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Magnetic dipole transitions of Pb-like ions from the multiconfiguration relativistic random-phase approximation

Hsiang-Shun Chou and Keh-Ning Huang
Institute of Atomic and Molecular Sciences, Academia Sinica, P. O. Box 23-166, Taipei, Taiwan 10764, Republic of China and Department of Physics, National Taiwan University, Taipei, Taiwan 10764, Republic of China

Walter R. Johnson
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
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The multiconfiguration relativistic random-phase-approximation theory is applied to magnetic dipole transitions in atoms. Excitation energies and oscillator strengths from the ground level $^3P_0$ to the excited level $^3P_1$ of Pb-like ions are calculated as prototypal examples. The first $^3P_1$ level for the neutral Pb atom, which is missing in the relativistic random-phase approximation, appears naturally in this theory, which accounts for two-particle–two-hole correlations.

A complete treatment of electron-electron correlations poses a formidable obstacle in high-precision theoretical calculations of excitation energies and transition rates in atoms. In recent years, the relativistic random-phase-approximation theory (RRPA) [1] and multiconfiguration Dirac-Fock (MCDF) calculations [2,3] have played two of the major roles in resolving 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 equation-of-motion approach [4], 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 theory (MCRRPA) [5]. In essence, it has certain features of the MCDF, while preserving all of the advantages, especially, the gauge invariance, of the RRPA. Applications of the MCRRPA to the resonance transitions of Be-, Mg-, and Zn-like ions [6,7] and to photoionization of Be, Mg, Zn, and Sr atoms [8–12] have been carried out and are in excellent agreement with experiment. In this paper we apply the MCRRPA to magnetic dipole transitions in Pb-like ions. The transitions are of great importance in the investigation of parity-nonconserving effects in atoms [13].

The MCRRPA theory is based on an approximate relativistic Hamiltonian

$$H(t)=\mathcal{H}+V(t)\,, \tag{1}$$

where

$$\mathcal{H}=\sum_{n=1}^{N} h_n+\sum_{\substack{n<m\\ n=1}}^{N} v_{nm}\,. \tag{2}$$

Here h_n is a single-electron Dirac Hamiltonian, and v_{nm}

TABLE I. MCRRPA excitation energies ω and oscillator strengths f for the transition $(6p^2)^3P_0 \rightarrow (6p^2)^3P_1$ in Pb-like ions. Numbers in square brackets indicate powers of ten: $x[y]=x\times 10^y$.

	ω (cm^{-1})		f	
Ions	MCRRPA	Expt.[a]	MCRRPA	Other theory[b]
Pb	7430	7819	5.152[−7]	5.152[−7]
Bi^+	12915	13324	8.669[−7]	
Po^{2+}	19107		1.245[−6]	
At^{3+}	26059		1.655[−6]	
Rn^{4+}	33796		2.100[−6]	
Fr^{5+}	42350		2.581[−6]	
Ra^{6+}	51762		3.100[−6]	
Ac^{7+}	62068		3.660[−6]	
Th^{8+}	73315		4.262[−6]	
Pa^{9+}	85552		4.909[−6]	
U^{10+}	98828		5.602[−6]	
Np^{11+}	113203		6.343[−6]	
Pu^{12+}	128730		7.134[−6]	
Am^{13+}	145482		7.978[−6]	
Cm^{14+}	163503		8.864[−6]	
Bk^{15+}	182844		9.717[−6]	
Cf^{16+}	203389		9.434[−6]	

[a]Reference 15.
[b]Reference 16.

are mutual Coulomb interactions between electrons,

$$v_{nm} = \frac{e^2}{r_{nm}} . \tag{3}$$

In Eq. (1), $V(t)$ is an external potential which induces transitions between atomic states,

$$V(t) = v_+ e^{-i\omega t} + v_- e^{i\omega t} , \tag{4}$$

with

$$v_\pm = \sum_{n=1}^{N} v_{n\pm} . \tag{5}$$

The Breit interaction is not considered here but may be easily included in the calculation if required.

Our point of departure is the time-dependent variational principle [14]. We describe the N-electron system as a superposition of configuration wave functions with time-dependent weights. Since the external perturbation may have components with nonvanishing angular momentum and with odd parity, the atomic wave function contains terms of mixed angular momentum and parity. Applying the variational principle we derive time-dependent multiconfiguration Dirac-Fock equations describing the response of the atom to the external field. Terms independent of the external field lead to the usual MCDF description of an atomic state. Those terms proportional to the external field lead to equations describing the linear response of the atomic state to the external field; in the sequel we refer to these linear response equations as the MCRRPA equations. If we start from a single-configuration reference state, the MCRRPA equations reduce to the usual RRPA equations. The MCRRPA equations may alternatively be derived from an equation-of-motion point of view [4]. In the MCRRPA formulation, the reference state of Pb-like ions is given by a multiconfiguration wave function of the form

$$\Psi = C_1 (6p_{1/2})^2 + C_2 (6p_{3/2})^2 , \tag{6}$$

where the symbol $(6l_j)^2$ designates a Slater determinant constructed from the $(6l_j)$ valence orbitals and twenty-two core orbitals. The parameters C_a $(a=1,2)$ in Eq. (6) are configuration weight coefficients. The core and valence orbitals and the configuration weights are determined by solving the MCDF equations numerically. 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 $6p_{1/2}$ or $6p_{3/2}$ ionic cores. These two-particle–two-hole final state correlations were omitted in previous RRPA studies. In fact, for the neutral Pb atom, the $(6p^2)^3P_1$ state is missing in the RRPA spectrum. Excitation energies and oscillator strengths for the transition $(6p^2)^3P_0 \rightarrow (6p^2)^3P_1$ in Pb-like ions are given in Table I. The excitation energies are in excellent agreement with available experimental results [15], and the oscillator strength is also consistent with the other theoretical result [16].

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