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Proposed Title

Ab-initio Structure Calculation of Few-Body Atomic Systems in Free and Plasma Environment

Abstract

The study of structural properties of few–body atomic systems (H–like, He–like etc.) provides a key testing ground for many quantum mechanical approximation methods such as perturbation, variation, WKB method etc. These theoretical studies have immense application in the field of confined systems, plasma diagnostics, astrophysical data analysis etc. In this course of studies, we focus on studying the structural properties of few-body atomic systems in free case (only Coulombic attraction and repulsion among the constituent particles) and also in plasma environment.

This dissertation's work has been organized into five chapters. The following paragraphs provide an outline of these chapters:

Chapter 1

At the beginning of the first chapter "Introduction", we have given a detailed account on the rapid growth towards the production of relatively long-lived plasma using tunable ultra-short intense X–ray free-electron laser (FEL) or orion laser etc. and the importance of accurate theoretical estimation of the structural and spectral properties of plasma embedded few–body systems for diagnostic determination of such plasmas. In this context, the progress of atomic structure calculation starting from the hydrogen atom problem to general three–body problem is discussed. The fundamental notions of classifying and defining the quantum states of a three–body or two–electron system have been given. In this chapter we have introduced 'plasma' by defining its salient features, controlling parameters (particle density, temperature etc.) and abundance in both laboratory and astrophysical environments. Classification of plasma has been made on the basis of plasma particle distribution function (*classical plasma* and *quantum plasma*) as well as plasma coupling parameter (*weakly coupled plasma* and *strongly coupled plasma*) defined as the ratio of the average electrostatic energy to the average kinetic energy of the plasma particles. As plasma contains a large number of charged particles, the collective interaction is very difficult to tackle theoretically. Hence, a suitable model potentials are considered which incorporate the collective behaviors of the plasma particles. The analytic expressions of the model potentials in case of classical weakly coupled plasma, classical strongly coupled plasma, quantum plasma and dusty plasma are given at the end of this chapter.

Chapter 2

In recent studies, H–like ions in motion within the plasma environment have become increasingly significant from an experimental standpoint. Depending on plasma parameters and ion velocity, a moving ion produces a 'wake' which alters the potential of the medium. This potential modifies the energy levels and transition properties of the ion. Firstly we give a detailed account of the works on structural properties of H–like ions under classical weakly coupled plasma, classical strongly coupled plasma, quantum plasma and dusty plasma environments. Starting from electrostatic considerations, we have presented the mathematical development of the model potential in plasma environment using Meijer's G

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function for an ion moving through classical weakly coupled plasma, classical dusty plasma and quantum plasma environments. We have used trial wavefuntion expanded in Slater-type orbitals and subsequently solved the Schrödinger equation under the framework of Ritz variational principle to estimate the energy eigenvalues of ions moving through plasma. The analytic forms of the matrix elements and relevant basis integrals are given in relevant sections of this chapter. In the subsequent section, the results and discussions are illustrated in detail. It is observed that the plasma potential removes the l–degeneracy of the energy levels and the motion of the ion removes the $|m|$–degeneracy ('Stark-like' splitting). The present work discusses how plasma density, temperature, and ion velocity affect hydrogenic energy levels and the transition wavelengths of π and σ components of Lyman-α lines.

Chapter 3

In this chapter we have discussed the variation of ground state energy of different quantum mechanical three–body systems with arbitrary comparable masses, embedded under classical weakly coupled plasma. We have also estimated the energy and width of resonance S^e state of free hadronic three–body systems. In first section an extensive literature review is given describing the works on both bound and resonance state properties of three–body systems under plasma environments. At the beginning of methodology section, the construction of trial wavefunction and variational equation are given in a most exhaustive way possible. The trial wavefunction is expanded in multi-exponent Hylleraas-type basis set. The analytic form of necessary basis integral is given and demonstrated with some practical examples. In the last part of the methodology section, we have made a detailed discussion on the theory of stabilization method to estimate resonance parameters (energy and width). The results are given separately for bound and resonance states. In case of bound state, we have reported "Borromean binding" for various three–body systems under classical WCP whereas resonance parameters of S^e state of three–body exotic ppY and pYY $[Y:\mu,\pi,K]$ ions in the free environment are given.

Chapter 4

In this chapter we focus on the determination of structural properties of doubly excited F^e state of two–electron systems under both free and plasma (WCP) environment. A detailed account on doubly excited states of two–electron systems under different plasma scenario is given at the starting of this chapter. In the next section we elaborate the present methodology in the following steps: formation of trial wavefunction, construction of variational equation, expansion of trial wavefunction in multi–exponent Hyllerass–type basis set and analytical formulation of the relevant basis integrals. A detailed discussion on different structural properties (energy eigenvalues, one– and two–particle moments, inter–electronic angles etc.) of both meta–stable bound and resonance F^e states of free two–electron systems is given in the next segment. The methodology established for free systems is then extended to estimate different structural properties of two–electron systems embedded in classical WCP environment. The study on the variation of transition energies for the dipole transitions $F^e \to D^o$ with respect to the plasma screening strength is also included in this section.

Chapter 5

In this chapter we finally conclude all the findings from the present dissertation's works as described in previous chapters. A consolidated account of the present work on the accurate determination of the structural properties of the few–body atomic systems which are necessary for astrophysical data analysis as well as in laboratory plasma diagnostics is presented. We also discuss the potential future scopes of these works involving atomic structure calculation in different external confining environment which may be significant in different fields of research.

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