

Fictitious-Time Wave-Packet Dynamics in Atomic Systems

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Gaussian wave packets (GWPs) are well suited as basis functions to describe the time evolution of arbitrary wave functions in systems with non-singular smooth potentials. They are rare in atomic systems on account of the singular behaviour of the Coulomb potential. We present a time-dependent variational method that makes the use of GWPs possible in the description of propagation of quantum states also in these systems. We use a regularization of the Coulomb potential and introduce a fictitious-time coordinate in which the evolution of an initial state can be calculated exactly and analytically for a pure Coulomb potential. Therefore, in perturbed atomic systems variational approximations only arise from those parts of the potentials which deviate from the Coulomb potential. The method is applied to the hydrogen atom in external magnetic and electric fields. It can be adapted to systems with definite symmetries and thus allows for a wide range of applications.

Key words: Hydrogen Atom in External Magnetic and Electric Fields; Coulomb Potential; Gaussian Wave Packets.

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