Relativistic many-body perturbation-theory calculations of transition rates for copperlike, silverlike, and goldlike ions

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We perform relativistic many-body perturbation theory calculations through third order to study amplitudes of the principal transitions in copperlike, silverlike, and goldlike ions. For low ionicities, semiempirical corrections are given for the omitted fourth- and higher-order terms. Comparisons with experiment are made. [S1050-2947(97)03809-2]

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In this paper, we perform third-order relativistic many-body perturbation theory (MBPT) calculations to obtain transition amplitudes for the principal transitions, $ns_{1/2}\rightarrow np_{1/2}$ and $ns_{1/2}\rightarrow np_{3/2}$, in Cu-like ($n=4$), Ag-like ($n=5$), and Au-like ($n=6$) ions. The spectra of these ions have aroused considerable interest in recent years. Both theoretical [1–4] and experimental [5–25] studies have been carried out. We note that these ions have electronic structures similar to the alkali-metal atoms, and that relativistic MBPT calculations have been applied with success to study transition rates for Li-like ions [26], Na-like ions [26], and for neutral alkali-metal atoms [26].

The MBPT formulas for energies and transition amplitudes in atoms with one valence electron were presented in Ref. [27]. The first-order MBPT amplitudes are identical to amplitudes obtained from Dirac-Hartree-Fock (DHF) calculations. The second-order MBPT calculations lead to the random-phase approximation (RPA) corrections to the DHF transition amplitudes. Iteration of the RPA equations yields the full RPA amplitudes. The third-order MBPT contributions to transition amplitudes include the third-order RPA corrections, the third-order Brueckner-orbital (BO) corrections, the structural radiation (SR) corrections, and the normalization (Norm.) corrections. For the first three members in the isoelectronic sequences, we scale the BO corrections to give semiempirical corrections for omitted fourth- and higher-order terms.

Contributions to the electric-dipole transition amplitudes for neutral copper are given in Table I. Atomic units (a.u.) are employed in this and all subsequent tables. The first three rows give the first-order transition amplitude, the second-order RPA (RPA2) correction, and the sum of higher-order RPA corrections (RPA3+). The fourth and the fifth rows give the unscaled and scaled BO corrections. The SR and Norm. corrections are tabulated in the sixth and seventh rows, respectively. The last row gives the total transition amplitude, which is the sum of all rows except BO. The first-order transition amplitudes from the present calculations agree well with previous DHF results by Cheng and Kim [1]. It is noticed that the RPA corrections and the BO corrections always reduce the transition amplitudes. A simple physical interpretation can be given. The transition amplitude is the reduced matrix element of the electromagnetic multipole potential. The RPA corrections account for the core-shielding effects in atoms. The external field induces an internal field inside the atom which shields the external field. Therefore, the core-shielding effects lead to an effective potential that weakens the electromagnetic multipole potential and reduces the transition amplitudes. The BO corrections account for the core-polarization effects. The core orbitals are polarized by the valence electrons in the absence of external fields. The core polarization gives rise to an additional attractive potential acting on the valence electrons. The larger effective nuclear charge in turn reduces the transition amplitudes. From the present calculations, we see that the BO corrections affect the heavier elements more strongly than the homologous light elements. In addition, the present calculations show that the percentages of BO corrections to the transition amplitudes decrease with increasing nuclear charge Z. Comparisons with previous MBPT calculations for alkali-metal-like ions [26] indicate that the BO corrections have larger influence on Cu, Ag, and Au than on the alkali-metal atoms.

In Table II, we compare the transition amplitudes from the present calculations with experiment. We present the scaled transition amplitudes for the first three members of the isoelectronic sequences. From the levels $(n-1)d^{10}np^2P^o_{1/2}$ and $(n-1)d^{10}np^2P^o_{3/2}$ the ions Cu ($n=4$), Ag ($n=5$), Au ($n=6$), and Hg^{1+} ($n=6$) can decay to the ground level $(n-1)d^{10}ns^2S_{1/2}$ or to the metastable levels (n

TABLE I. Contributions to the $E1$ transition amplitudes for copper.

	$4s_{1/2}\rightarrow 4p_{1/2}$	$4s_{1/2}\rightarrow 4p_{3/2}$
$Z(1)$	2.8992	4.0944
RPA2	−0.2072	−0.2896
RPA3+	−0.0320	−0.0463
BO	−0.3013	−0.4266
BO (scaled)	−0.3838	−0.5412
SR	0.0193	0.0276
Norm.	−0.0374	−0.0525
Z(tot)	2.2581	3.1923

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TABLE II. Transition amplitudes for the Cu-like ions, Ag-like ions, and Au-like ions.

Cu	$4s_{1/2}\rightarrow 4p_{1/2}$		$4s_{1/2}\rightarrow 4p_{3/2}$		
Z	Present	Expt.	Present	Expt.	Ref.
29	2.2581	2.18(1)	3.1923	3.07(1)	[5]
30	1.8931	1.86(8)	2.6800	2.56(10)	[6]
31	1.6425	1.72(14)	2.3267	2.33(9)	[7]
32	1.4629	1.42(4)	2.0733	2.01(6)	[8]
33	1.3255	1.26(8)	1.8793	1.88(5)	[8]
34	1.2162	1.24(7)	1.7249	1.74(9)	[8]
35	1.1262		1.5978		
36	1.0503	1.07(2)	1.4907	1.50(3)	[9]
37	0.9852		1.3987		
38	0.9284		1.3186		
39	0.8784		1.2480		
40	0.8339		1.1852		
41	0.7939	0.84(5)	1.1289	1.11(4)	[10]
42	0.7579	0.80(3)	1.0780	1.14(4)	[11]
50	0.5577		0.7961		
53	0.5075	0.55(1)	0.7255	0.73(1)	[12]
Ag	$5s_{1/2}\rightarrow 5p_{1/2}$		$5s_{1/2}\rightarrow 5p_{3/2}$		
47	2.2609	2.27(1)	3.1955	3.20(1)	[13]
48	1.9175	1.92(1)	2.7217	2.65(3)	[14]
49	1.6919	1.79(3)	2.4040	2.38(12)	[15]
50	1.5219	1.51(12)	2.1637	2.35(22)	[16]
51	1.3996	1.54(10)	1.9906	2.02(19)	[17]
52	1.3006	1.37(4)	1.8503	1.90(6)	[18]
53	1.2179	1.33(6)	1.7331	1.83(8)	[19]
54	1.1471		1.6328		
55	1.0856		1.5456		
56	1.0314		1.4687		
57	0.9830		1.4002		
58	0.9396		1.3386		
59	0.9002		1.2828		
60	0.8643		1.2319		
Au	$6s_{1/2}\rightarrow 6p_{1/2}$		$6s_{1/2}\rightarrow 6p_{3/2}$		
79	1.8300	1.83(9)	2.5942	2.56(9)	[20]
		1.75(3)		2.45(5)	[21]
80	1.6354	1.67(13)	2.3353		[22]
		1.58(3)		2.22(5)	[23]
81	1.4961		2.1346		
82	1.3795	1.42(6)	1.9680	2.03(8)	[24]
83	1.2924	1.29(7)	1.8434	2.06(5)	[25]
84	1.2187		1.7373		
85	1.1550		1.6455		

$-1)d^9ns^2\,{}^2D_{3/2}$ and $(n-1)d^9ns^2\,{}^2D_{5/2}$. The configurations differ in two orbitals for the latter transitions. Therefore the branching ratio for the decay branch to the ground level is expected to be much greater than that for the decay branch to the metastable levels. In Table II, we neglect the branch to the metastable levels and take the transition rate to be the reciprocal of the lifetime. The comparison of theory and experiment for the Cu-like, Ag-like, and Au-like ions is illustrated in Fig. 1. The experimental results in Fig. 1 are from the first experimental values we tabulated in Table II for each ion. For the $4s_{1/2}\rightarrow 4p_{1/2}$ transition in Cu-like ions, the transition amplitudes from the present calculations are consistent with experimental results except for Cu, Mo^{13+}, and I^{24+}. The MBPT transition amplitude for Cu, before scaling the BO contribution, is 7.4% greater than the experimental value. Inclusion of higher-order corrections by scaling the BO terms reduces the difference. However, a discrepancy of 3.6% still exists. The MBPT transition amplitudes for Mo^{13+} and I^{24+} are less than the experimental values by 5.3% and 7.7%, respectively. The discrepancy is not due to

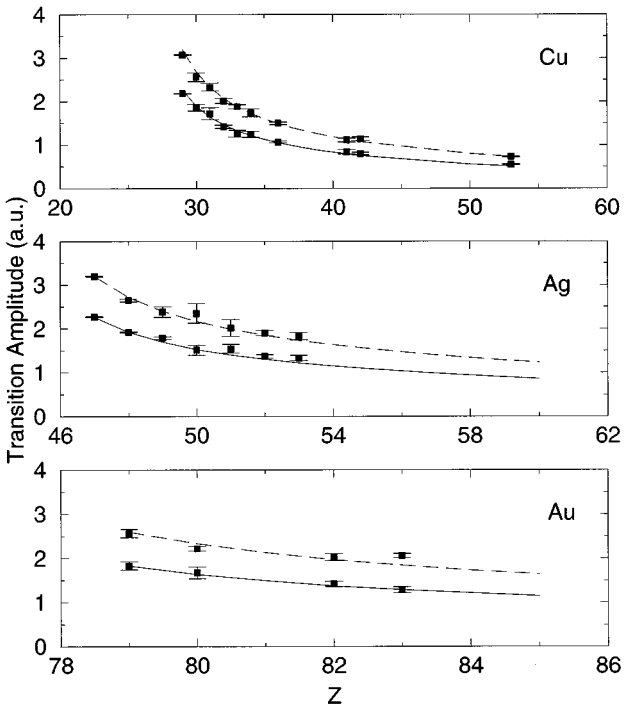

FIG. 1. Transition amplitudes vs Z for $ns_{1/2} \rightarrow np_{1/2}$ (solid line) and $ns_{1/2} \rightarrow np_{3/2}$ (dashed line) transitions in the Cu-like ions ($n=4$), Ag-like ions ($n=5$), and Au-like ions ($n=6$). The experimental values are denoted by squares.

our neglect of higher-order terms, as the higher-order corrections decrease rapidly with increasing Z. We believe that the experiments overestimate the transition amplitude. For the $4s_{1/2} \rightarrow 4p_{3/2}$ transition in Cu-like ions, the MBPT transition amplitudes agree well with experiment except for Cu, Zn^{1+}, and Mo^{13+}. The unscaled MBPT transition amplitude for Cu is greater than the experimental value by 7.7%. Scaling the BO terms removes half of the discrepancy. The MBPT amplitude for Zn^{1+} differs from the experimental result by 1.2 standard deviations. For Mo^{13+}, the MBPT calculations yield transition amplitude smaller than experimental results by 5.4%. Again, the neglect of higher-order terms is not responsible for the discrepancy.

The first-order amplitude for Ag-like ions from the present calculations are consistent with the DHF results by Cheng and Kim [2]. For the $5s_{1/2} \rightarrow 5p_{1/2}$ transition in the Ag-like ions, the MBPT amplitudes agree with experiment for Ag, Cd^{1+}, and Sn^{3+}, but disagree with experiment for In^{2+}, Sb^{4+}, Te^{5+}, and I^{6+}. The unscaled MBPT amplitudes for Ag differ from the experimental results by 0.7%. The discrepancy is resolved by scaling the Brueckner orbitals. The discrepancy between theory and experiment for In^{2+}, Sb^{4+}, Te^{5+}, and I^{6+} is unexpected, as the higher-order corrections decrease with increasing Z. Inspection of Fig. 1 helps us gain insight into the discrepancy. The theoretical amplitudes decrease smoothly with increasing Z, while irregularities are observed in the experimental results for In^{2+}, Sb^{4+}, Te^{5+}, and I^{6+}. The precise agreement between theory and experiment for Ag as well as the smoothness of the theoretical curve suggest that the theoretical values are reliable. The MBPT amplitudes for the $5s_{1/2} \rightarrow 5p_{3/2}$ transition in Ag-like ions are in satisfactory agreement with experiment except for Cd^{1+} and I^{6+}. Scaling the BO terms brings the MBPT transition amplitudes for Ag into excellent agreement with experiment but increases the difference between theory and experiment for Cd^{1+}. This suggests that the experimental result for Cd^{1+} underestimates the transition amplitude by about 3%. Again, the difference between theory and experiment for I^{6+} is unexpected. Apparently, the experiment overestimates the amplitude by about 6%.

For the Au-like ions, the MBPT transition amplitudes are within experimental uncertainties except for the $6s_{1/2} \rightarrow 6p_{3/2}$ transition in Hg^{1+} and Bi^{4+}. The theoretical transition amplitudes for Au differ by about 5% with the recent laser-induced fluorescence results [21], but are in excellent agreement with the measurement of Penkin and Slavenas [20] obtained by the hook method. It is noticed that scaling the BO corrections increases the differences between the MBPT values and the laser-induced fluorescence results for Au. Thus the present calculations are in favor of the measurement by the hook method. The same reasoning suggests that the experimental result in Ref. [23] underestimates the transition amplitude for Hg^{1+} by about 5%. In Fig. 1, an irregularity is observed in the experimental value for the $6s_{1/2} \rightarrow 6p_{3/2}$ transition in Bi^{4+}. In this case, we believe that the experiment overestimates the transition amplitude by about 10%.

In summary, we perform MBPT calculations to study the transition amplitudes for the principal transitions in Cu-like ions, Ag-like ions, and Au-like ions. The amplitudes for Cu disagree with experiment by about 4%, but agree well with experiment for Ag and Au. The accuracy of the present calculations is expected to increase at higher Z because of the rapid rate of convergence of MBPT. The discrepancies between theory and experiment for certain ions is a matter of concern. Further theoretical and experimental investigations are certainly needed to understand fully, and remove, the remaining discrepancies.

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