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Large-scale HFB calculations for deformed nuclei with the exact particle number projection

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Abstract. Recent theoretical advances in the large-scale HFBTHO calculations of nuclear ground-state properties are presented with the emphasis on the exact particle number projection. The applicability of the widely used Lipkin-Nogami procedure is discussed together with the analysis of the particle number projection after variation.

PACS. 21.10.Dr Binding energies and masses – 21.60.Jz Hartree-Fock and random-phase approximations

1 Introduction

Modern nuclear structure theory is rapidly expanding from the description of phenomena in stable nuclei toward regions of exotic short-lived nuclei far from stability. Stringent constraints on the microscopic approach to nuclear dynamics, effective nuclear interactions, and nuclear energy density functionals are obtained from studies of the structure and stability of exotic nuclei with extreme isospin values, as well as extended asymmetric nucleonic matter.

The Hartree-Fock-Bogoliubov (HFB) method is a reliable tool for a microscopic self-consistent description of nuclei, which can be used in the context of the density functional theory (DFT). We solve the HFB equations by using the Transformed Harmonic-Oscillator (THO) basis [1], which allows for a correct asymptotic behavior of single-quasiparticle wave functions. The method is adopted for performing massive calculations for many axially deformed nuclei including those which are weakly bound [2].

Recently, it has been shown [3] that the total energy in the particle-number–projected (PNP) HFB approach can be expressed as a functional of the unprojected HFB density matrix and pairing tensor. Its variation leads to a set of HFB-like equations with modified Hartree-Fock fields and pairing potentials. The method has been illustrated within schematic models [3], and also implemented in HFB calculations with the finite-range Gogny force [4]. In the present paper, we adopt it for the Skyrme functionals and zero-range pairing term; in this case the building blocks of the method are the local densities and mean fields. The HFB results using the Lipkin-Nogami (LN) approximation, followed by the particle-number projection *after variation* (PLN), are compared to the HFB results with projection *before variation* (PNP).

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2 Particle-number–projected Skyrme-HFB method

The particle-number–projected HFB state can be written as

$$|\Psi\rangle \equiv P^N|\Phi\rangle = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\phi\, e^{\imath\phi(\hat{N}-N)}|\Phi\rangle, \qquad (1)$$

where $\hat{N}$ is the number operator, N is the particle number, and $|\Phi\rangle$ is the HFB wave function which does not have a well-defined particle number. As shown in ref. [3], the PNP HFB energy

$$\mathsf{E}^N[\rho,\bar{\rho}] = \frac{\langle\Phi|HP^N|\Phi\rangle}{\langle\Phi|P^N|\Phi\rangle} = \frac{\int \mathrm{d}\phi\langle\Phi|He^{i\phi(\hat{N}-N)}|\Phi\rangle}{\int \mathrm{d}\phi\langle\Phi|e^{i\phi(\hat{N}-N)}|\Phi\rangle}, \qquad (2)$$

is an energy functional of the unprojected particle-hole and pairing densities ρ and $\bar{\rho}$, respectively. In the case of the Skyrme force, the projected energy (2) reads

$$\mathsf{E}^N[\rho,\tilde{\rho}] = \int \mathrm{d}\phi\; y(\phi) \int \mathrm{d}\mathbf{r} \left(H(\mathbf{r},\phi) + \tilde{H}(\mathbf{r},\phi)\right), \qquad (3)$$

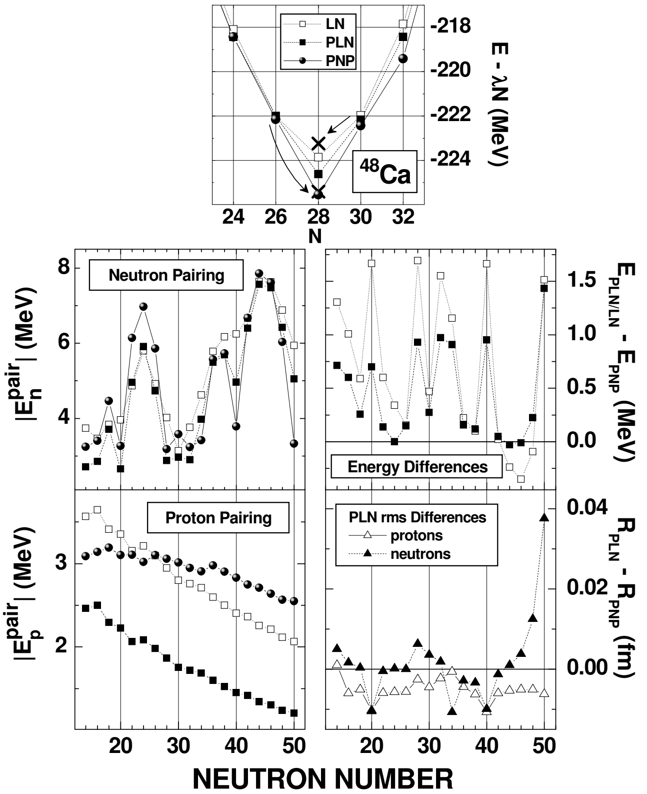

Fig. 1. The LN and PLN (projection after variation) and PNP HFB (projection before variation) results obtained for the SLy4 force and mixed delta pairing. Arrows in the top panel indicate projection results from the neighboring nuclei.

where

$$x(\phi) = \frac{1}{2\pi} \frac{e^{-i\phi N} \det(e^{i\phi} I)}{\sqrt{\det C(\phi)}}, \qquad y(\phi) = \frac{x(\phi)}{\int \mathrm{d}\phi' \, x(\phi')}, \tag{4}$$

I is the unit matrix, and the gauge-angle–dependent energy densities $H(\mathbf{r}, \phi)$ and $\tilde{H}(\mathbf{r}, \phi)$ are derived from the unprojected ones by simply replacing particle (pairing) local densities by their gauge-angle–dependent counterparts. The latter ones are defined by the gauge-angle–dependent density matrices.

Obviously, the projected energy (3) is a functional of the unprojected density matrices. Its derivatives with respect to $\rho_{n'n}$ and $\tilde{\rho}_{n'n}$ lead to the PNP Skyrme-HFB equations

$$\begin{pmatrix} h^N & \tilde{h}^N \\ \tilde{h}^N & -h^N \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E^N \begin{pmatrix} U \\ V \end{pmatrix}, \tag{5}$$

where

$$\begin{aligned} h^N &= \int \mathrm{d}\phi y(\phi) \left[Y(\phi) E(\phi) + e^{-2i\phi} C(\phi) h(\phi) C(\phi) \right] \\ &\quad - \left[\int \mathrm{d}\phi y(\phi) i e^{-i\phi} \sin(\phi) \tilde{\rho}(\phi) \tilde{h}(\phi) C(\phi) + \text{h.c.} \right], \quad (6) \\ \tilde{h}^N &= \frac{1}{2} \int \mathrm{d}\phi y(\phi) e^{-i\phi} \left\{ \tilde{h}(\phi) C(\phi) + (\tilde{h}(\phi) C(\phi))^T \right\}, \end{aligned}$$

and $Y(\phi) = ie^{-i\phi} \sin\phi C(\phi) - i \int \mathrm{d}\phi' y(\phi') e^{-i\phi'} \sin\phi' C(\phi')$ and $C(\phi) = e^{2i\phi} \left(1 + \rho(e^{2i\phi} - 1)\right)^{-1}$. The gauge-angle–dependent field matrices $h(\phi)$ and $\tilde{h}(\phi)$ are obtained by simply replacing the particle and pairing local densities in the unprojected fields with their gauge-angle–dependent counterparts.

3 Results

Figure 1 shows the PNP results for the complete chain of the calcium isotopes (from the proton drip to the neutron drip line), calculated with the SLy4 Skyrme functional and mixed delta pairing [1]. Comparison is also made with the LN and PLN results. One can conclude that the PLN approximation works best for open-shell nuclei, where the total energy differences between various variants of calculations are less than 250 keV. For closed-shell nuclei [5], however, the energy differences increase to more than 1 MeV. In such cases, one can improve the PLN results by applying the projection to the LN solutions obtained for the neighboring nuclei [6], as illustrated in the top panel of fig. 1.

In summary, the Skyrme HFBTHO PNP framework has been implemented and tested. The particle number corrections maximize for magic nuclei where the static pairing breaks down. It is to be noted that conceptual questions related to the notion of symmetry restoration in DFT still remain; those will be discussed in the following work [7].

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