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Constraining symmetry restoration within the nuclear energy density functional method

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We review the notion of symmetry breaking and restoration within the frame of nuclear energy density functional methods. We focus on key differences between wave-function- and energy-functional-based methods. In particular, we point to difficulties to formulate the restoration of symmetries within the energy functional framework.

1. Introduction

Symmetries are essential features of quantal systems as they characterize their energetics and provide transition matrix elements of operators with specific selection rules. However, certain emergent phenomena relate to the spontaneous breaking of those symmetries [1]. In nuclear systems, such spontaneously-broken symmetries (i) relate to specific features of the inter-particle interactions, (ii) characterize internal correlations and (iii) leave clear fingerprints in the excitation spectrum of the system. In finite systems though, quantum fluctuations cannot be ignored such that the concept of spontaneous symmetry breaking is only an intermediate description that arises within certain approximations. Eventually, symmetries must be restored to achieve a complete description of the system.

2. Wavefunction-based methods vs EDF-based method

In wave-functions based methods, the symmetry breaking step, e.g. the symmetry unrestricted Hartree-Fock-Bogoliubov approximation, relies on minimizing the average value of the Hamiltonian for a trial wave-function that does not carry good quantum numbers, i.e. which mixes irreducible representations of the symmetry group of interest. Restoring symmetries amounts to using an enriched trial wave-function that does carry good quantum numbers. One typical approach is to project out from the symmetry-breaking trial state the component that belongs to the

intended irreducible representation. Wave-function-based projection methods and their variants are well formulated quantum mechanically [2]. The goal of the Ref. 3 was to discuss their Energy Density Functional (EDF) counterparts [4] which have been *empirically adapted* from the former to deal quantitatively with properties of nuclei. The SR-EDF method (MR-EDF) relies on computing the analog to the symmetry-breaking average energy E (Energy *kernel* $E[g',g]$) as an a priori *general* functional $\mathcal{E}[\rho,\kappa,\kappa^*]$ ($\mathcal{E}[g',g] \equiv \mathcal{E}[\rho^{g'g},\kappa^{g'g},\kappa^{gg'*}]$) of the one-body density matrices (transition one-body matrices) computed from the symmetry breaking state (two transformed symmetry breaking state). As opposed to what was considered in Wavefunction-based methods, the symmetry-breaking energy (symmetr-restored energy) is *not* computed from the average value of a genuine operator H.

3. Questions

The question one may ask is : are the constraints imposed on the energy kernel $\mathcal{E}[\rho,\kappa,\kappa^*]$ at the SR level sufficient to making the MR-EDF method well defined? As a matter of fact, a set of physical constraints to be imposed on $\mathcal{E}[g',g]$ have already been worked out [5]. References [6,7,8,9] have already provided important elements in the case of $U(1)$, i.e. for particle-number restoration (PNR), about how to constrain more tightly MR-EDF calculations. Indeed, in the EDF context, it was demonstrated [8,9] that Fourier components $\mathcal{E}^N$ are a priori different from zero for $N \leq 0$, i.e. one usually obtains a non-zero symmetry-restored energy for negative particle numbers! In the wave-function-based method, the E^N is zero [8] for $N \leq 0$. Such a result is indeed obtained from the fact that E^N is computed as the average value of H in $|\Phi^N\rangle$. Applying the regularization method proposed in Ref. [7], the cancelation of non-physical Fourier components was recovered [8]. For an arbitrary symmetry group, the situation might not be as transparent as for $U(1)$. Indeed, it is unlikely in general that certain coefficients of the expansion of $\mathcal{E}[g',g]N[g',g]$ over irreducible representations of the group are zero based on physical arguments. Ref. 3 briefly introduces an example of such a property in the case of $SO(3)$, i.e. for angular momentum restoration. This kind of mathematical properties deduced from a wave-function-based method must be imposed on $\mathcal{E}[g',g]$ to make symmetry-restored energy physically sound.

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