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Ab Initio description of open-shell nuclei at polynomial cost

Content

Ab initio methods for the description of atomic nuclei have, in recent years, become state-of-the-art techniques for performing systematically improvable predictions of nuclear observables. While initially limited to a restricted set of nuclei, specifically doubly closed-shell systems, recent advancements have extended their applicability to open-shell nuclei.

Although ab initio methods capable of solving the many-body Schrödinger equation exactly do exist, their reach remains confined to few-body systems due to computational constraints. In my talk I will focus on a specific class of ab initio approaches known as correlation-expansion methods. These methods exhibit favorable computational scaling with respect to the system's mass, enabling calculations to be extended to heavy nuclei.

In doubly closed-shell systems, correlation-expansion methods follow a two-step process. First, a mean-field calculation is performed to capture the dominant correlations within the system under study, typically by solving the spherical Hartree-Fock (HF) equations. Then, a beyond-mean-field expansion is applied to the mean-field solution (the so-called reference state) to incorporate dynamical correlations.

When moving from doubly closed-shell to singly open-shell systems, two key challenges arise when employing the spherical HF method:
1. New static correlations introduced in open-shell systems are not efficiently captured at the mean-field level.
2. Zero-energy denominators can render the beyond-mean-field expansion ill-posed.

To address these issues, a well-established strategy involves breaking symmetries at the reference-state level. It has been shown that for singly open-shell systems, breaking particle-number symmetry U(1) is the most effective approach, while for doubly open-shell systems breaking rotational symmetry SU(2) provides an efficient way to incorporate static correlations into the mean-field description.

In my talk I will present key findings from a recent analysis [Eur. Phys. J. A 60, 209], which demonstrates the necessity of breaking SU(2) symmetry at the reference-state level to accurately describe open-shell nuclei using correlation-expansion methods.

The second part of the talk will focus on the development of a novel ab initio technique that is still unpublished: the second-order deformed Dyson Self-Consistent Green's Function (dDSCGF) method. This approach captures dynamical correlations in a non-perturbative fashion on top of an SU(2)-breaking reference state, leading to improved predictions of nuclear observables compared to perturbative techniques for open-shell nuclei and non-perturbative techniques for closed-shell nuclei.

Finally, I will present general conclusions and future perspectives on the ab initio study of deformed nuclear systems.

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