Relaxed relativistic random-phase-approximation calculations of photoionization amplitudes and phases for the 4d subshell of xenon

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Calculations of photoionization amplitudes and phases for the $4d$ subshell of xenon are carried out in the relativistic random-phase approximation for photon energies ranging from 80 to 140 eV. These calculations account for correlations within and between the $4d$, $5s$, and $5p$ subshells as well as relaxation of the $4d$ subshell. The resulting theoretical amplitudes are compared with a recent experimental measurement of photoionization amplitudes and phases for the $4d_{5/2}$ subshell at 94.5 eV.

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Recently, Kämmerling and Schmidt [1] reported a *complete* experimental measurement of the amplitudes and phases for photoionization of the $4d_{5/2}$ subshell of xenon at photon energy 94.5 eV. To determine these quantities, the angular correlation between the photoelectron and the $N_5O_{23}O_{23}$ $^1S_0$ Auger electron emitted in the decay of the residual Xe^+ ion was measured. This measurement was combined with experimental values of the $4d_{5/2}$ partial cross section $\sigma(4d_{5/2})$, the photoelectron angular distribution asymmetry parameter $\beta(4d_{5/2})$, and the noncoincident alignment parameter $\mathcal{A}_{20}(4d_{5/2})$ to determine the three amplitudes and two relative phases governing photoionization of the $4d_{5/2}$ subshell. In this report, we present results of a relativistic random-phase-approximation (RRPA) [2, 3] calculation (including corrections for core relaxation) of the amplitudes and phases for photoionization of the $4d_{3/2}$ and $4d_{5/2}$ subshells of xenon in the energy range 80–140 eV, and we compare the resulting theoretical amplitudes at 94.5 eV with the experimental values from [1].

Although the random-phase approximation with exchange (RPAE) [4] accounts for inter- and intrashell correlation corrections in atomic photoionization, it is necessary to go beyond the random-phase approximation and include corrections for relaxation of the ionic core to understand low-energy photoionization of the $4d$ subshells of xenon quantitatively [5, 6]. Nonrelativistic RPAE calculations of $4d$ photoionization cross sections, including core relaxation, have been reported previously by Amusia and co-workers [6–8], and the corresponding relaxed RRPA calculations have been given previously by Kutzner, Radojević, and Kelly [9]. These previous reports, however, do not give photoionization amplitudes and phases, and therefore cannot be directly compared with experiments such as those of Ref. [1].

Previously, we have carried out extensive RRPA calculations of cross sections, angular-distribution asymmetry parameters and spin-polarization parameters for the noble gases argon, krypton, and xenon [10]. For the xenon $4d$ subshell, these calculations covered the energy range 80–160 eV and included correlations between the following 13 coupled channels:

$$4d_{3/2} \to p_{1/2}, p_{3/2}, f_{5/2},$$
$$4d_{5/2} \to p_{3/2}, f_{5/2}, f_{7/2},$$
$$5p_{1/2} \to s_{1/2}, d_{3/2},$$
$$5p_{3/2} \to s_{1/2}, d_{3/2}, d_{5/2},$$
$$5s_{1/2} \to p_{1/2}, p_{3/2}.$$

In the present work, we repeat the RRPA calculation reported in [10] using relaxed orbitals instead of frozen-core Dirac-Fock (DF) orbitals, and replacing theoretical $4d$ thresholds (which are given by the DF eigenvalues in the RRPA) by Δ_{SCF} thresholds. (SCF denotes self-consistent field.) These Δ_{SCF} thresholds are obtained by subtracting the DF total energies of neutral Xe and Xe^+ with a hole in the $4d$ subshells. We find that length- and velocity-form results are in good agreement if *both* of the corrections described above are made, in accordance with the findings of Refs. [6, 9].

The present calculation is similar to the relaxed RRPA calculation reported in [9], except that we ignore excitations from the $4s$, $4p$, and $3d$ subshells as well as wave-function overlap factors. The omitted excitation channels have very little effect in the energy range considered here. All core orbitals in the present work are calculated using Desclaux's multiconfiguration DF code [11] for the Xe^+ ion with a hole in the $4d_{5/2}$ subshell. Replacing the hole in the $4d_{5/2}$ subshell with one in the $4d_{3/2}$ subshell has negligible effect on the final results. Regardless of which set of core orbitals is used, excited orbitals generated in our RRPA code are always orthogonal to the occupied ones.

In Fig. 1, we show the amplitudes and relative phases for the three $4d_{5/2}$ excitation channels, together with the experimental amplitudes at 94.5 eV reported in [1]. We

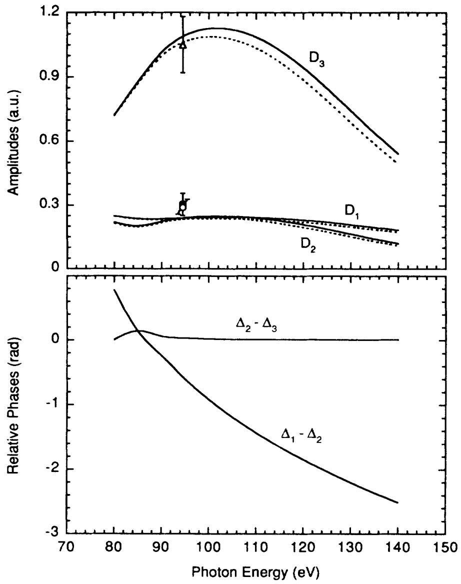

FIG. 1. Amplitudes D_i (upper panel) and relative phases $\Delta_i - \Delta_j$ (lower panel) for photoionization of the $4d_{5/2}$ subshell, where $i, j = 1, 2$, and 3 refer to the $p_{3/2}$, $f_{5/2}$, and $f_{7/2}$ channels, respectively. Experimental data from [1]: $D_1 = \bullet$, $D_2 = \circ$, $D_3 = \triangle$.

use the convention given in [2] to normalize our amplitudes. As can be seen from the figure, the length- and velocity-form amplitudes differ by only a few percent and there is essentially no difference between the relative phases calculated using the two forms for the dipole operator. Of course, differences between length- and velocity-form amplitudes and phases in frozen-core RRPA calculations are also negligible. At low energies, the relaxed

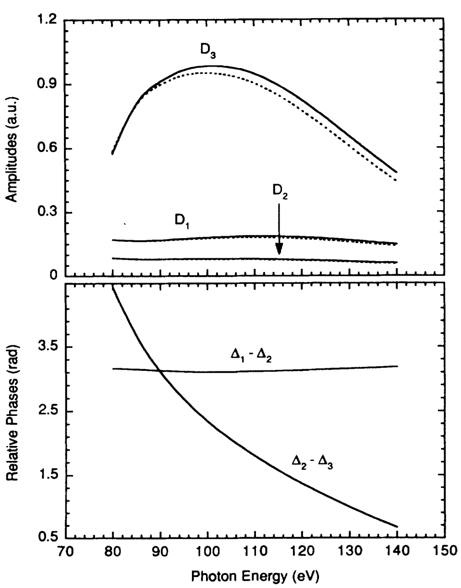

FIG. 2. Amplitudes D_i (upper panel) and relative phases $\Delta_i - \Delta_j$ (lower panel) for photoionization of the $4d_{3/2}$ subshell, where $i, j = 1, 2$, and 3 refer to the $p_{1/2}$, $p_{3/2}$, and $f_{5/2}$ channels, respectively.

TABLE I. Comparison of theoretical and experimental [1] photoionization amplitudes, D_i, and relative phases, $\Delta_i - \Delta_j$, for the $4d_{5/2}$ subshell of xenon at 94.5 eV, where i and $j = 1, 2, 3$ refer to the channels $4d_{5/2} \to p_{3/2}$, $4d_{5/2} \to f_{5/2}$, and $4d_{5/2} \to f_{7/2}$, respectively.

	Relaxed RRPA	Experiment
D_1	0.239 a.u.	0.306 ± 0.049 a.u.
D_2	0.239 a.u.	0.290 ± 0.038 a.u.
D_3	1.089 a.u.	1.05 ± 0.13 a.u.
$\Delta_1 - \Delta_2$	-0.570 rad	$\pm 0.10 \pm 0.10$ rad
$\Delta_2 - \Delta_3$	0.032 rad	$\pm 1.35 \pm 0.10$ rad

RRPA amplitudes in Fig. 1 are smaller than corresponding amplitudes from our previous frozen-core RRPA calculations [10], however, the relative phases from the present relaxed RRPA calculations agree well with those from the frozen-core RRPA calculations, except for small deviations near the thresholds. Since the relative phases are insensitive to relaxation, the angular-distribution asymmetry parameter β and the spin-polarization parameters δ, ξ, η, and ζ from the present relaxed RRPA calculation are very close to the frozen-core values given in [10]. The amplitudes and relative phases for photoionization of the $4d_{3/2}$ subshell are shown in Fig. 2.

The data at 94.5 eV shown in Fig. 1 and the corresponding experimental phase shift differences are also presented in Table I. Whereas the experimental amplitudes are seen to agree well with the theoretical ones, the experimental and theoretical phase differences are seen to be in serious disagreement. In particular, the phase shift difference between the two $4d_{5/2} \to f_{5/2}$, $f_{7/2}$ channels, $\Delta_2 - \Delta_3$ (which should vanish nonrelativistically) is found to be near 0 theoretically, but greater than 1 experimentally. The experimental phase shifts have been reanalyzed recently in light of the theoretical values, and larger error limits have been assigned to the measurements [12].

In Fig. 3 we present theoretical cross sections for the

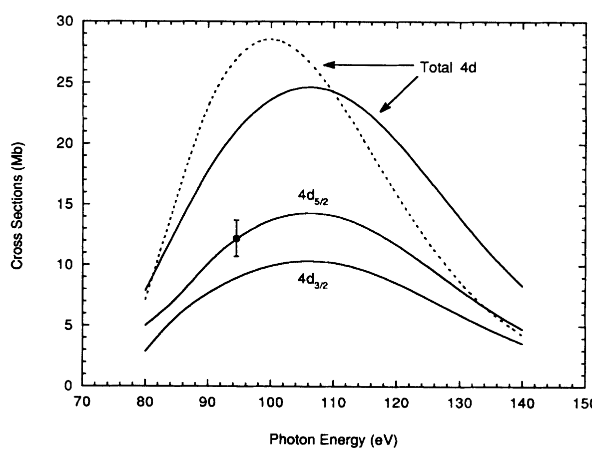

FIG. 3. Photoionization cross sections for the $4d_{3/2}$ and $4d_{5/2}$ subshells of xenon and the total $4d$ cross section as functions of photon energy. ——, relaxed RRPA values; – – –, frozen-core RRPA results. Experimental $4d_{5/2}$ cross section data from [1].

$4d_{3/2}$ and $4d_{5/2}$ subshells, together with the total $4d$ cross section. For comparison purposes, we also present the frozen-core RRPA results for the total $4d$ cross section. As can be seen from the figure, the cross section peak is reduced in the relaxed RRPA calculation and shifted to higher energy. Detailed comparisons of the relaxed RRPA cross section with experiment [13, 14] are given in [9] and will not be repeated here. It suffices to mention that the experimental cross sections agree quite precisely with the relaxed RRPA values below 100 eV, but agree somewhat better with frozen-core RRPA results above 120 eV. The relaxed RRPA values for the angular-distribution asymmetry parameter and the spin-polarization parameters are in good agreement with the frozen-core RRPA values presented in [10] and therefore will not be repeated here.

It should be noted that our theoretical value for the $4d_{5/2}$ cross section $\sigma(4d_{5/2}) = 12.1$ Mb at 94.5 eV agrees well with the experimental value $\sigma(4d_{5/2}) = 12.2(1.5)$ Mb used as input data in [1]. The theoretical value $\beta(4d_{5/2}) = 0.26$ at 94.5 eV from the present calculation is in precise agreement with the value determined in our previous frozen-core RRPA calculation [10], reflecting the fact that the relative phases in relaxed RRPA calculations are very close to those obtained in frozen-core RRPA calculations. This theoretical value can be compared to the experimental value $\beta(4d_{5/2}) = 0.35(1)$ used in [1]. Additionally, we obtain the value $\mathcal{A}_{20}(4d_{5/2}) = -0.232$ for the noncoincidence alignment parameter which can be compared with the value of $\mathcal{A}_{20}(4d_{5/2}) = -0.230(15)$ also used in [1].

In summary, relaxed RRPA calculations provide a quantitative description of low-energy photoionization. Moreover, the amplitudes and phases from such calculations can provide useful guides for *complete* experiments such as those reported in [1].

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[1] B. Kämmerling and V. Schmidt, Phys. Rev. Lett. **67**, 1848 (1991).
[2] W.R. Johnson and C.D. Lin, Phys. Rev. A **20**, 964 (1979).
[3] W.R. Johnson and K.T. Cheng, Phys. Rev. A **20**, 978 (1979).
[4] M.Ya. Amusia and N.A. Cherepkov, *Case Studies in Atomic Physics* (North-Holland, Amsterdam, 1975), Vol. 5, p. 47.
[5] G. Wendin, J. Phys. B **1**, 1080 (1971); Phys. Lett. **51A**, 291 (1975).
[6] M.Ya. Amusia, V.K. Ivanov, and L.V. Chernysheva, Phys. Lett. **59A**, 191 (1976).
[7] M.Ya. Amusia, V.K. Ivanov, S.A. Sheinerman, S.I. Sheftel, and A.F. Ioffe, Zh. Eksp. Teor. Fiz. **78**, 910 (1990) [Sov. Phys. JETP **51**, 458 (1980)].
[8] M.Ya. Amusia, L.V. Chernysheva, G.F. Gribakin, and K.L. Tsemekhman, J. Phys. B **23**, 393 (1990).
[9] M.Kutzner, V. Radojević, and H.P. Kelly, Phys. Rev. A **40**, 5052 (1989).
[10] K.-N. Huang, W.R. Johnson, and K.T. Cheng, At. Data Nucl. Data Tables **26**, 33 (1981).
[11] J.P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).
[12] V. Schmidt (private communication).
[13] B. Kämmerling, H. Kossman, and V. Schmidt, J. Phys. B **22**, 841 (1989).
[14] U. Becker, D. Szostak, H.G. Kerkhoff, M. Kupsch, B. Langer, R. Wehrlitz, A. Yagishita, and T. Hayaishi, Phys. Rev. A **39**, 3902 (1989).