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LETTER TO THE EDITOR

Allowed and forbidden transitions of helium-like ions

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Abstract. A relativistic generalization of the random phase approximation is used to study the response of helium-like ions to electromagnetic perturbations. The spectrum of the response function in this relativistic theory contains allowed and forbidden transitions. The computed E1($2^{1,3}P_1 - 1^1S_0$), M1($2^3S_1 - 1^1S_0$) and M2($2^3P_2 - 1^1S_0$) transition rates agree well with those obtained by refined calculations and with experiment. Accurate values are also obtained for the excitation energies of ions with large nuclear charges, where relativistic effects are of major importance.

Relativistic effects on the probabilities of allowed and forbidden transitions have assumed a new importance because of the observations in the solar corona and in high temperature plasmas generally of elements of high nuclear charge. In the few instances that have been examined theoretically, special perturbation treatments of restricted applicability have been used (Younger and Weiss 1975, Kim and Desclaux 1976). We have recently developed a relativistic version of the random phase approximation (RRPA) (Johnson and Dalgarno 1976) that should be generally applicable to many-electron systems. In this letter, we demonstrate its utility by solving the RRPA equations for helium-like systems to high accuracy and by comparing the resulting allowed and forbidden transition probabilities with established theoretical and experimental data.

We adopt as a starting point the particular formulation of the non-relativistic random phase approximation or time-dependent Hartree–Fock theory given by Dalgarno and Victor (1966). We generalize it to include relativistic effects by replacing the non-relativistic Hamiltonian by the Dirac–Breit Hamiltonian, consisting of a sum of Dirac single-electron terms, the electron–electron Coulomb interaction and the Breit interaction which must be treated as a perturbation. We neglect the electron self-energy and vacuum polarization and other higher order quantum electrodynamic effects.

With these assumptions, we can construct Dirac–Hartree–Fock (DHF) orbitals $u_i(r)$ from the Dirac–Breit equations (cf Grant 1970). We restrict consideration to a closed-shell system of N electrons whose ground state wavefunction can be described by a single determinant containing N DHF orbitals $u_i(r)$. The perturbations $w_i^{\pm}(r)$ of $u_i(r)$ induced by the external field $(A_-\exp(i\omega t) + A_+\exp(-i\omega t))$ satisfy the RPA equations

$$(h_0 + V - \epsilon_i \mp \omega)w_i^{\pm} = (A_{\pm} - V_{\pm}^{(1)})u_i \tag{1}$$

where h_0 is the single-electron Dirac Hamiltonian, V is the DHF potential, ϵ_i is the orbital energy of the ith electron and ω is the transition energy. If the right-hand side is put equal to zero, the equation reduces to the Dirac–Hartree–Fock equation for an excited orbital. The potential $V_{\pm}^{(1)}$ on the right represents the correlation effects included in the RPA. To obtain excitation energies ω and eigenfunctions $w_{i\pm}(r)$, we may set $A_{i\pm} = 0$. The eigenfunctions of (1) describe atomic states with definite angular momentum J, M and parity $\pi = \pm 1$. Such states can decay into the ground state by electric or magnetic multipole radiation. For electric multipole transitions the rates computed from (1) in the velocity and length forms are identical. The final state described by $w_{i\pm}(r)$ is an intermediate coupling state and the RRPA can be used to study the transition from LS coupling at low Z to jj coupling at high Z.

Equation (1) can be reduced to a set of coupled radial equations. We solved the resulting equation by iteration starting with the DHF orbitals in the zeroth approximation. The Breit interaction was included as a first order perturbation correction, by adding the extra term to the right of equation (1). The resulting equations were then solved by the same iterative technique. We shall describe the numerical methods in more detail elsewhere.

The solutions of (1) for E1 transitions consist of closely-spaced pairs of states which reduce to the $^1P_1$ and $^3P_1$ states in the non-relativistic limit. The calculation gives the allowed $2^1P_1 \rightarrow 1^1S_0$ and forbidden $2^3P_1 \rightarrow 1^1S_0$ transition rates. In table 1, we compare our computed oscillator strengths with some non-relativistic calculations. At low Z, our allowed rates compare very well with the refined calculations of Accad *et al* (1971). At high Z, our calculations depart from the non-relativistic calculations of Dalgarno and Parkinson (1967) because we include relativistic effects. For the forbidden transitions at low Z, our RPA results do not have high precision. At low Z, the intercombination rates are inversely proportional to the square of the fine structure splitting between the $^3P_1$ and $^1P_1$ states and the RPA energies are not accurate. If we replace the energy differences by the correct values (Accad *et al* 1971), the oscillator strengths, f_{emp}, compare favourably with the Hylleraas-type calculations of Drake and Dalgarno (1969). The forbidden transition rates are comparable to the allowed transition rates at high Z. Because of the energy dependence of the relativistic transition operator, the oscillator strengths for the allowed and the forbidden transitions at high Z are not consistent with a uniform statistical ratio.

For magnetic multipole transitions, equation (1) decouples and we can study separately the $^3S_1 \rightarrow {}^1S_0$ and $^3D_1 \rightarrow {}^1S_0$ transitions in the M1 case and the $^3P_2 \rightarrow {}^1S_0$ and $^3F_2 \rightarrow {}^1S_0$ transitions in the M2 case. In table 2, we compare the RPA results

Table 1. Electric dipole E1 transition oscillator strengths.

		$^1P_1 \rightarrow {}^1S_0$		$^3P_1 \rightarrow {}^1S_0$		
Z	Ion	f_{RPA}	f_{other}	f_{RPA}	f_{emp}	f_{other}
5	B	0·6042	0·6089†	5·13(−6)	7·31(−6)	7·10(−6)§
9	F	0·7070	0·7101†	1·99(−4)	2·39(−4)	2·39(−4)§
16	S	0·7514	0·759‡	6·13(−3)	6·77(−3)	
30	Zn	0·6661	0·808‡	0·105	0·105	
60	Nd	0·4737		0·236	0·236	
80	Hg	0·3937		0·234	0·234	

† Accad *et al* (1971). ‡ Dalgarno and Parkinson (1967). § Drake and Dalgarno (1969).

Table 2. Magnetic dipole (M1) and quadrupole (M2) transition probabilities in s^{-1}.

		$^3S_1 \rightarrow {}^1S_0$(M1)				$^3P_2 \rightarrow {}^1S_0$(M2)	
Z	Ion	A_{RPA}	A_{other}		A_{exp}	A_{RPA}	A_{other}
5	B	6·90	6·73†	6·70‡		5·08 (3)	5·01 (3)††
10	Ne	1·10 (4)	1·10(4)†	1·09 (4)‡		9·21 (5)	9·16 (5)††
16	S	1·43 (6)	1·43(6)†	1·41 (6)‡	1·42 ± 0·15 (6)§	1·19 (8)	1·19 (8)††
18	Ar	4·80 (6)			4·95 ± 0·4 (6)¶	3·16 (8)	3·18 (8)††
26	Fe	2·08 (8)			2 ± 0·2 (8)‖	6·56 (9)	
36	Kr	5·85 (9)			5 ± 0·7 (9)¶	9·44 (10)	
60	Nd	1·17 (12)	1·17 (12)†			6·17 (12)	

† Johnson and Lin (1974). ‡ Drake (1971). § Bednar *et al* (1975). ‖ Gould and Marrus (1974). ¶ Gould *et al* (1973), Gould and Marrus (1976). †† Drake (1969).

Table 3. Transition energies in wavelengths (Å) of helium-like ions.

		$2^1P_1 \rightarrow 1^1S_0$		$2^3P_1 \rightarrow 1^1S_0$		$2^3P_2 \rightarrow 1^1S_0$		$2^3S_1 \rightarrow 1^1S_0$	
Z	Ion	λ_{RRPA}	λ_{obs}	λ_{RRPA}	λ_{obs}	λ_{RRPA}	λ_{obs}	λ_{RRPA}	λ_{obs}
12	Mg	9·163	9·168	9·230	9·231	9·227	9·228	9·315	9·313
18	Ar	3·947	3·948	3·968	3·969	3·965	3·965	3·993	3·993
20	Ca	3·176	3·176	3·192	3·192	3·188	3·189	3·210	3·210
26	Fe	1·8493	1·8500	1·8585	1·8591	1·8545	1·8551	1·8674	1·8677
28	Ni	1·5873	1·5880	1·5956	1·5961	1·5914	1·5919	1·6028	1·6031

with other theoretical and experimental results. For the M1 transitions, our results agree well with the relativistic perturbation calculation of Johnson and Lin (1974) at all Z and the non-relativistic calculation of Drake (1971) at low Z. Our M1 results also agree with the beam–foil measurements (Bednar *et al* 1975, Gould *et al* 1973, Gould and Marrus 1974, 1976). For the M2 transitions, our RPA results agree with the non-relativistic calculation of Drake (1969) at low Z and we expect the results to be good at high Z also.

Unlike oscillator strengths, the RPA excitation energies are usually not of high accuracy. However, the RPA is in principle more accurate than excited DHF calculations. At higher Z where correlation is not very large, the RPA treatment represents a significant improvement over DHF theory. In table 3, the RRPA transition wavelengths for several cosmically abundant ions are compared with wavelengths obtained empirically by Gabriel (1972). The RRPA energies are accurate enough for purposes of identification of the emitting species.

In summary, the relativistic RPA calculations can provide accurate values of transition rates and useful values of excitation energies. Its computational simplicity suggests that it can be readily extended to treat many-electron atomic systems.

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