EXACT SEPARATION OF ANGULAR MOMENTUM IN WAVE FUNCTIONS OF FEW-PARTICLE SYSTEMS: APPLICATIONS

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Consider a quantum system (an atom or a small molecule) as a collection of N particles (electrons and nuclei), each of them carrying its own partial momentum and partial angular momentum. Since, the total momentum operator P and the total angular momentum operator L commute with the Hamiltonian H of the system, it is possible to identify three degrees of freedom associated with each of these operators. This identification allows us to reduce the dimentionality of the wave function by eliminating those degrees. While the separation of the degrees of freedom asociated with P is well-known (separation of the center of mass), the exact separation of the degrees of freedom associated with L is more complicated and consequently less-known.

The current paper is supposed to review the situation in the field and discuss in detail the family of minimal multipolar harmonics (see [1] for a thorough review of related topics) that can be used to derive a family of reduced Schrödinger equations in 3N-6 variables for systems with well-defined quantum numbers corresponding the definite arbitrary values of the total momentum P, the total angular momentum L, its projection M, and parity π. The derived formalism is used to compute very accurate energy levels of a few-particle systems.

REFERENCES

[1] A.V. Meremianin, J.S. Briggs „The irreducible tensor approach in the separation of collective angles in the quantum N-body problem“, *Phys. Rep*. **2003**, 384, 121–195.

[2] H. A. Witek, G. Pestka, A. Sadhukhan, R. Podeszwa, „Elimination of angular dependency in quantum three-body problem made easy“, arXiv:2506.23962v2 **2025**