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The Schrödinger equation on a Lagrange mesh

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Abstract content
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Atomic, molecular and nuclear systems are quantum mechanical systems that are accurately described by the Schrödinger equation. Theoretical studies of these systems require the solution of the many-body Schrödinger equation that involves realistic interactions in the systems. It is common knowledge that the Schrödinger equation can be solve exactly only for a few types of interaction potentials. Therefore, only numerical solutions of the equation are possible even for systems with few constituents. Although variational methods have been shown to generate accurate numerical solutions to the Schrödinger equation, such methods are computationally demanding. The Lagrange-mesh method is a semi-variational method that combines the Lagrange basis expansion with Gauss quadrature approximation. This combination leads to a set of simple algebraic equations that can be solved fast and accurately. In this work the Lagrange-mesh method is used to solve the two- and three-dimensional Schrödinger equation in polar coordinates. General matrix elements for the Hamiltonian depending only on the grid points and can be used with any system are presented for the first time. Results with selected Hamiltonian related to some few-body systems are within machine accuracy.

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