Centre for Theoretical Atomic, Molecular, and Optical Physics

Ph.D. Project 2022-2025

Quantum chaos in multicharged positive ions

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State of the art and motivations

Many-body quantum chaos is an area of research that spans the boundaries of atomic, nuclear and condensed matter physics [1]. Its starting point was a realisation by Wigner in the 1950's that the interaction between the nucleons in a heavy nucleus results in excited states of enormous complexity. This called for the development of a statistical theory that would describe the average properties of the spectrum and eigenstates: the level density, mean-squared amplitudes, etc. Notwithstanding the progress in computing power, the eigenstates of numerous many-particle systems still cannot be obtained by brute force methods.

The project focusses on one such system – open-shell positive ions. Chaotic multiply excited states in positive ions lead to observable effects, such as strongly enhanced electron-ion recombination rates [2, 3, 4, 5] and secondary threshold laws in multiple ionization [6].

A convenient starting point for describing many-electron systems, e.g., atoms or ions, is the mean-field approximation. In this approximation every electron in the system moves in the static field of the nucleus and all other electrons. Quantum-mechanically, this motion is described by single-particle wavefunctions. The total wavefunction of the system is then given by an antisymmetrised product of the individual electron's wavefunctions. Accordingly, the atom or ion is characterised by a certain electronic *configuration*, i.e., a list of single-particle states, or orbitals, occupied by the electrons. Besides the orbitals occupied by electrons in the lowest-energy (ground) state of the system, one can also consider orbitals with higher energies, which are normally empty. However, when energy is pumped into the system, electrons can be promoted into these orbitals, thereby creating an excited state of the atom or ion.

The above mean-field picture is only an approximation. In reality, when one electron changes its position, other electrons "notice" the change and respond to it, e.g., by changing their orbitals. This effect is known as electron correlations. It leads to a breakdown of the description based on fixed electron configurations. Different configurations become *mixed* by the residual electron interaction (i.e., that beyond the mean field). However, the configuration states can still be used as a basis for expanding the true eigenstates of the system. Their energies are found as eigenvalues of the Hamiltonian matrix in the space of configuration states.

The project focuses on atomic systems with extremely strong configuration mixing, in which all configurations with nearby energies are mixed together. Such mixing takes place in excited states of heavy nuclei, open-shell many-electron atoms, such as Ce, and multicharged many-electron ions, e.g., gold Au^{25+}, tungsten W^{20+}, etc. [2, 3, 4, 5, 8], and is termed *many-body quantum chaos*. Processes involving tungsten ions are of particular imporance, because of this metal is a major component of ITER and a major contaminant of the thermonuclear reactor plasma, with potentially drastic consequences for the feasibility of fusion [7]. The complexity of these systems prevents one from doing a full configuration-interaction calculation, as the size of

the corresponding Hamiltonian matrix is too large. However, this complexity also allows one to develop a *statistical* approach to the description of the system [2, 8, 9, 10].

Objectives & Methodology

The aim of the project is to develop further the ideas put forward in [2, 3, 4, 5, 8], focussing on the multicharged ions of tungsten, which is used as a wall material in nuclear fusion reactors.

The project will involve both analytical and numerical work, and will combine model calculations (e.g., random-matrix theory approaches) with realistic calculations for many-electron ions, based on the Dirac-Fock equation and configuration-interaction approaches. While full diagonalisation of the Hamiltonian matrix in this complex system is beyond reach, we can explore the mixing of individual important multiply excited configurations (along the lines of [3]). Particular attention should be given the so-called *doorway configurations* which provide a pathway for the initial excitation of the atomic system [9], such as the $4d$-$4f$ excitation in Xe ions [11].

A complimentary, and possibly more powerful, approach will be to construct the Hamiltonian matrix and investigate configuration mixing in the time domain by integrating the time-dependent Schrödinger equation. This procedure is computationally less expensive than the full diagonalisation, and can easily be used for Hamiltonian matrices of sizes up to 10^5. Such calculation can start with a simple single excited electron state, which would model electron-ion recombination or excitation by a photon. Its time evolution will the reveal the process of energy-sharing between this initial excitation and multiply excited many-electron states.

Such time-dependent approach will in some sense model the behaviour of atomic systems in short X-ray pulses, such as those created by the Linac Coherent Light Source (LCLS), the world's first hard hard X-ray free-electron laser (see, e.g., [12]).

This approach should give reliable quantitative information on the nature and extent of configuration mixing in many-electron multicharged ions. It should facilitate calculations of average values of observable quantities: recombination cross sections, radiative widths, etc. [4, 5]. From a broader perspective, the project will contribute to the theory of finite quantum systems of a few strongly-interacting particles [8], and understanding of many-body quantum chaos.

Collaborations

While the project will be based at Queen's, discussions, exchange of ideas and, possibly, joint work with the group of Prof. V. V. Flambaum and Dr. V. A. Dzuba at the School of Physics, UNSW (Sydney, Australia) is foreseen. This group is a world leader in applications of many-body theory in atomic physics and precise atomic calculations.

Required skills

The candidate is expected to have good working knowledge of and interest in Quantum Mechanics. He/she will be expected to learn and master many-body-theory methods and their application to many-electron systems. Running, modifying and developing computer codes is an integral and substantial part of the project. In spite of the complexity of the codes, the underlying many-body theory should allow great transparency and good physical understanding of the results.

Further information

While focussed on the problems of quantum chaos and multicharged ions, the project will inroduce the candidate to the general area of theoretical atomic physics, atomic structure calculations and computations methods. The experience of handling and writing computer codes, that will be acquired through the work on the project, will be useful in a wide range of future careers.

For further information, please contact Dr Gleb Gribakin.

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