Relativistic Pure Rotational Energy for Diatomic Molecules

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Abstract

This paper provides a simplified solution of the Dirac equation for the pure rotational energy of the diatomic molecules and a discussion of the non-relativistic limit. The last works [1-2] led to a complicated form of the relativistic energy of the molecular rotation-vibrational energy with high computational cost based on Schrodinger-like equation. The present work provides a way to determine the pure rotational energy without exclusion of the wavefunction components or using the Schrodinger-like equation, where the selection rule $\Delta J=\pm 1$, where J is the rotational quantum number, appears as a prerequisite for solving the equations. Based on the anti-hermitian spin-orbit operator (L) that been introduced in this paper, which excludes the derivatives, the computational cost expects to decrease.

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