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VI Time-dependent configuration interaction singles

Many-body effects are becoming more prominent and omnipresent as strong-field phenomena are studied in larger and more complex multielectron systems. Many-body effects such as multiorbital ionization or collective excitations can dramatically change the system response requiring a theoretical description that goes beyond the single-particle picture. In this chapter, we discuss a practically useful many-body method, time-dependent configuration interaction singles (TDCIS), and its specific implementation (grid representation, etc.) to describe strong-field processes. TDCIS captures a variety of many-body effects and at the same time keeps much of the single-particle picture making TDCIS a computationally very attractive approach.

1 Introduction

The absorption and emission of electromagnetic radiation have been the method of choice for over a century to access the quantum world of atoms, molecules, and solids. Since the invention of the laser in the 1960s and the possibility to produce well-defined pulses of radiation (laser pulses), the underlying structure and mechanisms in these microscopic systems can be studied in unprecedented detail. By knowing exactly the spectrum of the radiation pulse hitting the system, a direct connection between the final pulse spectrum (after passing through the system) and the internal structure of the system can be established. The kinetic energy distribution of electrons expelled from the system (the photoelectron spectrum) can be measured and contains quite complementary information on the system.

Atoms, molecules, and solids are all multielectron systems. The Coulomb interaction among the electrons causes them to become correlated, i.e., the behavior of any given electron can generally not be specified without specifying the behavior of all other electrons in the system. Even though the importance of electron correlations for physical or chemical properties has been realized in the early years of quantum mechanics, it remains a challenge to rigorously describe them. For any realistic

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