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A. Multielectron Correlation Effects in Collisions

A.1. *Probing Correlations through Spin-Orbit Interaction*

Recently, a new aspect of interchannel coupling has been found [1], known as spin-orbit activated interchannel coupling, stimulated by an experimental study on photoionization of Xe in the vicinity of the 3d threshold. This effect results only through the spin-orbit splitting of inner-shell thresholds. Effects of spin-orbit activated interchannel coupling on nondipole [2] photoelectron angular distribution asymmetry parameters have been discussed, including the spin-polarization of photoelectrons from 3d electrons of Xe, Cs and Ba, concluding that through spin-orbit interaction polarization can be achieved and correlation probed.

A.2. *Dramatic Distortion of the 4d Giant Resonance by the C₆₀ Fullerene Shell*

The recent encapsulation of molecular hydrogen in fullerene C₆₀ using a molecular surgical method and the possibility of preparing a series of C₆₀ fullerenes, encapsulating either small atoms or molecules [3], has prompted this study. The photoionization cross section for the endohedral Xe@C₆₀ atom has been investigated [4,5] within the framework of representing the C₆₀ by a delta-type potential with very interesting results. Results demonstrate that in Xe@C₆₀, the 4d giant resonance is distorted significantly when compared with that of the isolated Xe atom. The reflection of the photoelectron waves by the C₆₀ causes strong oscillations in the photoionization cross section resulting in the replacement of the Xe 4d giant resonance by four prominent peaks. The approximation of C₆₀ by an infinitely thin real potential preserves reasonably well the sum rule for the 4d electrons but modifies the dipole polarizability of the 4d shell.

A.3. *Giant Resonances in Xe⁺, I and I⁺*

We have utilized the recently developed RPAE method [6], which can be used to study the inner-shell electron transition of an open shell atom, to calculate the photoionization cross section of the Xe⁺ 4d - ϵf , so called giant resonance. We first create the ground state of Xe⁺ 4d¹⁰5s²5p⁵(²P) and core wave functions of 4d⁹5s²5p⁵(¹P, ¹D, ¹F, ³P, ³D, ³F) through self-consistent HF calculations. Then radial functions of the continuum electron are obtained by solving the linear HF equations without self-consistency using those core wave functions. The reduced dipole matrix elements for the relevant transitions are evaluated using our previous operator method. After evaluating the Coulomb matrix elements, the RPAE equation was solved and we obtained the ²S, ²P, and ²D partial cross sections. The maximum of the total cross section, 24.4 MB at the photon energy of 96.3 eV from our RPAE calculation agrees very well with the experimental maximum of (27 $\pm$ 3) MB at the photon energy of 95eV.

The 4d giant resonances of I and I⁺ have been calculated using our recently developed RPAE program [6]. The results for I⁺ agree quite well with the recent experimental data. However, for the I atom the RPAE results for the 4d giant resonance yields maxima at 102 eV of

23.8 MB (length) and 19.6 MB (velocity), which are still much higher than the experimental maximum of 6.5 MB at 91 eV

A.4 *Near Threshold Behavior of Angular Anisotropy Parameters in Negative Ions Photo-Detachment*

We have investigated the near threshold behavior of the dipole and nondipole angular anisotropy parameters in atomic photoionization by performing both analytical and numerical calculations. The numerical calculations of the angular asymmetry parameters were performed both in the one-electron Hartree-Fock (HF) approximation and with account of the many-electron correlations within the framework of the Random Phase Approximation with Exchange (RPAE). The results of our calculations are presented for the outer and intermediate subshells of the iodine negative ion I^- and contrasted with those of the neutral neighbor atom Xe. Essential differences in the HF and RPAE near threshold behavior of the angular distribution parameters between the negative ion and the neutral atom are demonstrated[7].

B. Complex Angular Momentum Methods for Regge-Poles Calculation

Recently, the complex angular momentum (CAM) theory for integral cross sections has been introduced and used to demonstrate the oscillations, a general feature of potential scattering, in the integral elastic scattering cross sections for proton impact on atomic hydrogen. The method avoids the details of Stokes' and anti-Stokes' lines, a draw-back of the semi-classical methods. The Padé-Regge approach has been illustrated with several one-particle potential problems [8]. We continue to develop methods that avoid the explicit use of Stokes' and anti-Stokes' lines [9], with the collaboration of Professor Sokolovski of Queen's University of Belfast.

Invitations

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