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Analytical Structure Matching and Very Precise Approach to the Coulombic Quantum Three-Body Problem

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Abstract: A powerful approach to solve the Coulombic quantum three-body problem is proposed. The approach is exponentially convergent and more efficient than the hyperspherical coordinate method and the correlation-function hyperspherical harmonic method. This approach is numerically competitive with the variational methods, such as that using the Hylleraas-type basis functions. Numerical comparisons are made to demonstrate the efficiency of this approach, by calculating the nonrelativistic and infinite-nuclear-mass limit of the ground state energy of the helium atom. The exponential convergency of this approach is due to the full matching between the analytical structure of the basis functions that are used in this paper and the true wavefunction. This full matching was not reached by most other methods. For example, the variational method using the Hylleraas-type basis does not reflects the logarithmic singularity of the true wavefunction at the origin as predicted by Bartlett and Fock. Two important approaches are proposed in this work to reach this full matching: the coordinate transformation method and the asymptotic series method. Besides these, this work makes use of the least square method to substitute complicated numerical integrations in solving the Schrödinger equation without much loss of accuracy, which is routinely used by people to fit a theoretical curve with discrete experimental data, but here is used to simplify the computation.

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Key words: quantum three-body problem, analytical structure, matching, the least square method, asymptotic series, Bartlett-Fock expansion

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