A Time-Dependent R-Matrix Approach for Molecular Systems

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Recent years have seen the development of ultra-fast light sources with durations in the attosecond regime [1]. These ultra-fast light sources open the possibility of directly observing ultra-fast dynamics, such as correlated electron motion in atoms and molecules.

The theoretical description of ultra-fast phenomena is a particularly challenging problem. The time scales involved require that a time dependent approach is adapted while the dynamics of interest in an atomic or molecular system on these time scales will involve multiple active electrons, further increasing the computational difficulty. Consequently a computational solution of the full dimensional time dependent Schrödinger equation is intractable.

Recent work in atomic systems has successfully employed time dependent R-Matrix techniques [2] and finite difference propagator methods [3] to describe correlated electron dynamics on an ultra-fast time scale [4]. The use of R-Matrix techniques reduces computational demands significantly due to the partition of configuration space into a highly detailed inner region and a reduced dimensionality outer region. More recently, the R-matrix and finite difference approaches have been combined in the RMT method [5].

The aim of the presented work is to combine the techniques employed in the RMT method with the highly successful molecular R-Matrix codes from the UK-RMol project [6,7]. Work is ongoing at the time of writing and the most recent results will be presented at the conference.

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