PHOTOIONIZATION DYNAMICS OF SOME FREE AND CONFINED ATOMIC SYSTEMS

A THESIS

Submitted by

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Dedicated to my family and friends

Declaration by the Research Scholar

This is to certify that the thesis entitled "**Photoionization Dynamics of Some Free and Confined Atomic Systems**", submitted by me to the Indian Institute of Technology Mandi for the award of the degree of Doctorate of Philosophy is a bonafide record of research work carried out by me under the supervision of **Dr. Hari Varma** and **Prof. P. C. Deshmukh**. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of degree or diploma.

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Thesis Certificate

This is to certify that the thesis entitled "**Photoionization Dynamics of Some Free and Confined Atomic Systems**" submitted by **Mr. Ashish Kumar** to the Indian Institute of Technology, Mandi for the award of the degree of Doctor of Philosophy is a bonafide record of research work carried out by him under our supervision. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma. In keeping with the general practice of reporting scientific observation, due acknowledgements have been made wherever the work described is based on the findings of other investigators.

Guide:

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ABSTRACT

The present thesis are reported the photoionization of free and confined atomic systems using the Relativistic Random Phase Approximation (RRPA) and Relativistic Multichannel Quantum Defect theory (RMQDT). The present thesis reports studies for outer shell of high-Z atoms like Radon (Z=86) and Radium (Z=88). The combined effects of interchannel coupling, relativistic interactions and confinement on the photoionization parameters of heavy atoms such as Radon (Rn) and Radium (Ra) have been carried out.

For this thesis work, a study of the outer 4s subshell of the Ca atom in a spherical attractive potential well (SAW) of variable depth is performed to determine the effect of an external potential on dipole (E1) and quadrupole (E2) photoionization processes. As the depth of the potential well increases, dramatic changes are observed in the 4s cross section, as well as in the photoelectron angular distribution. The existence of Cooper minima in the 4s dipole channels give rise to very significant effects of quadrupole interactions, even at extremely low energies, in the vicinity of the E1 Cooper minimum. It is shown that the entrapment of Ca in a spherical attractive well (Ca@SAW) *further* enhances the importance of quadrupole interactions determining the photoionization parameters. The complicated behavior of both dipole and quadrupole Cooper minima, as functions of well depth, is delineated, along with the importance of relativistic effects.

The present work reports an investigation of photoemission time delay from endohedral anions $A@C_{60}^{q}$. Photoionization of inner and outer subshells of the endohedral $Ne@C_{60}^{-5}$ near the 1s threshold is chosen as a case study. Significant enhancement of the time delay in the 1s dipole photoionization channels is found,

owing to the emergence of the *Coulomb* Confined Resonances (CRs). Moreover, by way of interchannel coupling, the inner-shell 1s Coulomb CRs induce a revival of these resonances in the 2s and 2p photoionization channels some 800 eV above their thresholds. These induced resonances, termed *correlation* Coulomb CR's, result in large time delay in the release of the 2s and 2p photoelectrons from Ne at these high energies. Furthermore, Coulomb CRs are found to emerge in the 1s quadrupole ionization channels as well, thereby also causing considerable time delays in 1s quadrupole photoemission.

In the present work, the photoionization time delay in photoionization of the 2p subshell in the energy region of the 2s→np autoionization resonances in atomic Neon have been analyzed. In this work, the expressions for the Breit-Wigner resonances developed in the context of scattering theory is used. Photoionization and electron-ion scattering have the same final state, but have different initial states. These two processes are related by the 'time reversal symmetry'. The Fano parameters for these resonances have been determined using RMQDT in which the quantum defect parameters were obtained *ab-initio* using the RRPA. The resonance lifetimes and the photoionization Wigner time delay through the autoionization resonances have been studied in the present thesis work.

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