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Bogoliubov many-body perturbation theory for open-shell nuclei

A. Tichai [a,f,*], P. Arthuis [b,c], T. Duguet [b,d], H. Hergert [e], V. Somà [b], R. Roth [f]

[a] ESNT, IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France
[b] IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France
[c] CEA, DAM, DIF, 91297 Arpajon, France
[d] KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium
[e] NSCL/FRIB Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824-1321, USA
[f] Institut für Kernphysik, Technische Universität Darmstadt, Schlossgartenstr. 2, 64289 Darmstadt, Germany

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ABSTRACT

A Rayleigh–Schrödinger many-body perturbation theory (MBPT) approach is introduced by making use of a particle-number-breaking Bogoliubov reference state to tackle (near-)degenerate open-shell fermionic systems. By choosing a reference state that solves the Hartree–Fock–Bogoliubov variational problem, the approach reduces to the well-tested Møller–Plesset, i.e., Hartree–Fock based, MBPT when applied to closed-shell systems. Due to its algorithmic simplicity, the newly developed framework provides a computationally simple yet accurate alternative to state-of-the-art non-perturbative many-body approaches. At the price of working in the quasi-particle basis associated with a single-particle basis of sufficient size, the computational scaling of the method is independent of the particle number. This paper presents the first realistic applications of the method ranging from the oxygen to the nickel isotopic chains on the basis of a modern nuclear Hamiltonian derived from chiral effective field theory.

1. Introduction

Over the past two decades the *ab initio* description of nuclear structure properties has extended significantly both with respect to accessible mass numbers and to the open-shell character of the targeted system. Simplest approaches applicable to closed-shell systems start from a single-determinantal, e.g., Hartree–Fock (HF), reference state and account for *dynamic correlations* via the inclusion of particle–hole excitations on top of it. In this context, a plethora of many-body frameworks have been developed to describe medium-mass systems, e.g., many-body perturbation theory (MBPT) [1–3], coupled-cluster (CC) theory [4–8], self-consistent Green's functions (SCGF) theory [9–11] or the in-medium similarity renormalization group (IMSRG) approach [12–15]. For doubly closed-shell nuclei, all of these methods agree well with quasi-exact no-core shell model (NCSM) calculations for ground-state energies of nuclei in the $A \sim 20$ regime [16].

However, when going away from nuclear shell closures, the single-determinantal description becomes qualitatively wrong because several determinants contribute strongly to a configuration interaction (CI) expansion, requiring a proper treatment of *static correlations*. In order to overcome this drawback, more general reference states are required, i.e., either *multi-determinantal* or *symmetry-broken* reference states. The latter were first used in nuclear structure through the Gorkov extension of SCGF (GSCGF) that relies on a particle-number-broken Hartree–Fock–Bogoliubov (HFB) vacuum to describe singly-open-shell nuclei [17,18]. A similar extension led to designing the Bogoliubov CC formalism, although only proof-of-principle calculations limited to small model spaces and two-body forces have actually been performed so far [19]. In parallel, multi-determinantal reference states were successfully applied in the multi-reference extension of the IMSRG (MR-IMSRG) [20]. The first MR-IMSRG applications used particle-number-projected (PNP) HFB states [16,20,21]. More recently, solutions of no-core shell model (NCSM) calculations [22–24] in a small model space were employed, leading to the so-called in-medium no-core shell model (IM-NCSM) [25], and proof-of-principle calculations with angular-momentum projected HFB states were presented in [26]. With the revival of perturbative techniques in nuclear structure theory [1,2] the concept of multi-determinantal reference states inspired the development of a MBPT variant based on a NCSM reference state in a small model space, yielding the perturbatively-improved no-core shell model (NCSM-PT). This method has allowed the first description of medium-mass

* Corresponding author.
E-mail addresses: alexander.tichai@cea.fr (A. Tichai), pierre.arthuis@cea.fr (P. Arthuis), thomas.duguet@cea.fr (T. Duguet), hergert@nscl.msu.edu (H. Hergert), vittorio.soma@cea.fr (V. Somà), robert.roth@physik.tu-darmstadt.de (R. Roth).

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nuclei with even and odd mass numbers on an equal footing [3]. In general the use of a perturbative framework is computationally advantageous since it obviates the storage of large tensors like, e.g., cluster amplitudes in CC theory or the flowing Hamiltonian in IM-SRG, and, furthermore, does not require a solution of a numerically more challenging non-linear set of equations.

Even though pioneering work based on symmetry-broken reference states was done within the GSCGF framework, similar ideas have scarcely been employed in *ab initio* calculations. One reason is that symmetry breaking cannot occur in finite quantum systems, hence the explicitly broken symmetry must eventually be restored, which has been a long-standing challenge already on a formal level. While the design of a proper symmetry-restoration protocol remains yet to be formulated within the GSCGF framework, full-fledged symmetry-broken and -restored MBPT and CC formalisms have been recently designed to consistently restore the symmetry at any truncation order [27,28]. The spin-projected CC version of this formalism [27] has been transferred and implemented successfully on the Hubbard model and on molecule dissociation [29].

While the full details of the newly derived Bogoliubov many-body perturbation theory (BMBPT) formalism will be described in a forthcoming publication [30], its first full-fledged implementation in large model spaces with an approximate inclusion of three-body forces via normal-ordering techniques is presented in this letter. We investigate ground-state energies along complete medium-mass isotopic chains with further emphasis on two-neutron separation energies to monitor footprints of nuclear shell closures. Whenever possible, BMBPT calculations are benchmarked against well-established non-perturbative IT-NCSM, GSCGF, and MR-IMSRG results for the same input Hamiltonian.

2. Many-body formalism

Bogoliubov MBPT is an expansion of the exact A-body ground-state energy in perturbations around a (possibly) symmetry-breaking reference state. In semi-magic nuclei, the relevant symmetry is the $U(1)$ global gauge symmetry associated with particle number conservation. Breaking $U(1)$ symmetry permits to efficiently deal with Cooper pair's instability associated with the superfluid character of open-shell nuclei. The degeneracy of a Slater determinant with respect to particle–hole excitations is lifted via the use of a Bogoliubov reference state and commuted into a degeneracy with respect to symmetry transformations of the group. As a consequence, the ill-defined (i.e. singular) expansion of exact quantities with respect to a Slater determinant is replaced by a well-behaved one.[1]

Eventually, the degeneracy with respect to $U(1)$ transformations must also be lifted by restoring the symmetry. However, BMBPT only restores the symmetry in the limit of an all-order resummation, and, therefore retains a symmetry contamination at any finite order. While BMBPT is presently used as a stand-alone approach it eventually provides the first step towards the implementation of the particle-number projected BMBPT (PNP-BMBPT) which exactly restores good particle number at any truncation order [28]. While the present focus is on BMBPT, the next step will consist of implementing PNP-BMBPT.

The formalism is based on the introduction of the Bogoliubov reference state

$$|\Phi\rangle \equiv \mathcal{C} \prod_k \beta_k |0\rangle \,, \tag{1}$$

where $\mathcal{C}$ is a complex normalization constant and $|0\rangle$ denotes the physical vacuum. The Bogoliubov state is a vacuum for the quasi-particle operators $\beta_k^\dagger, \beta_k$ that are obtained from the creation and annihilation operators of our chosen single-particle basis via the transformation

$$\beta_k \equiv \sum_p U_{pk}^* c_p + V_{pk}^* c_p^\dagger \,, \tag{2a}$$

$$\beta_k^\dagger \equiv \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \,. \tag{2b}$$

While other choices are possible [30], $|\Phi\rangle$ is presently obtained by solving the Hartree–Fock–Bogoliubov variational problem. The transformation matrices (U, V) consist of the eigenvectors of the HFB eigenvalue equation [31], and the quasi-particle energies $\{E_k > 0\}$ are the corresponding eigenvalues. This fixes the reference state and corresponds to the Møller–Plesset implementation of the otherwise more general Rayleigh–Schrödinger BMBPT formalism. We note that only like-particle pairing is included at the HFB level and, thus, proton–neutron pairing is absent from the formalism.

While the HFB reference state is not an eigenstate of the particle-number operator[2] A, the expectation value of A is constrained to match the number of particles A_0 of the targeted system. It is enforced in the HFB iteration via the use of a Lagrange multiplier λ in the minimization of the grand potential $\Omega \equiv H - \lambda A$ expectation value. In actual applications, separate Lagrange multipliers are used to constrain proton and neutron numbers separately.

In the next step, the grand potential Ω is normal ordered with respect to the HFB reference state

$$\Omega = \overbrace{\Omega^{00}}^{\Omega^{[0]}} + \overbrace{\Omega^{20} + \Omega^{11} + \Omega^{02}}^{\Omega^{[2]}} + \underbrace{\Omega^{40} + \Omega^{31} + \Omega^{22} + \Omega^{13} + \Omega^{04}}_{\Omega^{[4]}} \,, \tag{3}$$

where Ω^{ij} denotes the normal-ordered component involving i (j) quasi-particle creation (annihilation) operators, e.g.,

$$\Omega^{31} \equiv \frac{1}{3!} \sum_{k_1 k_2 k_3 k_4} \Omega^{31}_{k_1 k_2 k_3 k_4} \beta_{k_1}^\dagger \beta_{k_2}^\dagger \beta_{k_3}^\dagger \beta_{k_4} \,. \tag{4}$$

Thus, Ω^{00} is the expectation value of Ω in $|\Phi\rangle$, $\Omega^{[2]}$ is an effective, i.e., normal-ordered, one-body operator and $\Omega^{[4]}$ is an effective two-body one. Working in the normal-ordered two-body approximation (NO2B) [32] in the quasi-particle representation,[3] the residual three-body part $\Omega^{[6]}$ is presently discarded. Details on the normal-ordering procedure as well as expressions of the matrix elements of each operator Ω^{ij} in terms of the original matrix elements of the Hamiltonian and of the (U, V) matrices can be found in Ref. [19].

To set up the perturbation theory, the Hamiltonian (i.e. grand potential) must be partitioned into an one-body unperturbed part Ω_0 and a residual part Ω_1, i.e.,

$$\Omega = \Omega_0 + \Omega_1 \,. \tag{5}$$

[1] Extending the treatment to doubly open-shell nuclei also requires a treatment of the $SU(2)$ symmetry associated with the conservation of angular momentum.

[2] In practice the constraint has to be done for neutron and proton-number operators N and Z, respectively by introducing two separate chemical potentials λ_N and λ_Z. In our formalism A stands for either one of them.

[3] We emphasize that the NO2B approximation does not break particle number itself, i.e., the truncated grand potential does commute with A.