Resonance Transitions of Be-like Ions from Multiconfiguration Relativistic Random-Phase Approximation

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Relativistic excitation energies and transition rates from the $^1S_0$ ground states to the first $^3P_1$ and $^1P_1$ excited states of berylliumlike ions are determined by using the newly developed multiconfiguration relativistic random-phase approximation (MCRRPA). Results from the MCRRPA theory are compared with those from other theories and experiments. The large discrepancies between the single-configuration RRPA predictions of excitation energies and the precise experimental values are resolved.

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Excitation energies and oscillator strengths for resonance transitions in highly stripped ions are needed for estimating the energy loss through impurity ions in plasmas and for plasma diagnostics. Precision spectroscopy both in astrophysical and in laboratory beam-foil measurements also demands accurate theoretical values. At present, a complete treatment of electron-electron correlations poses a formidable obstacle in high-precision theoretical calculations. In recent years, the relativistic random-phase approximation (RRPA)[1] and multiconfiguration Dirac-Fock (MCDF) calculations[2] have played two of the major roles in attacking the correlation problem in relativistic calculations and have produced extensive data on a variety of atoms and ions. The MCDF approach has the merit of being applicable to arbitrary systems and being capable of treating certain correlations not included in the RRPA approach. The RRPA can be applied only to closed-shell systems, and only a single configuration is allowed to describe the reference state of the system. Nevertheless, the RRPA approach does have several advantages: First, the RRPA results are gauge independent; there is no arbitrariness in choosing the gauge as in the case of the MCDF. Second, both discrete and continuum correlations can be dealt with in the RRPA. Third, core polarization can be treated readily in the RRPA.

Although it is possible to treat open-shell systems from the relativistic equations-of-motion approach,[3] where the RRPA type as well as other correlations can be accounted for, the associated numerical techniques are still under development. In the meantime, the RRPA can be improved upon by using a multiconfiguration wave function as the reference state. The electron-electron correlation effects due to the presence of "real" doubly excited configurations in the initial state are thereby included. This approach is called the multiconfiguration relativistic random-phase approximation (MCRRPA). In essence, it has certain features of the MCDF, while preserving all of the advantages, especially, the gauge invariance, of the RRPA. A detailed derivation of the MCRRPA theory is given in a separate paper.[4] Here we report only a prototypal application of this new theory to Be-like ions and make comparisons with RRPA[5] and MCDF[6-9] calculations and with experiment[10-21] to demonstrate the practical merits of this approach.

In previous applications of the RRPA to the Be-like ions,[5] single-configuration wave functions constructed from $1s_{1/2}$ and $2s_{1/2}$ orbitals have served as reference states for describing one-particle excitation spectra. However, because of the near degeneracy of $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ orbitals, the $^1S_0$ ground states of the Be-like ions are not described well by such single-configuration wave functions. Therefore, the RRPA predictions of excitation energies are in rather poor agreement with precise experimental values. In the present MCRRPA formulation, the reference state is given by a multiconfiguration wave function of the form

$$\Psi = C_1(2s_{1/2})^2 + C_2(2p_{1/2})^2 + C_3(2p_{3/2})^2, \tag{1}$$

where the symbol $(2l_j)^2$ designates a Slater determinant constructed from the $(2l_j)$ valence orbitals and two $(1s_{1/2})$ core orbitals. The parameters C_a $(a=1,2,3)$ in Eq. (1) are configuration weight coefficients. The core and valence orbitals and the configuration weights are determined by solving MCDF equations numerically.

We restrict our attention in the present study to electric dipole excitations of the multiconfiguration ground state given in Eq. (1) to the first $^1P_1$ and $^3P_1$ excited states. Since the MCRRPA equations include all one-particle excitations of the ground state, they automatically include, in addition to the usual RRPA correlation effects, the important final-state correlations between an excited electron and excited $2p_{1/2}$ or $2p_{3/2}$ ionic cores. These two-particle–two-hole final-state correlations were omitted in previous RRPA studies. Therefore, it is not surprising that the corresponding predictions of excitation energies were poor. In fact, for neutral Be, the first triplet P state, $(2s2p)^3P_1$, is missing from the RRPA spectrum,[5] while the excitation energy of the first singlet P state, $(2s2p)^1P_1$, is in error by about 9%. This situation does not improve substantially for other more highly ionized members of the Be sequence.

Because we are most interested in highly ionized species where both relativistic and correlation effects play important roles, we compare only with other relativistic calculations. In this context, we note that the correlation problem in nonrelativistic atomic systems has been studied extensively, especially for Be and Be-like ions of low nuclear charge. Among others, several approaches are many-body perturbation theory,[22] large-scale configuration-interaction calculations,[23-26] variational configuration-interaction techniques,[27] variational Bethe-Goldstone calculations,[28] non-closed-shell many-electron theory,[29,30] Z-expansion methods,[31,32] model-potential calculations,[33] and the multiconfiguration time-dependent Hartree-Fock method.[34] The present approach with use of a multiconfiguration wave function as the reference state is related to the multiconfiguration time-dependent Hartree-Fock method.[34,35]

In Tables I and II, excitation energies and oscillator strengths of the Be-like ions from the MCRRPA theory are compared with those from other relativistic theories and experiment. While consistent with other relativistic predictions, the

TABLE I. Excitation energies and oscillator strengths of the transition $(2s^2)\,^1S_0 \rightarrow (2s2p)\,^1P_1{}^\circ$ for Be-like ions.

Ion	$\omega_{\mathrm{MCDF}}{}^a$	$\omega_{\mathrm{RRPA}}{}^b$	$\omega_{\mathrm{MCRRPA}}{}^c$	$\omega_{\mathrm{exp}}{}^d$ (au)	$f_{\mathrm{MCDF}}{}^a$	$f_{\mathrm{RRPA}}{}^b$	$f_{\mathrm{MCRRPA}}{}^c$	f_{exp}
Be	0.222	0.177	0.201	0.19394^e	1.28	1.38	1.42	1.38 ± 0.12^f
								1.34 ± 0.05^g
B^+			0.347	0.33442^e			1.05	0.83 ± 0.09^h
								0.73 ± 0.07^i
								0.9 ± 0.2^j
C^{2+}	0.520	0.428	0.484	0.46635	0.794	0.753	0.797	0.65 ± 0.03^k
N^{3+}	0.652		0.617	0.59549	0.634		0.641	
O^{4+}	0.782	0.658	0.749	0.72354	0.529	0.499	0.536	0.42 ± 0.05$^\ell$
F^{5+}	0.911		0.879	0.85132	0.454		0.460	
Ne^{6+}	1.04	0.885	1.01	0.97939	0.399	0.375	0.404	0.336 ± 0.025^m
								0.60^n
Mg^{8+}	1.30	1.12	1.27	1.2379	0.321	0.304	0.326	0.32 ± 0.03^p
Si^{10+}	1.56	1.35	1.54	1.5021	0.270	0.256	0.274	0.28 ± 0.02^p
Si^{12+}	1.84	1.60	1.81	1.7751	0.235	0.223	0.238	0.23 ± 0.03^p
Ar^{14+}	2.12	1.86	2.10	2.0604	0.209	0.198	0.212	
Ca^{16+}	2.42	2.14	2.40	2.3625	0.190	0.181	0.192	
Ti^{18+}	2.75	2.44	2.73	2.6868	0.175	0.167	0.177	
Cr^{20+}	3.10		3.08	3.0401	0.164		0.166	
Fe^{22+}	3.49	3.15	3.47	3.4303	0.155	0.150	0.157	
Ni^{24+}	3.92	3.57	3.90	3.8673	0.148	0.144	0.151	

[a] Ref. 9.
[b] Ref. 5.
[c] Present calculations.
[d] Cited in Ref. 10 unless otherwise noted.
[e] Ref. 11.
[f] Ref. 12.
[g] Ref. 13.
[h] Ref. 14.
[i] Ref. 15.
[j] Ref. 16.
[k] Ref. 17.
[l] Ref. 18.
[m] Ref. 19
[n] Ref. 20.
[p] Ref. 21

TABLE II. Excitation energies and oscillator strengths of the transition $(2s^2)^1S_0 \rightarrow (2s2p)^3P_1^\circ$ for Be-like ions. Numbers in parentheses represent powers of 10.

Ion	$\omega_{\rm MCDF}$[a]	$\omega_{\rm RRPA}$[b]	$\omega_{\rm MCRRPA}$[c]	$\omega_{\rm exp}$[d] (au)	$f_{\rm MCDF}$[a]	$f_{\rm RRPA}$[b]	$f_{\rm MCRRPA}$[c]
Be	0.105		0.101	0.10015[e]	1.14 (-9)		3.41 (-9)
B^+			0.172	0.17013[e]			3.48 (-8)
C^{2+}	0.246	0.109	0.243	0.23871	1.23 (-7)	4.29 (-8)	1.83 (-7)
N^{3+}	0.314		0.312	0.30651	4.46 (-7)		6.17 (-7)
O^{4+}	0.382	0.200	0.381	0.37398	1.23 (-6)	5.55 (-7)	1.63 (-6)
F^{5+}	0.450		0.450	0.44142	2.87 (-6)		3.64 (-6)
Ne^{6+}	0.517	0.298	0.519	0.50902	5.89 (-6)	3.04 (-6)	7.27 (-6)
Mg^{8+}	0.653	0.396	0.657	0.64532	1.92 (-5)	1.07 (-5)	2.28 (-5)
Si^{10+}	0.792	0.498	0.797	0.78433	4.99 (-5)	2.91 (-5)	5.75 (-5)
S^{12+}	0.935	0.605	0.941	0.92710	1.11 (-4)	6.71 (-5)	1.25 (-4)
Ar^{14+}	1.08	0.717	1.09	1.0747	2.18 (-4)	1.35 (-4)	2.43 (-4)
Ca^{16+}	1.24	0.842	1.24	1.2280	3.94 (-4)	2.55 (-4)	4.32 (-4)
Ti^{18+}	1.39	0.974	1.40	1.3877	6.59 (-4)	4.40 (-4)	7.15 (-4)
Cr^{20+}	1.56		1.57	1.5543	1.03 (-3)		1.11 (-3)
Fe^{22+}	1.73	1.27	1.74	1.7275	1.53 (-3)	1.08 (-3)	1.63 (-3)
Ni^{24+}	1.91	1.43	1.92	1.9066	2.14 (-3)	1.55 (-3)	2.26 (-3)

[a] Ref. 9

[b] Ref. 5

[c] Present calculations.

[d] Cited in Ref. 10 unless otherwise noted.

[e] Ref. 11.

MCRRPA excitation energies give the best agreement with experiment in the low-Z region, where the electron-electron correlations are most important. The errors in RRPA and MCRRPA excitation energies, as determined by comparison with precise experimental measurements, are plotted against nuclear charges in Fig. 1. One sees that the substantial errors in RRPA calculations are dramatically reduced in the corresponding MCRRPA calculations. The remaining small discrepancy between the MCRRPA results and experiment is probably due to the relaxation and further correlation effects which were omitted in the present calculation. The MCRRPA $^1P_1$ oscillator strengths agree very well with available experimental values. For neutral Be, the better agreement of the RRPA oscillator strength with experiment are fortuitous; on the other hand, further correlations would reduce the MCRRPA value. The $^3P_1$ oscillator strengths are consistent with MCDF values, resolving the large discrepancy between RRPA and MCDF calculations. The present method offers the promise of obtaining precise information on discrete transitions for various highly charged systems where both relativistic and correlation effects play important roles. This method may be readily extended to

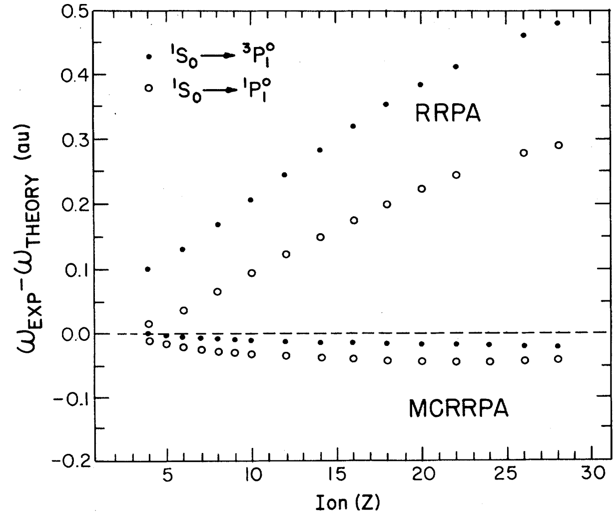

FIG. 1. Comparison of RRPA and MCRRPA excitation energies with experiment.

study photoionization spectra or to calculate properties of atomic ground states such as susceptibilities and shielding factors. Work on such extensions is already in progress.

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