Hole dynamics and coherence

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I. Introduction

Photoionization of an atom or a molecule leads, in general, to the formation of a superposition of ionic eigenstates. That superposition cannot, in general, be described in terms of a wave function, but a description in terms of a reduced density matrix (a statistical mixture) is required.

II. Hole dynamics driven by spin-orbit coupling

In the first part of the talk, ultrafast, partially coherent hole dynamics driven by spin-orbit coupling will be analyzed in terms of a time-dependent multichannel mean-field theory [1]. This theory will be compared with the results of an attosecond transient absorption experiment on strong-field-ionized krypton atoms [2].

III. Decoherence in attosecond photoionization

In the second part of the talk, a new implementation of time-dependent configuration interaction singles (TDCIS) will be discussed [3]. Using TDCIS calculations, it will be shown that photoelectron-mediated interchannel coupling causes ion decoherence in attosecond photoionization. As a consequence, even if the spectral bandwidth of the ionizing pulse exceeds the energy splittings among the hole states involved, perfectly coherent hole wave packets cannot be formed [4].

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