

**PARTICLE-NUMBER-PROJECTED HFB METHOD WITH
SKYRME FORCES AND DELTA PAIRING**

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Particle-number restoration before variation is implemented in the HFB method employing the Skyrme force and zero-range delta pairing. Results are compared with those obtained within the Lipkin-Nogami method, with or without the particle-number projection after variation. Shift invariance property is proven to be valid also in the case of density functional calculations which allows the well known singularity ($u_n^2 = v_n^2$) in PNP HFB calculations to be safely avoided.

1. Introduction

Pairing correlations play a central role in describing properties of atomic nuclei. In mean-field approaches, they are best treated in the Hartree-Fock-Bogoliubov (HFB) approximation¹. The HFB ansatz for the nuclear wave function, however, breaks the particle-number symmetry. The symmetry needs to be restored, in principle, especially if one looks at observables that strongly vary as functions of particle number.

Recently, it has been shown² 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 models², and also implemented in HFB calculations with the finite-range Gogny force³. In the present paper we adopt it for the Skyrme functional and delta pairing, where the method must rely on the spatial locality of 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).

2. Particle-Number-Projected Skyrme-HFB Method

2.1. Skyrme-HFB method

Due to the zero-range character of the Skyrme force, the Skyrme-HFB energy is an energy functional,

$$E[\rho, \tilde{\rho}] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \int d\mathbf{r} \left[H(\mathbf{r}) + \tilde{H}(\mathbf{r}) \right], \quad (1)$$

of *local* particle and pairing densities, where $H(\mathbf{r})$ and $\tilde{H}(\mathbf{r})$ are normal and pairing energy densities, respectively. Their explicit expressions⁴ are given in terms of particle (pairing) local densities and currents. All local densities and currents are completely determined by particle $\rho_{n'n}$ and pairing $\tilde{\rho}_{n'n}$ density-matrix elements in the configurational space, i.e.,

$$\begin{aligned} \rho(\mathbf{r}\sigma, \mathbf{r}'\sigma') &= \sum_{nn'} \rho_{nn'} \psi_n^*(\mathbf{r}', \sigma') \psi_n(\mathbf{r}, \sigma), \\ \tilde{\rho}(\mathbf{r}\sigma, \mathbf{r}'\sigma') &= \sum_{nn'} \tilde{\rho}_{nn'} \psi_n^*(\mathbf{r}', \sigma') \psi_n(\mathbf{r}, \sigma). \end{aligned} \quad (2)$$

The use of the pairing density matrix $\tilde{\rho}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -2\sigma'\kappa(\mathbf{r}, \sigma, \mathbf{r}', -\sigma')$ instead of the pairing tensor κ is convenient when the time-reversal symmetry is assumed⁴.

The derivatives of the energy (1) with respect to $\rho_{nn'}$ and $\tilde{\rho}_{nn'}$ define

the particle-hole and particle-particle matrices

$$h_{nn'} = \frac{\partial E(\rho, \tilde{\rho})}{\partial \rho_{n'n}} = \sum_{\sigma\sigma'} \int d\mathbf{r} \psi_n^*(\mathbf{r}, \sigma) h(\mathbf{r}, \sigma, \sigma') \psi_{n'}(\mathbf{r}, \sigma'),$$

$$\tilde{h}_{nn'} = \frac{\partial E(\rho, \tilde{\rho})}{\partial \tilde{\rho}_{n'n}} = \sum_{\sigma\sigma'} \int d\mathbf{r} \psi_{n'}^*(\mathbf{r}, \sigma) \tilde{h}(\mathbf{r}, \sigma, \sigma') \psi_n(\mathbf{r}, \sigma'),$$
(3)

respectively, which enter the Skyrme-HFB equations

$$\begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h} & -h + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}.$$
(4)

2.2. Particle-number-projection

Let us consider, in the context of HFB theory, the PNP state:

$$|\Psi\rangle \equiv P^N |\Phi\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{i\phi(\hat{N}-N)} |\Phi\rangle,$$
(5)

where \hat{N} is the number operator, N is the particle number, and $|\Phi\rangle$ is the HFB wavefunction which does not have a well-defined particle number. As shown in Ref. ², the PNP HFB energy

$$E^N[\rho, \tilde{\rho}] = \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle} = \frac{\int d\phi \langle \Phi | H e^{i\phi(\hat{N}-N)} | \Phi \rangle}{\int d\phi \langle \Phi | e^{i\phi(\hat{N}-N)} | \Phi \rangle},$$
(6)

is again an energy functional of the unprojected densities ρ and $\tilde{\rho}$.

The situation, however, is not so simple in the case when the energy is deduced from an energy density functional. The source of the problem lies in the fact that the unprojected energy (1) is defined only in connection with one mean field state, i.e., one identifies formally $E[\rho, \tilde{\rho}] \iff \langle \Phi | \hat{H} | \Phi \rangle$ where $\rho(\mathbf{r}\sigma, \mathbf{r}'\sigma')$ and $\tilde{\rho}(\mathbf{r}\sigma, \mathbf{r}'\sigma')$ are densities associated with $|\Phi\rangle$.

The question is how to use the energy-density functionals in projection techniques which require the knowledge of off-diagonal (or “transitional”) expectation values:

$$\langle \Phi(0) | \hat{H} | \Phi(\phi) \rangle, \quad |\Phi(\phi)\rangle = e^{i\phi(\hat{N}-N)} |\Phi\rangle.$$
(7)

These are not automatically given by DFT. Extensions of the formalism are necessary and they are not unique. Various recipes are discussed in Ref. ³.

Let us consider in particular the “mixed density” recipe that treats all local densities as “mixed” (or “transitional”) ones defined between the

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states $\Phi(0)$ and $\Phi(\phi)$. In the case of the Skyrme force, the projected energy (6) reads:

$$E^N[\rho, \tilde{\rho}] = \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle} = \int d\phi y(\phi) \int d\mathbf{r} \left(H(\mathbf{r}, \phi) + \tilde{H}(\mathbf{r}, \phi) \right), \quad (8)$$

where

$$x(\phi) = \frac{1}{2\pi} \frac{e^{-i\phi N} \det(e^{i\phi} I)}{\sqrt{\det C(\phi)}}, \quad y(\phi) = \frac{x(\phi)}{\int d\phi' x(\phi')}, \quad (9)$$

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 “mixed” density matrices

$$\begin{aligned} \rho(\mathbf{r}\sigma, \mathbf{r}'\sigma', \phi) &= \sum_{nn'} \rho_{nn'}(\phi) \psi_{n'}^*(\mathbf{r}', \sigma') \psi_n(\mathbf{r}, \sigma), \\ \tilde{\rho}(\mathbf{r}\sigma, \mathbf{r}'\sigma', \phi) &= \sum_{nn'} \tilde{\rho}_{nn'}(\phi) \psi_{n'}^*(\mathbf{r}', \sigma') \psi_n(\mathbf{r}, \sigma), \end{aligned} \quad (10)$$

where

$$\begin{aligned} \rho_{n'n}(\phi) &= \frac{\langle \Phi | c_n^\dagger c_{n'} e^{i\phi \hat{N}} | \Phi \rangle}{\langle \Phi | e^{i\phi \hat{N}} | \Phi \rangle} = \sum_m C_{nm}(\phi) \rho_{mn'}, \\ \tilde{\rho}_{n'n}(\phi) &= e^{-i\phi} \sum_m C_{nm}(\phi) \tilde{\rho}_{mn'}, \\ C(\phi) &= e^{2i\phi} (1 + \rho(e^{2i\phi} - 1))^{-1}. \end{aligned} \quad (11)$$

Obviously, the projected energy (8) is again a functional of the unprojected density matrices ρ and $\tilde{\rho}$. Its derivatives with respect to $\rho_{n'n}$ and $\tilde{\rho}_{n'n}$ lead to the PNP Skyrme-HFB equations

$$\begin{pmatrix} h^N & \tilde{h}^N \\ \tilde{h}^N & -h^N \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E^N \begin{pmatrix} U \\ V \end{pmatrix}, \quad (12)$$

where

$$\begin{aligned}
 h^N &= \int d\phi y(\phi) Y(\phi) E(\phi) + \int d\phi y(\phi) e^{-2i\phi} C(\phi) h(\phi) C(\phi) \\
 &\quad - \frac{1}{2} \left[\int d\phi y(\phi) 2ie^{-i\phi} \sin(\phi) \tilde{\rho}(\phi) \tilde{h}(\phi) C(\phi) + \text{h.c.} \right], \\
 \tilde{h}^N &= \frac{1}{2} \int d\phi y(\phi) e^{-i\phi} \{ \tilde{h}(\phi) C(\phi) + (\tilde{h}(\phi) C(\phi))^T \}
 \end{aligned} \tag{13}$$

$$Y(\phi) = ie^{-i\phi} \sin \phi C(\phi) - i \int d\phi' y(\phi') e^{-i\phi'} \sin \phi' C(\phi').$$

The gauge-angle dependent field matrices $h(\phi)$ and $\tilde{h}(\phi)$ are obtained by simply replacing in the unprojected fields (3) the particle and pairing local densities with their gauge-angle dependent counterparts.

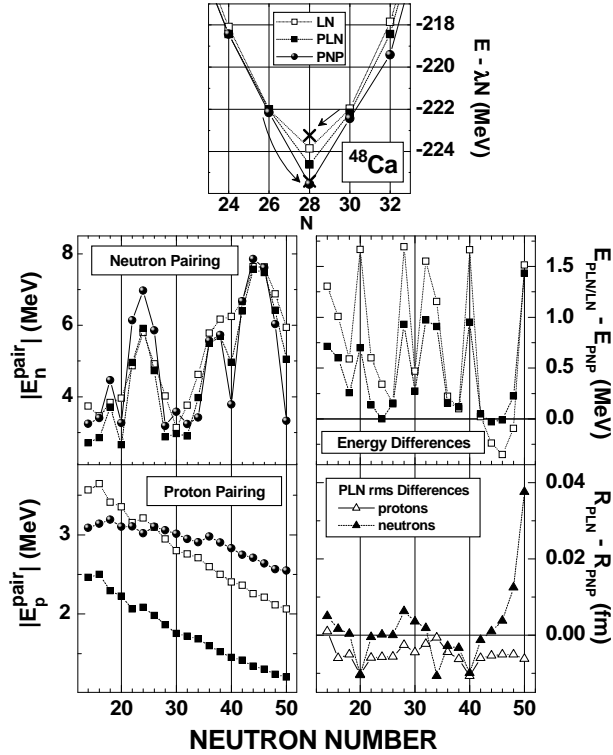


Figure 1. The LN and PLN (projection after variation), and PNP HFB (projection before variation) results obtained for the SLy4 force and mixed delta pairing. Arrows in the top panel indicate projection results from the neighboring nuclei.

2.3. Delta pairing forces

When using delta pairing forces, one has to restrict the quasiparticle space in order to avoid the divergences associated with the zero range. Within the unprojected HFB calculations, a pairing cut-off is introduced by using the so-called equivalent single-particle spectrum^{4,5}. After each iteration performed with a given chemical potential λ , one calculates an equivalent spectrum $\bar{\epsilon}_n$ and pairing gaps $\bar{\Delta}_n$:

$$\bar{\epsilon}_n = (1 - 2P_n)E_n + \lambda, \quad \bar{\Delta}_n = 2E_n\sqrt{P_n(1 - P_n)}, \quad (14)$$

where E_n are the quasiparticle energies and P_n denotes the norms of the lower HFB wave function. Due to the similarity between $\bar{\epsilon}_n$ and the single-particle energies, one can take into account only those quasiparticle states for which $\bar{\epsilon}_n$ is less than the cut-off energy ϵ_{cut} (usually around 60 MeV).

One can see that this procedure cannot be directly applied to the PNP HFB calculations, because the Lagrange multiplier λ entering the unprojected HFB Eqs. (4) is no longer available in Eq. (12). This means that the local densities emerging after each HFB diagonalization (12) are not automatically normalized to the particle number N . As a result, all auxiliary quantities, as e.g. the analogues of the quasiparticle energies, E_n^N , and probabilities, P_n^N , do not have the usual meaning. However, one can always reintroduce the Lagrange multiplier λ into Eq. (12) without changing the results, and adjust it to give a correct *average* particle number in the *unprojected* state. In practice, it is enough to calculate for the solutions of Eq. (12) the average values E_n of the unprojected HFB matrix and use them in Eq. (14) together with $P_n \equiv P_n^N$. This allows for defining the Lagrange multiplier and implementing the cut-off procedure.

2.4. Sample PNP HFB results

Figure 1 gives the PNP HFB results for the complete chain of the calcium isotopes (proton-neutron drip to drip line), calculated for the Sly4 force⁶ and mixed delta pairing⁵. Comparison is also made with the HFB Lipkin-Nogami (LN) results and projected (after variation) Lipkin-Nogami results (PLN). One can conclude that the PLN approximation works good for open-shell nuclei, where the total energy differences between various variants of calculations are less than 250 keV. For closed-shell nuclei⁷, 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 nuclei⁸, as illustrated in the top panel of

Fig. 1.

3. Shift Invariance Within DFT

Important consequences for the PNP HFB expectation values follow from the obvious shift invariance property ⁹

$$\underbrace{e^{\psi(\hat{N}-N)}}_{\hat{S}_\psi} |\Psi\rangle = |\Psi\rangle \quad (15)$$

of the PNP wave function (5), where ψ is an arbitrary number. For example, the energy (6) is obviously shift-invariant under the transformation \hat{S}_ψ since

$$E^N = \frac{\langle \Phi | \hat{H} | \Psi \rangle}{\langle \Phi | \Psi \rangle} = \frac{\langle \Phi | \hat{H} \hat{S}_\psi | \Psi \rangle}{\langle \Phi | \hat{S}_\psi | \Psi \rangle}. \quad (16)$$

Again, the situation becomes more complicated when the energy is deduced from an energy density functional.

3.1. The shift invariance under the “mixed density” recipe

In order to prove the shift invariance under the “mixed density” recipe, let us introduce the “mixed local densities” in their canonical representation

$$\begin{aligned} \rho_\phi(\mathbf{r}) &= \sum_n \frac{v_n^* v_n e^{2i\phi}}{u_n^* u_n + v_n^* v_n e^{2i\phi}} \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}), \\ \kappa_\phi(\mathbf{r}) &= \sum_n \frac{u_n^* v_n e^{2i\phi}}{u_n^* u_n + v_n^* v_n e^{2i\phi}} \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}), \\ \bar{\kappa}_\phi(\mathbf{r}) &= \sum_n \frac{u_n v_n^*}{u_n^* u_n + v_n^* v_n e^{2i\phi}} \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}). \end{aligned} \quad (17)$$

The energy (8) can be rewritten as

$$E^N = \frac{\int d\phi e^{-i\phi N} \mathbb{I}(\phi) \mathbb{E}(\kappa_\phi, \bar{\kappa}_\phi, \rho_\phi)}{\int d\phi e^{-i\phi N} \mathbb{I}(\phi)}, \quad \mathbb{I}(\phi) = \langle \Phi(0) | \Phi(\phi) \rangle. \quad (18)$$

As a rule of thumb, we note that the phase factor $e^{2i\phi}$ is always linked to v_n , considering v_n^* as an independent variable.

In order to check whether the definition (17)-(18) does also guarantees the shift invariance (16), one needs to show that $E^N = E^{(\text{shift})}$ where

$$E^{(\text{shift})} = \frac{\int d\phi e^{-i\phi N - \psi N} \mathbb{I}(\phi, \psi) \mathbb{E}(\kappa_{\phi\psi}, \bar{\kappa}_{\phi\psi}, \rho_{\phi\psi})}{\int d\phi e^{-i\phi N - \psi N} \mathbb{I}(\phi, \psi)}, \quad (19)$$

$$\mathbb{I}(\phi, \psi) = \langle \Phi(0) | e^{-\psi N} | \Phi(\phi) \rangle \quad (20)$$

and

$$\begin{aligned} \rho_{\phi\psi}(\mathbf{r}) &= \sum_n \frac{v_n^* v_n e^{2i\phi+2\psi}}{u_n^* u_n + v_n^* v_n e^{2i\phi+2\psi}} \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}), \\ \kappa_{\phi\psi}(\mathbf{r}) &= \sum_n \frac{u_n^* v_n e^{2i\phi+2\psi}}{u_n^* u_n + v_n^* v_n e^{2i\phi+2\psi}} \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}), \\ \bar{\kappa}_{\phi\psi}(\mathbf{r}) &= \sum_n \frac{u_n v_n^*}{u_n^* u_n + v_n^* v_n e^{2i\phi+2\psi}} \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}). \end{aligned} \quad (21)$$

The shift invariance is trivially maintained for the kinetic energy because this quantity is given by expectation value of an operator such that a reasoning as in Eq. (16) applies. To prove the invariance for other terms, we start from the observation that the shift is tightly linked to the r.h.s. occupation amplitude, i.e.

$$v_n \longleftrightarrow v_n e^{2i\phi+2\psi}. \quad (22)$$

Now we make the strong assumption that the energy expectation value can be expanded into a mixed power series with respect to v_n , v_n^* , u_n , and u_n^* . We collect terms having the same number of v_n . The numerator in the energy expression will then contain a kernel as

$$E^{(\text{num})} = \int d\phi e^{-i\phi N - \psi N} \sum_{N_v} \underbrace{v_{n_1} \dots v_{n_{N_v}}}_{N_v \text{ terms}} e^{i\phi N_v + \psi N_v} \sum_{\text{anything}} v_m^* \dots u_k \dots u_l^* \dots \quad (23)$$

The ϕ integration filters the term $N = N_v$, yielding

$$\int d\phi e^{-i\phi N} e^{i\phi N_v} \implies N = N_v \implies e^{-\psi N} e^{\psi N_v} = 1.$$

The same reasoning applies to the denominator. Thus both the numerator and the denominator in the projected energy expression are separately shift-invariant. This holds for DFT with the extension recipe (17).

The above demonstration relies on a power series expansion in order v^N . But such an expansion will not converge just around the critical point $u_n = v_n$. However, as we discuss later, one can always avoid the case containing the critical point $u_n = v_n$, and one indeed does not need such a proof expansion.

3.2. Other extensions of DFT

There are alternatives to the recipe((17)-(18)) suggested in Ref. ¹⁰. For example, one may use the projected densities as, e.g., $\rho^N(\mathbf{r})$ in the DFT energy expectation value. This reads, e.g., for the potential energy

$$E_{\text{pot}}^N = E_{\text{pot}}[\rho^N]. \quad (24)$$

With the same reasoning as above, one can show that $\rho^N(r)$ is shift invariant. The recipe (24) is then also shift-invariant. There are, however, objections for other reasons. For example, this recipe can be shown to be wrong in the simple case of a two-body point coupling force.

There is a proposal from ¹⁰ to extend the DFT definition just by adding two densities $\bar{\rho}_\phi(\mathbf{r})$ and $\bar{\rho}_0(\mathbf{r})$ associated with $\Phi(0)$ and $\Phi(\phi)$, respectively. The recipe consists in using an average value

$$E_{\text{pot}}(\rho) \longrightarrow \frac{1}{2} (E_{\text{pot}}[\bar{\rho}_0] + E_{\text{pot}}[\bar{\rho}_\phi]) \quad (25)$$

in the projection kernel. But note that $\bar{\rho}_\phi(r) = \bar{\rho}_0(r) = \rho(r)$ for that particular case of particle number projection. The phase factors $e^{2i\phi}$ just cancel out if used on bra and ket simultaneously. One then obtain

$$\frac{1}{2} (E_{\text{pot}}[\bar{\rho}_0] + E_{\text{pot}}[\bar{\rho}_\phi]) = E_{\text{pot}}[\rho], \quad (26)$$

i.e., one obtains the unprojected energy.

3.3. The innocent singularity in DFT applications

At first glance, the mixed density recipe (17)-(18) also has a problem. Looking at the denominator of the spatial densities (17), one notices a possible singularity at $u_n^2 = v_n^2 = 1/2$ for a gauge-angle $\phi \rightarrow \pi/2$. The shift invariance allows to show that this singularity is unimportant.

We assume that we have a discrete spectrum with a finite set of v_n and u_n . Now let it happen that $u_n^2 = v_n^2$. We apply a shift $v_n \longrightarrow v_n e^{2\psi}$ which guarantees that $u_n^2 \neq v_n^2$. In a discrete spectrum, one can always find a ψ such that all other amplitudes u_m and v_m stay different. We then can evaluate the projected energy without having dealt with singularity.

In numerical applications one can easily implement the shift $v_n \longrightarrow v_n e^{2\psi}$ by changing the normalization of the internal density

$$\int \bar{\rho}(\mathbf{r}) d\mathbf{r} = \bar{N}, \quad \bar{\rho}(\mathbf{r}) = \sum_n v_n^2 \varphi_n^\dagger(\mathbf{r}) \varphi_n(\mathbf{r}). \quad (27)$$

Different values of ψ correspond to different values of the normalization constant \bar{N} . Therefore, instead of ψ , one can keep the internal normalization constant \bar{N} fixed during the PNP HFB iterations. This could be achieved by introducing a Lagrange multiplier μ by means of Eq. (27), and μ always goes to zero when the PNP HFB solution is achieved.

Indeed, all the numerical tests we have performed have shown that the PNP HFB results do not depend on the particular values of \bar{N} , and perfect shift invariance is always achieved. Changing the intrinsic normalization \bar{N} in a wide range, occupation probability v^2 , which is closer to the critical value $1/2$, varies from 0.076 to 0.945, but all nuclear characteristics remain unchanged.

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