COMMENTS

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Comment on "Relativistic excitation energies and oscillator strengths for the $6s^2\,{}^1S_0 \rightarrow 6s6p\,{}^1P_1, {}^3P_1$ transitions in Hg-like ions"

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In a recent paper, Chou and Huang [Phys. Rev. A **45**, 1403 (1992)] employ the multiconfiguration relativistic random-phase approximation (MCRRPA) in an attempt to remove discrepancies between experimental and theoretical oscillator strengths for the $6s^2\,{}^1S_0 \rightarrow 6s6p\,{}^1P_1, {}^3P_1$ transitions in mercurylike ions. Their MCRRPA results are found to be still in poor agreement with beam-foil measurements, and the authors suggest that a significant part of this disagreement may arise from "an improper account of the cascade effects in beam-foil lifetime measurements." However, Chou and Huang have overlooked several, more recent beam-foil measurements in which "proper" account has been taken of cascading by the application of an arbitrarily-normalized-decay-curve technique with which their MCRRPA results are still in poor agreement. We conclude that this disagreement is mainly due to the omission by Chou and Huang from their calculation of core-polarization effects. In fact, calculations in which such effects are included show quite satisfactory agreement with the beam-foil measurements in which an account of cascade effects has been taken.

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Chou and Huang have recently employed the multiconfiguration relativistic random-phase approximation (MCRRPA) to calculate f values for the $6s^2\,{}^1S_0 \rightarrow 6s6p\,{}^1P_1, {}^3P_1$ transitions in Hg-like ions [1]. The aim of the work was to provide a reliable atomic calculation, which would remove the discrepancy between previous calculations [2,3] and experimental results [4–8]. The only experimental values quoted are for the singlet-triplet transition in Hg I [4–7] and from a beam-foil experiment for the singlet-singlet transitions in Tl II, Pb III, and Bi IV[8]. The f values calculated by Chou and Huang are actually in significantly worse agreement with experiment than were the results of previous calculations. The ratio of the MCRRPA and experimental f values for the singlet-singlet transition increases from about 2 in Tl II to about 3 in Bi IV. The authors suggest that a substantial part of this disagreement may arise from "an improper account of the cascade effects in beam-foil lifetime measurements." In fact, recent experiments [9–12], in which "proper" account is taken of cascade effects, have shown that, while correcting for cascading in the beam-foil measurements does tend to increase the measured oscillator strength, the change is nowhere near enough to account for the discrepancy with the Chou and Huang MCRRPA calculations. On the other hand, the beam-foil measurements incorporating cascade correction do give results in fair agreement with the calculations of Migdalek and Baylis [2]. We will now give some further details to support these statements.

It is certainly true that cascade repopulation is a major source of potential error in beam-foil lifetime measurements. The problem has been understood for over 20 years, during which time several methods have been suggested to overcome the problem. The most successful of these, the so-called ANDC method, was first suggested by Curtis and his colleagues [13], although use of the technique has only become routine more recently with the advent of various computer programs [14–16]. (The acronym ANDC signifies that the method relies on the simultaneous analysis of arbitrarily normalized decay curves for both a transition from the level for which the lifetime is required, and for all the transitions that significantly and directly repopulate that level, according to the set of differential equations that relate the population of the various levels involved in the cascade scheme.) The method has been demonstrated to be very effective in spectra involving one [17] or two [18] active electrons, and useful for three-electron spectra [19]. Since Hg-like

TABLE I. Oscillator strengths for Hg-like ions.

		Experiment		Theory			
				Ref. [1][c]	Ref. [2][d]		
Transition	Ion	Beam foil[a]	Beam foil[b]		A	B	C
$^1S_0$-$^1P_1$	Hg I		1.14±0.05		1.526	1.257	1.176
	Pb III	1.01±0.20	1.30±0.07	2.455	2.498	1.640	1.419
	Bi IV	0.88±0.15	1.41±0.08	2.515	2.576	1.694	1.387
$^1S_0$-$^3P_1$	Hg I		0.029±0.006[e]	0.0160	0.0113	0.0198	0.0254
			0.073±0.005	0.0615	0.0489	0.0544	0.0644
			0.098±0.007	0.0867	0.0714	0.0725	0.0870

[a]Results not allowing for cascade effects [8].
[b]Results incorporating ANDC analyses [9–12].
[c]Multiconfiguration relativistic random-phase approximation.
[d]Multiconfiguration Dirac-Fock calculation (see discussion in text).
[e]In agreement with the more precise value (0.0241±0.002) obtained by King and Adams [4] using electron-photon delayed coincidences.

ions give spectra in which two electrons are active, we can be reasonably confident of the f values derived from ANDC analyses of beam-foil decay curves for these ions, provided that the ANDC method is rigorously applied.

In Table I we show the f values for the three Hg-like ions for which beam-foil measurements incorporating ANDC analyses to correct for cascade effects have been published, and we compare these results with those obtained by Chou and Huang [1] and by Migdalek and Baylis [2]. It is clear that the most recent beam-foil measurement for the resonance transition in Pb III and Bi IV give f values that are significantly larger than were obtained from the early measurements [8]. However, the disagreement with the MRRPA results of Chou and Huang is still more than 70%. On the other hand, the relativistic Dirac-Fock calculations including core-polarization effects [2] are in much closer agreement with experiment. We now discuss this in more detail.

Although the MCRRPA method has the capacity to include valence-core correlation, the implementation by Chou and Huang [1] neglected virtual excitations of the core electrons and thereby excluded all core-polarization effects. The importance of such effects can be seen by a comparison of columns A and C of the theory by Migdalek and Baylis [2]: both columns are from multiconfiguration Dirac-Fock calculations, but column A is without core polarization, whereas columns B and C include core-polarization effects in both the wave functions and in the dipole-moment operator by means of a model potential that represents the polarization of the closed-shell ion core by the two valence electrons. In column C, the core-size parameter r_0 of the model is adjusted by fitting the theoretical ionization energies to experiment, whereas in column B, r_0 is simply set equal to the mean radius of the $5d_{5/2}$ orbital. We view the column-C results as most reliable, since the adjustment can compensate for inaccuracies in the core polarizability and for the effects of intracore correlation. The results of Chou and Huang are in reasonable agreement with the values in column A, for which core polarization has been neglected.

As Chou and Huang state, one expects the core-polarization effects to become less important as the charge of the ion increases. However, it is evident from Table I that for the heavy ions of the Hg isoelectronic sequence, such correlation effects are still large even for the triply charged ion (Bi IV). It is interesting to note that the correlation effects are different for the triplet and singlet states. As discussed in Ref. [20], Sec. 3.2.2, the dielectric term greatly strengthens the polarization effects in the singlet states and weakens them in the triplet states. (Unfortunately, some papers on core polarization have ignored the effects of this important two-electron term.) Physically, the two valence electrons stay closer together in the singlet state and further apart in the triplet state, so that their combined effect in the singlet (triplet) state is greater (less) than for two independent electrons. As a result, the core-valence correlation lowers the $6s6p\ ^1P$ state almost as much as it does the ground state, whereas the energy shift in the triplet state is much less. Thus core polarization affects the excitation energy of the intercombination line (^1S-^3P) more strongly than the resonance line (^1S-^1P), but it affects the oscillator strength more for the resonance transition.

We conclude that (i) the valence-core correlation is important for the excitation energies of the intercombination lines and for the oscillator strengths of the resonance transitions, at least through Bi IV in the mercury isoelectronic sequence, and (ii) there is already satisfactory agreement between those calculations which adequately include core-polarization effects as well as intravalance correlation and those beam-foil results which account for cascades through rigorous application of the ANDC procedure.

[1] H.-S. Chou and K. N. Huang, Phys. Rev. A **45**, 1403 (1992).
[2] J. Migdalek and W. E. Baylis, J. Phys. B **18**, 1533 (1985).
[3] J. Migdalek and A. Bojara, J. Phys. B **21**, 2221 (1988).
[4] G. C. King and A. Adams, J. Phys. B **7**, 1712 (1974).
[5] J. A. Halstead and R. R. Reeves, J. Quant. Spectrosc. Radiat. Transfer **28**, 289 (1982).
[6] K. A. Mohammed, J. Quant. Spectrosc. Radiat. Transfer **30**, 225 (1983).
[7] J. S. Deech and W. E. Baylis, Can. J. Phys. **40**, 90 (1970).
[8] T. Andersen, A. K. Nielsen and G. Sørensen, Phys. Scr. **6**, 122 (1972).
[9] E. H. Pinnington, W. Ansbacher, J. A. Kernahan, T. Ahmad, and Z. -Q. Ge, Can. J. Phys. **66**, 960 (1988).
[10] E. H. Pinnington, W. Ansbacher, J. A. Kernahan, Z. -Q. Ge, and A. S. Ismamdar, Nucl. Instrum. Methods Phys. Res. B **31**, 206 (1988).
[11] W. Ansbacher, E. H. Pinnington, and J. A. Kernahan, Can. J. Phys. **66**, 402 (1988).
[12] W. Ansbacher, E. H. Pinnington, A. Tauheed, and J. A. Kernahan, Phys. Scr. **40**, 454 (1989).
[13] L. J. Curtis, H. G. Berry, and J. Bromander, Phys. Lett. **34A**, 169 (1971).
[14] E. H. Pinnington, R. N. Gosselin, J. A. O'Neill, J. A. Kernahan, K. E. Donnelly, and R. L. Brooks, Phys. Scr. **20**, 151 (1979).
[15] L. Engström, Nucl. Instrum. Methods **202**, 369 (1982).
[16] W. Ansbacher, E. H. Pinnington, J. A. Kernahan, and R. N. Gosselin, Can. J. Phys. **64**, 1365 (1986).
[17] E. H. Pinnington, J. L. Bahr, D. J. G. Irwin, and J. A. Kernahan, Nucl. Instrum. Methods **202**, 67 (1982).
[18] E. H. Pinnington, Nucl. Instrum. Methods Phys. Res. B **9**, 549 (1985).
[19] E. H. Pinnington, W. Ansbacher, A. Tauheed, E. Träbert, P. H. Heckmann, G. Möller, and J. H. Blanke, Z. Phys. D **17**, 5 (1990).
[20] J. Migdalek and W. E. Baylis, J. Phys. B **19**, 1 (1986).