Computer Physics Communications 253 (2020) 107184

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Implementation of the quasiparticle finite amplitude method within the relativistic self-consistent mean-field framework: The program DIRQFAM☆,☆☆

A. Bjelčić, T. Nikšić*

University of Zagreb, Faculty of Science, Physics Department, Croatia

ARTICLE INFO

Article history:
Received 1 August 2019
Received in revised form 25 December 2019
Accepted 8 January 2020
Available online 25 January 2020

Keywords:
Relativistic quasiparticle random-phase approximation
Finite amplitude method
Multipole response
Dirac–Hartree–Bogoliubov
Nuclear energy density functional

ABSTRACT

The DIRQFAM code calculates the multipole response of even–even axially symmetric deformed nuclei using the framework of relativistic self-consistent mean-field models. The response is calculated by implementing the finite amplitude method for relativistic quasiparticle random phase approximation.

Program summary

Program Title: DIRQFAM
Program Files doi: http://dx.doi.org/10.17632/6gv8nxg4ns.1
Licensing provisions: GPLv3
Programming language: Fortran 90/95, easily downgradable to FORTRAN 77.
External routines/libraries: BLAS/LAPACK, version 3.6.0. or higher.
Nature of problem: Multipole response of deformed even–even open-shell nuclei can be calculated using the quasiparticle finite amplitude method (QFAM), based on the relativistic self-consistent mean-field models. The particle–hole channel is described by a zero-range relativistic effective interaction, while the particle–particle channel of the effective inter-nucleon interaction is described by a separable finite-range pairing force. The method can be applied to perform systematic studies of collective modes even in heavy deformed nuclei.
Solution method: The current implementation computes the multipole response by solving the QFAM equations in a self-consistent iteration scheme. At each iteration the QFAM solutions are updated using the modified Broyden's method. The QFAM amplitudes are expanded in the simplex-y harmonic oscillator basis.
Restrictions: Open-shell even–even nuclei with axially symmetric ground states are considered. An electric multipole operator with $J \leq 3$ is used to calculate the response function.
Unusual features: The code should be recompiled before running it with different values of one of the following input parameters: number of oscillator shells in the expansion of nucleon spinors (`n0f`), number of Gauss–Hermite (`NGH`) or Gauss–Laguerre nodes (`NGL`), the multipolarity values that define the external perturbation operator (`J_multipole`, `K_multipole`).

1. Introduction

Energy density functionals (EDF) provide an accurate description of ground-state properties and collective excitations of atomic nuclei, from relatively light systems to superheavy nuclei, and from the valley of β-stability to the particle drip-lines [1–4]. One of the most interesting topics for this type of research is studies of multipole response in nuclei far from stability with possible occurrence of exotic modes of excitation [5,6]. Theoretical studies of collective vibrations in heavy nuclei are commonly performed within the framework of quasiparticle random-phase approximation [7] (QRPA), most often in a matrix form. However, the dimension of the QRPA matrices increases rapidly for deformed heavy systems and such calculations have become possible only during the past decade [8–12].

In order to bypass problems of practical implementation of matrix QRPA in deformed heavy systems, a finite amplitude method (FAM) was introduced as an alternative way to compute the multipole response functions. The FAM has been successfully applied in a number of studies both in the coordinate space and in the harmonic oscillator basis [13–22].

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).
☆☆ The review of this paper was arranged by Prof. Z. Was.
* Corresponding author.
E-mail address: tniksic@phy.hr (T. Nikšić).

https://doi.org/10.1016/j.cpc.2020.107184
0010-4655/

A particular class of self-consistent mean-field models (SCMF) are those based on zero-range relativistic (covariant) energy density functionals. These models have been successfully applied to the analysis of a variety of nuclear structure phenomena, with accuracy comparable to the nonrelativistic Hartree–Fock–Bogoliubov approach based on Skyrme functionals or Gogny effective interactions (see Ref. [4] and references cited therein). We have presented the DIRHB program package [23] for the solution of the stationary relativistic Hartree–Bogoliubov equations for even–even open-shell nuclei with spherical symmetry, axially symmetric quadrupole deformation, and triaxial quadrupole shapes. Here we would like to complement this package with the QFAM solver to calculate the multipole response for systems with axially symmetric quadrupole deformation. The present version of the code is restricted to zero-range effective interaction, however we plan to upgrade this in the near future.

The paper is organized as follows. Section 2 includes a brief overview of the small amplitude limit of the time-dependent relativistic Hartree–Bogoliubov model and the finite amplitude method, some details of practical implementation are described in Section 3, and the structure of the program is explained in Section 4. Short summary is provided in Section 5 and further mathematical details can be found in appendices.

2. Small amplitude limit of the time-dependent relativistic Hartree–Bogoliubov model and the finite amplitude method

The relativistic Hartree–Bogoliubov (RHB) model [2,24] provides a unified description of nuclear particle–hole (ph) and particle–particle (pp) correlations on a mean-field level by combining two average potentials: the self-consistent nuclear mean field h that encloses all the long range ph correlations, and a pairing field Δ which sums up the pp-correlations. In the RHB framework the nuclear single-reference state is described by a generalized Slater determinant $|\Phi\rangle$ that represents a vacuum with respect to independent quasiparticles. The quasiparticle operators are defined by the unitary Bogoliubov transformation, and the corresponding Hartree–Bogoliubov wave functions U and V are determined by the solution of the RHB equation:

$$\begin{pmatrix} h_D - m - \lambda & \Delta \\ -\Delta^* & -h_D^* + m + \lambda \end{pmatrix} \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} . \tag{1}$$

In the relativistic case the self-consistent mean-field is included in the single-nucleon Dirac Hamiltonian h_D, Δ is the pairing field, and U and V denote Dirac spinors. In the formalism of supermatrices introduced by Valatin [25], the RHB functions are determined by the Bogoliubov transformation which relates the original basis of particle creation and annihilation operators c_k, $c_k^\dagger$ (e.g. an oscillator basis), to the quasiparticle basis α_μ, $\alpha_\mu^\dagger$ [1]:

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \mathcal{W} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \qquad \text{with} \qquad \mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} . \tag{2}$$

In this notation a single-particle operator can be represented in the matrix form:

$$F = \frac{1}{2} \begin{pmatrix} \alpha^\dagger & \alpha \end{pmatrix} \mathcal{F} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} + const, \tag{3}$$

with:

$$\mathcal{F} = \begin{pmatrix} F^{11} & F^{20} \\ -F^{02} & -(F^{11})^T \end{pmatrix} . \tag{4}$$

In particular, for the generalized density $\mathcal{R}$:

$$\mathcal{R} = \mathcal{W}^\dagger \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} \mathcal{W}, \tag{5}$$

where the density matrix and pairing tensor read: $\rho = V^* V^T$ and $\kappa = V^* U^T$. The RHB Hamiltonian is given by a functional derivative of a given energy density functional with respect to the generalized density:

$$\mathcal{H} = \frac{\delta E[\mathcal{R}]}{\delta \mathcal{R}} = \mathcal{W}^\dagger \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \mathcal{W}. \tag{6}$$

The evolution of the quasiparticle operator $\alpha_\mu(t)$ subject to time-dependent external perturbation $F(t)$ is determined by the equation:

$$i\partial_t \alpha_\mu(t) = \left[H(t) + F(t), \alpha_\mu(t) \right]. \tag{7}$$

For a weak harmonic external field:

$$F(t) = \eta (F(\omega) e^{-i\omega t} + F^\dagger(\omega) e^{+i\omega t}), \tag{8}$$

characterized by the small real parameter η, the $F(\omega)$ operator reads:

$$F(\omega) = \frac{1}{2} \sum_{\mu\nu} F^{20}_{\mu\nu} \alpha^\dagger_\mu \alpha^\dagger_\nu + F^{02}_{\mu\nu} \alpha_\nu \alpha_\mu . \tag{9}$$

The $F^{11}_{\mu\nu}$ term that would appear in the previous equation does not contribute in linear response and thus can be safely omitted. The external harmonic field $F(t)$ induces a small-amplitude oscillations of the $\alpha_\mu(t)$ operator around the ground-state solution with the same energy:

$$\alpha_\mu(t) = \left(\alpha_\mu + \delta\alpha_\mu(t) \right) e^{iE_\mu t} . \tag{10}$$

E_μ denotes the quasiparticle energies (see Eq. (1)). The oscillating part of the $\alpha_\mu(t)$ operator is expanded in terms of quasiparticle creation operators [2]:

$$\delta\alpha_\mu(t) = \eta \sum_\nu \alpha^\dagger_\nu \left(X_{\nu\mu}(\omega) e^{-i\omega t} + Y^*_{\nu\mu}(\omega) e^{+i\omega t} \right). \tag{11}$$

The oscillations of the density matrix and the pairing tensor produce the induced oscillating fields in the single-particle Hamiltonian $h(t) = h_0 + \delta h(t)$ and the pairing field $\Delta(t) = \Delta_0 + \delta\Delta(t)$. h_0 and Δ_0 denote the ground state values. The Hamiltonian $H(t)$ can also be decomposed into static and oscillating terms:

$$H(t) = H_0 + \delta H(t) = H_0 + \eta \left[\delta H(\omega) e^{-i\omega t} + \delta H^\dagger(\omega) e^{+i\omega t} \right]. \tag{12}$$

The $\delta H(\omega)$ operator is decomposed:

$$\delta H(\omega) = \frac{1}{2} \sum_{\mu\nu} \delta H^{20}_{\mu\nu}(\omega) \alpha^\dagger_\mu \alpha^\dagger_\nu + \delta H^{02}_{\mu\nu}(\omega) \alpha_\nu \alpha_\mu . \tag{13}$$

By inserting Eqs. (10)–(13) into Eq. (7) and retaining only linear terms, we obtain the QFAM equations:

$$\left(E_\mu + E_\nu - \omega \right) X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) = -F^{20}_{\mu\nu}, \tag{14}$$

$$\left(E_\mu + E_\nu + \omega \right) Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) = -F^{02}_{\mu\nu}. \tag{15}$$

We notice that $\delta H^{20}_{\mu\nu}(\omega)$ and $\delta H^{02}_{\mu\nu}(\omega)$ depend on the induced fields which in turn depend on the induced densities, i.e., on the amplitudes $X_{\mu\nu}(\omega)$ and $Y_{\mu\nu}(\omega)$. Therefore, Eqs. (14)–(15) represent a set of equations that can be solved self-consistently. The expansion of $\delta H^{20}_{\mu\nu}(\omega)$ and $\delta H^{02}_{\mu\nu}(\omega)$ in terms of $X_{\mu\nu}(\omega)$ and $Y_{\mu\nu}(\omega)$ up to linear order leads to the conventional QRPA equations. These equations contain second derivatives of the density functional

[1] In the following, the Roman alphabet characters will denote the particle basis states, while the Greek will denote the quasiparticle basis states.

[2] We notice that including the annihilation operators in the expansion would not alter the density matrix or the pairing tensor.

$E[\mathcal{R}]$ with respect to $\mathcal{R}$ as matrix elements. For deformed nuclei in particular, the number of two-quasiparticle configurations can become very large and the evaluation of matrix elements requires a considerable, and in many cases prohibitive, numerical effort. In many cases this has prevented systematic applications of the conventional QRPA method to studies of the multipole response of medium-heavy and heavy deformed nuclei.

In order to use the stationary RHB code as a starting point for the evaluation of the $\mathcal{H}(\mathcal{R})$, the generalized density should be transformed back to the original single-particle basis by using the Bogoliubov transformation:

$$\alpha_\mu(t) = \sum_k \left(U^*_{k\mu}(t) c_k + V^*_{k\mu}(t) c^\dagger_k \right). \tag{16}$$

Eqs. (10) and (11) lead to the following expressions for the $U(t)$ and $V(t)$ coefficients:

$$U_{k\mu}(t) = U_{k\mu} e^{-iE_\mu t} + \eta e^{-iE_\mu t} \sum_\nu \left(V^*_{k\nu} Y_{\nu\mu}(\omega) e^{-i\omega t} + V^*_{k\nu} X^*_{\nu\mu}(\omega) e^{+i\omega t} \right), \tag{17}$$

$$V_{k\mu}(t) = V_{k\mu} e^{-iE_\mu t} + \eta e^{-iE_\mu t} \sum_\nu \left(U^*_{k\nu} Y_{\nu\mu}(\omega) e^{-i\omega t} + U^*_{k\nu} X^*_{\nu\mu}(\omega) e^{+i\omega t} \right). \tag{18}$$

$V_{k\mu}$ and $U_{k\mu}$ denote the stationary Bogoliubov coefficients. The induced density matrix $\rho(t) = V^*(t) V^T(t)$ reads:

$$\rho(t) = V^* V^T + \eta \left(\delta\rho(\omega) e^{-i\omega t} + \delta\rho^\dagger(\omega) e^{+i\omega t} \right), \tag{19}$$

with $\delta\rho(\omega) = UX(\omega)V^T + V^* Y^T(\omega) U^\dagger$. The induced pairing tensor $\kappa(t) = V^*(t) U^T(t)$ reads:

$$\kappa(t) = V^* U^T + \eta \left(\delta\kappa^{(+)}(\omega) e^{-i\omega t} + \delta\kappa^{(-)}(\omega) e^{+i\omega t} \right), \tag{20}$$

with $\delta\kappa^{(+)}(\omega) = UX(\omega)U^T + V^* Y^T(\omega) V^\dagger$ and $\delta\kappa^{(-)}(\omega) = V^* X^\dagger(\omega) V^\dagger + UY^*(\omega) U^T$. It should be noted that although $\delta\rho(\omega)$ matrix is not necessarily Hermitian, the matrices $\delta\kappa^{(+)}(\omega)$ and $\delta\kappa^{(-)}(\omega)$ are still antisymmetric. The induced single-particle Hamiltonian:

$$\delta h(t) = \eta \left(\delta h(\omega) e^{-i\omega t} + \delta h^\dagger(\omega) e^{+i\omega t} \right), \tag{21}$$

is linearized explicitly in the coordinate space, while the induced pairing field reads:

$$\delta\Delta(t) = \eta \left(\delta\Delta^{(+)}(\omega) e^{-i\omega t} + \delta\Delta^{(-)}(\omega) e^{+i\omega t} \right), \tag{22}$$

with

$$\delta\Delta^{(\pm)}_{lm}(\omega) = \frac{1}{2} \sum_{pq} \bar{v}_{lmpq} \delta\kappa^{(\pm)}_{pq}(\omega). \tag{23}$$

$\bar{v}_{lmpq}$ are the antisymmetrized matrix elements of the pairing interaction. The $\delta H^{20}(\omega)$ and $\delta H^{02}(\omega)$ are calculated by transforming back to the quasiparticle basis:

$$\delta\mathcal{H}(\omega) = \mathcal{W}^\dagger \begin{pmatrix} \delta h(\omega) & \delta\Delta^{(+)}(\omega) \\ -\delta\Delta^{(-)}(\omega)^* & -\delta h^T(\omega) \end{pmatrix} \mathcal{W}. \tag{24}$$

The explicit expressions for $\delta H^{20}(\omega)$ and $\delta H^{02}(\omega)$ read:

$$\delta H^{20}(\omega) = + U^\dagger \delta h(\omega) V^* - V^\dagger \delta h^T(\omega) U^* + U^\dagger \delta\Delta^{(+)}(\omega) U^* - V^\dagger [\delta\Delta^{(-)}(\omega)]^* V^*, \tag{25}$$

$$\delta H^{02}(\omega) = - V^T \delta h(\omega) U + U^T \delta h^T(\omega) V - V^T \delta\Delta^{(+)}(\omega) V + U^T [\delta\Delta^{(-)}(\omega)]^* U. \tag{26}$$

The transition strength for each particular energy is calculated from:

$$\frac{dB}{d\omega}(f, \omega) = S(f, \omega) = -\frac{1}{\pi} \operatorname{Im} \operatorname{Tr}[f^\dagger \delta\rho(\omega)], \tag{27}$$

where $\delta\rho(\omega)$ denotes the induced density matrix and f_{kl} are the matrix elements of the operator $F(\omega)$ in the single-particle basis:

$$F(\omega) = \sum_{kl} f_{kl} c^\dagger_k c_l. \tag{28}$$

3. Practical implementation

3.1. Point-coupling models

The energy density functional (EDF) for the relativistic point-coupling model is built from densities and currents bilinear in the Dirac spinor field of the nucleon:

$$E_{RMF}[\psi, \bar{\psi}, A^\mu] = \sum_{i=1}^{A} \int d^3r \, \psi_i^\dagger \left(\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m \right) \psi_i + \frac{e}{2} \int d^3r j^p_\mu A^\mu + \frac{1}{2} \int d^3r \left[\alpha_s \rho_s^2 + \alpha_v j_\mu j^\mu + \alpha_{tv} \vec{j}_\mu \cdot \vec{j}^\mu + \delta_s \rho_s \triangle \rho_s \right]. \tag{29}$$

Vectors in isospin space are denoted by arrows, and boldfaced symbols will indicate vectors in ordinary three-dimensional space. The Dirac spinor ψ denotes the nucleon with mass m. The strength parameters α_i, $i \in \{s, v, tv\}$ of the interaction terms are functions of the nucleon 4-current:

$$j^\mu = \bar{\psi} \gamma^\mu \psi = \hat{\rho} u^\mu, \tag{30}$$

where u^μ is the 4-velocity defined as $(1 - \boldsymbol{v}^2)^{-1/2}(1, \boldsymbol{v})$. In the rest-frame of homogeneous nuclear matter $\boldsymbol{v} = 0$. The variation of the EDF (29) with respect to the Dirac spinors $\bar{\psi}$ leads to the Dirac equation:

$$h_D \psi_i(\boldsymbol{r}) = \epsilon_i \psi_i(\boldsymbol{r}), \tag{31}$$

where h_D denotes the single-nucleon Dirac Hamiltonian:

$$h_D = \boldsymbol{\alpha} \cdot (\boldsymbol{p} - \boldsymbol{\Sigma}) + \Sigma_0 + \beta(m + \Sigma_s). \tag{32}$$

The nuclear self-energies Σ are defined by the following expressions:

$$\Sigma_s = \alpha_s \rho_s + \delta_s \triangle \rho_s, \tag{33}$$

$$\Sigma^\mu = \alpha_v j^\mu + e \frac{1 + \tau_3}{2} A^\mu + \alpha_{tv} \vec{\tau} \cdot \vec{j}^\mu + \Sigma^\mu_R. \tag{34}$$

The density dependence of the vertex functions α_s, α_v and α_{tv}, produces the rearrangement contribution to the vector self-energy:

$$\Sigma^\mu_R = \frac{1}{2} \frac{j^\mu}{\rho_v} \left(\frac{\partial \alpha_s}{\partial \rho_v} \rho_s^2 + \frac{\partial \alpha_v}{\partial \rho_v} j_\mu j^\mu + \frac{\partial \alpha_{tv}}{\partial \rho_v} \vec{j}_\mu \cdot \vec{j}^\mu \right). \tag{35}$$

The `DIRQFAM` code includes density-dependent point-coupling interaction DD-PC1 [26] where the following ansatz was used for the functional form of the couplings:

$$\alpha_s(\rho_v) = a_s + (b_s + c_s x) e^{-d_s x}, \tag{36}$$

$$\alpha_v(\rho_v) = a_v + b_v e^{-d_v x}, \tag{37}$$

$$\alpha_{tv}(\rho_v) = b_{tv} e^{-d_{tv} x}, \tag{38}$$

with $x = \rho_v / \rho_{sat}$. ρ_{sat} denotes the nucleon density at saturation in symmetric nuclear matter. Because of the charge conservation, only 3rd component of the isovector current contributes. Furthermore, in the ground-state solution for an even–even nucleus there are no currents (time-reversal invariance), and the corresponding spatial components of the currents vanish. Finally, the electromagnetic field is determined by solving the Poisson equation:

$$- \triangle A^0 = e \rho^p_v, \tag{39}$$

where ρ_v^p denotes the proton vector density. The induced single-particle Dirac Hamiltonian is obtained by calculating the functional derivative of the Dirac Hamiltonian with respect to the density:

$$\delta h_D = \begin{pmatrix} \delta V + \delta S & -\boldsymbol{\sigma}\cdot\delta\boldsymbol{\Sigma} \\ -\boldsymbol{\sigma}\cdot\delta\boldsymbol{\Sigma} & \delta V - \delta S \end{pmatrix}, \tag{40}$$

where $\delta S = \delta\Sigma_s$, $\delta V = \delta\Sigma^0 + \delta\Sigma_R^0 + \frac{1+\tau_3}{2}\delta V_C$ and $\delta\boldsymbol{\Sigma}$ denote the induced scalar, time-like and space-like components of the induced vector potential, respectively. The detailed expressions for $\delta\Sigma_s$, $\delta\Sigma^0$, $\delta\Sigma_R^0$ and $\delta\boldsymbol{\Sigma}$ are listed below.

$$\delta\Sigma_s = \left\{\alpha_s'(\rho_v^0)\rho_s^0\right\}\delta\rho_v + \left\{\alpha_s(\rho_v^0)\right\}\delta\rho_s + \delta_s\triangle\delta\rho_s, \tag{41}$$

$$\delta\Sigma^0 = \left\{\alpha_v'(\rho_v^0)\rho_v^0 + \alpha_v(\rho_v^0) + \tau_3\alpha_{tv}'(\rho_v^0)\rho_{tv}^0\right\}\delta\rho_v + \left\{\tau_3\alpha_{tv}(\rho_v^0)\right\}\delta\rho_{tv}, \tag{42}$$

$$\delta\Sigma_R^0 = \frac{1}{2}\left\{\alpha_s''(\rho_v^0)(\rho_s^0)^2 + \alpha_v''(\rho_v^0)(\rho_v^0)^2 + \alpha_{tv}''(\rho_v^0)(\rho_{tv}^0)^2\right\}\delta\rho_v + \left\{\alpha_s'(\rho_v^0)\rho_s^0\right\}\delta\rho_s + \left\{\alpha_v'(\rho_v^0)\rho_v^0\right\}\delta\rho_v + \left\{\alpha_{tv}'(\rho_v^0)\rho_{tv}^0\right\}\delta\rho_{tv}, \tag{43}$$

$$\delta\boldsymbol{\Sigma} = \left\{\alpha_v(\rho_v^0)\right\}\delta\boldsymbol{j}_v + \left\{\tau_3\alpha_{tv}(\rho_v^0)\right\}\delta\boldsymbol{j}_{tv}. \tag{44}$$

ρ_s^0, ρ_v^0 and ρ_{tv}^0 denote the isoscalar–scalar, isoscalar–vector and isovector–vector ground state densities. We notice that the expression for $\delta\boldsymbol{\Sigma}$ is simplified considerably due to the fact that the single-nucleon currents vanish in the time-reversal invariant ground-state.

The induced Coulomb field δV_C is calculated by solving the standard Poisson equation (39) with the induced proton density as the source term. In the current implementation of the code, we omit the space-like components of the induced Coulomb field since their contribution should be negligible in comparison to the other terms.

Finally, we have also implemented the method proposed in [13] to separate the spurious response related to the breaking of the translation symmetry from the physical response. Although the zero-energy modes and the physical modes should be decoupled exactly within the random phase approximation [7,27], in practice there is always some mixing mostly due to the finite size of the oscillator basis used in the calculation. Other numerical inaccuracies also contribute to the mixing of the spurious and physical modes, but their contribution is less pronounced in comparison to the finite size of the basis. For example, the finite size of the harmonic oscillator basis certainly violates the translational invariance thus causing admixtures of the zero-energy mode within the physical modes. We have verified that the method proposed in Ref. [13] removes such unphysical admixtures.

3.2. Separable pairing interaction

Pairing correlations in nuclei are restricted to an energy window of a few MeV around the Fermi level, and their scale is well separated from the scale of binding energies, that are in the range from several hundred to thousand MeV. There is no empirical evidence for any relativistic effect in the nuclear pairing field Δ and, therefore, a hybrid RHB model [28] with a non-relativistic pairing interaction can be formulated. For a general two-body interaction, the matrix elements of the relativistic pairing field read:

$$\Delta_{n_1p_1,n_1'p_1'} = \frac{1}{2}\sum_{n_2p_2,n_2'p_2'}\langle n_1p_1, n_1'p_1'|V^{pp}|n_2p_2, n_2'p_2'\rangle_a\kappa_{n_2p_2,n_2'p_2'}. \tag{45}$$

The indices p_1, p_1', p_2 and p_2' refer to the large and small components of the quasiparticle Dirac spinors:

$$U_k = \begin{pmatrix} f_k^{(U)} \\ ig_k^{(U)} \end{pmatrix}, \qquad V_k = \begin{pmatrix} f_k^{(V)} \\ ig_k^{(V)} \end{pmatrix}. \tag{46}$$

In practical applications of the RHB model only the large components of the spinors U_k and V_k are used to build the pairing tensor κ. The resulting pairing field reads:

$$\Delta_{n_1f,n_1'f} = \frac{1}{2}\sum_{n_2n_2'}\langle n_1f, n_1'f|V^{pp}|n_2f, n_2'f\rangle_a\,\kappa_{n_2f,n_2'f}. \tag{47}$$

The other components: Δ_{fg}, Δ_{gf}, and Δ_{gg} can be safely omitted [29].

In order to reduce the computational effort, a separable form of the pairing force has been introduced for RHB calculations in spherical and deformed nuclei [30–32]. The force is separable in momentum space, and is completely determined by two parameters that are adjusted to reproduce the pairing gap of the Gogny force in symmetric nuclear matter. The gap equation in the $^1S_0$ channel reads:

$$\Delta(k) = -\int_0^\infty \frac{k'^2dk'}{2\pi^2}\langle k|V^{^1S_0}|k'\rangle\frac{\Delta(k')}{2E(k')}, \tag{48}$$

and the pairing force is separable in momentum space:

$$\langle k|V^{^1S_0}|k'\rangle = -Gp(k)p(k'). \tag{49}$$

By assuming a simple Gaussian ansatz $p(k) = e^{-a^2k^2}$, the two parameters G and a have been adjusted to reproduce the density dependence of the gap at the Fermi surface, calculated with a Gogny force. For the D1S parameterization [33] of the Gogny force the following values were determined: $G = 728$ MeV fm^3 and $a = 0.644$ fm. When the pairing force equation (49) is transformed from momentum to coordinate space, it takes the form:

$$V^{pp}(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_1',\boldsymbol{r}_2') = -\frac{G}{2}(1-P_\sigma)\delta^3\left(\boldsymbol{R}-\boldsymbol{R}'\right)P(\boldsymbol{r})P(\boldsymbol{r}'), \tag{50}$$

where $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_1+\boldsymbol{r}_2)$ and $\boldsymbol{r} = \boldsymbol{r}_2-\boldsymbol{r}_1$ denote the center-of-mass and the relative coordinates, respectively, and $P(\boldsymbol{r})$ is the Fourier transform of the $p(k)$ function:

$$P(\boldsymbol{r}) = \frac{1}{\left(4\pi a^2\right)^{3/2}}e^{-\boldsymbol{r}^2/4a^2}. \tag{51}$$

The pairing force has a finite range and, because of the presence of the factor $\delta^3\left(\boldsymbol{R}-\boldsymbol{R}'\right)$, it preserves translational invariance. Even though $\delta^3\left(\boldsymbol{R}-\boldsymbol{R}'\right)$ implies that this force is not completely separable in coordinate space, the corresponding antisymmetrized pp matrix elements:

$$\langle n_1n_2|V^{pp}|n_1'n_2'\rangle_a = \langle n_1n_2|V^{pp}|n_1'n_2'\rangle - \langle n_1n_2|V^{pp}|n_2'n_1'\rangle, \tag{52}$$

can be represented as a sum of a finite number of separable terms in the harmonic oscillator basis. Detailed expressions can be found in Appendix E. Finally, the induced pairing field is calculated according to Eq. (23).

3.3. Numerical details

The current version of the code supports the electric isoscalar and isovector multipole operators, defined as:

$$f_{JK}^{IS} = \sum_{i=1}^{A} f_{JK}(\boldsymbol{r}_i), \quad f_{JK}^{IV} = \sum_{i=1}^{Z} f_{JK}(\boldsymbol{r}_i) - \sum_{i=1}^{N} f_{JK}(\boldsymbol{r}_i). \tag{53}$$

The summations in the expression for the f_{JK}^{IV} operator run over protons and neutrons, respectively. In general, the operator $f_{JK}(\boldsymbol{r}) = r^JY_{JK}(\theta,\phi)$. However, for the monopole excitations, the operator is defined as $f_{00}(\boldsymbol{r}) = r^2$, while for the isovector dipole excitation ($D_K = rY_{1K}$, $K = 0,\pm1$), the following definition is employed:

$$D_K = e\frac{NZ}{A}\left[\frac{1}{Z}\sum_{i=1}^{Z}D_K(\boldsymbol{r}_i) - \frac{1}{N}\sum_{i=1}^{N}D_K(\boldsymbol{r}_i)\right]. \tag{54}$$

Since for an even–even axially symmetric nucleus the operators f_{JK} and f_{J-K} produce identical strength functions, in the code we employ the $f^{(+)}_{JK} = (f_{JK} + (-1)^K f_{J-K})/\sqrt{2+2\delta_{K0}}$ operator and assume $K \geq 0$. Detailed expressions can be found in Appendix B.1.

The QFAM equations (14) and (15) are solved iteratively by employing the modified Broyden's method [34]. The mth Broyden vector $\boldsymbol{V}^{(m)}$ in the DIRQFAM code contains the matrix elements of the induced fields $\boldsymbol{V} \equiv \{\delta h(\omega), \delta\Delta^{(+)}(\omega), \delta\Delta^{(-)}(\omega)\}$. The default value for the number of Broyden vectors retained in the Broyden memory is 30 (broyd_m variable located in the prep.f file) and the convergence criterion is the relative error between two consecutive Broyden vectors:

$$\frac{\left\|\boldsymbol{V}^{(m)} - \boldsymbol{V}^{(m-1)}\right\|_2}{\left\|\boldsymbol{V}^{(m-1)}\right\|_2} < \texttt{tol}, \tag{55}$$

where $\|\cdot\|_2$ denotes the Euclidean norm and tol is small value, defined in the iter_fam subroutine. We have verified that for most cases already the value $\texttt{tol} = 10^{-5}$ produces satisfactory precision of transition strength (4–5 correct most significant digits). However, if higher precision is required, one should reduce the default value (10^{-5}) for the tol parameter.

In order to prevent that the QFAM solutions diverge in the vicinity of the QRPA state Ω_i, we add a small imaginary part to the energy $\omega \to \omega + i\gamma$. This procedure corresponds to the folding of the QRPA strength function with a Lorentzian of width $\Gamma = 2\gamma$ [16].

In order to solve Eqs. (14) and (15), the QFAM amplitudes are expanded in a basis of the eigenstates of the axially symmetric harmonic oscillator and the simplex-y operator. The choice of this basis is motivated by the fact that the $f^{(+)}_{JK}$ operator does not connect the basis states with the opposite simplex quantum numbers, i.e., the $f^{(+)}_{JK}$ operator is block-diagonal in the basis of the eigenstates of the simplex-y operator. In the following we will refer to this basis as the simplex-y harmonic oscillator (simplex-y HO) basis. The induced currents and densities are first computed in the simplex-y HO basis and after that they are transformed in the coordinate space to calculate the induced fields. Spatial integrals needed to calculate the matrix elements of the induced single-particle Hamiltonian $\delta h(\omega)$ are computed using cylindrical coordinates $r_\perp$ and z. The integration is carried out by using Gaussian quadratures with NGH Gauss–Hermite nodes in the $z > 0$ direction and NGL Gauss–Laguerre nodes in the $r_\perp$ direction, while the angular part is calculated analytically. The default values for both NGH and NGL is 48.

4. Description of the DIRQFAM code

4.1. Structure of the DIRQFAM code

The DIRQFAM code consists of a Fortran source code and two additional files: dirqfam.par and dirqfam.dat. The dirqfam.par file contains the relevant information about the dimensions of the arrays, depending on the multipolarity K of the excitation, the number of oscillator shells selected for the expansion of nucleon spinors (n0f), and the number of Gaussian quadrature nodes in the $r_\perp$ (NGL) and the $z > 0$ direction (NGH). This file is generated prior to the compilation process based on the data from the dirqfam.dat file by invoking the make prep command. In addition to the n0f, NGH and NGL parameters, the dirqfam.dat file includes the data for the specific nucleus being calculated and the information related to the multipole response calculation.

The main program calls various subroutines that read the data and perform the computation. The execution essentially consists of three parts. The first part uses the file dirqfam.dat to start the program, initializes and generates all the relevant information. The second part of the code carries out the self-consistent ground-state (GS) computation as described in Ref. [23].

The third part of the code performs the computation of the multipole response upon achieving the convergence of the ground-state calculation. Below we specify the subroutines related to this part of the code.

- main_fam: Main QFAM subroutine that calls the subroutines listed below.
  - base_simplex: Constructs the configuration space and the arrays of quantum numbers for the HO simplex-y basis.
  - construct_u and construct_v: Transforms the Bogoliubov U and V matrices from the HO to the HO simplex-y basis according to Eqs. (A.17) and (A.18) given in Appendix A.
  - check_gs_dens and check_unitarity: Verifies the previous transformation by recalculating the ground-state density and calculating the unitarity conditions for the U and V matrices ($\mathcal{W}\mathcal{W}^\dagger = \mathbb{1}$, where the matrix $\mathcal{W}$ is defined in Eq. (2)).
  - init_fam: Reads relevant QFAM input data and initializes QFAM submodule:
    - init_basis: Calculates the basis wave functions in the coordinate space (see Appendix A).
    - init_multipole: Calculates the matrix elements of the multipole operator (see Appendix B).
    - init_spurious: Calculates the matrices relevant for eliminating the translational Nambu–Goldstone mode.
    - init_coulomb: Calculates the Green's function for the induced Coulomb interaction (see Appendix D).
    - init_pairing: Calculates the W coefficients for the pairing matrix elements (see Appendix E).
  - start_fam: Determines whether the user wants to calculate the fully self-consistent or the free response for some predefined range of energies or to calculate self-consistent response and print induced density for some selected value of energy. If the user chooses to calculate the self-consistent response function over the range of energies, the code loops over the predefined energy range and executes the following subroutines:
    - iter_fam: Performs QFAM iterations for single energy until self-consistency is reached by calling the following sequence of subroutines:
      - fam_drhodkappa: Calculates the induced density matrix $\delta\rho(\omega)$ and pairing tensor $\delta\kappa^{(\pm)}(\omega)$ using the induced single-particle Hamiltonian $\delta h(\omega)$ and pairing field $\delta\Delta^{(\pm)}(\omega)$ from previous iteration.
      - fam_ddensdcurr: Calculates the induced densities and currents in the coordinate space (see Appendix C).
      - fam_dpotentials: Calculates the induced potentials in the coordinate space according to Eqs. (41)–(44).
      - fam_dh1: Calculates the induced single-particle Hamiltonian $\delta h(\omega)$ in simplex-y basis.
      - fam_ddelta: Calculates the induced pairing field $\delta\Delta^{(\pm)}(\omega)$.

Table 1
Total running time per iteration and the required amount of memory for QFAM calculation of $J = 3$, $K = 1$ response in the ^{20}Ne atomic nucleus with NGH $= 48$, NGL $= 48$ Gaussian quadrature nodes. Test was performed on the Intel® NUC Kit NUC8i7HVK machine with OpenBLAS [37] implementation on single thread.

Number of oscillator shells	Total time per iteration (s)	Required amount of memory (GiB)
12	1.5	1.53
14	3.1	2.64
16	5.5	4.55
18	9.5	7.63
20	16	12.3
22	25	19.4

· `fam_broyden`: Performs the Broyden mixing step.

∗ `fam_strength`: Calculates the transition strength $S(f, \omega)$ after the convergence of the QFAM calculation has been achieved.

If the user chooses to calculate free response, then $\delta h(\omega)$ and $\delta\Delta^{(\pm)}(\omega)$ are set to zero, `fam_drhodkappa` is invoked followed by immediate calculation of transition strength. If the user chooses to calculate the self-consistent response for a selected value of energy, the code executes the `fam_iter` routine for this particular value of energy followed by the `print_dens` routine in order to print out the induced density. The code prints out both the real and imaginary parts of the induced density together with the ground-state density so that the user can easily generate a movie showing the density oscillations.

4.2. Compilation and code execution

The programming language of the DIRQFAM code is Fortran and the user should provide an implementation of the BLAS and LAPACK (version 3.6.0. or higher) linear-algebra libraries [35,36]. Since the code depends heavily on `zgemm`, `dgemm` and `dgemv` subroutines, we recommend that the user provides an efficient implementation of the BLAS library. The code is compiled by standard Makefile build automation which is set to work with the GFortran compiler. If the user invokes `make prep` command, an auxiliary code will generate `dirqfam.par` file that contains the relevant information about the dimension of various arrays used in the code. The `make run` command compiles the code and produces the executable file `run`. The code is executed by the `./run` command. If the size of the `common` blocks and local data exceeds 2 GB, the code should be compiled using the `-mcmodel` option with values `-mcmodel=medium` or `-mcmodel=large`. Otherwise, `-mcmodel=small` will be sufficient. The default option `-mcmodel=medium` can easily be modified by editing the Makefile.

In order to illustrate the computational resources required to run the QFAM calculations, in Table 1 we present the total running time per QFAM iteration and the required amount of memory for a calculation of $J = 3, K = 1$ response of ^{20}Ne nucleus with NGH $= 48$ and NGL $= 48$. Typically, in order to obtain converged solution, one has to perform 30–60 iterations at each energy. We would also like to emphasize that QFAM calculation can be parallelized very easily, thus reducing the time required to perform such calculations.

4.3. Input data

The input data can be divided into two parts: (i) input related to the ground state calculation, (ii) input related to the QFAM calculation. The input data needed by the ground state part of the code includes:

- Number of oscillator shells used in the expansion of nucleon spinors (`n0f`). In the current implementation of the code `n0f` should be even.
- Number of Gauss–Hermite nodes (`NGH`).
- Number of Gauss–Laguerre nodes (`NGL`).
- β-deformation parameter of the harmonic oscillator basis (`beta0`). We recommend that the user chooses the value that is close to the actual deformation of the considered atomic nucleus.
- β-deformation parameter for the initial Woods–Saxon potentials (`betai`). We recommend that the user chooses the value that is close to the actual deformation of the considered atomic nucleus.
- The starting parameter for the potentials (`inin`). If the parameter `inin` is set to 1, the code starts from a default Woods–Saxon potentials predefined in the code. If the parameter `inin` is set to 0, the initial potentials are read from the file `dirhb.wel`.
- The starting parameter for the pairing field (`inink`). If `inink` is set to 1, the code starts with the diagonal pairing field with equal matrix elements `delta0`. If `inink` is set to 0, the initial pairing matrix elements are read from the file `dirhb.del`.
- The nuclide to be computed: the element name (`nucnam`) followed by the mass number (`nama`). If the element name has only one character, it should begin with an underscore, e.g. `_C 12, _O 16, _U 238`.
- Neutron and proton initial pairing gaps (`delta0`).
- Acronym of the parameter set of the selected energy density functional (`parname`). Current implementation of the code supports DD-PC1 effective interaction.
- The quadrupole constraint control parameter `icstr`. If `icstr` is set to 0, the quadrupole constraint is not included, and the parameters `betac` and `cqad` are not used. If `icstr` is set to 1, then `betac` denotes the constrained value of the quadrupole deformation.
- Constrained value of the β-deformation parameter (`betac`).
- Stiffness constant for the quadrupole constraint (`cqad`). The default value is 0.1, but if the iteration starts diverging it should be reduced.

The input parameters used to calculate multipole response include:

- The calculation type flag (`i_calculation_type`). Value 0: free response is calculated for a given range of energies. Value 1: Self-consistent response is calculated for a given range of energies. Value 2: Self-consistent response is calculated for a given energy (`omega_print`) and the induced density is outputted.
- The Coulomb flag (`i_coulomb`). Value 0: Coulomb interaction is omitted both in the ground state and the QFAM calculation. Value 1: Coulomb interaction is included both in the ground state and the QFAM calculation.
- The pairing flag (`i_pairing`). Value 0: pairing interaction is omitted both in the ground state and the QFAM calculation by setting the pairing strength constant G to zero. Value 1: pairing interaction is included both in the ground state and the QFAM calculation.
- J (`J_multipole`) and K (`K_multipole`) multipolarity values that define the multipole operator f_{JK}. In the current implementation of the code their values are restricted to $0 \leq J \leq 3$, $0 \leq K \leq J$.
- The isospin `ISO` flag that determines whether the excitation is isoscalar (`ISO` $= 0$) or isovector (`ISO` $= 1$).

- The smearing width γ (in MeV) used in the QFAM calculation (`gamma_smear`).
- Parameters that control the starting point (`omega_start`), the ending point (`omega_end`) and the increment (`delta_omega`) of the energy range over which the response is calculated. Relevant only if the calculation type flag is set to 0 or 1.
- If the user chooses to calculate the response and print the induced density for some particular value of energy (calculation type flag set to 2), this value of energy is also provided in the input file (`omega_print`).

4.4. Output data

The output of the calculation is divided into two parts. The first output file `dirhb.out` located in the `GS_output` directory contains the information on the ground state calculation. Detailed description of this file can be found in Ref. [23]. The second part of the output relevant for the QFAM calculation is located in the `QFAM_output` directory. The calculated strength function is written to the `strength.out` file. If the calculation type flag is set to 2, an additional file `rhov.out` is generated which contains the ground state vector density $\rho_v^0(\boldsymbol{r})$ and the induced vector density $\delta\rho_v(\boldsymbol{r},\omega)$ for the selected energy (`omega_print`). The values printed in the `rhov.out` file are suitable for visualizing the time dependent density calculated by using the following relation:

$$\rho_v(\boldsymbol{r},t) = \rho_v^0(\boldsymbol{r}) + 2\eta\,\mathrm{Re}\left[e^{-i\omega t}\delta\rho_v(\boldsymbol{r},\omega)\right]. \tag{56}$$

4.5. Test calculations

As a benchmark after the code has been installed on a particular computer, we provide three test calculations along with the code. The `test1` directory contains the fully self-consistent calculation of the $J = 3$, $K = 1$ response built on top of the deformed ground state of the ^{20}Ne isotope. The `test2` directory contains the calculation for the same configuration only for fixed energy and in this case the induced vector density is printed. Finally, the `test3` directory contains the free response for the same configuration as the one described in the `test1` directory case. Examples of dirqfam.dat files for three test calculations can be found in the test directory together with the expected output files.

Finally, we have also performed the fully self-consistent calculation of the $J = 2$, ($K = 0$, $K = 1$, $K = 2$) response built on top of the spherical configuration of the ^{84}Zr isotope. Due to the Wigner–Eckart theorem, spherical nuclei should exhibit the strength function response invariant to the quantum number K for the fixed value of the angular momentum J. In Table 2 we display the results of this calculation thus demonstrating the agreement within 7 most significant digits in the strength response function. In this calculation, we set Broyden's iteration tolerance to a slightly lower value (`tol` $= 10^{-8}$, located in the `iter_fam` subroutine) in order to achieve better level of agreement between various K quantum numbers.

Table 2
Isoscalar quadrupole response in the spherical configuration of the ^{84}Zr atomic nucleus. Calculation was performed in a space of 10 harmonic oscillator shells with dense Gaussian quadrature mesh: `NGH` = 48, `NGL` = 48. The value of `tol` parameter was decreased to `tol` = 10^{-8} in order to improve the level of agreement between various K quantum numbers.

Energy [MeV]	$S(f,\omega)$ [fm^4 MeV^{-1}]		
	$K = 0$	$K = 1$	$K = 2$
5	**31.5919**694917	**31.5919**710786	**31.5919**715257
10	**24.7155**886321	**24.7155**875415	**24.7155**892845
15	**107.0087**945746	**107.0087**760979	**107.0087**950602
20	**39.7574**698943	**39.7574**764571	**39.7574**725327
25	**8.918110**4468	**8.918111**1725	**8.918110**2475
30	**3.184910**2533	**3.184910**6081	**3.184910**2773
35	**1.334428**3637	**1.334428**3202	**1.334428**2347
40	**0.781888**53950	**0.781888**6118	**0.781888**5252

5. Summary

We have developed a computer code to calculate the multipole response of even–even axially symmetric deformed nuclei by using the quasiparticle finite amplitude method built on top of the self-consistent mean-field models based on the relativistic nuclear energy density functional. The particle–hole channel is described by a zero-range relativistic effective interaction, while the particle–particle channel is described by a separable finite-range pairing force.

The present version of the code solves the QFAM equations by expanding the QFAM amplitudes in a basis of eigenstates of axially symmetric harmonic oscillator and the simplex-y operator. The execution time of the code depends heavily on the number of oscillator shells used in this expansion. However, the calculation can be trivially parallelized by calculating the response for each particular value of the energy on a different node. This would allow systematic studies of collective model even in medium-heavy and heavy deformed nuclei.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work has been supported in part by the Croatian Science Foundation project Structure and Dynamics of ExoticFemtosystems (IP-2014-09-9159) and the QuantiXLie Centre of Excellence, a project cofinanced by the Croatian Government and European Union through the European Regional Development Fund - the Competitiveness and Cohesion Operational Programme (KK.01.1.1.01). A.B. would like to thank Zlatko Drmač for sharing his immense knowledge and expertise on numerical algorithms. T.N. gratefully acknowledges many helpful discussions with Peter Ring, Nobuo Hinohara and Markus Kortelainen.

Appendix A. Single-nucleon basis

In this section we first briefly describe the single-particle basis of eigenfunctions of a single-particle Hamiltonian for an axially symmetric deformed harmonic oscillator (HO) potential:

$$V_{osc}(z,r_\perp) = \frac{1}{2}m\omega_z^2 z^2 + \frac{1}{2}m\omega_\perp^2 r_\perp^2, \tag{A.1}$$

used in the ground-state calculations. $(z, r_\perp, \phi)$ denote the standard cylindrical coordinates:

$$x = r_\perp\cos\phi, \quad y = r_\perp\sin\phi, \quad z = z. \tag{A.2}$$

Imposing volume conservation, the two oscillator frequencies $\hbar\omega_z$ and $\hbar\omega_\perp$ can be expressed in terms of a deformation parameter β_0:

$$\hbar\omega_z = \hbar\omega_0 e^{-\sqrt{\frac{5}{4\pi}}\beta_0}, \quad \hbar\omega_\perp = \hbar\omega_0 e^{\frac{1}{2}\sqrt{\frac{5}{4\pi}}\beta_0}. \tag{A.3}$$

The corresponding oscillator length parameters are:

$$b_z = \sqrt{\frac{\hbar}{m\omega_z}}, \quad b_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}}. \tag{A.4}$$

$b_\perp^2 b_z = b_0^3$ because of the volume conservation. The basis is now determined by the two constants $\hbar\omega_0$ and β_0. Current implementation of the code uses the following estimate for the HO frequency: $\hbar\omega_0 = 41A^{1/3}$ MeV. The eigenfunctions of the deformed harmonic oscillator potential are labeled by the set of quantum numbers:

$$|\alpha\rangle = |n_z n_r \Lambda m_s\rangle, \tag{A.5}$$

where $n_z, n_r \in \mathbb{N}_0$, are the number of nodes in the z and $r_\perp$ directions, respectively. $\Lambda \in \mathbb{Z}$ and $m_s \in \{\pm\frac{1}{2}\}$ are projections of the orbital angular momentum and spin on the intrinsic z-axis, respectively. Making use of the dimensionless variables:

$$\xi = z/b_z, \quad \eta = r_\perp^2/b_\perp^2, \tag{A.6}$$

the harmonic oscillator eigenvectors read:

$$|\alpha\rangle = |n_z n_r \Lambda m_s\rangle = \varphi_{n_z}(z, b_z)\varphi_{n_r}^{\Lambda}(r_\perp, b_\perp)\frac{e^{i\Lambda\phi}}{\sqrt{2\pi}}\chi_{m_s}(s), \tag{A.7}$$

where:

$$\varphi_{n_z}(z, b_z) = b_z^{-1/2}\mathcal{N}_{n_z}H_{n_z}(\xi)e^{-\xi^2/2}, \tag{A.8}$$

$$\varphi_{n_r}^{\Lambda}(r_\perp, b_\perp) = b_\perp^{-1}\mathcal{N}_{n_r}^{\Lambda}\sqrt{2}\eta^{|\Lambda|/2}L_{n_r}^{|\Lambda|}(\eta)e^{-\eta/2}. \tag{A.9}$$

$H_{n_z}(\xi)$ and $L_{n_r}^{|\Lambda|}(\eta)$ denote the Hermite and associated Laguerre polynomials, respectively. The normalization factors are:

$$\mathcal{N}_{n_z} = (\sqrt{\pi}2^{n_z}n_z!)^{-1/2} \quad \text{and} \quad \mathcal{N}_{n_r}^{\Lambda} = (n_r!/(n_r+|\Lambda|)!)^{1/2}. \tag{A.10}$$

The large and small components of a Dirac spinor are expanded independently in terms of the oscillator eigenfunctions:

$$f_k(\boldsymbol{r}, m_s, t_z) = \sum_{\substack{\text{Shell}(\alpha)\le N_{max}\\ \Omega=\Lambda+m_s>0}} f_\alpha^{(k)}|\alpha\rangle\chi_{t_z}(t), \tag{A.11}$$

$$g_k(\boldsymbol{r}, m_s, t_z) = \sum_{\substack{\text{Shell}(\tilde\alpha)\le N_{max}+1\\ \tilde\Omega=\tilde\Lambda+\tilde m_s>0}} g_{\tilde\alpha}^{(k)}|\tilde\alpha\rangle\chi_{t_z}(t). \tag{A.12}$$

To avoid the appearance of spurious states, the quantum numbers α and $\tilde\alpha$ are chosen in such a way that the corresponding shell they belong to: $\text{Shell}(\alpha) = n_z + 2n_r + |\Lambda|$ and $\text{Shell}(\tilde\alpha) = \tilde n_z + 2\tilde n_r + |\tilde\Lambda|$, are not larger than N_{max} and $N_{max}+1$ for the large and small components, respectively.[3] Due to the time-reversal symmetry of the ground state solution, only positive eigenvalues $\Omega = \Lambda + m_s > 0$ of the J_z symmetry operator are retained in the expansion.

The HO basis states are used to build the eigenfunctions of the simplex-y operator $S_y = Pe^{-i\pi J_y}$, where P denotes the parity operator.[4] One can easily verify that the following combinations are eigenstates of the S_y operator with eigenvalues $s = +i$ and $s = -i$:

$$|n_z n_r \Lambda;\ s = +i\rangle = \frac{1}{\sqrt{2}}\left(i|n_z n_\perp \Lambda\uparrow\rangle + |n_z n_r - \Lambda\downarrow\rangle\right), \tag{A.13}$$

$$|n_z n_r \Lambda;\ s = -i\rangle = \frac{1}{\sqrt{2}}\left(|n_z n_\perp \Lambda\uparrow\rangle + i|n_z n_r - \Lambda\downarrow\rangle\right). \tag{A.14}$$

Furthermore, these states are related by the time-reversal operator T:

$$T|n_z n_r \Lambda;\ s = \pm i\rangle = \mp|n_z n_r \Lambda;\ s = \mp i\rangle. \tag{A.15}$$

Due to the time-reversal symmetry of the ground state solution, for each solution with $\Omega > 0$, there is a degenerate time-reversed solution with $\Omega < 0$. These two states can be used to construct the eigenstates of the RHB Hamiltonian that are simultaneously also the eigenfunctions of the simplex-y operator. The HO basis states used to expand the ground state quasiparticle spinors are ordered in the following way: basis states with $\Omega > 0$ are listed first followed by their time-reversed pairs. The simplex-y HO basis states used in the QFAM calculations are ordered into two blocks: basis states with $s = +i$ are listed first followed by the $s = -i$ pairs of states. By ordering the single-quasiparticle states in the same manner, the Bogoliubov matrices U and V acquire the following block structure:

$$U = \begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix}, \quad V = \begin{pmatrix} 0 & -v^* \\ v & 0 \end{pmatrix}. \tag{A.16}$$

Furthermore, the following transformation between the quasiparticle spinors in simplex-y HO and HO basis holds:

$$\begin{aligned}
f^{(u_\mu)}_{\left(n_z,n_r,+\Omega-\frac{1}{2}\right)} &= +1\times f^{(U_\mu)}_{\left(n_z,n_r,\Omega-\frac{1}{2},m_s=+\frac{1}{2}\right)}\\
f^{(u_\mu)}_{\left(n_z,n_r,-\Omega-\frac{1}{2}\right)} &= +i\times f^{(U_\mu)}_{\left(n_z,n_r,\Omega+\frac{1}{2},m_s=-\frac{1}{2}\right)}\\
g^{(u_\mu)}_{\left(n_z,n_r,+\Omega-\frac{1}{2}\right)} &= +i\times g^{(U_\mu)}_{\left(n_z,n_r,\Omega-\frac{1}{2},m_s=+\frac{1}{2}\right)}\\
g^{(u_\mu)}_{\left(n_z,n_r,-\Omega-\frac{1}{2}\right)} &= +1\times g^{(U_\mu)}_{\left(n_z,n_r,\Omega+\frac{1}{2},m_s=-\frac{1}{2}\right)}
\end{aligned}, \tag{A.17}$$

$$\begin{aligned}
f^{(v_\mu)}_{\left(n_z,n_r,+\Omega-\frac{1}{2}\right)} &= -1\times f^{(V_\mu)}_{\left(n_z,n_r,\Omega-\frac{1}{2},m_s=+\frac{1}{2}\right)}\\
f^{(v_\mu)}_{\left(n_z,n_r,-\Omega-\frac{1}{2}\right)} &= -i\times f^{(V_\mu)}_{\left(n_z,n_r,\Omega+\frac{1}{2},m_s=-\frac{1}{2}\right)}\\
g^{(v_\mu)}_{\left(n_z,n_r,+\Omega-\frac{1}{2}\right)} &= -i\times g^{(V_\mu)}_{\left(n_z,n_r,\Omega-\frac{1}{2},m_s=+\frac{1}{2}\right)}\\
g^{(v_\mu)}_{\left(n_z,n_r,-\Omega-\frac{1}{2}\right)} &= -1\times g^{(V_\mu)}_{\left(n_z,n_r,\Omega+\frac{1}{2},m_s=-\frac{1}{2}\right)}
\end{aligned}. \tag{A.18}$$

The wave functions on the left-hand side of Eqs. (A.17) and (A.18) are expanded in the basis defined in Eqs. (A.13)–(A.14), while those on the right-hand side are expanded in the HO basis. Therefore, one can easily construct the U and V matrices in the HO simplex-y basis from the ground-state solution represented in HO basis. We emphasize that the large and small components of the Dirac spinors in particular simplex block are expanded in the simplex-y eigenfunctions of opposite eigenvalues.

Appendix B. QFAM equations in the simplex-y HO basis

B.1. External perturbation operator in the HO simplex-y basis

The matrix element of the multipole operator $f_{JK} = r^J Y_{JK}(\theta,\phi)$ calculated in the HO basis reads:

$$\begin{aligned}
&\langle n_z n_r \Lambda m_s|r^J Y_{JK}(\theta,\phi)|n_z' n_r' \Lambda' m_s'\rangle = \delta_{m_s,m_s'}\delta_{\Lambda-\Lambda',K}\\
&\times\sqrt{\frac{2J+1}{4\pi}\frac{(J-K)!}{(J+K)!}}\langle n_z n_r|\Lambda||r^J P_{JK}(\cos\theta)|n_z' n_r'|\Lambda'|\rangle,
\end{aligned} \tag{B.1}$$

where $P_{JK}(\cos\theta)$ denotes the associated Legendre polynomial. Due to the selection rule $m_s = m_s'$ in the previous expression, the f_{JK} operator is block diagonal in the simplex-y basis:

$$\begin{aligned}
&\langle n_z n_r \Lambda; s = \pm i|r^J Y_{JK}(\theta,\phi)|n_z' n_r' \Lambda'; s = \pm i\rangle = \left(\delta_{\Lambda'-\Lambda,K} + \delta_{\Lambda-\Lambda',K}\right)\\
&\times\sqrt{\frac{2J+1}{4\pi}\frac{(J-K)!}{(J+K)!}}\langle n_z n_r|\Lambda||r^J P_{JK}(\cos\theta)|n_z' n_r'|\Lambda'|\rangle.
\end{aligned} \tag{B.2}$$

[3] N_{max} parameter corresponds to the `n0f` parameter from the input file `dirqfam.dat`.

[4] Notice that the parity operator acting on Dirac spinors is given by γ^0 matrix.

For $K \geq 0$ we have:

$$\langle n_z n_r \Lambda; s = \pm i | f_{JK}^{(+)} | n_z' n_r' \Lambda'; s = \pm i \rangle = \sqrt{\frac{1+\delta_{K,0}}{2}} \delta_{|\Lambda'-\Lambda|,K} \times \sqrt{\frac{2J+1}{4\pi}\frac{(J-K)!}{(J+K)!}} \langle n_z n_r |\Lambda| | r^J P_{JK}(\cos\theta) | n_z' n_r' |\Lambda|' \rangle, \tag{B.3}$$

$$f_{JK}^{(+)} = \begin{pmatrix} f_1 & 0 \\ 0 & f_2 \end{pmatrix}. \tag{B.4}$$

For this particular operator the following relation holds: $f_1 = f_2$, where f_1 (and f_2) are real and symmetric matrices.

B.2. QFAM matrices in the simplex-y basis

The single-quasiparticle states are ordered so that we first list states with $s = +i$, and then states with $s = -i$. The corresponding U and V matrices read:

$$U = \begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix}, \quad V = \begin{pmatrix} 0 & -v^* \\ v & 0 \end{pmatrix}, \tag{B.5}$$

while the F^{20} and F^{02} matrices for the external operator f read:

$$F^{20} = \begin{pmatrix} 0 & f^{20} \\ -[f^{20}]^T & \end{pmatrix}, \quad F^{02} = \begin{pmatrix} 0 & f^{02} \\ -[f^{02}]^T & \end{pmatrix}, \tag{B.6}$$

with $f^{20} = -\left(u^\dagger f_1 v + \left(u^\dagger f_2^* v\right)^\dagger\right)$ and $f^{02} = -\left(v^\dagger f_1 u + \left(v^\dagger f_2^* u\right)^\dagger\right)^T$. In the initial step of the QFAM iteration, we set the matrix elements of the induced Hamiltonian to zero, i.e. $\delta H_{\mu\nu}^{20}(\omega) = \delta H_{\mu\nu}^{02}(\omega) = 0$, and the initial QFAM matrices $X(\omega)$ and $Y(\omega)$ inherit the structure of the F^{20} and F^{02} matrices (see Eq. (B.6)). This structure is retained in all subsequent QFAM iterations:

$$X(\omega) = \begin{pmatrix} 0 & x(\omega) \\ -x^T(\omega) & 0 \end{pmatrix}, \quad Y(\omega) = \begin{pmatrix} 0 & y(\omega) \\ -y^T(\omega) & 0 \end{pmatrix}. \tag{B.7}$$

The induced density matrix is block diagonal:

$$\delta\rho(\omega) = UX(\omega)V^T + V^*Y^T(\omega)U^\dagger = \begin{pmatrix} \delta\rho_1(\omega) & 0 \\ 0 & \delta\rho_2(\omega) \end{pmatrix}, \tag{B.8}$$

with $\delta\rho_1(\omega) = -\left(ux(\omega)v^\dagger + vy^T(\omega)u^\dagger\right)$ and $\delta\rho_2(\omega) = -\left(vx(\omega)u^\dagger + uy^T(\omega)v^\dagger\right)^T$. The induced single-particle Hamiltonian is also block diagonal:

$$\delta h(\omega) = \begin{pmatrix} \delta h_1(\omega) & 0 \\ 0 & \delta h_2(\omega) \end{pmatrix}. \tag{B.9}$$

The pairing tensors $\delta\kappa^{(+)}(\omega)$ and $\delta\kappa^{(-)}(\omega)$ are skew symmetric:

$$\delta\kappa^{(+)}(\omega) = UX(\omega)U^T + V^*Y^T(\omega)V^\dagger = \begin{pmatrix} 0 & \delta\kappa_1{}^{(+)}(\omega) \\ -\left[\delta\kappa_1{}^{(+)}(\omega)\right]^T & 0 \end{pmatrix}, \tag{B.10}$$

$$\delta\kappa^{(-)}(\omega) = V^*X^\dagger(\omega)V^\dagger + UY^*(\omega)U^T = \begin{pmatrix} 0 & \delta\kappa_1{}^{(-)}(\omega) \\ -\left[\delta\kappa_1{}^{(-)}(\omega)\right]^T & 0 \end{pmatrix}, \tag{B.11}$$

with $\delta\kappa_1{}^{(+)}(\omega) = ux(\omega)u^\dagger - vy^T(\omega)v^\dagger$ and $\delta\kappa_1{}^{(-)}(\omega) = -vx^\dagger(\omega)v^\dagger + uy^*(\omega)u^\dagger$. Consequently, the pairing field acquires analogous form:

$$\delta\Delta^{(\pm)}(\omega) = \begin{pmatrix} 0 & \delta\Delta_1^{(\pm)}(\omega) \\ -\left[\delta\Delta_1^{(\pm)}(\omega)\right]^T & 0 \end{pmatrix}. \tag{B.12}$$

Finally, the induced Hamiltonian elements $\delta H^{20}(\omega)$ and $\delta H^{02}(\omega)$ read:

$$\delta H^{20}(\omega) = \begin{pmatrix} 0 & \delta h^{20}(\omega) \\ -\left[\delta h^{20}(\omega)\right]^T & 0 \end{pmatrix}, \quad \delta H^{02}(\omega) = \begin{pmatrix} 0 & \delta h^{02}(\omega) \\ -\left[\delta h^{02}(\omega)\right]^T & 0 \end{pmatrix}, \tag{B.13}$$

with:

$$\delta h^{20}(\omega) = -\Big(u^\dagger \delta h_1(\omega) v + v^\dagger \delta h_2^T(\omega) u - u^\dagger \delta\Delta_1^{(+)}(\omega) u + v^\dagger \left[\delta\Delta_1^{(-)}(\omega)\right]^\dagger v\Big), \tag{B.14}$$

$$\delta h^{02}(\omega) = -\Big(v^\dagger \delta h_1(\omega) u + u^\dagger \delta h_2^T(\omega) v + v^\dagger \delta\Delta_1^{(+)}(\omega) v - u^\dagger \left[\delta\Delta_1^{(-)}(\omega)\right]^\dagger u\Big)^T. \tag{B.15}$$

Eqs. (14) and (15) are reduced to the following form:

$$(E_\mu + E_\nu - \omega) x_{\mu\nu}(\omega) + \delta h_{\mu\nu}^{20}(\omega) + f_{\mu\nu}^{20} = 0, \tag{B.16}$$

$$(E_\mu + E_\nu + \omega) y_{\mu\nu}(\omega) + \delta h_{\mu\nu}^{02}(\omega) + f_{\mu\nu}^{02} = 0. \tag{B.17}$$

Appendix C. Induced densities and currents in the coordinate space

In order to calculate the matrix elements of the induced single-particle Hamiltonian Eq. (B.9), we have to calculate the induced densities and currents in the coordinate space. The scalar and vector densities read:

$$\begin{aligned} \delta\rho_{v,s}(\boldsymbol{r},\omega) = &\sum_{kl} (\delta\rho_1(\omega))_{kl} \Phi_{k,s=+i}^\dagger(\boldsymbol{r},s)\Phi_{l,s=+i}(\boldsymbol{r},s) \\ &+ \sum_{kl} (\delta\rho_2(\omega))_{kl} \Phi_{k,s=-i}^\dagger(\boldsymbol{r},s)\Phi_{l,s=-i}(\boldsymbol{r},s) \\ &\pm \sum_{\tilde{k}\tilde{l}} (\delta\rho_1(\omega))_{\tilde{k}\tilde{l}} \Phi_{\tilde{k},s=-i}^\dagger(\boldsymbol{r},s)\Phi_{\tilde{l},s=-i}(\boldsymbol{r},s) \\ &\pm \sum_{\tilde{k}\tilde{l}} (\delta\rho_2(\omega))_{\tilde{k}\tilde{l}} \Phi_{\tilde{k},s=+i}^\dagger(\boldsymbol{r},s)\Phi_{\tilde{l},s=+i}(\boldsymbol{r},s), \end{aligned} \tag{C.1}$$

with positive sign for vector and negative sign for scalar density. The $\Phi_{k,s=\pm i}(\boldsymbol{r},s)$ are eigenvectors of the simplex-y operator (A.13)–(A.14). Indices (k, l) and $(\tilde{k}, \tilde{l})$ denote summations over large and small components of the Dirac spinor, respectively. For both eigenvalues of the simplex-y operator, the product of wave functions reads:

$$\Phi_{k,s=\pm i}^\dagger(\boldsymbol{r},s)\Phi_{l,s=\pm i}(\boldsymbol{r},s) = \frac{1}{2\pi}\varphi_k(z,r_\perp)\varphi_l(z,r_\perp)\cos\left[(\Lambda_k - \Lambda_l)\phi\right], \tag{C.2}$$

where $\varphi_k(z,r_\perp)$ denotes the product of functions (A.8)–(A.9). The sums of the matrix elements $(\delta\rho_1(\omega))_{kl} + (\delta\rho_2(\omega))_{kl}$ and $(\delta\rho_1(\omega))_{\tilde{k}\tilde{l}} + (\delta\rho_2(\omega))_{\tilde{k}\tilde{l}}$ vanish for combinations k $(\tilde{k})$ and l $(\tilde{l})$ with $|\Lambda_k - \Lambda_l| \neq K$ $(|\Lambda_{\tilde{k}} - \Lambda_{\tilde{l}}| \neq K)$. This ensures that the induced density in the coordinate space has the following angular dependence: $\delta\rho(\boldsymbol{r},\omega) = \delta\rho(z,r_\perp,\omega)\cos K\phi$, which is preserved in all subsequent iterative steps of solving Eqs. (B.16)–(B.17).

The time-odd current in the coordinate space reads:

$$\begin{aligned} \delta\boldsymbol{j}(\boldsymbol{r},\omega) = &i\sum_{k\tilde{l}} (\delta\rho_1^T(\omega))_{k\tilde{l}} \Phi_{k,s=+i}^\dagger(\boldsymbol{r},s)\boldsymbol{\sigma}\Phi_{\tilde{l},s=-i}(\boldsymbol{r},s) \\ &- i\sum_{k\tilde{l}} (\delta\rho_1(\omega))_{k\tilde{l}} \Phi_{\tilde{l},s=-i}^\dagger(\boldsymbol{r},s)\boldsymbol{\sigma}\Phi_{k,s=+i}(\boldsymbol{r},s) \end{aligned}$$

$$+ i\sum_{k\tilde{l}}(\delta\rho_2^T(\omega))_{k\tilde{l}}\Phi^\dagger_{k,s=-i}(\boldsymbol{r},s)\boldsymbol{\sigma}\Phi_{\tilde{l},s=+i}(\boldsymbol{r},s)$$
$$- i\sum_{k\tilde{l}}(\delta\rho_2(\omega))_{k\tilde{l}}\Phi^\dagger_{\tilde{l},s=+i}(\boldsymbol{r},s)\boldsymbol{\sigma}\Phi_{k,s=-i}(\boldsymbol{r},s). \tag{C.3}$$

The spin operator $\boldsymbol{\sigma}$ can be decomposed in the cylindrical coordinates:

$$\boldsymbol{\sigma} = \sigma_+ e^{-i\phi}(\boldsymbol{e}_\perp - i\boldsymbol{e}_\phi) + \sigma_- e^{+i\phi}(\boldsymbol{e}_\perp + i\boldsymbol{e}_\phi) + \sigma_3\boldsymbol{e}_z, \tag{C.4}$$

leading to the following relation:

$$\Phi^\dagger_{k,s=\pm i}(\boldsymbol{r},s)\boldsymbol{\sigma}\Phi_{l,s=\mp i}(\boldsymbol{r},s) = \frac{1}{2\pi}\varphi_k(z,r_\perp)\varphi_l(z,r_\perp)$$
$$\times\Big[\cos\big((\Lambda_k+\Lambda_l+1)\phi\big)\boldsymbol{e}_\perp - \sin\big((\Lambda_k+\Lambda_l+1)\phi\big)\boldsymbol{e}_\phi$$
$$\mp i\cos\big((\Lambda_k-\Lambda_l)\phi\big)\boldsymbol{e}_z\Big]. \tag{C.5}$$

The sum of the matrix elements $(\delta\rho_1(\omega))_{k\tilde{l}} - (\delta\rho_1^T(\omega))_{k\tilde{l}} + (\delta\rho_2(\omega))_{k\tilde{l}} - (\delta\rho_2^T(\omega))_{k\tilde{l}}$ vanishes for combinations of the k and $\tilde{l}$ indices with $|\Lambda_k + \Lambda_{\tilde{l}} + 1| \neq K$. On the other hand, the sum of the matrix elements $(\delta\rho_1(\omega))_{k\tilde{l}}+(\delta\rho_1^T(\omega))_{k\tilde{l}}-(\delta\rho_2(\omega))_{k\tilde{l}}-(\delta\rho_2^T(\omega))_{k\tilde{l}}$ vanishes for combinations of the k and $\tilde{l}$ indices with $|\Lambda_k - \Lambda_{\tilde{l}}| \neq K$. Finally, the induced current can be cast into the following form:

$$\delta\boldsymbol{j}(\boldsymbol{r},\omega) = \delta j_z(\boldsymbol{r},\omega)\boldsymbol{e}_z + \delta j_\perp(\boldsymbol{r},\omega)\boldsymbol{e}_\perp + \delta j_\phi(\boldsymbol{r},\omega)\boldsymbol{e}_\phi, \tag{C.6}$$

with:

$$\delta j_z(\boldsymbol{r},\omega) = \delta j_z(z,r_\perp,\omega)\cos K\phi, \tag{C.7}$$
$$\delta j_\perp(\boldsymbol{r},\omega) = \delta j_\perp(z,r_\perp,\omega)\cos K\phi, \tag{C.8}$$
$$\delta j_\phi(\boldsymbol{r},\omega) = \delta j_\phi(z,r_\perp,\omega)\sin K\phi. \tag{C.9}$$

Subroutine that calculates the induced densities and currents has been implemented using low-rank approximation techniques. A brief overview of such methods are described in Ref. [38].

We notice that the induced potentials equations (41)–(44) depend linearly on the induced densities and currents and as a consequence they inherit the $\cos K\phi$ or $\sin K\phi$ angular dependence. Therefore, the angular integrals that appear in the calculation of the matrix elements of the induced single-particle Hamiltonian $\delta h(\omega)$ can be carried out analytically thus reducing the computational cost and improving the accuracy of the calculation. In Appendix D we show that the induced Coulomb potential δV_C also inherits the $\cos K\phi$ angular dependence.

Appendix D. Induced coulomb potential

The induced potential for protons includes the direct Coulomb field:

$$\delta V_C(\boldsymbol{r},\omega) = e^2\int d^3r'\frac{\delta\rho_v^p(\boldsymbol{r}',\omega)}{|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{D.1}$$

where $\delta\rho_v^p(\boldsymbol{r},\omega)$ denotes the induced proton vector density. The logarithmic singularity in the integrand at the point $\boldsymbol{r}=\boldsymbol{r}'$ can be eliminated by using the identity [39]:

$$\triangle_{\boldsymbol{r}'}|\boldsymbol{r}-\boldsymbol{r}'| = \frac{2}{|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{D.2}$$

that together with an integration by parts, gives:

$$\delta V_C(\boldsymbol{r},\omega) = \frac{e^2}{2}\int d^3r'|\boldsymbol{r}-\boldsymbol{r}'|\triangle_{\boldsymbol{r}'}\delta\rho_v^p(\boldsymbol{r}',\omega). \tag{D.3}$$

Since the induced proton density can be written as $\delta\rho_v^p(\boldsymbol{r},\omega) = \delta\rho_v^p(z,r_\perp,\omega)\cos K\phi$, this angular dependence also holds for the Laplacian:

$$\triangle_{\boldsymbol{r}}\delta\rho_v^p(\boldsymbol{r},\omega) = \big[\triangle_{z,r_\perp,K}\delta\rho_v^p(z,r_\perp,\omega)\big]\cos K\phi, \tag{D.4}$$

with:

$$\triangle_{z,r_\perp,K} = \frac{1}{r_\perp}\partial_{r_\perp}\left(r_\perp\partial_{r_\perp}\right) - \frac{K^2}{r_\perp^2} + \partial_z^2. \tag{D.5}$$

The angular part of the integral (D.3) can be solved analytically. We insert the following relation into Eq. (D.3):

$$|\boldsymbol{r}-\boldsymbol{r}'| = \sqrt{(r_\perp+r'_\perp)^2+(z-z')^2}\sqrt{1-a\cos^2\frac{\phi-\phi'}{2}}, \tag{D.6}$$

with:

$$a = \frac{4r_\perp r'_\perp}{(r_\perp+r'_\perp)^2+(z-z')^2}. \tag{D.7}$$

Next, we substitute $\phi-\phi' = 2x$ and use the symmetry properties of the integrand to reduce the integration interval. Finally, we obtain the following integral:

$$I_K(a) = \int_0^{\pi/2}\sqrt{1-a\cos^2 x}\cos(2Kx)dx. \tag{D.8}$$

We notice that $K \geq 0$ and $a \in [0,1]$. For the $K=0$ value Eq. (D.8) is reduced to the definition of the complete elliptic integral of the second kind:

$$I_0(a) = E(a) = \int_0^{\pi/2}\sqrt{1-a\cos^2 x}dx, \tag{D.9}$$

while for the $K=1$ value it can be written as:

$$I_1(a) = \left(\frac{2-2a}{3a}\right)K(a) - \left(\frac{2-a}{3a}\right)E(a), \tag{D.10}$$

where $K(a)$ denotes the complete elliptic integral of the first kind:

$$K(a) = \int_0^{\pi/2}\frac{dx}{\sqrt{1-a\cos^2 x}}. \tag{D.11}$$

Finally, for $K \geq 2$ the following recursive relation can be used to calculate $I_K(a)$:

$$I_K(a) = \left(\frac{(4K-4)(2-a)}{(2K+1)a}\right)I_{K-1}(a) - \left(\frac{2K-5}{2K+1}\right)I_{K-2}(a). \tag{D.12}$$

The entire problem of calculating the I_K is reduced to computation of the complete elliptic integrals $E(a)$ and $K(a)$ and this can be accomplished easily by using a polynomial approximation or any other well established numerical method. The induced Coulomb field also inherits the $\cos K\phi$ angular dependence:

$$\delta V_C(\boldsymbol{r},\omega) = \delta V_C(z,r_\perp,\omega)\cos K\phi, \tag{D.13}$$

with:

$$\delta V_C(z,r_\perp,\omega) = \int_{-\infty}^{+\infty}dz'\int_0^{+\infty}dr'_\perp r'_\perp G(z',r'_\perp,z,r_\perp)$$
$$\times\triangle_{z',r'_\perp,K}\delta\rho_v^p(z',r'_\perp,\omega). \tag{D.14}$$

The Green's function $G(z',r'_\perp,z,r_\perp)$ reads:

$$G(z',r'_\perp,z,r_\perp) = 2e^2\sqrt{(r_\perp+r'_\perp)^2+(z-z')^2}$$
$$\times I_K\left(\frac{4r_\perp r'_\perp}{(r_\perp+r'_\perp)^2+(z-z')^2}\right). \tag{D.15}$$

Appendix E. Induced pairing field

In the following sections, for a given set $A \subseteq \mathbb{R}$, we use $\mathbf{1}_A(\cdot)$ to denote the characteristic function of the set A, and $\mathrm{sgn}(\cdot)$ to denote the signum function. The induced pairing field in the HO simplex-y basis takes the following form:

$$\delta\Delta^{(\pm)}(\omega) = \begin{pmatrix} 0 & \delta\Delta_1^{(\pm)}(\omega) \\ -\left[\delta\Delta_1^{(\pm)}(\omega)\right]^T & 0 \end{pmatrix}. \tag{E.1}$$

In this section, we give an efficient formula for calculating $\delta\Delta_1^{(\pm)}(\omega)$ obtained from formula (23). Suppose we have N_z, N_r, $n_{z1}, n_{z2}, n_{r1}, n_{r2} \in \mathbb{N}_0$ and $\Lambda_1, \Lambda_2 \in \mathbb{Z}$. We will use the shorthand $k = (n_z, n_r, \Lambda)$ for triples of large component expansion of the Dirac spinor just as we did in Appendix C. First we define:

$$\begin{aligned} W^{N_z,N_r}_{(n_{z1},n_{r1},\Lambda_1),(n_{z2},n_{r2},\Lambda_2)} =& \mathbf{1}_{\mathbb{N}_0\cap[0,n_{z1}+n_{z2}]}(N_z) \times \delta_{\mathrm{mod}(n_{z1}+n_{z2},2),\mathrm{mod}(N_z,2)} \times \\ & \mathbf{1}_{\mathbb{N}_0\cap\left[0,n_{r1}+n_{r2}+\frac{|\Lambda_1|+|\Lambda_2|-|\Lambda_1-\Lambda_2|}{2}\right]}(N_r) \times \\ & M^{n_{z1},n_{z2}}_{N_z,n_z} \times M^{n_{r1},\Lambda_1,n_{r2},-\Lambda_2}_{N_r,\Lambda_1-\Lambda_2,n_r,0} \times \\ & \frac{b_\perp\sqrt{b_z}}{(2\pi)^{3/4}} \times \frac{\sqrt{n_z!}}{2^{\frac{n_z}{2}}\left(\frac{n_z}{2}\right)!} \times \frac{\left(a^2-b_z^2\right)^{\frac{n_z}{2}}}{\left(a^2+b_z^2\right)^{\frac{n_z+1}{2}}} \\ & \times \frac{\left(b_\perp^2-a^2\right)^{n_r}}{\left(b_\perp^2+a^2\right)^{n_r+1}}, \end{aligned} \tag{E.2}$$

where we used the shorthand: $n_z = n_{z1}+n_{z2}-N_z$ and $n_r = n_{r1}+n_{r2}-N_r+\frac{|\Lambda_1|+|\Lambda_2|-|\Lambda_1-\Lambda_2|}{2}$. Coefficients $M^{n_{z1},n_{z2}}_{N_z,n_z}$ and $M^{n_{r1},\Lambda_1,n_{r2},\Lambda_2}_{N_r,\Lambda,n_r,\lambda}$ are Talmy–Moshinsky brackets, and are given in Appendix F. Notice that $W^{N_z,N_r}_{k,l}$ enjoy symmetry property: $W^{N_z,N_r}_{l,k} = W^{N_z,N_r}_{k,l}$.

Next, for any $N_z, N_r \in \mathbb{N}_0$, we define:

$$P^{(\pm)}_{N_z,N_r}(\omega) = \sum_{\substack{\mathrm{Shell}(k')\le N_{max}\\ \mathrm{Shell}(l')\le N_{max}}} W^{N_z,N_r}_{k',l'} \left(\delta\kappa_1^{(\pm)}(\omega)\right)_{k'l'}. \tag{E.3}$$

Similar to the selection rules governed in $\delta\rho_1(\omega)$ and $\delta\rho_2(\omega)$ from Appendix C, one can show that the following selection rule is fulfilled in the induced pairing tensor: $\left(\delta\kappa_1^{(\pm)}(\omega)\right)_{kl} + \left(\delta\kappa_1^{(\pm)}(\omega)\right)_{lk} \propto \delta_{|\Lambda_k-\Lambda_l|,K}$. Therefore, if we rewrite (E.3) as:

$$P^{(\pm)}_{N_z,N_r}(\omega) = \sum_{\substack{\mathrm{Shell}(k')\le N_{max}\\ \mathrm{Shell}(l')\le N_{max}}} W^{N_z,N_r}_{k',l'} \frac{1}{2}\left[\left(\delta\kappa_1^{(\pm)}(\omega)\right)_{k'l'} + \left(\delta\kappa_1^{(\pm)}(\omega)\right)_{l'k'}\right], \tag{E.4}$$

we see that the sum in (E.3) can be constrained by the additional selection rule: $|\Lambda_{k'} - \Lambda_{l'}| = K$. Finally, for any $k_1 = (n_{z1}, n_{r1}, \Lambda_1), k_2 = (n_{z2}, n_{r2}, \Lambda_2)$, the following formula holds:

$$\begin{aligned} \left(\delta\Delta_1^{(\pm)}(\omega)\right)_{k_1k_2} =& -G \times \frac{1+\delta_{K,0}}{2} \times \delta_{|\Lambda_1-\Lambda_2|,K} \\ & \times \sum_{N_z'}\sum_{N_r'} W^{N_z',N_r'}_{k_1,k_2} P^{(\pm)}_{N_z',N_r'}(\omega), \end{aligned} \tag{E.5}$$

where the first summation is over all $0 \le N_z' \le n_{z1}+n_{z2}$, satisfying $\mathrm{mod}(N_z', 2) = \mathrm{mod}(n_{z1}+n_{z2}, 2)$, and the second summation is over all $0 \le N_r' \le n_{r1}+n_{r2}+\frac{|\Lambda_1|+|\Lambda_2|-|\Lambda_1-\Lambda_2|}{2}$. We see that the tedious summation over all quantum numbers has been separated in two independent parts: $\{k', l'\}$ and $\{N_z, N_r\}$ by means of coefficients W which can be easily pre-calculated.

Appendix F. Talmy–Moshinsky brackets

F.1. One dimensional Talmy–Moshinsky brackets

For a given scale parameter $b_0 \ge 0$, and for any $n_z \in \mathbb{N}_0$, we introduce a sequence of functions:

$$\phi_{n_z}(z) = \frac{1}{\sqrt{b_0}}\frac{1}{\sqrt{\sqrt{\pi}2^{n_z}n_z!}} H_{n_z}\left(\frac{z}{b_0}\right)\exp\left(-\frac{1}{2}\left(\frac{z}{b_0}\right)^2\right), \quad \forall z \in \mathbb{R}, \tag{F.1}$$

where $H_n(\cdot)$ denotes nth-degree Hermite polynomial. For any non-negative integers: $n_{z1}, n_{z1}, N_z, n_z \in \mathbb{N}_0$, we define one dimensional Talmy–Moshinsky bracket $M^{n_{z1},n_{z2}}_{N_z,n_z}$ as follows:

$$\begin{aligned} M^{n_{z1},n_{z2}}_{N_z,n_z} =& \mathbf{1}_{\mathbb{N}_0\cap[0,n_{z1}+n_{z2}]}(N_z) \times \delta_{n_{z1}+n_{z2},N_z+n_z} \times \\ & \frac{1}{\sqrt{2^{n_{z1}+n_{z2}}}} \times \sqrt{\frac{n_{z1}!n_{z2}!}{N_z!n_z!}} \times \\ & \sum_{p=\max\{0,n_{z1}-N_z\}}^{\min\{n_z,n_{z1}\}} (-1)^p \binom{n_z}{p}\binom{N_z}{n_{z1}-p}. \end{aligned} \tag{F.2}$$

Then, for any fixed $n_{z1}, n_{z2} \in \mathbb{N}_0$, and $z_1, z_2 \in \mathbb{R}$, it holds that:

$$\phi_{n_{z1}}(z_1)\phi_{n_{z2}}(z_2) = \sum_{N_z=0}^{+\infty}\sum_{n_z=0}^{+\infty} M^{n_{z1},n_{z2}}_{N_z,n_z}\phi_{N_z}\left(\frac{z_1+z_2}{\sqrt{2}}\right)\phi_{n_z}\left(\frac{z_2-z_1}{\sqrt{2}}\right). \tag{F.3}$$

Previous equation has been numerically verified for various combinations of $n_{z1}, n_{z2} \in \mathbb{N}_0, z_1, z_2 \in \mathbb{R}$. Notice that due to the constraints on N_z and n_z in (F.2), infinite series in (F.3) reduces to finite sum. Also notice that from Eq. (F.3), one can easily see the following symmetry:

$$M^{n_{z2},n_{z1}}_{N_z,n_z} = (-1)^{n_z} M^{n_{z1},n_{z2}}_{N_z,n_z}. \tag{F.4}$$

F.2. Two dimensional Talmy–Moshinsky brackets

Let us assume that $b_0 > 0$ is a scale parameter, and for any $n_r \in \mathbb{N}_0, m \in \mathbb{Z}$, we define a sequence of functions:

$$\begin{aligned} \phi_{n_r,m}(\boldsymbol{\rho}) =& \frac{1}{b_0}\sqrt{\frac{2n_r!}{(n_r+|m|)!}}\left(\frac{|\boldsymbol{\rho}|}{b_0}\right)^{|m|} L_{n_r}^{|m|}\left(\frac{|\boldsymbol{\rho}|^2}{b_0^2}\right) \\ & \times \exp\left(-\frac{1}{2}\frac{|\boldsymbol{\rho}|^2}{b_0^2}\right)\frac{e^{im\varphi}}{\sqrt{2\pi}}. \end{aligned} \tag{F.5}$$

$\boldsymbol{\rho} = (|\boldsymbol{\rho}|\cos\varphi, |\boldsymbol{\rho}|\sin\varphi) \in \mathbb{R}^2$, where $L_n^\alpha(\cdot)$ denotes associated Laguerre polynomial. For any $n_{r1}, n_{r2}, N_r, n_r \in \mathbb{N}_0$ and $m_1, m_2, M, m \in \mathbb{Z}$, we define two dimensional Talmy–Moshinky bracket $M^{n_{r1},m_1,n_{r2},m_2}_{N_r,M,n_r,m}$ as follows:

$$\begin{aligned} M^{n_{r1},m_1,n_{r2},m_2}_{N_r,M,n_r,m} =& \mathbf{1}_{\mathbb{N}_0\cap\left[0,n_{r1}+n_{r2}+\frac{|m_1|+|m_2|-|M|-|m|}{2}\right]}(N_r) \times \\ & \mathbf{1}_{\mathbb{Z}\cap\left[-\frac{2n_{r1}+|m_1|+2n_{r2}+|m_2|}{2},+\frac{2n_{r1}+|m_1|+2n_{r2}+|m_2|}{2}\right]} \\ & \times \left(M-\frac{m_1+m_2}{2}\right) \times \\ & \delta_{m_1+m_2,M+m} \times \delta_{2n_{r1}+|m_1|+2n_{r2}+|m_2|,2N_r+|M|+2n_r+|m|} \times \\ & \frac{(-1)^{N_r+n_r+n_{r1}+n_{r2}}}{\sqrt{2^{2N_r+|M|+2n_r+|m|}}} \\ & \times \sqrt{\frac{n_{r1}!(n_{r1}+|m_1|)!n_{r2}!(n_{r2}+|m_2|)!}{N_r!(N_r+|M|)!n_r!(n_r+|m|)!}} \times \\ & \sum_{\substack{0\le p,q,r,s\le n_r\\ 0\le P,Q,R,S\le N_r\\ 0\le t\le|m|\\ 0\le T\le|M|\\ (C1),(C2),(C3),(C4)}} (-1)^{t+r+s}\binom{n_r}{p\ q\ r\ s}\binom{N_r}{P\ Q\ R\ S} \\ & \times \binom{|M|}{T}\binom{|m|}{t}, \end{aligned} \tag{F.6}$$

where the summation over $p, q, r, s, P, Q, R, S, t, T \in \mathbb{N}_0$, is performed with four additional constraints:

(C1) : $p+q+r+s=n_r$
(C2) : $P+Q+R+S=N_r$
(C3) : $(2n_{r1}+|m_1|)-(2n_{r2}+|m_2|)+|m|+|M|=2(p+P)-2(q+Q)+2(t+T)$
(C4) : $m_1=(r+R)-(s+S)+\mathrm{sgn}(m)t+\mathrm{sgn}(M)T$.

In (F.6), we use standard notation for the multinomial coefficients. Then, for any $n_{r1}, n_{r2} \in \mathbb{N}_0$ and $m_1, m_2 \in \mathbb{Z}$, there holds:

$$\phi_{n_{r1},m_1}(\boldsymbol{\rho}_1)\phi_{n_{r2},m_2}(\boldsymbol{\rho}_2) = \sum_{M=-\infty}^{+\infty}\sum_{N_r=0}^{+\infty}\sum_{m=-\infty}^{+\infty}\sum_{n_r=0}^{+\infty} M_{N_r,M,n_r,m}^{n_{r1},m_1,n_{r2},m_2} \times \phi_{N_r,M}\left(\frac{\boldsymbol{\rho}_1+\boldsymbol{\rho}_2}{\sqrt{2}}\right)\phi_{n_r,m}\left(\frac{\boldsymbol{\rho}_2-\boldsymbol{\rho}_1}{\sqrt{2}}\right), \quad \text{(F.7)}$$

for all $\boldsymbol{\rho_1}, \boldsymbol{\rho_2} \in \mathbb{R}^2$. Previous equation has also been proven correct and numerically verified. Again, constraints on $N_r, n_r \in \mathbb{N}_0$ and $M, m \in \mathbb{Z}$ in (F.6) result in truncation of the infinite series in (F.7) to finite sum. Notice that from (F.7), one can easily confirm the following symmetry properties:

$$M_{N_r,M,n_r,m}^{n_{r2},m_2,n_{r1},m_1} = (-1)^m M_{N_r,M,n_r,m}^{n_{r1},m_1,n_{r2},m_2}, \quad \text{(F.8)}$$

$$M_{N_r,-M,n_r,-m}^{n_{r1},-m_1,n_{r2},-m_2} = M_{N_r,M,n_r,m}^{n_{r1},m_1,n_{r2},m_2}. \quad \text{(F.9)}$$

References

[1] M. Bender, P.-H. Heenen, P.-G. Reinhard, Rev. Modern Phys. 75 (2003) 121.
[2] D. Vretenar, A.V. Afanasjev, G.A. Lalazissis, P. Ring, Phys. Rep. 409 (2005) 101.
[3] J.R. Stone, P.-G. Reinhard, Prog. Part. Nucl. Phys. 58 (2007) 587.
[4] T. Nikšić, D. Vretenar, P. Ring, Prog. Part. Nucl. Phys. 66 (2011) 519.
[5] N. Paar, D. Vretenar, E. Khan, G. Colo, Rep. Progr. Phys. 70 (2007) 691.
[6] D. Savran, T. Aumann, A. Zilges, Prog. Part. Nucl. Phys. 70 (2013) 210.
[7] P. Ring, P. Schuck, The Nuclear Many-Body Problem, Springer-Verlag, Berlin, 1980.
[8] S. Péru, H. Goutte, Phys. Rev. C 77 (2008) 044313.
[9] K. Yoshida, N.V. Giai, Phys. Rev. C 78 (2008) 064316.
[10] D. Pena Arteaga, E. Khan, P. Ring, Phys. Rev. C 79 (2009) 034311.
[11] J. Terasaki, J. Engel, Phys. Rev. C 82 (2010) 034326.
[12] C. Losa, A. Pastore, T. Dossing, E. Vigezzi, R.A. Broglia, Phys. Rev. C 81 (2010) 064307.
[13] T. Nakatsukasa, T. Inakura, K. Yabana, Phys. Rev. C 76 (2007) 024318.
[14] T. Inakura, T. Nakatsukasa, K. Yabana, Phys. Rev. C 80 (2009) 044301.
[15] T. Inakura, T. Nakatsukasa, K. Yabana, Phys. Rev. C 84 (2011) 021302.
[16] P. Avogadro, T. Nakatsukasa, Phys. Rev. C 84 (2011) 014314.
[17] M. Stoitsov, M. Kortelainen, T. Nakatsukasa, C. Losa, W. Nazarewicz, Phys. Rev. C 84 (2011) 041305(R).
[18] N. Hinohara, M. Korelainen, W. Nazarewicz, Phys. Rev. C 87 (2013) 064309.
[19] H. Liang, T. Nakatsukasa, Z. Niu, J. Meng, Phys. Rev. C 87 (2013) 054310.
[20] T. Nikšić, N. Kralj, T. Tutiš, D. Vretenar, P. Ring, Phys. Rev. C 88 (2013) 044327.
[21] M. Kortelainen, N. Hinohara, W. Nazarewicz, Phys. Rev. C 92 (2015) 051302.
[22] X. Sun, D. Lu, Phys. Rev. C 96 (2017) 024614.
[23] T. Nikšić, N. Paar, D. Vretenar, P. Ring, Comput. Phys. Comm. 185 (2014) 1808.
[24] J. Meng, H. Toki, S.-G. Zhou, S.Q. Zhang, W.H. Long, L.S. Geng, Prog. Part. Nucl. Phys. 57 (2006) 470.
[25] J.G. Valatin, Phys. Rev. 122 (1961) 1012.
[26] T. Nikšić, D. Vretenar, P. Ring, Phys. Rev. C 78 (2008) 034318.
[27] J.-P. Blaizot, G. Ripka, Quantum Theory of Finite Systems, MIT, Cambridge, MA, 1986.
[28] T. Gonzalez-Llarena, J. Egido, G. Lalazissis, P. Ring, Phys. Lett. B 379 (1996) 13.
[29] M. Serra, P. Ring, Phys. Rev. C 65 (2002) 064324.
[30] Y. Tian, Z.Y. Ma, P. Ring, Phys. Lett. B 676 (2009) 44.
[31] Y. Tian, Z.Y. Ma, P. Ring, Phys. Rev. C 79 (2009) 064301.
[32] Y. Tian, Z.Y. Ma, P. Ring, Phys. Rev. C 80 (2009) 024313.
[33] J.F. Berger, M. Girod, D. Gogny, Comput. Phys. Comm. 61 (1991) 365.
[34] A. Baran, A. Bulgac, M. McNeil Forbes, G. Hagen, W. Nazarewicz, N. Schunck, M. Stoitsov, Phys. Rev. C 78 (2008) 014318.
[35] http://www.netlib.org/blas/.
[36] http://www.netlib.org/lapack/.
[37] http://www.openblas.net/.
[38] M. Berry, Z. Drmač, E. Jessup, SIAM Rev. 41 (2) (1999).
[39] D. Vautherin, Phys. Rev. C 7 (1973) 296.