Time-dependent unitary transformation method to numerically solve the strong-field-ionization dynamics in the Kramers-Henneberger frame

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Time-dependent unitary transformation (TDUT) method has been employed in quantum mechanical system composed of discrete states by the authors [1, 2]. It has been proved to be especially helpful to solve molecular rotational dynamics in the quasi-adiabatic regime, because the literally strict unitary nature of the propagation operator allows us to set the temporal step size larger; a rigid limitation on the temporal step size ($dt << 1$) can be alleviated due to the strict unitary nature.

On the other hand, in a strongly ionizing system where the Hamiltonian is not Hermitian, the same approach cannot be directly applied because it is demanding to define a set of field-dressed eigenstates. In this work, by employing the Kramers-Henneberger (KH) frame [3], in which the strong-field-dressed discrete eigenstates are given by the field-free discrete eigenstates in a moving frame, we have successfully implemented the TDUT method in the ionizing regime. In the KH frame, the eigenstates of a field-dressed Hamiltonian are equivalent to the field-free eigenstates except that they are uniformly displaced from the origin as illustrated in Fig. 1. Once the field-free eigenstates of an atom or a molecule are accurately obtained, we can apply a TDUT method.

While the present work verifies the method for a one-dimensional atom as a prototype, the method can be applied to three-dimensional atoms and molecules as well as solid materials exposed to strong laser fields.

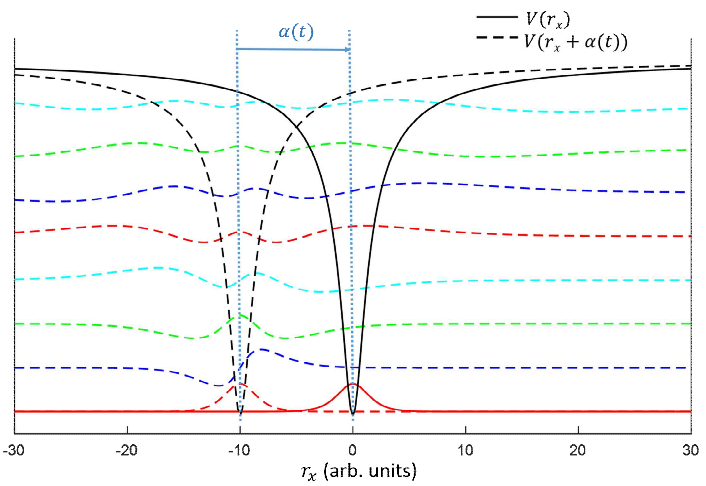

Figure 1 Representation of the two frames converted by a translation operator. The black-solid and black-dashed lines are atomic potentials in the field-free and the field-dressed KH frames, respectively, while the red solid line is the ground state of the atom, and the other colored-dashed-lines are eigenstates of the field-dressed KH Hamiltonian. The initial ground state can be expanded by the field-dressed Hamiltonian.

References

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