Chapter 11

RESONANCE STATES OF ATOMS

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Introduction

This chapter is concerned with the use of explicitly correlated functions for the description of the autoionizing states of atoms. Such states are multiply excited. In the one-electron picture they correspond to multiply-excited electron configurations. If the description of electron correlation is considered, that of a highly excited system is much more demanding than for the ground or singly excited state of the same system. In a multiply excited state the electron correlations contribute strongly to the binding of the system: to the energy and to the electron density distribution — to the localization of the state.

The states under consideration here are localized. But on the other hand, they are autoionizing. At least one of the electrons can escape to infinity without an exchange of energy with the surrounding environment. This is possible since the energy level of the multiply excited autoionizing state is embedded in a continuum of scattering states; there are unbound states of the system corresponding to the same energy.

\[1\] This is because the excited electrons move much slower than in the ground state and thus their response to the Coulomb repulsion from other electrons is much stronger [1]. Banyard, Keeble and Drake [1] investigated the correlation effects for the doubly excited two-electron \(2p^2\) state of He-like systems for \(1 \leq Z \leq 4\) in terms of the Coulomb hole and partial Coulomb holes. They found that the correlation effect in a doubly excited state exceeds that of the ground or singly excited states of a given system.
Hence, the system being initially in the localized state can autoionize by internal Coulomb repulsion between electrons\(^2\).

The existence of autoionizing states in the continuum background of scattering states causes the appearance of resonant structures in the observed quantities, measured as a function of energy, in various experiments. Therefore, the states are called resonance states or simply resonances.

Both of the above mentioned resonance state features, \textit{localization} and \textit{autoionization}, are due to the electron correlation effects. They fight for their place in the wave function. In order to describe well the localization and decay of the state one has to account for the correlation effects. This can be done to high accuracy by using basis sets of functions dependent on interelectronic distances \(r_{ij}\). In fact, such bases have been used for investigations of autoionizing states.

The chapter is organized as follows: First, certain general properties of resonance states are presented. Then, several explicitly correlated expansions are given, as they were used for the resonance state computations. This is a list of trial functions which is referred to in further sections. General properties of \(r_{ij}\)-dependent expansions are not discussed here. They are elaborated in other chapters of this book. Instead, some aspects of using such expansions within methods dedicated to resonances are presented. Separate sections are devoted to the stabilization, the Feshbach-projection, the complex coordinate rotation and to the variational scattering methods. Among these special attention is paid to the Feshbach-projection operator method and to the complex coordinate rotation technique. The former one is very important for understanding the resonance phenomenon. The latter method is the most frequently used one, also within explicitly correlated functions.

1. **Nature of autoionizing resonances**

Resonance states are \textit{quasi}–bound. Their energy levels are diluted in continua of scattering energies. Below, their general features, similarities to- and differences from- bound and scattering states are briefly

\(^2\)Autoionization is also possible via the relativistic coupling of a bound state to a continuum of different symmetry in the \(LS\) approximation. Such a relativistic autoionization will not be discussed here. First, because the application of \(r_{ij}\)-dependent functions for such bound (in the \(LS\) approximation) states does not differ from the ground or singly-excited state case, e.g. see the above mentioned computations of Banyard, Keeble, and Drake [1], the computations of Bylicki and Pestka [2] for the only two bound states of He\(^-\), and the work of Woźnicki et al. [3] on doubly-excited \(2P^e\) states of the lithium isoelectronic series. Second, no papers on application of explicitly correlated functions for determination of the widths of such states (coupling to the continuum) are known to the authors.