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Axially deformed solution of the Skyrme–Hartree–Fock–Bogolyubov equations using the transformed harmonic oscillator basis. The program HFBTHO (v1.66p) ☆

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Abstract

We describe the program HFBTHO for axially deformed configurational Hartree–Fock–Bogolyubov calculations with Skyrme-forces and zero-range pairing interaction using Harmonic-Oscillator and/or Transformed Harmonic-Oscillator states. The particle-number symmetry is approximately restored using the Lipkin–Nogami prescription, followed by an exact particle number projection after the variation. The program can be used in a variety of applications, including systematic studies of wide ranges of nuclei, both spherical and axially deformed, extending all the way out to nucleon drip lines.

Program summary

Title of the program: HFBTHO (v1.66p)
Catalogue number: ADUI
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADUI
Licensing provisions: none
Computers on which the program has been tested: Pentium-III, Pentium-IV, AMD-Athlon, IBM Power 3, IBM Power 4, Intel Xeon

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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doi:10.1016/j.cpc.2005.01.001

Operating systems: LINUX, Windows
Programming language used: FORTRAN-95
Memory required to execute with typical data: 59 MB when using $N_{\mathrm{sh}} = 20$
No. of bits in a word: 64
No. of processors used: 1
Has the code been vectorized?: No
No. of bytes in distributed program, including test data, etc.: 195 285
No. of lines in distributed program: 12 058
Distribution format: tar.gz
Nature of physical problem: The solution of self-consistent mean-field equations for weakly bound paired nuclei requires a correct description of the asymptotic properties of nuclear quasiparticle wave functions. In the present implementation, this is achieved by using the single-particle wave functions of the Transformed Harmonic Oscillator, which allows for an accurate description of deformation effects and pairing correlations in nuclei arbitrarily close to the particle drip lines.
Method of solution: The program uses the axially Transformed Harmonic Oscillator (THO) single-particle basis to expand quasiparticle wave functions. It iteratively diagonalizes the Hartree–Fock–Bogolyubov Hamiltonian based on the Skyrme-forces and zero-range pairing interaction until a self-consistent solution is found.
Restrictions on the complexity of the problem: Axial-, time-reversal-, and space-inversion symmetries are assumed. Only quasiparticle vacua of even–even nuclei can be calculated.
Typical running time: 4 s per iteration on an Intel Xeon 2.8 GHz processor when using $N_{\mathrm{sh}} = 20$
Unusual features of the program: none

PACS: 07.05.T; 21.60.-n; 21.60.Jz

Keywords: Hartree–Fock; Hartree–Fock–Bogolyubov; Nuclear many-body problem; Skyrme interaction; Self-consistent mean-field; Quadrupole deformation; Constrained calculations; Energy surface; Pairing; Particle number projection; Nuclear radii; Quasiparticle spectra; Harmonic oscillator; Coulomb field

1. Introduction

Nuclear structure theory strives to build a comprehensive microscopic framework in which bulk nuclear properties, nuclear excitations, and nuclear reactions can all be described. Exotic radioactive nuclei are the critical new focus in this quest. The extreme isospin of these nuclei and their weak binding bring new phenomena that amplify important features of the nuclear many-body problem.

A proper theoretical description of such weakly bound systems requires a careful treatment of the asymptotic part of the nucleonic density. An appropriate framework for these calculations is Hartree–Fock–Bogolyubov (HFB) theory, solved in the coordinate representation [1,2]. This method has been used extensively in the treatment of spherical nuclei [3], but is much more difficult to implement for systems with deformed equilibrium shapes. There have been three ways of implementing deformation effects into the coordinate-space HFB. The oldest method, the so-called two-basis method [4–6], is based on the diagonalization of the particle–particle part of the HFB Hamiltonian in the self-consistent basis, obtained by solving the HF problem with box boundary conditions. The disadvantage of this method is the appearance of a large number of positive-energy free-particle (box) states, which limits the number of discretized continuum states (the maximum single-particle energy taken in this method is usually less than 10 MeV).

The second, very promising strategy, the so-called canonical-basis HFB method, utilizes the spatially localized eigenstates of the one-body density matrix without explicitly going to the quasiparticle representation [7–9]. Finally, an approach to axial coordinate-space HFB has recently been developed that uses a basis-spline method [10,11]. While precise, these two latter methods are not easy to implement and, because they are time-consuming, cannot be used in large-scale calculations in which a crucial factor is the ability to perform quick calculations for many nuclei.

In the absence of fast coordinate-space solutions to the deformed HFB equations, it is useful to consider instead the configuration-space approach, whereby the HFB solution is expanded in some single-particle basis. In this context, the basis of a harmonic oscillator (HO) turned out to be particularly useful. Over the years, many configuration-space HFB+HO codes have been developed, either employing Skyrme forces or the Gogny effective interaction [12–16], or using a relativistic Lagrangian [17] in the context of the relativistic Hartree–Bogolyubov theory. For nuclei at the drip lines, however, the HFB+HO expansion converges slowly as a function of the number of oscillator shells [3], producing wave functions that decay too rapidly at large distances.

A related alternative approach that has recently been proposed is to expand the quasiparticle HFB wave functions in a complete set of transformed harmonic oscillator (THO) basis states [18], obtained by applying a local-scaling coordinate transformation (LST) [19,20] to the standard HO basis. Applications of this HFB+THO methodology have been reported both in the nonrelativistic [21] and relativistic domains [22]. In all of these calculations, specific global parameterizations were employed for the scalar LST function that defines the THO basis. There are several limitations in such an approach, however. For example, the minimization procedure that is needed in such an approach to optimally define the basis parameters is computationally very time-consuming, making it very difficult to apply the method systematically to nuclei across the periodic table.

Recently, a new prescription for choosing the THO basis has been proposed and employed in self-consistent large-scale calculations [23]. For a given nucleus, the new prescription requires as input the results from a relatively simple HFB+HO calculation, with no variational optimization. The resulting THO basis leads to HFB+THO results that almost exactly reproduce the coordinate-space HFB results for spherical nuclei [24]. Because the new prescription requires no variational optimization of the LST function, it can be applied in systematic studies of nuclear properties. In order to correct for the particle number nonconservation inherent to the HFB approach, the Lipkin–Nogami prescription for an approximate particle number projection, followed by an exact particle number projection after the variation has been implemented in the code HFBTHO (v1.66p) [25,26].

The paper is organized as follows. Section 2 gives a brief summary of the HFB formalism. The implementation of the method to the case of the Skyrme energy density functional is discussed in Section 3, together with the overview of the THO method and the treatment of pairing. Section 4 describes the code HFBTHO (v1.66p). Finally, conclusions are given in Section 5.

2. Hartree–Fock–Bogolyubov method

A two-body Hamiltonian of a system of fermions can be expressed in terms of a set of annihilation and creation operators $(c, c^\dagger)$:

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c^\dagger_{n_1} c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c^\dagger_{n_1} c^\dagger_{n_2} c_{n_4} c_{n_3}, \tag{1}$$

where $\bar{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle$ are anti-symmetrized two-body interaction matrix-elements. In the HFB method, the ground-state wave function $|\Phi\rangle$ is defined as the quasiparticle vacuum $\alpha_k |\Phi\rangle = 0$, where the quasiparticle operators $(\alpha, \alpha^\dagger)$ are connected to the original particle operators via a linear Bogolyubov transformation

$$\alpha_k = \sum_n \left(U^*_{nk} c_n + V^*_{nk} c^\dagger_n \right), \qquad \alpha^\dagger_k = \sum_n \left(V_{nk} c_n + U_{nk} c^\dagger_n \right), \tag{2}$$

which can be rewritten in the matrix form as

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^{\mathrm{T}} & U^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}. \tag{3}$$

The matrices U and V satisfy the relations:

$$U^\dagger U + V^\dagger V = I, \qquad U U^\dagger + V^* V^{\mathrm{T}} = I, \qquad U^{\mathrm{T}} V + V^{\mathrm{T}} U = 0, \qquad U V^\dagger + V^* U^{\mathrm{T}} = 0. \tag{4}$$

In terms of the normal ρ and pairing κ one-body density matrices, defined as

$$\rho_{nn'} = \left\langle \Phi \left| c^{\dagger}_{n'} c_n \right| \Phi \right\rangle = (V^* V^{\mathrm{T}})_{nn'}, \qquad \kappa_{nn'} = \langle \Phi | c_{n'} c_n | \Phi \rangle = (V^* U^{\mathrm{T}})_{nn'}, \tag{5}$$

the expectation value of the Hamiltonian (1) is expressed as an energy functional

$$E[\rho,\kappa] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \mathrm{Tr}\left[\left(e + \frac{1}{2}\Gamma\right)\rho\right] - \frac{1}{2}\,\mathrm{Tr}[\Delta\kappa^*], \tag{6}$$

where

$$\Gamma_{n_1 n_3} = \sum_{n_2 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \rho_{n_4 n_2}, \qquad \Delta_{n_1 n_2} = \frac{1}{2} \sum_{n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4}. \tag{7}$$

The variation of the energy (6) with respect to ρ and κ results in the HFB equations:

$$\begin{pmatrix} e + \Gamma - \lambda & \Delta \\ -\Delta^* & -(e+\Gamma)^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}, \tag{8}$$

where the Lagrange multiplier λ has been introduced to fix the correct average particle number.

It should be stressed that the modern energy functionals (6) contain terms that cannot be simply related to some prescribed effective interaction, see, e.g., Refs. [27,28] for details. In this respect the functional (6) should be considered in the broader context of the energy density functional theory.

3. Skyrme Hartree–Fock–Bogolyubov method

3.1. Skyrme energy density functional

For Skyrme forces, the HFB energy (6) has the form of a local energy density functional,

$$E[\rho,\tilde{\rho}] = \int \mathrm{d}^3\mathbf{r}\, \mathcal{H}(\mathbf{r}), \tag{9}$$

where

$$\mathcal{H}(\mathbf{r}) = H(\mathbf{r}) + \tilde{H}(\mathbf{r}) \tag{10}$$

is the sum of the mean-field and pairing energy densities. In the present implementation, we use the following explicit forms:

$$\begin{aligned} H(\mathbf{r}) = {} & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_q \rho_q^2\right] \\ & + \frac{1}{2}t_1\left[\left(1+\frac{1}{2}x_1\right)\rho\left(\tau - \frac{3}{4}\Delta\rho\right) - \left(\frac{1}{2}+x_1\right)\sum_q \rho_q\left(\tau_q - \frac{3}{4}\Delta\rho_q\right)\right] \\ & + \frac{1}{2}t_2\left[\left(1+\frac{1}{2}x_2\right)\rho\left(\tau + \frac{1}{4}\Delta\rho\right) - \left(\frac{1}{2}+x_2\right)\sum_q \rho_q\left(\tau_q + \frac{1}{4}\Delta\rho_q\right)\right] \\ & + \frac{1}{12}t_3\rho^{\alpha}\left[\left(1+\frac{1}{2}x_3\right)\rho^2 - \left(x_3+\frac{1}{2}\right)\sum_q \rho_q^2\right] \\ & - \frac{1}{8}(t_1x_1 + t_2x_2)\sum_{ij}\mathbf{J}_{ij}^2 + \frac{1}{8}(t_1 - t_2)\sum_{q,ij}\mathbf{J}_{q,ij}^2 - \frac{1}{2}W_0\sum_{ijk}\varepsilon_{ijk}\left[\rho\nabla_k\mathbf{J}_{ij} + \sum_q \rho_q \nabla_k \mathbf{J}_{q,ij}\right] \end{aligned} \tag{11}$$

and

$$\tilde{H}(\mathbf{r}) = \frac{1}{2}V_0\left[1 - V_1\left(\frac{\rho}{\rho_0}\right)^{\gamma}\right]\sum_q \tilde{\rho}_q^2. \tag{12}$$

The index q labels the neutron ($q = n$) or proton ($q = p$) densities, while densities without index denote the sums of proton and neutron densities. $H(\mathbf{r})$ and $\tilde{H}(\mathbf{r})$ depend on the local particle density $\rho(\mathbf{r})$, local pairing density $\tilde{\rho}(\mathbf{r})$, kinetic energy density $\tau(\mathbf{r})$, and spin-current density $\mathbf{J}_{ij}(\mathbf{r})$:

$$\begin{aligned}
&\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}), \qquad \tilde{\rho}(\mathbf{r}) = \tilde{\rho}(\mathbf{r},\mathbf{r}),\\
&\tau(\mathbf{r}) = \nabla_{\mathbf{r}}\nabla_{\mathbf{r}'}\rho(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}}, \qquad \mathbf{J}_{ij}(\mathbf{r}) = \frac{1}{2i}(\nabla_i - \nabla_i')\rho_j(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}},
\end{aligned} \tag{13}$$

where $\rho(\mathbf{r},\mathbf{r}')$, $\rho_i(\mathbf{r},\mathbf{r}')$, $\tilde{\rho}(\mathbf{r},\mathbf{r}')$, $\tilde{\rho}_i(\mathbf{r},\mathbf{r}')$ are defined by the spin-dependent one-body density matrices in the standard way:

$$\begin{aligned}
\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma') &= \frac{1}{2}\rho(\mathbf{r},\mathbf{r}')\delta_{\sigma\sigma'} + \frac{1}{2}\sum_i(\sigma|\sigma_i|\sigma')\rho_i(\mathbf{r},\mathbf{r}'),\\
\tilde{\rho}(\mathbf{r}\sigma,\mathbf{r}'\sigma') &= \frac{1}{2}\tilde{\rho}(\mathbf{r},\mathbf{r}')\delta_{\sigma\sigma'} + \frac{1}{2}\sum_i(\sigma|\sigma_i|\sigma')\tilde{\rho}_i(\mathbf{r},\mathbf{r}').
\end{aligned} \tag{14}$$

We use the pairing density matrix $\tilde{\rho}$,

$$\tilde{\rho}(\mathbf{r}\sigma,\mathbf{r}'\sigma') = -2\sigma'\kappa(\mathbf{r},\sigma,\mathbf{r}',-\sigma'), \tag{15}$$

instead of the pairing tensor κ. This is convenient for describing time-even quasiparticle states when both ρ and $\tilde{\rho}$ are hermitian and time-even [2]. In the pairing energy density (12), we have restricted our consideration to contact (delta) pairing forces in order to reduce the complexity of the general expressions [2,28].

3.2. Skyrme Hartree–Fock–Bogolyubov equations

The variation of the energy (9) with respect to ρ and $\tilde{\rho}$ results in the Skyrme HFB equations:

$$\sum_{\sigma'}\begin{pmatrix} h(\mathbf{r},\sigma,\sigma') & \tilde{h}(\mathbf{r},\sigma,\sigma') \\ \tilde{h}(\mathbf{r},\sigma,\sigma') & -h(\mathbf{r},\sigma,\sigma')\end{pmatrix}\begin{pmatrix} U(E,\mathbf{r}\sigma') \\ V(E,\mathbf{r}\sigma')\end{pmatrix} = \begin{pmatrix} E+\lambda & 0 \\ 0 & E-\lambda\end{pmatrix}\begin{pmatrix} U(E,\mathbf{r}\sigma) \\ V(E,\mathbf{r}\sigma)\end{pmatrix}, \tag{16}$$

where local fields $h(\mathbf{r},\sigma,\sigma')$ and $\tilde{h}(\mathbf{r},\sigma,\sigma')$ can be easily calculated in the coordinate space by using the following explicit expressions:

$$\begin{aligned}
h_q(\mathbf{r},\sigma,\sigma') &= -\nabla M_q\nabla + U_q + \frac{1}{2i}\sum_{ij}(\nabla_i\sigma_j B_{q,ij} + B_{q,ij}\nabla_i\sigma_j t),\\
\tilde{h}_q(\mathbf{r},\sigma,\sigma') &= V_0\left(1 - V_1\left(\frac{\rho}{\rho_0}\right)^{\gamma}\right)\tilde{\rho}_q,
\end{aligned} \tag{17}$$

where

$$\begin{aligned}
M_q &= \frac{\hbar^2}{2m} + \frac{1}{4}t_1\left[\left(1+\frac{1}{2}x_1\right)\rho - \left(x_1+\frac{1}{2}\right)\rho_q^2\right] + \frac{1}{4}t_2\left[\left(1+\frac{1}{2}x_2\right)\rho + \left(x_2+\frac{1}{2}\right)\rho_q^2\right],\\
B_{q,ij} &= -\frac{1}{4}(t_1x_1 + t_2x_2)\mathbf{J}_{ij} + \frac{1}{4}(t_1 - t_2)\mathbf{J}_{q,ij} + \frac{1}{2}W_0\sum_{ijk}\varepsilon_{ijk}\nabla_k(\rho + \rho_q),
\end{aligned}$$

$$
\begin{aligned}
U_q = {} & t_0\left[\left(1+\frac{1}{2}x_0\right)\rho - \left(x_0+\frac{1}{2}\right)\rho_q\right] \\
& + \frac{1}{4}t_1\left[\left(1+\frac{1}{2}x_1\right)\left(\tau - \frac{3}{2}\Delta\rho\right) - \left(x_1+\frac{1}{2}\right)\left(\tau_q - \frac{3}{2}\Delta\rho_q\right)\right] \\
& + \frac{1}{4}t_2\left[\left(1+\frac{1}{2}x_2\right)\left(\tau + \frac{1}{2}\Delta\rho\right) + \left(x_2+\frac{1}{2}\right)\left(\tau_q + \frac{1}{2}\Delta\rho_q\right)\right] \\
& + \frac{1}{12}t_3\rho^\alpha\left[\left(1+\frac{1}{2}x_3\right)(2+\alpha)\rho - \left(x_3+\frac{1}{2}\right)\left(2\rho_q + \frac{\alpha}{\rho}\sum_{q'}\rho_{q'}^2\right)\right] \\
& - \frac{\gamma V_0 V_1}{2\rho}\left(\frac{\rho}{\rho_0}\right)^\gamma \sum_q \tilde{\rho}_q^2 - \frac{1}{2}W_0\sum_{ijk}\varepsilon_{ijk}\nabla_k[\mathbf{J}_{ij} + \mathbf{J}_{q,ij}].
\end{aligned}
\tag{18}
$$

The properties of the HFB equation in spatial coordinates, Eq. (16), have been discussed in Ref. [2]. In particular, it has been shown that the spectrum of eigenenergies E is continuous for $|E| > -\lambda$ and discrete for $|E| < -\lambda$. In the present implementation, we solve the HFB equations by expanding quasiparticle wave functions in a finite basis; therefore, the quasiparticle spectrum E_k becomes discretized. Hence in the following we use the notation $V_k(\mathbf{r}\sigma) = V(E_k, \mathbf{r}\sigma)$ and $U_k(\mathbf{r}\sigma) = U(E_k, \mathbf{r}\sigma)$. Since for $E_k > 0$ and $\lambda < 0$ the lower components $V_k(\mathbf{r}\sigma)$ are localized functions of $\mathbf{r}$, the density matrices,

$$
\rho(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \sum_k V_k(\mathbf{r}\sigma)V_k^*(\mathbf{r}'\sigma'), \tag{19}
$$

$$
\tilde{\rho}(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\sum_k V_k(\mathbf{r}\sigma)U_k^*(\mathbf{r}'\sigma'), \tag{20}
$$

are always localized. The orthogonality relation for the single-quasiparticle HFB wave functions reads

$$
\int \mathrm{d}^3\mathbf{r}\sum_\sigma\left[U_k^*(\mathbf{r}\sigma)U_{k'}(\mathbf{r}\sigma) + V_k^*(\mathbf{r}\sigma)V_{k'}(\mathbf{r}\sigma)\right] = \delta_{k,k'}, \tag{21}
$$

and the norms of the lower components N_k,

$$
N_k = \int \mathrm{d}^3\mathbf{r}\sum_\sigma \left|V_k(\mathbf{r}\sigma)\right|^2, \tag{22}
$$

define the total number of particles

$$
N = \int \mathrm{d}^3\mathbf{r}\rho(\mathbf{r}) = \sum_n N_k. \tag{23}
$$

3.3. Axially deformed nuclei

For spherical nuclei, the Skyrme HFB equations are best solved in the coordinate space, because Eq. (16) reduces in this case to a set of radial differential equations [29]. In the case of deformed nuclei, however, the solution of a deformed HFB equation in coordinate space is a difficult and time-consuming task. For this reason, here we use the method proposed by Vautherin [30], which combines two different representations. The solution of the deformed HFB equation is carried out by diagonalizing the HFB Hamiltonian in the configurational space of wave-functions with appropriate symmetry, while evaluation of the potentials and densities is performed in coordinate space. Such a method is applicable to nonaxial deformations [16], but typical computation times for large-scale mass-table calculations are prohibitively large. In the present implementation, we make the restriction to axially-symmetric and reflection-symmetric shapes in order to obtain HFB solutions within a much shorter CPU time.

In the case of axial symmetry, the third component J_z of the total angular momentum is conserved and provides a good quantum number Ω_k. Therefore, quasiparticle HFB states can be written in the following form:

$$\begin{pmatrix} U_k(\mathbf{r},\sigma,\tau) \\ V_k(\mathbf{r},\sigma,\tau) \end{pmatrix} = \chi_{q_k}(\tau)\left[\begin{pmatrix} U_k^+(r,z) \\ V_k^+(r,z) \end{pmatrix} \mathrm{e}^{\mathrm{i}\Lambda^-\varphi}\chi_{+1/2}(\sigma) + \begin{pmatrix} U_k^-(r,z) \\ V_k^-(r,z) \end{pmatrix} \mathrm{e}^{\mathrm{i}\Lambda^+\varphi}\chi_{-1/2}(\sigma)\right], \tag{24}$$

where $\Lambda^\pm = \Omega_k \pm 1/2$ and r, z, and φ are the standard cylindrical coordinates defining the three-dimensional position vector as $\mathbf{r} = (r\cos\varphi, r\sin\varphi, z)$, while z is the chosen symmetry axis. The quasiparticle states (24) are also assumed to be eigenstates of the third component of the isospin operator with eigenvalues $q_k = +1/2$ for protons and $q_k = -1/2$ for neutrons.

By substituting ansatz (24) into Eq. (16), the HFB equation reduces to a system of equations involving the cylindrical variables r and z only. The same is also true for the local densities, i.e.

$$\begin{aligned}
\rho(r,z) &= \sum_k \left(\left|V_k^+(r,z)\right|^2 + \left|V_k^-(r,z)\right|^2\right), \\
\tau(r,z) &= \sum_k \Bigg(\left|\nabla_r V_k^+(r,z)\right|^2 + \left|\nabla_r V_k^-(r,z)\right|^2 + \frac{1}{r^2}\left|\Lambda^+ V_k^-(r,z)\right|^2 \\
&\quad + \left|\nabla_z V_k^+(r,z)\right|^2 + \left|\nabla_z V_k^-(r,z)\right|^2 + \frac{1}{r^2}\left|\Lambda^- V_k^+(r,z)\right|^2\Bigg), \\
(\nabla\cdot\mathbf{J})(r,z) &= \sum_k \Bigg(\nabla_r V_k^+(r,z)\nabla_z V_k^-(r,z) + \frac{\Lambda^-}{r} V_k^+(r,z)\left[\nabla_r V_k^+(r,z) - \nabla_z V_k^-(r,z)\right] \\
&\quad - \nabla_r V_k^-(r,z)\nabla_z V_k^+(r,z) - \frac{\Lambda^+}{r} V_k^-(r,z)\left[\nabla_r V_k^-(r,z) + \nabla_z V_k^+(r,z)\right]\Bigg), \\
\tilde\rho(r,z) &= -\sum_k \left(V_k^+(r,z)U_k^+(r,z) + V_k^-(r,z)U_k^-(r,z)\right),
\end{aligned} \tag{25}$$

where $\nabla_r = \partial/\partial r$ and $\nabla_z = \partial/\partial z$. When tensor forces are considered, the following additional densities have to be calculated:

$$\begin{aligned}
J_{r\varphi}(r,z) &= \sum_k \left(\nabla_r V_k^+(r,z)V_k^-(r,z) - \nabla_r V_k^-(r,z)V_k^+(r,z)\right), \\
J_{\varphi r}(r,z) &= \sum_k \left(\frac{\Lambda^-}{r} V_k^+(r,z)V_k^-(r,z) + \frac{\Lambda^+}{r} V_k^-(r,z)V_k^+(r,z)\right), \\
J_{z\varphi}(r,z) &= \sum_k \left(\nabla_z V_k^+(r,z)V_k^-(r,z) - \nabla_z V_k^-(r,z)V_k^+(r,z)\right), \\
J_{\varphi z}(r,z) &= \sum_k \left(\frac{\Lambda^-}{r} V_k^+(r,z)V_k^+(r,z) - \frac{\Lambda^+}{r} V_k^-(r,z)V_k^-(r,z)\right),
\end{aligned} \tag{26}$$

where indices denote the cylindrical components of the tensor $\mathbf{J}_{ij}$, while all remaining components vanish due to the cylindrical symmetry, i.e. $J_{rr}(r,z) = J_{zz}(r,z) = J_{\varphi\varphi}(r,z) = J_{rz}(r,z) = J_{zr}(r,z) = 0$.

Due to the time-reversal symmetry, if the kth state, defined by the set $\{U_k^+, U_k^-, V_k^+, V_k^-, \Omega_k\}$, satisfies the HFB equation (16), then the $\bar{k}$th state, corresponding to the set defined by $\{U_k^+, -U_k^-, V_k^+, -V_k^-, -\Omega_k\}$, also satisfies the HFB equation for the same quasiparticle energy E_k. Moreover, all wave functions in cylindrical coordinates are real. The contributions from the time-reversed states k and $\bar{k}$ are identical (we assume that the set of occupied states is invariant with respect to the time-reversal), and we can restrict all summations to positive values of Ω_k

while multiplying total results by a factor two. In a similar way, one can see that due to the assumed reflection symmetry, only positive values of z need to be considered.

3.4. HO and THO wave functions

The solution of the HFB equation (16) is obtained by expanding the quasiparticle function (24) in a given complete set of basis wave functions that conserve axial symmetry and parity. The program HFBTHO (v1.66p) is able to do so for the two basis sets of wave functions: HO and THO.

The HO set consists of eigenfunctions of a single-particle Hamiltonian for an axially deformed harmonic oscillator potential. By using the standard oscillator constants:

$$\beta_z = \frac{1}{b_z} = \left(\frac{m\omega_z}{\hbar}\right)^{1/2}, \qquad \beta_\perp = \frac{1}{b_\perp} = \left(\frac{m\omega_\perp}{\hbar}\right)^{1/2}, \tag{27}$$

and auxiliary variables

$$\xi = z\beta_z, \qquad \eta = r^2\beta_\perp^2, \tag{28}$$

the HO eigenfunctions are written explicitly as

$$\Phi_\alpha(\mathbf{r},\sigma) = \psi_{n_r}^{\Lambda}(r)\psi_{n_z}(z)\frac{\mathrm{e}^{\mathrm{i}\Lambda\varphi}}{\sqrt{2\pi}}\chi_\Sigma(\sigma), \tag{29}$$

where

$$\begin{aligned}\psi_{n_r}^{\Lambda}(r) &= \beta_\perp\tilde{\psi}_{n_r}^{\Lambda}(\eta) = N_{n_r}^{\Lambda}\beta_\perp\sqrt{2}\eta^{|\Lambda|/2}\mathrm{e}^{-\eta/2}L_{n_r}^{|\Lambda|}(\eta),\\ \psi_{n_z}(z) &= \beta_z^{1/2}\tilde{\psi}_{n_z}(\xi) = N_{n_z}\beta_z^{1/2}\mathrm{e}^{-\xi^2/2}H_{n_z}(\xi).\end{aligned} \tag{30}$$

$H_{n_z}(\xi)$ and $L_{n_r}^{\Lambda}(\eta)$ denote the Hermite and associated Laguerre polynomials [31], respectively, and the normalization factors read

$$N_{n_z} = \left(\frac{1}{\sqrt{\pi}2^{n_z}n_z!}\right)^{1/2} \quad \text{and} \quad N_{n_r}^{\Lambda} = \left(\frac{n_r!}{(n_r+|\Lambda|)!}\right)^{1/2}. \tag{31}$$

The set of quantum numbers $\alpha = \{n_r, n_z, \Lambda, \Sigma\}$ includes the numbers of nodes, n_r and n_z, in the r- and z-directions, respectively, and the projections on the z-axis, Λ and Σ, of the angular momentum operator and the spin.

The HO energy associated with the HO state (29) reads

$$\epsilon_\alpha = \big(2n_r + |\Lambda| + 1\big)\hbar\omega_\perp + \left(n_z + \frac{1}{2}\right)\hbar\omega_z, \tag{32}$$

and the basis used by the code consists of $M_0 = (N_{\mathrm{sh}}+1)(N_{\mathrm{sh}}+2)(N_{\mathrm{sh}}+3)/6$ states having the lowest energies ϵ_α for the given frequencies $\hbar\omega_\perp$ and $\hbar\omega_z$. In this way, for the spherical basis, i.e. for $\hbar\omega_\perp = \hbar\omega_z$, all HO shells with the numbers of quanta $N = 0, \ldots, N_{\mathrm{sh}}$ are included in the basis. When the basis becomes deformed, $\hbar\omega_\perp \neq \hbar\omega_z$, the code selects the lowest-HO-energy basis states by checking the HO energies of all states up to 50 HO quanta. Note that in this case the maximum value of the quantum number Ω_k, and the number of blocks in which the HFB equation is diagonalized, see Section 3.5, depend on the deformation of the basis.

The THO set of basis wave functions consists of transformed harmonic oscillator functions, which are generated by applying the local scale transformation (LST) [19,20,32] to the HO single-particle wave functions (29). In the

axially deformed case, the LST acts only on the cylindrical coordinates r and z, i.e.

$$\begin{aligned} r \to r' \equiv r'(r,z) &= r\frac{f(\mathcal{R})}{\mathcal{R}}, \\ z \to z' \equiv z'(r,z) &= z\frac{f(\mathcal{R})}{\mathcal{R}}, \end{aligned} \tag{33}$$

and the resulting THO wave functions read

$$\Phi_\alpha(\mathbf{r},\sigma) = \sqrt{\frac{f^2(\mathcal{R})}{\mathcal{R}^2}\frac{\partial f(\mathcal{R})}{\partial \mathcal{R}}}\psi^{\Lambda}_{n_r}\left(\frac{r}{\mathcal{R}}f(\mathcal{R})\right)\psi_{n_z}\left(\frac{z}{\mathcal{R}}f(\mathcal{R})\right)\frac{\mathrm{e}^{\mathrm{i}\Lambda\varphi}}{\sqrt{2\pi}}\chi_\Sigma(\sigma), \tag{34}$$

where

$$\mathcal{R} = \sqrt{\frac{z^2}{b_z^2} + \frac{r^2}{b_\perp^2}}, \tag{35}$$

and $f(\mathcal{R})$ is a scalar LST function. In the code HFBTHO (v1.66p), the function $f(\mathcal{R})$ is chosen as in Ref. [23]. It transforms the incorrect Gaussian asymptotic behavior of deformed HO wave functions into the correct exponential form. Below, we keep the same notation $\Phi_\alpha(\mathbf{r},\sigma)$ for both HO and THO wave functions, because expressions in which they enter are almost identical in both cases and are valid for both HO and THO variants.

3.5. HFB diagonalization in configurational space

We use the same basis wave functions to expand upper and lower components of the quasiparticle states, i.e.

$$\begin{aligned} U_k(\mathbf{r},\sigma,\tau) &= \chi_{q_k}(\tau)\sum_\alpha U_{k\alpha}\Phi_\alpha(\mathbf{r},\sigma), \\ V_k(\mathbf{r},\sigma,\tau) &= \chi_{q_k}(\tau)\sum_\alpha V_{k\alpha}\Phi_\alpha(\mathbf{r},\sigma), \end{aligned} \tag{36}$$

where $\Phi_\alpha(\mathbf{r},\sigma)$ are the HO or THO basis states. Note that the same basis $\Phi_\alpha(\mathbf{r},\sigma)$ is used for protons and neutrons.

Inserting expression (36) into the HFB equation (16) and using the orthogonality of the basis states, we find that the expansion coefficients have to be eigenvectors of the HFB Hamiltonian matrix

$$\begin{pmatrix} h^{(q_k)} - \lambda^{(q_k)} & \tilde{h}^{(q_k)} \\ \tilde{h}^{(q_k)} & -h^{(q_k)} + \lambda^{(q_k)} \end{pmatrix}\begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k\begin{pmatrix} U_k \\ V_k \end{pmatrix}, \tag{37}$$

where the quasiparticle energies E_k, the chemical potential $\lambda^{(q_k)}$, and the matrices

$$h^{(q)}_{\alpha\beta} = \langle\Phi_\alpha|h_q|\Phi_\beta\rangle \quad \text{and} \quad \tilde{h}^{(q)}_{\alpha\beta} = \langle\Phi_\alpha|\tilde{h}_q|\Phi_\beta\rangle \tag{38}$$

are defined for a given proton ($q_k = +1/2$) or neutron ($q_k = -1/2$) block.

Proton and neutron blocks are decoupled and can be diagonalized separately. Furthermore, in the case of axially deformed nuclei considered here, $\Omega_k = \Lambda_k + \Sigma_k$ is a good quantum number and, therefore, the matrices $h^{(q)}_{\alpha\beta}$ and $\tilde{h}^{(q)}_{\alpha\beta}$ are block diagonal, each block being characterized by a given value of Ω. Moreover, for the case of conserved parity considered here, $\pi = (-1)^{n_z+\Lambda}$ is also a good quantum number, and each of the Ω_k blocks falls into two sub-blocks characterized by the values of $\pi = \pm 1$. Finally, due to the time-reversal symmetry, the Hamiltonian matrices need to be constructed for positive values of Ω_k only.

3.6. Calculations of matrix elements

As discussed in Section 3.2, local densities (25) and average fields, (17) and (18), are calculated in coordinate space. Therefore, the calculation of matrix elements (38) amounts to calculating appropriate spatial integrals in the cylindrical coordinates r and z. In practice, the integration is carried out by using Gaussian quadratures [31] for 22 Gauss–Hermite points in the $z > 0$ direction and 22 Gauss–Laguerre points in the r-direction. This gives a sufficient accuracy for calculations up to $N_{\rm sh} = 40$.

In the case of the HO basis functions, the integration is performed by using the Gauss integration points, ξ_n and η_m, for which the local densities and fields have to be calculated at the mesh points of $z_n = b_z\xi_n$ and $r_m = b_\perp \eta_m^{1/2}$. As an example, consider the following diagonal matrix element of the potential $U_q(r,z)$ (18),

$$U^q_{\alpha\alpha} = \int_{-\infty}^{\infty} \mathrm{d}z \int_0^{\infty} r\,\mathrm{d}r\, U_q(z,r)\psi^2_{n_z}(z)\psi^{\Lambda\,2}_{n_r}(r). \tag{39}$$

Inserting here the HO functions $\psi^2_{n_z}(z)$ and $\psi^{\Lambda\,2}_{n_r}(r)$ (29), and changing the integration variables to dimensionless variables ξ and η, the above matrix element reads

$$U^q_{\alpha\alpha} = \int_{-\infty}^{\infty} \mathrm{d}\xi \int_0^{\infty} \mathrm{d}\eta\, \tilde{U}_q(\xi,\eta)\tilde{\psi}^2_{n_z}(\xi)\tilde{\psi}^{\Lambda 2}_{n_r}(\eta), \tag{40}$$

where

$$\tilde{U}_q(\xi,\eta) = \frac{1}{2}U_q(\xi b_z, \sqrt{\eta}\, b_\perp). \tag{41}$$

Here, Gaussian quadrature can be applied directly, because the HO wave functions contain appropriate exponential profile functions.

The situation is a little bit more complicated in the case of the THO basis states where, before calculating, one has to change variables with respect to the LST functions $f(\mathcal{R})$. For example, let us consider the same matrix elements (39) but in THO representation:

$$U^q_{\alpha\alpha} = \int_{-\infty}^{\infty} \mathrm{d}z \int_0^{\infty} r\,\mathrm{d}r\, U_q(z,r)\left[\frac{f^2(\mathcal{R})}{\mathcal{R}^2}\frac{\mathrm{d}f(\mathcal{R})}{\mathrm{d}\mathcal{R}}\right]\psi^2_{n_z}\left(\frac{zf(\mathcal{R})}{\mathcal{R}}\right)\psi^{\Lambda\,2}_{n_r}\left(\frac{r^2 f^2(\mathcal{R})}{\mathcal{R}^2}\right). \tag{42}$$

Introducing new dimensionless variables

$$\xi = \frac{z}{b_z}\frac{f(\mathcal{R})}{\mathcal{R}}, \qquad \eta = \frac{r^2}{b_\perp^2}\frac{f^2(\mathcal{R})}{\mathcal{R}^2}, \tag{43}$$

for which we have

$$\mathrm{d}\xi\,\mathrm{d}\eta = \frac{2}{b_z b_\perp^2}\left[\frac{f^2(\mathcal{R})}{\mathcal{R}^2}\frac{\mathrm{d}f(\mathcal{R})}{\mathrm{d}\mathcal{R}}\right] r\,\mathrm{d}r\,\mathrm{d}z, \tag{44}$$

the matrix elements have the form of integrals, which are exactly identical to those in the HO basis (40), after changing the function $\tilde{U}_q(\xi,\eta)$ to

$$\tilde{U}_q(\xi,\eta) = \frac{1}{2}U_q\left(\xi b_z\frac{\mathcal{R}}{f(\mathcal{R})}, \sqrt{\eta}\, b_\perp\frac{\mathcal{R}}{f(\mathcal{R})}\right). \tag{45}$$

The calculation of matrix elements corresponding to derivative terms in the Hamiltonian (17) can be performed in an analogous way, after the derivatives of the Jacobian, $\frac{f^2(\mathcal{R})}{\mathcal{R}^2}\frac{\mathrm{d}f(\mathcal{R})}{\mathrm{d}\mathcal{R}}$, are taken into account.

3.7. Calculation of local densities

After diagonalizing the HFB equation (37), local densities are calculated as

$$\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \sum_{\alpha\beta}\rho_{\alpha\beta}\Phi^*_\alpha(\mathbf{r}\sigma)\Phi_\beta(\mathbf{r}'\sigma'), \qquad \tilde{\rho}(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \sum_{\alpha\beta}\tilde{\rho}_{\alpha\beta}\Phi^*_\alpha(\mathbf{r}\sigma)\Phi_\beta(\mathbf{r}'\sigma'), \tag{46}$$

where $\Phi_\alpha(\mathbf{r}\sigma)$ denotes the HO or THO basis wave functions, and the matrix elements of mean-field and pairing density matrices read

$$\rho_{\alpha\beta} = \sum_k V^*_{\alpha k}V_{\beta k}, \qquad \tilde{\rho}_{\alpha\beta} = -\sum_k V^*_{\alpha k}U_{\beta k}. \tag{47}$$

The HFB calculations for a zero-range pairing interaction give divergent energies when increasing the number of quasiparticle states in the sums of Eq. (47) (see the discussion in Ref. [3]). Therefore, they invariably require a truncation of the quasiparticle basis by introducing a cut-off for the quasiparticle energy and including only all quasiparticle states up to this value.

The choice of an appropriate cut-off procedure has been discussed in [2]. After each iteration, performed with a given Fermi energy λ, one calculates an equivalent spectrum $\bar{e}_k$ and pairing gaps $\bar{\Delta}_k$:

$$\bar{e}_k = (1-2N_k)E_k, \qquad \bar{\Delta}_k = 2E_k\sqrt{N_k(1-N_k)}, \tag{48}$$

where N_k denotes the norm (23) of the lower HFB wave function. Using this spectrum and pairing gaps, the Fermi energy is readjusted to obtain the correct value of particle number, and this new value is used in the next HFB iteration.

Due to the similarity between the equivalent spectrum $\bar{e}_k$ and the single-particle energies, one can take into account only those quasiparticle states for which

$$\bar{e}_k \leqslant \bar{e}_{\max}, \tag{49}$$

where $\bar{e}_{\max} > 0$ is a parameter defining the amount of the positive-energy phase space taken into account. Since all hole-like quasiparticle states, $N_k < 1/2$, have negative values of $\bar{e}_k$, condition (49) guarantees that they are all taken into account. In this way, a global cut-off prescription is defined which fulfills the requirement of taking into account the positive-energy phase space as well as all quasiparticle states up to the highest hole-like quasiparticle energy. In the code, a default value of $\bar{e}_{\max} = 60$ MeV is used.

3.8. Coulomb interaction

In the case of proton states, one has to add to the central potential the direct Coulomb field

$$V^C_d(\mathbf{r}) = e^2\int \mathrm{d}^3\mathbf{r}'\,\frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \tag{50}$$

as well as the exchange Coulomb field, which in the present implementation is treated within the Slater approximation:

$$V^C_{\mathrm{ex}}(\mathbf{r}) = -e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{1/3}(\mathbf{r}). \tag{51}$$

The integrand in the direct term (50) has a logarithmic singularity at the point $\mathbf{r} = \mathbf{r}'$. A way to bypass this difficulty is to use the Vautherin prescription [30], i.e. to employ the identity

$$\triangle_{\mathbf{r}'}|\mathbf{r}-\mathbf{r}'| = 2/|\mathbf{r}-\mathbf{r}'|, \tag{52}$$

and then integrate by parts the integral in Eq. (50). As a results, one obtains a singularity-free expression

$$V_d^C(\mathbf{r}) = \frac{e^2}{2}\int \mathrm{d}^3\mathbf{r}'|\mathbf{r}-\mathbf{r}'|\triangle_{\mathbf{r}'}\rho_p(\mathbf{r}'). \tag{53}$$

In cylindrical coordinates, after integrating over the azimuthal angle φ, one finds

$$V_d^C(r',z') = 2e^2\int_0^\infty r\,\mathrm{d}r\int_{-\infty}^\infty \mathrm{d}z\,\sqrt{d(r,z)}E\left(\frac{4rr'}{d(r,z)}\right)\triangle\rho_p(r,z), \tag{54}$$

where $d(r,z) = [(z-z')^2+(r+r')^2]$ and $E(x)$ is the complete elliptic integral of the second kind that can be approximated by a standard polynomial formula [31].

Equivalently, one can use the prescription developed originally for calculations with the finite-range (Gogny) force [3]. It consists of expressing the Coulomb force as a sum of Gaussians:

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\mathrm{d}\mu}{\mu^2}\mathrm{e}^{-(\mathbf{r}-\mathbf{r}')^2/\mu^2}, \tag{55}$$

which gives

$$V_d^C(\mathbf{r}) = e^2\frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\mathrm{d}\mu}{\mu^2}I_\mu(\mathbf{r}), \tag{56}$$

where the integral

$$I_\mu(\mathbf{r}) = \int \mathrm{d}^3\mathbf{r}'\mathrm{e}^{-(\mathbf{r}-\mathbf{r}')^2/\mu^2}\rho(\mathbf{r}') \tag{57}$$

can be easily calculated in cylindrical coordinates. After integrating over the azimuthal angle φ, one finds

$$I_\mu(r',z') = 2\pi\int_0^\infty r\,\mathrm{d}r\int_{-\infty}^\infty \mathrm{d}z\,\mathrm{e}^{-(r^2+r'^2+(z-z')^2)/\mu^2}I_0\left(\frac{2rr'}{\mu^2}\right)\rho_p(r,z), \tag{58}$$

where $I_0(x)$ is the Bessel function that can also be approximated by a standard polynomial formula [31].

In order to perform the remaining one-dimensional integration in Eq. (56), the variable μ is changed to

$$\xi = b/\sqrt{b^2+\mu^2}, \tag{59}$$

where b is the largest of the two HO lengths b_z and $b_\perp$. This change of variable is very convenient, since then the range of integration becomes $[0,1]$. The integral (56) is accurately computed by using a 30-point Gauss–Legendre quadrature with respect to ξ.

We have tested the precision of both prescriptions, Eqs. (53) and (56), and checked that the second one gives better results within the adopted numbers of Gauss–Hermite and Gauss–Laguerre points that are used for calculating proton densities. Therefore, in the code HFBTHO (v1.66p) this second prescription is used, while the first one remains in the code, but is inactive.

3.9. Lipkin–Nogami method

The LN method constitutes an efficient method for approximately restoring the particle numbers before the variation [33]. With only a slight modification of the HFB procedure outlined above, it is possible to obtain a very good approximation for the optimal HFB state, on which an exact particle number projection then has to be performed [34,35].

In more detail, the LN method is implemented by performing the HFB calculations with an additional term included in the HF Hamiltonian,

$$h' = h - 2\lambda_2(1-2\rho), \tag{60}$$

and by iteratively calculating the parameter λ_2 (separately for neutrons and protons) so as to properly describe the curvature of the total energy as a function of particle number. For an arbitrary two-body interaction $\hat{V}$, λ_2 can be calculated from the particle-number dispersion according to [33],

$$\lambda_2 = \frac{\langle 0|\hat{V}|4\rangle\langle 4|\hat{N}^2|0\rangle}{\langle 0|\hat{N}^2|4\rangle\langle 4|\hat{N}^2|0\rangle}, \tag{61}$$

where $|0\rangle$ is the quasiparticle vacuum, $\hat{N}$ is the particle number operator, and $|4\rangle\langle 4|$ is the projection operator onto the 4-quasiparticle space. On evaluating all required matrix elements, one obtains [36]

$$\lambda_2 = \frac{4\,\mathrm{Tr}\,\Gamma'\rho(1-\rho) + 4\,\mathrm{Tr}\,\Delta'(1-\rho)\kappa}{8[\mathrm{Tr}\,\rho(1-\rho)]^2 - 16\,\mathrm{Tr}\,\rho^2(1-\rho)^2}, \tag{62}$$

where the potentials

$$\Gamma'_{\alpha\alpha'} = \sum_{\beta\beta'} V_{\alpha\beta\alpha'\beta'}\big(\rho(1-\rho)\big)_{\beta'\beta}, \qquad \Delta'_{\alpha\beta} = \frac{1}{2}\sum_{\alpha'\beta'} V_{\alpha\beta\alpha'\beta'}(\rho\kappa)_{\alpha'\beta'}, \tag{63}$$

can be calculated in full analogy to Γ and Δ by replacing ρ and κ by $\rho(1-\rho)$ and $\rho\kappa$, respectively. In the case of the seniority-pairing interaction with strength G, Eq. (62) simplifies to

$$\lambda_2 = \frac{G}{4}\frac{\mathrm{Tr}(1-\rho)\kappa\,\mathrm{Tr}\,\rho\kappa - 2\,\mathrm{Tr}(1-\rho)^2\rho^2}{[\mathrm{Tr}\,\rho(1-\rho)]^2 - 2\,\mathrm{Tr}\,\rho^2(1-\rho)^2}. \tag{64}$$

An explicit calculation of λ_2 from Eq. (62) requires calculating new sets of fields (63), which is rather cumbersome. However, we have found [25] that Eq. (62) can be well approximated by the seniority-pairing expression (64) with the effective strength

$$G = G_{\mathrm{eff}} = -\frac{\bar{\Delta}^2}{E_{\mathrm{pair}}} \tag{65}$$

determined from the pairing energy

$$E_{\mathrm{pair}} = -\frac{1}{2}\,\mathrm{Tr}\,\Delta\kappa \tag{66}$$

and the average pairing gap

$$\bar{\Delta} = \frac{\mathrm{Tr}\,\Delta\rho}{\mathrm{Tr}\,\rho}. \tag{67}$$

Such a procedure is implemented in the code HFBTHO (v1.66p).

3.10. *Particle-number projection after variation*

Introducing the particle-number projection operator for N particles,

$$P^N = \frac{1}{2\pi}\int \mathrm{d}\phi\, \mathrm{e}^{\mathrm{i}\phi(\hat{N}-N)}, \tag{68}$$

where $\hat{N}$ is the number operator, the average HFB energy of the particle-number projected state can be expressed as an integral over the gauge angle ϕ of the Hamiltonian matrix elements between states with different gauge angles

[37,38]. In particular, for the Skyrme-HFB method implemented here, the particle-number projected energy can be written as [25,26]

$$\mathsf{E}^N[\rho,\tilde{\rho}] = \frac{\langle\Phi|HP^N|\Phi\rangle}{\langle\Phi|P^N|\Phi\rangle} = \int \mathrm{d}\phi\, y(\phi) \int \mathrm{d}^3\mathbf{r}\,\mathcal{H}(\mathbf{r},\phi), \tag{69}$$

where the gauge-angle dependent energy density $\mathcal{H}(\mathbf{r},\phi)$ is derived from the unprojected energy density $\mathcal{H}(\mathbf{r})$ (10) by simply substituting the particle and pairing local densities $\rho(\mathbf{r})$, $\tilde{\rho}(\mathbf{r})$, $\tau(\mathbf{r})$, and $\mathbf{J}_{ij}(\mathbf{r})$ by their gauge-angle dependent counterparts $\rho(\mathbf{r},\phi)$, $\tilde{\rho}(\mathbf{r},\phi)$, $\tau(\mathbf{r},\phi)$, and $\mathbf{J}_{ij}(\mathbf{r},\phi)$, respectively. The latter densities are calculated from the gauge-angle dependent density matrices as

$$\begin{aligned}
\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma',\phi) &= \sum_{\alpha\alpha'} \rho_{\alpha\alpha'}(\phi)\Phi^*_{\alpha'}(\mathbf{r}',\sigma')\Phi_\alpha(\mathbf{r},\sigma),\\
\tilde{\rho}(\mathbf{r}\sigma,\mathbf{r}'\sigma',\phi) &= \sum_{\alpha\alpha'} \tilde{\rho}_{\alpha\alpha'}(\phi)\Phi^*_{\alpha'}(\mathbf{r}',\sigma')\Phi_\alpha(\mathbf{r},\sigma),
\end{aligned} \tag{70}$$

where the gauge-angle dependent matrix elements read

$$\rho_{\alpha'\alpha}(\phi) = \sum_\beta C_{\alpha\beta}(\phi)\rho_{\beta\alpha'}, \qquad \tilde{\rho}_{\alpha'\alpha}(\phi) = \mathrm{e}^{-\mathrm{i}\phi}\sum_\beta C_{\alpha\beta}(\phi)\tilde{\rho}_{\beta\alpha'}, \tag{71}$$

and depend on the unprojected matrix elements (47) and on the gauge-angle dependent matrix

$$C(\phi) = \mathrm{e}^{2\mathrm{i}\phi}\big[1+\rho(\mathrm{e}^{2\mathrm{i}\phi}-1)\big]^{-1}. \tag{72}$$

Function $y(\phi)$ appearing in Eq. (69) is defined as

$$y(\phi) = \frac{x(\phi)}{\int \mathrm{d}\phi'\, x(\phi')} \quad \text{for } x(\phi) = \frac{1}{2\pi}\frac{\mathrm{e}^{-\mathrm{i}\phi N}\det(\mathrm{e}^{\mathrm{i}\phi}I)}{\sqrt{\det C(\phi)}}, \tag{73}$$

where I is the unit matrix.

Since the gauge-angle dependent matrices (70) and (71) are all diagonal in the same canonical basis that diagonalizes the unprojected density matrices (47), all calculations are very much simplified when they are performed in the canonical basis. In particular, in the canonical basis the matrices (71) read

$$\rho_\mu(\phi) = \frac{\mathrm{e}^{2\mathrm{i}\phi}v_\mu^2}{u_\mu^2+\mathrm{e}^{2\mathrm{i}\phi}v_\mu^2} \quad \text{and} \quad \tilde{\rho}_\mu(\phi) = \frac{\mathrm{e}^{\mathrm{i}\phi}u_\mu v_\mu}{u_\mu^2+\mathrm{e}^{2\mathrm{i}\phi}v_\mu^2}, \tag{74}$$

while the function $x(\phi)$ can be calculated as

$$x(\phi) = \mathrm{e}^{-\mathrm{i}N\phi}\prod_{\mu>0}\big(u_\mu^2+\mathrm{e}^{2\mathrm{i}\phi}v_\mu^2\big), \tag{75}$$

where v_μ and u_μ ($v_\mu^2+u_\mu^2=1$) are the usual canonical basis occupation amplitudes.

All the above expressions apply to independently restoring the proton and neutron numbers, so, in practice, integrations over two gauge angles have to be simultaneously implemented. In practice, these integrations are carried out by using a simple discretization method, which amounts to approximating the projection operator (68) by a double sum [39], i.e.

$$P^{NZ} = \frac{1}{L}\sum_{l_n=0}^{L-1}\mathrm{e}^{\mathrm{i}\phi_n(\hat{N}-N)}\frac{1}{L}\sum_{l_p=0}^{L-1}\mathrm{e}^{\mathrm{i}\phi_p(\hat{Z}-Z)}, \tag{76}$$

where

$$\phi_q = \frac{\pi}{L}l_q, \qquad q=n,p. \tag{77}$$

Usually no more than $L=9$ points are required for a precise particle number restoration.

3.11. Constraints

In the code HFBTHO (v1.66p), the HFB energy (9) can be minimized under the constraint of a fixed quadrupole moment. This option should be used if one is interested in the potential energy surface of a nucleus along the quadrupole collective coordinate. The quadrupole constraint is assumed in the standard quadratic form [40]:

$$E^Q = C_Q\big(\langle\hat{Q}\rangle - \bar{Q}\big)^2, \tag{78}$$

where $\langle\hat{Q}\rangle$ is the average value of the mass-quadrupole-moment operator,

$$\hat{Q} = 2z^2 - r^2, \tag{79}$$

$\bar{Q}$ is the constraint value of the quadrupole moment, and C_Q is the stiffness constant.

4. Program HFBTHO (v1.66p)

The code HFBTHO (v1.66p) is written in Fortran 95 with `MODULE` definitions that specify all common arrays and variables for other subroutines by using the `USE` statements. Integer and real types of variables are automatically detected for the particular computer through the `KIND` statements. The code is entirely portable. It contains all initial data and no references to external subroutines or libraries are made.

The code requires one input data file (`tho.dat`). Optionally, in case one wants to restart calculations from a previous run, two more files, `dnnn_zzz.hel` and/or `dnnn_zzz.tel`, are required as described below. Also optionally, if one wants to run the code for user-defined Skyrme-force parameters, file `forces.dat` is required.

The results are printed on the standard output and also recorded in the file `thoout.dat`. The main results are also recorded in the files `hodef.dat` (HO basis) and `thodef.dat` (THO basis), where one line is written for every nucleus calculated, producing a concise table of results suitable for further analyses. Files `hodef.dat` and `thodef.dat` are also used when restarting the given calculation after an abnormal termination (CPU time limit or system crash). Namely, before performing a given run, the code always checks if the line corresponding to this run is present or not in the file `hodef.dat` or `thodef.dat`. If this is the case, the code does not repeat the calculation for the given run, and only the runs which have not been completed are executed. Due to this implementation, if the user wishes to rerun the same input data file, files `hodef.dat` and `thodef.dat` have to be first removed from the current directory.

4.1. General structure of the code

The code runs, in sequence, the set of main subroutines listed in Table 1. If multiple runs are requested in a single input data file, the code always repeats the whole sequence of calls from the beginning to end, including an initialization of all variables and data.

4.2. Input data file

Input data are read from file `tho.dat`, which is shown in Table 2. The file consists of the first line, which contains only two numbers, referred to as I1 and I2 below, followed by a sequence of identical lines, each of them defining one specific run of the code. All numbers containing a dot are type real, and those without a dot are type integer. In quotations there are four-character strings giving acronyms of the Skyrme forces. The code uses free format, so at least one space is needed in order to separate the input numbers.

The code has three main modes:

Table 1
List of main subroutines constituting the code HFBTHO (v1.66p)

Subroutine	Task
DEFAULT	Initializes all variables (initially, or after the previous run).
read input	Reads parameters from the input data file tho.dat.
PREPARER	Initializes variables according to the user's request defined in the input data file.
BASE0	Determines the HO configurational space and dimensions of allocatable arrays.
THOALLOC	Allocates memory required for the given run of the code.
BASE	Calculates and stores properties of the configurational space and all associated quantum numbers.
GAUPOL	Calculates and stores the HO basis wave functions.
INOUT	Sets or reads (optional) initial densities, fields, and matrix elements.
ITER	Main iteration loop for the HFB+HO calculation, which is repeated until convergence is met. It includes the following subroutines:
	DENSIT Calculates densities in coordinate space.
	FIELD Calculates mean fields in coordinate space.
	GAMDEL Calculates the particle-hole and pairing Hamiltonian matrices.
	EXPECT Calculates average values of observables.
	HFBDIAG Diagonalizes the HFB equation.
F01234	After the HFB+HO solution is found, calculates the THO basis wave functions, which replace the HO ones.
ITER	Main iteration loop for the HFB+THO calculation, which is repeated until convergence is met. The same subroutine and sequence of calls is used as above.
RESU	Calculates all required physical characteristics and canonical basis properties, and performs the particle number projection.
INOUT	Records the final densities, fields, and matrix elements for feature use (optional).

Table 2
Input data file tho.dat

(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)	(j)	(k)	(l)	(m)	(n)	(o)	(p)	(q)	(r)	(s)
−20	20																	
20	−2.	0.	−1	300	1	70	50	'SLY4'	−1	1	0	0.26	0.5	9	0	2	2	0.0001
20	−2.	0.	−1	300	1	72	50	'SLY4'	−1	1	0	0.26	0.5	9	0	2	−2	0.0001
20	−2.	0.	−1	300	1	74	50	'SLY4'	−1	1	0	0.26	0.5	9	0	−2	2	0.0001
20	−2.	0.	−1	300	1	76	50	'SLY4'	−1	1	0	0.26	0.5	9	0	−2	−2	0.0001
−14	−2.	0.	−1	300	1	78	50	'SKP'	−1	1	0	0.26	0.5	9	0	4	4	0.0001
0	−2.	0.	−1	300	1	70	50	'SLY4'	−1	1	0	0.26	0.5	9	0	0	0	0.0001

(i) **nucleus-after-nucleus**, defined by $I1 < 0$,
(ii) **file-after-file**, defined by $I1 = 0$,
(iii) **chain-after-chain**, defined by $I1 > 0$.

In the **nucleus-after-nucleus** mode, the code ignores the values of |I1| and I2, and then performs one run for each line of the input data file that follows the first line. This is the simplest and most often used mode, illustrated by the example given in Table 1.

In the **file-after-file** mode, the code ignores the value of I2, and then reads the second line of the input data file, from where it takes all fields except from the values of ININ, N, and Z. Then it performs one run for each dnnn_zzz file found in the current directory. Files dnnn_zzz contain results of previous runs and are described below.

In the **chain-after-chain** mode, the code reads the second line of the input data file, from where it takes all fields except from the values of N, and Z. Then it performs one run for each nucleus in the chain of isotones or

isotopes located between the bottom of the stability valley and the drip line. The bottom of the stability valley is parametrically defined as

$$f(N,Z) \equiv N - Z - 0.006(N+Z)^{5/3} = 0. \tag{80}$$

- If I2 > 0, the code calculates the chain of isotopes for the proton number $Z = \mathrm{I1}$, starting with the lowest even neutron number N satisfying $f(N,Z) > 0$, and then step-by-step increasing the number of neutrons by two. Calculations continue until the neutron drip line is reached, and then the program stops.
- If I2 < 0, the code calculates the chain of isotones for the neutron number $N = \mathrm{I1}$, starting with the lowest even proton number Z satisfying $f(N,Z) < 0$, and then step-by-step increasing the number of protons by two. Calculations continue until the proton drip line is reached, and then the program stops.

All lines of the input data file, after the first line, contain 19 fields each. Below we denote these fields by letters (a)–(s), as shown in the header of Table 2. The description of the fields is as follows:

- (a) Number of oscillator shells N_{sh}:
  - If $N_{\mathrm{sh}} > 0$, the code prints intermediate results at every iteration.
  - If $N_{\mathrm{sh}} < 0$, the code prints results at the first and last iterations only, and the modulus of the input value is used for N_{sh}.
  - If $N_{\mathrm{sh}} = 0$, the code stops. This value is used to indicate the end of the input data file.

  For $N_{\mathrm{sh}} > 14$, the code always begins with a short, 20-iteration run using $N_{\mathrm{sh}} = 14$, and the resulting fields then serve as a starting point for the calculation with the requested value of N_{sh}. For the THO-basis calculations, use of $N_{\mathrm{sh}} < 14$ is not recommended, because precision of the HO density profile can be insufficient for a reliable determination of the LST function.
- (b) Oscillator basis parameter $b_0 = \sqrt{b_z^2 + b_\perp^2}$:
  - If $b_0 > 0$, the code uses this given value of b_0.
  - If $b_0 < 0$, the code uses the default value of $b_0 = \sqrt{2(\hbar^2/2m)/(41 f A^{-1/3})}$ for $f = 1.2$.
- (c) Deformation β_0 of the HO basis. The value of β_0 defines the HO oscillator lengths through $b_\perp = b_0 q^{-1/6}$, $b_z = b_0 q^{1/3}$, and $q = \exp(3\sqrt{5/(16\pi)}\beta_0)$. In particular, the value of $\beta_0 = 0$ corresponds to the spherical HO basis.
- (d) The THO basis control parameter `ILST`:
  - If `ILST` $= 0$, the code performs the HO basis calculation only. If `ININ` < 0, the file `dnnn_zzz.hel` is used as the starting point. If `MAXI` > 0, at the end of the given run file `dnnn_zzz.hel` is written.
  - If `ILST` $= -1$, the code performs the HO basis calculation followed by the THO basis calculation. If `ININ` < 0, the file `dnnn_zzz.hel` is used as the starting point. If `MAXI` > 0, at the end of the given run files `dnnn_zzz.hel` and `dnnn_zzz.tel` are written.
  - If `ILST` $= 1$, the code performs the THO basis calculation only. File `dnnn_zzz.tel` must exist and is used as the starting point (only `ININ` < 0 is allowed). If `MAXI` > 0, at the end of the given run file `dnnn_zzz.tel` is written.
- (e) Maximal number of iterations `MAXI`. If the negative number is read, the absolute value is used.
  - If `MAXI` > 0, at the end of the given run files `dnnn_zzz.hel` and/or `dnnn_zzz.tel` are written,
  - If `MAXI` < 0, files `dnnn_zzz.hel` and `dnnn_zzz.tel` are not written, and the modulus of the input value is used for `MAXI`.
- (f) The starting-point control parameter `ININ`:
  - If `ININ` $= 1$, the code starts from a default spherical field predefined within the code,
  - If `ININ` $= 2$, the code starts from a default prolate field predefined within the code,
  - If `ININ` $= 3$, the code starts from a default oblate field predefined within the code,

Table 3
User-defined parameters of the Skyrme force, as given in the file `forces.dat`

Value	Description
'SLY4'	Skyrme-force acronym
0	Tensor term (0—excluded, 1—included)
−0.2488913d+04	t_0
0.4868180d+03	t_1
−0.5463950d+03	t_2
0.1377700d+05	t_3
0.8340000d0	x_0
−0.3440000d0	x_1
−1.0000000d0	x_2
1.3540000d0	x_3
0.1230000d+03	W_0
6.0d0	$1/\alpha$
20.735530d0	$\hbar^2/2\mathrm{m}$
0.160d0	ρ_0 (saturation density for pairing)
1.0d0	γ (power of density for pairing)
60.0d0	$\bar{e}_{\max}$ (pairing cut-off energy)
0.5d0	V_1 (0—volume, 1—surface, 0.5—mixed)
−244.7200d0	V_0 (pairing strength)

  - If `ININ` $= -1$, the code starts from file `snnn_zzz.hel` or `snnn_zzz.tel`,
  - If `ININ` $= -2$, the code starts from file `pnnn_zzz.hel` or `pnnn_zzz.tel`,
  - If `ININ=` -3, the code starts from file `onnn_zzz.hel` or `onnn_zzz.tel`.
- (g) Number of neutrons N.
- (h) Number of protons Z.
- (i) Skyrme force character*4 acronym, e.g., 'SIII', 'SKP', 'SLY4', or 'SKM*'. If value 'READ' is read, the code reads the Skyrme force parameters from file `forces.dat`. An example of the file `forces.dat` is presented in Table 3.
- (j) The Lipkin–Nogami control parameter `KINDHFB`:
  - If `KINDHFB` $= 1$, Lipkin–Nogami correction not included,
  - If `KINDHFB` $= -1$, Lipkin–Nogami correction included.
- (k) The pairing-force control parameter `IPPFORCE`:
  - If `IPPFORCE` $= 0$, no pairing correlations (Hartree–Fock calculation),
  - If `IPPFORCE` $= 1$, calculation for the density-dependent delta pairing force,
  - If `IPPFORCE` $= 2$, calculation for the density-independent delta pairing force.
- (l) The quadrupole-constraint control parameter `ICSTR`. If `ICSTR` $= 0$, the quadrupole constraint is not included, and the next two fields (m) and (n) are not used. If `ICSTR` $= 1$, then:
  - (m) Constrained value of the quadrupole deformation $\bar{\beta}$. The value of $\bar{\beta}$ defines the constrained quadrupole moment $\bar{Q}$ in Eq. (78) through: $\bar{Q} = \sqrt{\frac{5}{\pi}}\langle r^2\rangle\bar{\beta}$.
  - (n) Parameter η defining the stiffness C_Q of the quadratic quadrupole constraint constant by $C_Q = \eta(41A^{-1/3})/(8Ab_0^2\langle r^2\rangle)$.
- (o) The number of gauge-angle points L used for the particle number projection. Note that the code always performs the PNP, even if pairing correlations are not included.
- (p) The particle number shift control parameter `ISHIFT`. If, `ISHIFT` $= 0$, the particle number projection is performed on N and Z, and the next two fields (q) and (r) are not used. If `ISHIFT` $= 1$, then:
  - (q) Neutron number shift `KDN`, i.e. the projection is performed on neutron number $N +$ `KDN`,
  - (r) Proton number shift `KDZ`, i.e. the projection is performed on proton number $Z +$ `KDZ`.

- (s) Requested precision of convergence `SI` (in MeV). Iterations stop when changes of all mean-field and pairing matrix elements between two consecutive iterations become smaller than the value of `SI`. Recommended value is 0.0001.

After the solution is found, and if `MAXI` > 0, the code writes files `dnnn_zzz.hel` (if the HO-basis run has been performed) and/or `dnnn_zzz.tel` (if the THO-basis run has been performed). Names of these files are automatically constructed based on the input-data parameters `ININ`, N, and Z, namely:

- `d` = 's', 'p', or 'o', for |`ININ`| = 1, 2, or 3, respectively,
- `nnn` = three-digit value of N with leading zeros included,
- `zzz` = three-digit value of Z with leading zeros included.

These files can be used in a later run to restart calculations from previously found solutions. For example, file `s070_050.tel` contains results of the THO-basis calculation for ^{120}Sn, which has been obtained by starting from a spherical field. Note that the name of the file reflects the starting deformation only, while it may, in fact, contain results for another deformation that has been obtained during the iteration.

4.3. Output files

The results are printed on the standard output file. Each run produces a separate part of the output file; also the HO run preceding a THO run produces one such part. A test run output is included in the directory./compareoutput. Note that the output data may differ in the final decimal places depending on the compiler used. Below we briefly describe different sections of the output file.

- *Header*. Contains the version number of the code, date and time of execution, name of the element, and its particle, neutron, and proton numbers.
- *Input data*. Contains a short summary of the input data for the requested run.
- *Force*. Lists the acronym and parameters of the Skyrme force, as well as parameters of the pairing force.
- *Numerical*. Contains some information on numerical parameters and options used for the given run.
- *Mode*. Gives the mode in which the code is run.
- *Iterations*. Shows brief information about iterations performed. One line of the output file per each iteration is printed and contains the following columns:
  - Iteration number `i`.
  - Accuracy `si`.
  - Current mixing parameter between the previous and current fields `mix`.
  - Quadrupole deformation `beta`, $\beta = \sqrt{\frac{\pi}{5}}\frac{\langle\hat{Q}\rangle}{\langle r^2\rangle}$, for $\hat{Q}$ given in Eq. (79).
  - Total energy `Etot`.
  - Particle number `A`.
  - Neutron rms radius `rn`.
  - Proton rms radius `rp`.
  - Neutron pairing energy `En`.
  - Neutron pairing gap `Dn`.
  - Proton pairing energy `Ep`.
  - Proton pairing gap `Dp`.
  - Neutron Fermi energy `Ln`.
  - Proton Fermi energy `Lp`.

- *Files*. Contains information on the `dnnn_zzz.hel` or `dnnn_zzz.tel` file written.
- *Observables*. Lists values of various observables calculated for the HFB state without PNP and with the Lipkin–Nogami corrections, and then those calculated for the PNP HFB state.

The same information, plus more results on the quasiparticle and canonical states, is also written to the file `thoout.dat`. However, this file is rewound after each run, so it contains results of only the last run executed for the given input data file.

Files `hodef.dat` and `thodef.dat` contain synthetic results of all runs, printed in the form of a single line per each performed run. If the given run performs only an HO-basis calculation, or only a THO-basis calculation, then only an entry in file `hodef.dat` or `thodef.dat` is produced, respectively. On the other hand, runs that perform both HO and THO calculations produce entries in both these files. Lines in the files `hodef.dat` and `thodef.dat` contain 105 columns each, and each column is described by a name printed in the first header line. The names are self-explanatory, and most often they correspond to the names used in the present write-up. Names preceded by `U:` pertain to results obtained for the HFB states before PNP, while those beginning with `L` pertain to the results containing the Lipkin–Nogami corrections. Names ending with `t`, `n`, or `p` give total, neutron, or proton observables, respectively.

5. Conclusions

The code HFBTHO (v1.66p) is a tool of choice for self-consistent calculations for a large number of even–even nuclei. Several examples of deformed HFBTHO calculations, recently implemented on parallel computers, are given in Ref. [23]. By creating a simple load-balancing routine that allows one to scale the problem to 200 processors, it was possible to calculate the entire deformed even–even nuclear mass table in a single 24 wall-clock hour run (or approximately 4800 processor hours).

The crucial input for such calculations, which determines the quality of results, is the nuclear energy density functional. The development of the "universal" nuclear energy density functional still remains one of the major challenges for nuclear theory. While self-consistent HFB methods have already achieved a level of sophistication and precision which allows analyses of experimental data for a wide range of properties and for arbitrarily heavy nuclei (see, e.g., Refs. [41–43] for deformed HFB mass table), much work remains to be done. Developing a universal nuclear density functional will require a better understanding of the density dependence, isospin effects, and pairing, as well as an improved treatment of symmetry-breaking effects and many-body correlations.

In addition to systematic improvements of the nuclear energy density functional, there are several anticipated extensions of HFBTHO itself. The future enhancements to HFBTHO will include the implementation of the full particle-number projection *before* variation, extension of code to odd particle numbers, implementation of non-standard spin-orbit term and two-body center-of-mass correction, and evaluation of dynamical corrections representing correlations beyond the mean field.

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