

VI. RESULTS AND CONCLUSIONS

The $E1$ excitation spectrum consists of closely spaced pairs of states which reduce to singlets and triplets with $L = 1$ in the nonrelativistic limit. We retain the nonrelativistic nomenclature ${}^1P_1$ and ${}^3P_1$ to label the intermediate coupling solutions to Eqs. (10) and (11).

In Table I we collect energies and oscillator strengths for the resonance transition $2\,{}^1P_1 \rightarrow 1\,{}^1S_0$ ($E1$). The RPA energies given in column 2 include the Breit correction. Comparison values gleaned from various sources are listed in column 3. At low values of $Z (\leq 10)$ we compare our energies with those of Accad, Pekeris, and Schiff[16]; these comparison calculations contain corrections beyond those included in the relativistic RPA, such as the Lamb shift and the mass polarization effect. For Z between 10 and 50 we compare with the recent calculations of Scofield,[17] who determined energies from the Dirac-Breit equation supplemented by the Lamb shift. For $Z > 50$ our energies are compared with those of Ivanov *et al.*,[18] who included the Breit term but omitted the Lamb shift. In columns 4 and 5 of Table I the resonance oscillator strengths from the present calculation are compared with nonrelativisitic values. For low Z (≤ 10) the comparison oscillator strengths are from Schiff, Pekeris, and Accad,[19] while for $Z = 10-18$ the values of Dalgarno and Drake[20] are used. A few comparison values for $Z = 20$ and $Z = 30$ are taken from the $1/Z$ expansion of Dalgarno and Parkinson.[21] This latter formula gives remarkably accurate oscillator strengths for lower values of Z but breaks down at higher Z, where the ${}^3P$ channel begins to open. For high-Z atoms the present oscillator strengths are in general agreement with the rough relativistic Coulomb field calculations of Safronova *et al.*[22]

In Table II the $2\,{}^3P_1 \rightarrow 1\,{}^1S_0$ forbidden $E1$ transition energies and rates from the relativistic RPA are compared with the nonrelativistic calculations of Drake and Dalgarno[23] at low Z. The energy comparison parallels that of Table I. Excitation energies for the ${}^1P_1$ and ${}^3P_1$ are in general agreement with comparison calculations, but the RPA energy difference $\Delta = {}^1P - {}^3P$ is significantly too large at smaller values of Z. The ${}^3P_1 \rightarrow {}^1S_0$ rate is inversely proportional to Δ^2 in perturbation theory; consequently, the overestimate of Δ produces an underestimate of the transition rate. If

TABLE II. $1\,^1S_0 \rightarrow 2\,^3P_1$ ($E1$). Excitation energies (in a.u.) and transition rates (in sec^{-1}) including Breit correction, compared with other values. R is the ratio of RPA to exact $^1P_1$-$^3P_1$ energy separation. $A_{\text{emp}}=R^2 A_{\text{RPA}}$ corrects empirically for poor values of $^1P_1$-$^3P_1$ determined by the RPA. The notation $A(B)$ means $A\times 10^B$.

Z	ω_{RPA}	ω_{other}	R^2	A_{RPA}	A_{emp}	A_{other}
2	0.780	0.770 [a]	3.440	6.785(1)	2.33(2)	1.80(2) [b]
3	2.256	2.252	1.964	1.008(4)	1.98(4)	1.81(4)
4	4.483	4.481	1.592	2.648(5)	4.21(5)	4.01(5)
5	7.460	7.459	1.425	3.059(6)	4.36(6)	4.23(6)
6	11.188	11.187	1.331	2.170(7)	2.89(7)	2.84(7)
7	15.667	15.667	1.271	1.112(8)	1.41(8)	1.40(8)
8	20.898	20.898	1.230	4.520(8)	5.56(8)	5.53(8)
9	26.883	26.882	1.199	1.542(9)	1.85(9)	1.85(9)
10	33.621	33.620	1.177	4.586(9)	5.40(9)	5.43(9)
12	49.365	49.358 [c]	1.143	2.970(10)	3.40(10)	
14	68.138	68.125	1.121	1.410(11)	1.58(11)	
16	89.953	80.930	1.106	5.309(11)	5.87(11)	
18	114.822	114.786	1.094	1.664(12)	1.82(12)	
20	142.760	142.707	1.084	4.477(12)	4.85(12)	
30	329.119	328.894		1.224(14)		
40	595.512	594.900		6.976(14)		
50	946.357	945.043		2.122(15)		
60	1388.113	1388.050 [d]		4.863(15)		
70	1930.012	1929.923		9.510(15)		
80	2585.381	2585.237		1.678(16)		
90	3374.082	3373.823		2.754(16)		
100	4327.452	4326.390		4.273(16)		

[a] Accad *et al.*, Ref. 16.
[b] Drake and Dalgarno, Ref. 23.
[c] Scofield, Ref. 17.
[d] Ivanov *et al.*, Ref. 18.

we modify the RPA transition rate by a factor equal to the square of the ratio of the RPA value of Δ to its correct value, the resulting empirical rate is in general agreement with that determined by nonrelativistic calculations. For low values of Z the forbidden rate grows approximately as Z^{10}, while for high values the rate slows to approximately Z^6.

To illustrate the relative importance of various contributions to the energy and oscillator strength we list in Table III intermediate coupling DHF values, together with values determined from the

TABLE III. Intermediate coupling DHF values of excitation energy (in a.u.) and oscillator strengths compared with RPA calculations without Breit interaction (No-Br) and with final RPA values including Breit interaction. f^l_{DHF} and f^v_{DHF} are the length and velocity values of the DHF oscillator strengths. The length and velocity are equal in the RPA. $A(B)=A\times 10^B$.

Z	ω_{DHF}	$\omega_{\text{No-Br}}$	ω_{RPA}	f^l_{DHF}	f^v_{DHF}	$f_{\text{No-Br}}$	f_{RPA}
				$2\,^1P_1 \rightarrow 1\,^1S_0$			
10	33.925	33.920	33.908	0.751	0.744	0.7189	0.7190
20	143.591	143.586	143.483	0.765	0.762	0.7492	0.7470
30	331.269	331.263	330.921	0.685	0.683	0.6756	0.6661
40	601.086	601.080	600.275	0.593	0.592	0.5875	0.5764
50	959.308	959.303	957.718	0.531	0.530	0.5268	0.5175
				$2\,^3P_1 \rightarrow 1\,^1S_0$			
10	33.637	33.632	33.621	0.307(−3)	0.304(−3)	0.2942(−3)	0.3788(−3)
20	142.858	142.852	142.760	0.180(−1)	0.179(−1)	0.1765(−1)	0.2051(−1)
30	329.456	329.450	329.119	0.963(−1)	0.961(−1)	0.9505(−1)	0.1055
40	596.340	596.334	595.152	0.173	0.173	0.1714	0.1837
50	948.024	948.018	946.357	0.212	0.212	0.2106	0.2213

TABLE IV. RPA excitation energies (in a.u.) and oscillator strengths for $E1$ transitions from higher-excited states to the ground state. $A(B)=A\times10^{B}$.

Z	n	$\omega(n\,^1P_1)$	$\omega(n\,^3P_1)$	$f(n\,^1P_1\rightarrow1\,^1S_0)$	$f(n\,^3P_1\rightarrow1\,^1S_0)$
10	2	33.908	33.621	0.7190	0.3788(−3)
	3	39.476	39.399	0.1488	0.8744(−4)
	4	41.435	41.403	0.5586(−1)	0.3403(−4)
	5	42.343	42.327	0.2714(−1)	0.1683(−4)
20	2	142.483	142.760	0.7470	0.2051(−1)
	3	168.482	168.283	0.1477	0.4589(−2)
	4	177.255	177.174	0.5467(−1)	0.1769(−2)
	5	181.319	181.278	0.2639(−1)	0.8702(−3)
30	2	330.921	329.119	0.6661	0.1055
	3	389.369	388.853	0.1293	0.2164(−1)
	4	409.884	409.669	0.4760(−1)	0.8106(−2)
	5	419.382	419.273	0.2291(−1)	0.3931(−2)

RPA without the Breit interaction, and final RPA values, including the Breit correction for $Z=10$–50. The Breit correction to the allowed oscillator strengths are of minor importance, while the Breit correction to the forbidden transition oscillator strengths are very important. The DHF values improve with increasing Z, because of the diminishing importance of correlations. In our calculations the oscillator strengths are evaluated in both the velocity and length forms (f_v and f_l). We list both f_v and f_l for the DHF calculations; as Z increases the agreement between f_v and f_l improves. The two forms are of course equal for all Z in the relativistic RPA, before and after the Breit correction is applied.

Energies of higher-excited $n\,^1P_1$ and $n\,^3P_1$ states are listed along with their oscillator strengths in Table IV. For $Z=10$ nonrelativistic comparison values[19] of 0.1492, 0.0560, and 0.0274 are in good agreement with the allowed oscillator strengths listed in Table IV.

Results for magnetic dipole transitions $2\,^3S_1\rightarrow1\,^1S_0$ ($M1$) are presented in Table V. The energies are compared with those found by Accad, Pekeris, and Schiff[16] for $Z\leqslant10$, and with results of Ivanov *et al.*[18] for $Z\geqslant20$. The DHF rates are listed together with RPA values in column 4 and 5 of Table V. The agreement between DHF and RPA improves as Z increases and correlation decreases. The RPA transition rate is about 25% too large at $Z=2$ compared with Drake's nonrelativistic calculation[24] and agrees with an alternative relativistic calculation[25] for all but the lowest few Z values. For $Z=8$–18 the RPA also agrees well with the nonrelativistic calculation of Drake. An alternative calculation of the $M1$ transition given by Feinberg and Sucher[26] supports the Drake result at small

TABLE V. $2\,^3S_1\rightarrow1\,^1S_0$ ($M1$). Excitation energies (in a.u.) and transition rates (in sec^{-1}). $A(B)=A\times10^{B}$.

Z	ω_{RPA}	ω_{other}	A_{DHF}	A_{RPA}	A_{other}	
2	0.724	0.728 [a]	5.962(−5)	1.728(−4)	1.253(−4) [b]	1.272(−4) [c]
3	2.163	2.169	1.274(−2)	2.254(−2)	2.037(−2)	2.039(−2)
4	4.351	4.358	3.996(−1)	5.905(−1)	5.638(−1)	5.618(−1)
5	7.290	7.298	5.128(0)	6.902(0)	6.731(0)	6.695(0)
6	10.979	10.987	3.902(1)	4.959(1)	4.887(1)	4.856(1)
7	15.419	15.428	2.105(2)	2.574(2)	2.551(2)	2.532(2)
8	20.612	20.619	8.903(2)	1.058(3)	1.052(3)	1.044(3)
9	26.557	26.564	3.138(3)	3.653(3)	3.640(3)	3.608(3)
10	33.255	33.261	9.609(3)	1.100(4)	1.098(4)	1.087(4)
12	48.915		6.561(4)	7.333(4)	7.327(4)	7.243(4)
14	67.601		3.288(5)	3.614(5)	3.614(5)	3.563(5)
16	89.324		1.319(6)	1.431(6)	1.432(6)	1.408(6)
18	114.096		4.469(6)	4.804(6)	4.808(6)	4.709(6)
20	141.931	141.904 [d]	1.328(7)	1.417(7)	1.418(7)	1.383(7)
30	327.706	327.591	8.640(8)	9.013(8)	9.023(8)	
40	593.445	593.159	1.674(10)	1.727(10)	1.729(10)	
50	943.563	942.988	1.694(11)	1.736(11)	1.737(11)	
60	1384.476	1383.451	1.146(12)	1.169(12)	1.171(12)	
70	1925.355	1923.659	5.925(12)	6.028(12)	6.032(12)	
80	2579.437	2576.767	2.537(13)	2.575(13)	2.577(13)	
90	3366.445	3362.372	9.506(13)	9.633(13)	9.639(13)	
100	4317.456	4311.334	3.249(14)	3.289(14)		

[a] Accad *et al.*, Ref. 16.

[b] Johnson and Lin, Ref. 25.

[c] Drake, Ref. 24.

[d] Ivanov *et al.*, Ref. 18.

TABLE VI. $2\,^3P_2 \rightarrow 1\,^1S_0$ ($M2$). Excitation energies (in a.u.) and transition rates (in sec^{-1}). $A(B) = A \times 10^B$.

Z	ω_{RPA}	ω_{other}	A_{DHF}	A_{RPA}	A_{other}	
2	0.779	0.770[a]	2.949(−1)	3.935(−1)	3.27(−1)[b]	4.00(−1)[c]
3	2.257	2.252	3.240(1)	3.692(1)	3.50(1)	3.60(1)
4	4.483	4.481	5.838(2)	6.328(2)	6.17(2)	
5	7.460	7.459	4.805(3)	5.088(3)	5.01(3)	
6	11.188	11.188	2.534(4)	2.648(4)	2.62(4)	
7	15.688	15.668	1.001(5)	1.038(5)	1.03(5)	
8	20.901	20.901	3.230(5)	3.329(5)	3.31(5)	
9	26.887	26.887	8.968(5)	9.205(5)	9.16(5)	
10	33.628	33.627	2.217(6)	2.269(6)	2.26(6)	
12	49.380		1.045(7)	1.065(7)	1.06(7)	
14	68.169		3.830(7)	3.892(7)	3.87(7)	
16	90.010		1.170(8)	1.187(8)	1.19(8)	
18	114.920		3.119(8)	3.158(8)	3.18(8)	
20	142.919	142.909[d]	7.468(8)	7.555(8)		
30	330.144	330.110	2.104(10)	2.122(10)		
40	599.274	599.197	2.217(11)	2.235(11)		
50	956.450	956.318	1.375(12)	1.386(12)		
60	1410.651	1410.441	6.126(12)	6.174(12)		
70	1974.821	1974.512	1.981(13)	2.194(13)		
80	2667.844	2667.515	6.572(13)	6.628(13)		
90	3518.188	3517.606	1.756(14)	1.772(14)		
100	4571.316	4570.547	4.274(14)	4.316(14)		

[a] Accad *et al.*, Ref. 16.

[b] Drake, Ref. 27, variational values and Jacobs, Ref. 30.

[c] Drake, Ref. 27, $1/Z$ expansion values.

[d] Ivanov *et al.*, Ref. 18.

Z. The calculated $M1$ decay rates have been confirmed by accurate beam-foil measurements for elements ranging up to $Z = 36$.

Table VI lists energies and rates for the $2\,^3P_2 \rightarrow 1\,^1S_0$ ($M2$) transition. The DHF rates and RPA rates listed together in columns 4 and 5 of Table VI again agree more and more as Z increases. The RPA calculations of the decay rates agree well with nonrelativistic values of Drake[27] for Z up to 18, being about 20% too large at $Z = 2$.

To give some notion of the usefulness of the RPA energies for predictive purposes, in Table VII we compare wavelengths determined by the RPA with values determined from measurements.[28] We see that in the range of elements considered, $Z = 12-30$, the comparison with the semiempirical values is close, a feature which is of course shared by the comparison calculations used herein, and by other calculations in which relativistic corrections are included.[29]

In Table VIII we collect together recent experimental values of metastable transition probabilities determined mainly by beam-foil spectroscopy. The agreement between theory and experimental is seen to be good for the $M1$ transition but only fair for the $E1$ and $M2$ transition. In the

TABLE VII. Comparison of RPA wavelengths with observation (by Gabriel, Ref. 28). All values in Å.

	$2\,^1P_1 \rightarrow 1\,^1S_0$ ($E1$)		$2\,^3P_1 \rightarrow 1\,^1S_0$ ($E1$)		$2\,^3P_2 \rightarrow 1\,^1S_0$ ($M2$)		$2\,^3S_1 \rightarrow 1\,^1S_0$ ($M1$)	
Z	λ_{obs}	λ_{RPA}	λ_{obs}	λ_{RPA}	λ_{obs}	λ_{RPA}	λ_{obs}	λ_{RPA}
12 (Mg)	9.168	9.163	9.231	9.230	9.228	9.227	9.313	9.315
14 (Si)	6.647	6.644	6.688	6.687	6.685	6.684	6.739	6.740
16 (S)	5.038	5.036	5.066	5.065	5.063	5.062	5.101	5.101
18 (Ar)	3.948	3.947	3.969	3.968	3.965	3.965	3.993	3.993
20 (Ca)	3.176	3.176	3.192	3.192	3.189	3.188	3.210	3.210
26 (Fe)	1.8500	1.8493	1.8591	1.8585	1.8551	1.8545	1.8677	1.8674
28 (Ni)	1.5880	1.5873	1.5961	1.5956	1.5919	1.5914	1.6031	1.6028
29 (Ci)	1.4771	1.4768	1.4849	1.4844	1.4807	1.4802	1.4913	1.4910

TABLE VIII. Comparison of RPA predictions with experimental measurements of metastable transition probabilities. Theoretical $E1$ transition rates to $2\,^3S_1$ states are subtracted from the experimental $2\,^3P$ decay rates. $A(B)=A\times 10^B$.

	$2\,^3S_1\rightarrow 1\,^1S_0$ $(M1)$			$2\,^3P_1\rightarrow 1\,^1S_0$ $(E1)$			$2\,^3P_2\rightarrow 1\,^1S_0$ $(M2)$	
Z	τ_{RPA} (nsec)	τ_{expt} (nsec)	Z	A_{RPA} (sec^{-1})	A_{expt} (sec^{-1})	Z	A_{RPA} (sec^{-1})	A_{expt} (sec^{-1})
2	5.79(12)	9 ± 3(12) [a]	7	1.41(8)	1.7 ± 0.3(8) [f]	16	1.19(8)	1.7 ± 0.3(8) [m]
16	699	706 ± 83 [b]	8	5.56(8)	5.8 ± 0.6(8) [g]	17	1.96(8)	2.7 ± 0.3(8) [n]
17	374	354 ± 24 [b]	8		6.0 ± 0.4(8) [h]	18	3.16(8)	2.3 ± 1(8) [o]
18	208	202 ± 20 [c]	8		5.99 ± 0.09(8) [i]	26	6.55(9)	7.5 ± 2(9) [e]
22	26.6	25.8 ± 1.3 [d]	9	1.85(9)	1.77 ± 0.10(9) [j]			
23	16.9	16.9 ± 0.7 [e]	9		1.77 ± 0.07(9) [k]			
26	4.80	4.8 ± 0.6 [e]	16	5.87(11)	5.9 ± 1.0(11) [l]			
36	0.171	0.20 ± 0.06 [c]						

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latter cases two competing channels are involved in the decays; one channel leads to the ground state and the other leads to the $2\,^3S_1$ state. In quoting experimental rates to the ground state in Table VIII we have subtracted the theoretical $E1$ rate[20] to the $2\,^3S_1$ state from the $E1$ and $M2$ measurements. It is apparent from the comparison that the relativistic RPA has the power to follow the rapid Z-dependence characteristic of metastable decay probabilities.

The virtues of RPA appear to be its simplicity and versatility. On the basis of the present calculations it appears worthwhile to undertake studies of more complex ions where reliable relativistic values are not easily available from alternative calculations.

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APPENDIX

The Breit corrections $B(r)$ and $B_{\kappa\pm}(r)$ introduced in Eqs. (17) and (18) are two-component functions of r defined in terms of the ground-state DHF radial functions $G_0(r)$ and $F_0(r)$ and the unperturbed RPA radial functions $S_{\kappa\pm}(r)$ and $T_{\kappa\pm}(r)$. Let us introduce the two-component functions

$$\tilde{\mathfrak{F}}_0(r)=\begin{pmatrix} F_0(r) \\ G_0(r) \end{pmatrix};$$

then setting

$$W(r)=2e^2\int_0^\infty dr'\,\frac{r_<}{r_>^2}F_0(r')G_0(r'),$$

we have

$$B(r)=\tfrac{2}{3}W(r)\tilde{\mathfrak{F}}_0(r). \tag{A1}$$

Now for convenience let

$$\tilde{\mathfrak{S}}_{\kappa\pm}(r)=\begin{pmatrix} T_{\kappa\pm}(r) \\ S_{\kappa\pm}(r) \end{pmatrix},$$

and introduce the matrices

$$M_{\kappa}^{J}=\begin{pmatrix}1-(1+\kappa)/J & 0\\ 0 & -1-(1+\kappa)/J\end{pmatrix},$$

$$N_{\kappa}^{J}=\begin{pmatrix}-1-(1+\kappa)/(J+1) & 0\\ 0 & 1-(1+\kappa)/(J+1)\end{pmatrix}.$$

Define the functions

$$P_{\kappa\pm}(r)=S_{\kappa\pm}F_0-T_{\kappa\pm}G_0-[(\kappa+1)/J](S_{\kappa\pm}F_0+T_{\kappa\pm}G_0),$$

$$Q_{\kappa\pm}(r)=-S_{\kappa\pm}F_0+T_{\kappa\pm}G_0-[(\kappa+1)/(J+1)](S_{\kappa\pm}F_0+T_{\kappa\pm}G_0),$$

$$V_{\kappa\pm}(r)=S_{\kappa\pm}F_0+T_{\kappa\pm}G_0,$$

and introduce

$$\mathcal{E}_J(\kappa,\pm,r)=\frac{J(J+1)}{2J+1}\left\{\left[\frac{1}{2J-1}\int_0^\infty dr'\frac{r_<^{J-1}}{r_>^{J}}P_{\kappa\pm}(r')-\frac{1}{2}\int_r^\infty dr'\left(\frac{r_<^{J-1}}{r_>^{J}}-\frac{r_<^{J+1}}{r_>^{J+2}}\right)Q_{\kappa\pm}(r')\right]M_{\kappa}^{J}\right.$$
$$\left.+\left[\frac{1}{2J+3}\int_0^\infty dr'\frac{r_<^{J+1}}{r_>^{J+2}}Q_{\kappa\pm}(r')-\frac{1}{2}\int_0^r dr'\left(\frac{r_<^{J-1}}{r_>^{J}}-\frac{r_<^{J+1}}{r_>^{J+2}}\right)P_{\kappa\pm}(r')\right]N_{\kappa}^{J}\right\}, \tag{A2}$$

$$\mathfrak{M}_J(\kappa,\pm,r)=\int dr'\frac{r_<}{r_>^{J+1}}V_{\kappa\pm}(r'). \tag{A3}$$

In terms of $\mathcal{E}_J$ and $\mathfrak{M}_J$ one has the following for the Breit correction:

Electric excitations EJ:

$$B_{J\pm}(r)=-\frac{2}{3}\left(\frac{J}{2J+1}\tilde{\mathfrak{S}}^{\pm}_{J}+\frac{J+1}{2J+1}\tilde{\mathfrak{S}}^{\pm}_{-J-1}\right)W(r)-\frac{(J-1)e^2}{J(2J-1)}[\mathfrak{M}_{J-1}(J,\pm,r)+\mathfrak{M}_{J-1}(J,\mp,r)]\tilde{\mathfrak{F}}_0$$
$$+\frac{e^2}{(2J+1)^2}[-\mathcal{E}_J(J,\pm,r)+(2J+2)\mathcal{E}_J(-J-1,\pm,r)-(2J+1)\mathcal{E}_J(J,\mp,r)]\tilde{\mathfrak{F}}_0, \tag{A4}$$

$$B_{-J-1\pm}(r)=-\frac{2}{3}\left(\frac{J}{2J+1}\tilde{\mathfrak{S}}^{\pm}_{J}+\frac{J+1}{2J+1}\tilde{\mathfrak{S}}^{\pm}_{-J-1}\right)W(r)-\frac{(J+2)e^2}{(J+1)(2J+3)}[\mathfrak{M}_{J+1}(-J-1,\pm,r)+\mathfrak{M}_{J+1}(-J-1,\mp,r)]\tilde{\mathfrak{F}}_0$$
$$+\frac{e^2}{(2J+1)^2}[\mathcal{E}_J(-J-1,\pm,r)+2J\mathcal{E}_J(J,\pm,r)-(2J+1)\mathcal{E}_J(-J-1,\mp,r)]\tilde{\mathfrak{F}}_0. \tag{A5}$$

Magnetic excitations MJ:

$$B_{-J\pm}=\frac{2}{3}\left(\frac{J}{2J+1}\tilde{\mathfrak{S}}_{-J\pm}+\frac{J+1}{2J+1}\tilde{\mathfrak{S}}_{J+1\pm}\right)W(r)-\frac{e^2}{2J-1}[\mathcal{O}_{J-1}(-J,\pm,r)-\mathcal{E}_{J-1}(-J,\mp,r)]\tilde{\mathfrak{F}}_0$$
$$+\frac{(J+1)e^2}{J(2J+1)^2}[-\mathfrak{M}_J(-J,\pm,r)-2J\mathfrak{M}_J(J+1,\pm,r)+(2J+1)\mathfrak{M}_J(-J,\mp,r)]\tilde{\mathfrak{F}}_0, \tag{A6}$$

$$B_{J+1\pm}=\frac{2}{3}\left(\frac{J}{2J+1}\tilde{\mathfrak{S}}_{-J\pm}+\frac{J+1}{2J+1}\tilde{\mathfrak{S}}_{J+1\pm}\right)W(r)-\frac{e^2}{2J+3}[\mathcal{E}_{J+1}(J+1,\pm,r)-\mathcal{E}_{J+1}(J+1,\mp,r)]\tilde{\mathfrak{F}}_0$$
$$+\frac{Je^2}{(J+1)(2J+1)^2}[\mathfrak{M}_J(J+1,\pm,r)-(2J+2)\mathfrak{M}_J(-J,\pm,r)+(2J+1)\mathfrak{M}_J(J+1,\mp,r)]\tilde{\mathfrak{F}}_0. \tag{A7}$$

In applications Eqs. (A4)–(A7) are evaluated only once after the RPA equations have been solved, and the resulting functions $B_{\kappa\pm}(r)$ are used as driving terms in the inhomogeneous equations (18).

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