

Gamow-Hartree-Fock-Bogoliubov method: Representation of quasiparticles with Berggren sets of wave functions

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Single-particle resonant states, also called Gamow states, as well as bound and scattering states of complex energy form a complete set, the Berggren completeness relation. It is the building block of the recently introduced Gamow shell model, where weakly bound and resonant nuclear wave functions are expanded with a many-body basis of Slater determinants generated by this set of single-particle states. However, Gamow states have never been studied in the context of Hartree-Fock-Bogoliubov theory, except in the Bardeen-Cooper-Schrieffer (BCS) approximation, where both the upper and lower components of a quasiparticle wave function are assumed to possess the same radial dependence with that of a Gamow state associated with the Hartree-Fock potential. Hence, an extension of the notion of Gamow state has to be effected in the domain of quasiparticles. It is shown theoretically and numerically that bound, resonant and scattering quasiparticles are well defined and form a complete set, by which bound Hartree-Fock-Bogoliubov ground states can be constructed. It is also shown that the Gamow-Hartree-Fock single-particle basis can be used to solve the Gamow-Hartree-Fock-Bogoliubov problem. As an illustration, the proposed method is applied to neutron-rich nickel isotopes close to the neutron drip-line.

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I. INTRODUCTION

One of the current challenges of nuclear theory is the quantitative description of nuclei situated near and beyond drip-lines. Powerful facilities are being built in several countries in order to create these very short-lived states. For a long time, microscopic theories of nuclear structure have been developed for describing ground states of nuclei close to the valley of stability. For describing stable nuclei which are well localized, the harmonic oscillator (HO) bases are useful for both shell model [1] and Hartree-Fock Bogoliubov (HFB) calculations [2–6]; the HO bases converge quickly therein. However, it possesses poor convergence properties for weakly bound nuclei bearing large spatial extensions, which lie very close to neutron drip lines.

A promising approach to this problem has been proposed in Refs. [7–9] within a shell model framework; namely, the Gamow shell model (GSM). The fundamental idea is to replace the HO basis by the Berggren basis consisting of bound states, resonance states and continuum scattering states of complex energy, generated by a single-particle potential. It has been shown numerically that this basis has the ability to expand both halo nuclei and many-body resonant states precisely. The latter indeed belongs to a rigged Hilbert space [10,11], which is an extension of the notion of Hilbert space to non-square integrable wave functions. However, the dimension of the Berggren Slater determinants represented by the GSM

basis increase very quickly with increasing number of valence particles; it increases much faster than in standard shell model due to the presence of occupied scattering states. Hence, the GSM is a tool mainly dedicated to the study of light nuclei. For medium and heavy nuclei, a method of choice is the HFB, which can be followed by quasiparticle random phase approximation (QRPA). As pairing correlations are absorbed in the HFB ground state, one-body nature of the HFB framework enables fast evaluations of ground states of medium and heavy nuclei, and it is in fact the only method suitable for systematic calculations; see Ref. [12] for an evaluation of even-even nuclei in the whole nuclear chart with the HFB formalism. In order to properly treat drip-line nuclei within the HFB framework, the real-space coordinate-mesh method has been applied using box boundary conditions [13,14]. Extension of this approach to deformed nuclei is difficult and has been carried out only recently [15,16]. As an alternative more convenient approach, one can adopt basis expansion methods, where direct integration procedure is replaced by matrix diagonalization. A first amelioration of the HO basis had been proposed with the transformed harmonic oscillator (THO) basis [12,17]. Applying unitary transformations to the HO basis, one obtains the THO basis, in which Gaussian fall-off of the HO wave functions is replaced by physical exponential decrease of the THO basis wave functions. However, the THO basis always dictates exponential decrease

in expanding quasiparticle wave functions, for both upper and lower components, even when they are part of scattering states, so that unsatisfactory basis dependence remains. In order to solve this problem, a new basis has been introduced very recently, which consists in using bound and continuum basis states generated by the analytic Pöschl-Teller-Ginocchio (PTG) potential [18]. The PTG basis introduced in this paper [19] possesses a peculiarity to bear no narrow resonance states; those are replaced by bound PTG states. Thus, PTG continuum set of basis states can be discretized very effectively with Gauss-Legendre quadrature, as they contain no resonant structure. It has been shown that they can provide a good description of spatially extended nuclear ground states of both spherical and axially deformed nuclei [19]. On the other hand, the PTG basis formed by bound and real scattering states is not a Berggren complete set of states, so that it would be more convenient to use a Berggren quasiparticle basis set, when we are interested in describing particle-decaying excited states. Up to now, however, resonant quasiparticle states have been studied in the context of Berggren completeness relation only within the BCS approximation [20,21]. The last approach is indeed not satisfactory due to the well-known gas problem arising from the occupation of the continuum: In fact, densities are not localized in the BCS approach, because the lower components of scattering quasiparticle states are of scattering type as well. Contrary to what is stated in Ref. [20], it cannot be regularized using complex scaling because it does not have pure outgoing asymptotic. Use of continuum level density in Ref. [21] is also problematic, even though it suppresses the gas problem. Indeed, it is not part of continuum HFB theory [19], so that its introduction in HFB equations strongly modifies quasiparticle coupling to the continuum. In particular, it suppresses a large part of nonresonant continuum, and thus important physical properties of drip-line nuclei as well. Hence, with this approach, weakly bound systems cannot be studied properly. Only a full application of the HFB framework can unambiguously solve this problem, where densities are localized by construction for bound HFB ground states.

The major purpose of this paper is to develop a new method of solving the continuum HFB equations utilizing the Berggren basis, called Gamow-HFB method, by which bound, resonant and continuum quasiparticle states are provided. It allows expansion of QRPA excited states having escaping widths in terms of the Berggren quasiparticle basis associated with the bound HFB ground state. This is very important because, in weakly bound unstable nuclei, low-lying collective excited states may acquire particle-decay widths.

This paper is organized as follows. Firstly, the standard HFB formalism is briefly summarized. As we use the Skyrme interactions [22], it is effected in the context of density functional theory (DFT). Secondly, we define quasiparticle S-matrix poles and scattering states of complex energy; these are direct extensions of their single-particle counterparts. We then present the quasiparticle Berggren completeness relation generated by those states. Numerical methods to calculate Gamow and complex scattering quasiparticle states are described; they differ significantly from the scattering quasiparticle states discretized by box boundary conditions. We also present another method of solving the continuum HFB

equations in which the HFB quasiparticle wave functions are expanded in terms of the Gamow-Hartree-Fock (GHF) basis; this approach may be regarded as an extension of the standard two-basis method [23–25] to complex energy plane. Feasibility of the proposed methods is illustrated for neutron-rich nickel isotopes close to the drip line. Perspectives for unbound HFB theory and QRPA calculations using the Gamow-HFB quasiparticle basis will then be discussed.

II. GENERAL HFB FORMALISM WITH DFT

The HFB equations are expressed in supermatrix form constituted by particle-hole field Hamiltonian h , particle-particle pairing Hamiltonian \tilde{h} and chemical potential λ guaranteeing conservation of particle number in average:

$$\begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h} & \lambda - h \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}. \quad (1)$$

Using Skyrme and density-dependent contact interactions for the particle-hole and pairing channels, respectively, h and \tilde{h} are expressed in terms of local normal density $\rho(r)$ and pairing density $\tilde{\rho}(r)$. Formulas providing ρ , $\tilde{\rho}$, h , and \tilde{h} can be found in [14,26]. As h and \tilde{h} depend on ρ and $\tilde{\rho}$, determined from quasiparticles eigenvectors of Eq. (1), the HFB equations must be solved in a self-consistent manner [27].

Let us consider the HFB equations with the Skyrme energy density functionals and density-dependent contact pairing interactions assuming spherical symmetry. Fixing orbital and total angular momentum ℓ and j , as well as proton or neutron nature of the wave functions, Eq. (1) becomes a system of radial differential equations [14]:

$$\begin{aligned} & \left(\frac{d}{dr} \frac{\hbar^2}{2m^*(r)} \frac{d}{dr} \right) u(k, r) \\ &= \left[\frac{\hbar^2 \ell(\ell + 1)}{2m^*(r)r^2} + V(r) - (\lambda + E) \right] u(k, r) + W(r)v(k, r), \\ & \left(\frac{d}{dr} \frac{\hbar^2}{2m^*(r)} \frac{d}{dr} \right) v(k, r) \\ &= \left[\frac{\hbar^2 \ell(\ell + 1)}{2m^*(r)r^2} + V(r) - (\lambda - E) \right] v(k, r) - W(r)u(k, r), \end{aligned} \quad (2)$$

where

- (i) $u(k, r)$ and $v(k, r)$ are respectively the upper and lower components of quasiparticle wave function with energy E , and $k = \sqrt{2mE}/\hbar$ with the nucleon mass m ,
- (ii) $m^*(r)$, $V(r)$ and $W(r)$ are respectively the effective mass, the particle-hole (field) and particle-particle (pairing) potentials of the HFB Hamiltonian.

Because nuclear interactions are finite range, only Coulomb and centrifugal parts remain for $r \rightarrow +\infty$, so that Eq. (2)

becomes asymptotically:

$$\begin{aligned} \frac{d^2 u}{dr^2}(k, r) &= \left(\frac{\ell(\ell+1)}{r^2} + \frac{2\eta_u k_u}{r} - k_u^2 \right) u(k, r), \\ \frac{d^2 v}{dr^2}(k, r) &= \left(\frac{\ell(\ell+1)}{r^2} + \frac{2\eta_v k_v}{r} - k_v^2 \right) v(k, r), \end{aligned} \quad (3)$$

where the generalized momenta k_u, k_v and their associated Sommerfeld parameters η_u, η_v are defined by

$$k_u = \sqrt{\frac{2m}{\hbar^2}(\lambda + E)}, \quad k_v = \sqrt{\frac{2m}{\hbar^2}(\lambda - E)}, \quad (4)$$

$$\eta_{u(v)} = \frac{mZC_c}{\hbar^2 k_{u(v)}} \text{ (proton)}, \quad \eta_{u(v)} = 0 \text{ (neutron)} \quad (5)$$

with the number of protons Z and the Coulomb constant C_c . Hence, $u(k, r)$ and $v(k, r)$ are linear combinations of the Hankel or Coulomb wave functions $H_{\ell\eta_{u(v)}}^{\pm}(k_{u(v)}r)$ for $r \rightarrow +\infty$. Note that k_v is always imaginary provided the HFB ground state is bound ($\lambda < 0$), while k_u is real (imaginary) for $E > -\lambda$ ($E < -\lambda$).

The chemical potentials λ for neutrons and protons are determined from the requirement of conservation of their number in average:

$$\langle \hat{N} \rangle = \sum_i N_i = N, \quad N_i = \int_0^{+\infty} v_i^2(r) dr, \quad (6)$$

(and similar equations for protons). Here the sum runs over all quasiparticle states, N is the number of neutrons and $\langle \hat{N} \rangle$ is the expectation value in the HFB ground state. For a given particle-hole field Hamiltonian h , the chemical potential λ could be calculated in principle exactly at each iteration, recalculating all quasiparticle wave functions from Eq. (1) and updating λ until Eq. (6) is verified. However, in practice, it is much faster to use instead an approximate chemical potential issued from the BCS formulas, which will converge self-consistently to the exact chemical potential along with the HFB Hamiltonian [14]. For that, one defines auxiliary single-particle energies \bar{e}_i and auxiliary pairing gaps $\bar{\Delta}$ by

$$\bar{e}_i = \lambda + E_i(1 - 2N_i), \quad \bar{\Delta}_i = 2E_i\sqrt{N_i(1 - N_i)}, \quad (7)$$

which are defined by applying the BCS type formula to the HFB quasiparticle energies E_i , the average particle number N_i defined in Eq. (6) and the chemical potential λ issued from the previous iteration. While \bar{e}_i and $\bar{\Delta}_i$ correspond to the single-particle energy and the pairing gap in the BCS approximation, they are used here as auxiliary variables to solve the HFB equations. The approximate chemical potential λ is obtained by solving its associated BCS equation:

$$\sum_i \left(1 - \frac{\bar{e}_i - \lambda}{\sqrt{(\bar{e}_i - \lambda)^2 + \bar{\Delta}_i^2}} \right) = 2N. \quad (8)$$

III. S-MATRIX POLES AND SCATTERING QUASIPARTICLE STATES

A. Boundary conditions

The upper and lower components, $u(k, r)$ and $v(k, r)$, of the quasiparticle wave function satisfy the following boundary conditions:

$$u(k, r) \sim C_u^0 r^{\ell+1}, \quad v(k, r) \sim C_v^0 r^{\ell+1}, \quad r \rightarrow 0, \quad (9)$$

$$u(k, r) \sim C_u^+ H_{\ell\eta_u}^+(k_u r) + C_u^- H_{\ell\eta_u}^-(k_u r), \quad r \rightarrow +\infty, \quad (10)$$

$$v(k, r) \sim C_v^+ H_{\ell\eta_v}^+(k_v r), \quad r \rightarrow +\infty. \quad (11)$$

Equation (9) is required by regularity of wave functions at $r = 0$. Equations (10) and (11) determine the nature of quasiparticle state, which can be a bound, resonant ($C_u^- = 0$) or scattering ($C_u^- \neq 0$) state, and are generalizations of the boundary conditions defining single-particle states using the Berggren completeness relation. Equation (11) demands outgoing wave function behavior of $v(r)$ for all quasiparticle states. If its energy E is real and positive, as in the standard HFB approach, Eq. (11) is equivalent to the asymptotic condition $v(k, r) \rightarrow 0$ for $r \rightarrow +\infty$; the condition arising from integrability of nuclear density over all space [14]. Extension to complex energies follows from analyticity of the $v(k, r)$ function in the complex k -plane. Equation (10) with $C_u^- = 0$ then defines quasiparticle S-matrix poles, as it is equivalent to $u(k, r) \rightarrow 0$ for $r \rightarrow +\infty$ for bound quasiparticle states with $E < |\lambda|$, and provides resonant quasiparticle states if E is complex. Equation (10) with $C_u^- \neq 0$ represents standard scattering quasiparticle states for real and positive E , but they are extended to complex energies by analyticity arguments.

B. Normalization of quasiparticle states

Bound HFB quasiparticle states with energy E_n are normalized by

$$\int_0^{+\infty} [u(k_n, r)^2 + v(k_n, r)^2] dr = 1, \quad (12)$$

where $k_n = \sqrt{2mE_n}/\hbar$. For resonant quasiparticle states, the integral in the above equation diverges, so that this normalization condition cannot be used. The complex scaling method has been known as a practical means to normalize single-particle resonance states [28]. Convergence of integrals is obtained therein integrating up to a finite radius R situated in the asymptotic region, after which the interval $[R : +\infty]$ is replaced by a complex contour defined by a rotation angle $\theta > 0$, allowing exponential decrease of the integrand. Owing to Eqs. (10) and (11), the same method can be used to normalize resonant quasiparticle states, so that Eq. (12) becomes

$$\begin{aligned} & \int_0^R [u(k_n, r)^2 + v(k_n, r)^2] dr \\ & + \int_0^{+\infty} [C_u^+ H_{\ell\eta_u}^+(k_u(R + xe^{i\theta_u}))]^2 e^{i\theta_u} dx \\ & + \int_0^{+\infty} [C_v^+ H_{\ell\eta_v}^+(k_v(R + xe^{i\theta_v}))]^2 e^{i\theta_v} dx = 1, \end{aligned} \quad (13)$$

where $\theta_u > 0$ and $\theta_v > 0$ are chosen such that improper integrals converge. Hence, as in the single-particle case, normalization of quasiparticle S-matrix poles presents no other difficulty. As in Ref. [8], complex-scaled integrals will be denoted $\text{Reg}[\int_0^{+\infty} f(r) dr]$, i.e., the regularized value of the diverging integral.

Scattering quasiparticle states must be orthonormalized with the Dirac delta distribution:

$$\int_0^{+\infty} [u(k_a, r)u(k_b, r) + v(k_a, r)v(k_b, r)] dr = \delta(k_a - k_b), \quad (14)$$

for those with momenta k_a and k_b . From Eqs. (10) and (11), assuming that Eq. (3) is obtained for $r \geq R$, Eq. (14) becomes

$$\begin{aligned} & \int_0^R [u(k_a, r)u(k_b, r) + v(k_a, r)v(k_b, r)] dr \\ & + C_{u_a}^+ C_{u_b}^+ \text{Reg} \left[\int_R^{+\infty} H_{\ell\eta_{u_a}}^+(k_{u_a} r) H_{\ell\eta_{u_b}}^+(k_{u_b} r) dr \right] \\ & + C_{u_a}^- C_{u_b}^- \text{Reg} \left[\int_R^{+\infty} H_{\ell\eta_{u_a}}^-(k_{u_a} r) H_{\ell\eta_{u_b}}^-(k_{u_b} r) dr \right] \\ & + C_{v_a}^+ C_{v_b}^+ \text{Reg} \left[\int_R^{+\infty} H_{\ell\eta_{v_a}}^+(k_{v_a} r) H_{\ell\eta_{v_b}}^+(k_{v_b} r) dr \right] \\ & + C_{u_a}^- C_{u_b}^+ \int_R^{+\infty} H_{\ell\eta_{u_a}}^-(k_{u_a} r) H_{\ell\eta_{u_b}}^+(k_{u_b} r) dr \\ & + C_{u_a}^+ C_{u_b}^- \int_R^{+\infty} H_{\ell\eta_{u_a}}^+(k_{u_a} r) H_{\ell\eta_{u_b}}^-(k_{u_b} r) dr \\ & = \delta(k_a - k_b). \end{aligned} \quad (15)$$

The divergence of the Dirac delta function at $k_a = k_b$ occurs by way of the two last integrals of Eq. (15), as no complex scaling can make them converge if $k_a = k_b$ [8]. The Dirac delta normalization of the Coulomb wave functions implies, as in the single-particle case:

$$\begin{aligned} & C_{u_a}^- C_{u_b}^+ \int_R^{+\infty} H_{\ell\eta_{u_a}}^-(k_{u_a} r) H_{\ell\eta_{u_b}}^+(k_{u_b} r) dr \\ & + C_{u_a}^+ C_{u_b}^- \int_R^{+\infty} H_{\ell\eta_{u_a}}^+(k_{u_a} r) H_{\ell\eta_{u_b}}^-(k_{u_b} r) dr \\ & = 2\pi C_{u_a}^+ C_{u_a}^- \delta(k_{u_a} - k_{u_b}) + f(k_{u_a}, k_{u_b}), \end{aligned} \quad (16)$$

where $f(k_{u_a}, k_{u_b})$ is finite for all (k_{u_a}, k_{u_b}) . The relation between $\delta(k_a - k_b)$ and $\delta(k_{u_a} - k_{u_b})$ is easily obtained from Eq. (4):

$$\delta(k_{u_a} - k_{u_b}) = \left[\frac{\partial k_{u_a}}{\partial k_a}(k_a) \right]^{-1} \delta(k_a - k_b) = \frac{k_{u_a}}{k_a} \delta(k_a - k_b). \quad (17)$$

This a direct application of the standard Dirac delta distribution property stating that $\delta(f(k)) = f'(k_0)^{-1} \delta(k - k_0)$ for a given function $f(k)$ bearing a unique simple zero at $k = k_0$ [29]. Note that k_b is fixed while k_a is varied to obtain Eq. (17).

Inserting Eqs. (16) and (17) into Eq. (15), one obtains

$$\begin{aligned} & \int_0^{+\infty} [u(k_a, r)u(k_b, r) + v(k_a, r)v(k_b, r)] dr \\ & = \delta(k_a - k_b) \Leftrightarrow \frac{2\pi k_{u_a}}{k_a} C_{u_a}^+ C_{u_a}^- \delta(k_a - k_b) \\ & = \delta(k_a - k_b) + g(k_a, k_b), \end{aligned} \quad (18)$$

where $g(k_a, k_b)$ bears the same properties as $f(k_{u_a}, k_{u_b})$. As quasiparticle scattering states are orthogonal for $k_a \neq k_b$, $g(k_a, k_b) = 0$ therein, so that $\delta(k_a - k_b) + g(k_a, k_b) = \delta(k_a - k_b)$ in all cases.

Dirac delta distribution normalization for scattering states $|k\rangle$ and $|k'\rangle$ immediately follows:

$$\langle k|k'\rangle = \delta(k - k') \Leftrightarrow C_u^+ C_u^- = \frac{k}{2\pi k_u}. \quad (19)$$

Hence, besides the additional factor k/k_u , the normalization condition for quasiparticle scattering states is the same as that for single-particle scattering states [8].

C. Completeness of quasiparticle states of real and complex energy

The HFB supermatrix defined in Eq. (1) is Hermitian, so that it possesses a spectral decomposition [30]:

$$\begin{aligned} & \sum_{n \in b} [u(k_n, r)u(k_n, r') + v(k_n, r)v(k_n, r')] \\ & + \int_{k_\lambda}^{+\infty} [u(k, r)u(k, r') + v(k, r)v(k, r')] dk \\ & = \delta(r - r'), \end{aligned} \quad (20)$$

where $k_n = \sqrt{2mE_n}/\hbar$ for a bound quasiparticle state with energy E_n , k is a linear momentum for a continuum quasiparticle state, $u(\kappa, r)$, $v(\kappa, r)$ ($\kappa = k_n$ or k) are respectively the upper and lower components of a quasiparticle wave function with quantum numbers ℓ and j (here implicit), and $k_\lambda = \sqrt{-2m\lambda}/\hbar$. All quasiparticle states must be normalized to one (bound) or to a Dirac delta (scattering) (see Sec. III B). Equation (20) can also be demonstrated extending the method of Ref. [31] to quasiparticle states.

In order to obtain Berggren completeness of quasiparticle states, one can proceed as in Ref. [32], deforming the real energy contour in the complex plane. Resonant quasiparticle states appear therein, due to the Cauchy theorem, as S-matrix poles [32]. Hence, Eq. (20) becomes after contour deformation:

$$\begin{aligned} & \sum_{n \in (b,d)} [u(k_n, r)u(k_n, r') + v(k_n, r)v(k_n, r')] \\ & + \int_{L^+}^{+\infty} [u(k, r)u(k, r') + v(k, r)v(k, r')] dk \\ & = \delta(r - r'), \end{aligned} \quad (21)$$

where k_n refers now to a bound (b) or resonant (d) (decaying) quasiparticle state and k is complex as it follows the deformed contour in the complex plane, denoted as L^+ . Resonant

quasiparticle states are normalized with complex scaling (see Sec. III B).

IV. NUMERICAL DETERMINATION OF QUASIPARTICLE ENERGIES AND WAVE FUNCTIONS WITH DIRECT INTEGRATION

A. Quasiparticle Jost functions

In Eqs. (9), (10), and (11), constants and momenta of S-matrix poles are determined by the requirement of continuity of both the $u(k, r)$ and $v(k, r)$ functions and associated derivatives. These conditions can be expressed in a form of quasiparticle Jost functions, defined as a generalization of the Jost function for single-particle problems, whose zeroes correspond to S-matrix poles [33]. They read

$$\begin{aligned} J_u \left(k, \frac{C_v^0}{C_u^0}, \frac{C_v^+}{C_u^+} \right) &= \frac{u'(k, R_0^+)}{u(k, R_0^+)} - \frac{u'(k, R_0^-)}{u(k, R_0^-)}, \\ J_v \left(k, \frac{C_v^0}{C_u^0}, \frac{C_v^+}{C_u^+} \right) &= \frac{v'(k, R_0^+)}{v(k, R_0^+)} - \frac{v'(k, R_0^-)}{v(k, R_0^-)}, \\ J_m \left(k, \frac{C_v^0}{C_u^0}, \frac{C_v^+}{C_u^+} \right) &= \frac{u(k, R_0^+)}{u(k, R_0^-)} - \frac{v(k, R_0^+)}{v(k, R_0^-)}, \end{aligned} \quad (22)$$

where R_0 is a radius typically chosen around the nuclear surface and one can demand arbitrarily that $C_u^0 = C_u^+ = 1$ in Eqs. (9) and (10). The functions, $u(k, R_0^+)$, $v(k, R_0^+)$ and their derivatives, are obtained by forward integration of Eq. (2) using Eq. (9) as initial conditions, while $u(k, R_0^-)$, $v(k, R_0^-)$ and their derivatives are calculated by backward integration of Eq. (2) from the initial conditions provided by Eqs. (10) and (11). In Eq. (22), one can clearly see that $u(k, r)$ and $v(k, r)$ will have continuous logarithmic derivatives if $J_u = 0$ and $J_v = 0$, respectively. However, these two equalities are not sufficient to uniquely determine the quasiparticle state. Indeed, they imply that one can choose a set of constants so that either $u(k, r)$, $u'(k, r)$, or $v(k, r)$, $v'(k, r)$ are continuous, but not necessarily both of them. The condition $J_m = 0$ is thus enforced in Eq. (22). The set of three equations, $J_u = 0$, $J_v = 0$ and $J_m = 0$, uniquely determine quasiparticle S-matrix poles.

For quasiparticle scattering states, the linear momentum k is fixed, but constants have to be calculated with a matching procedure. One starts with imposing the condition $C_u^0 = 1$, as for S-matrix poles. As the $u(k, r)$ component is of scattering type, the condition $J_u = 0$ can always be fulfilled with appropriately chosen C_u^+ and C_u^- constants. Thus, it is sufficient to deal only with J_v and J_m :

$$\begin{aligned} J_v \left(\frac{C_v^0}{C_u^0}, C_v^+ \right) &= \frac{v'(k, R_0^+)}{v(k, R_0^+)} - \frac{v'(k, R_0^-)}{v(k, R_0^-)}, \\ J_m \left(\frac{C_v^0}{C_u^0}, C_v^+ \right) &= \frac{u(k, R_0^+)}{u(k, R_0^-)} - \frac{v(k, R_0^+)}{v(k, R_0^-)}, \end{aligned} \quad (23)$$

the difference with Eq. (22) being that J_v and J_m now depend on two parameters instead of three. As in the S-matrix pole equations, $u(k, R_0^+)$, $v(k, R_0^+)$ and their derivatives are generated by forward integration of Eq. (2). Concerning the implementation of $u(k, R_0^-)$, $v(k, R_0^-)$ and their derivatives, however, one first continues integrating forward in order to

obtain $u(k, R)$, $u'(k, R)$, R being in the asymptotic region. At this point R , $u(k, R)$, $u'(k, R)$ provide an initial condition for backward integration, while Eq. (11) is used to initialize $v(k, R)$, $v'(k, R)$. In this way, we obtain $u(k, R_0^-)$, $v(k, R_0^-)$ and their derivatives. Thus, the equations $J_v = 0$ and $J_m = 0$ provide the matching constants rendering $v(k, r)$, $v'(k, r)$ continuous.

The conditions, $J_u = 0$ (for S-matrix poles), $J_v = 0$ and $J_m = 0$, form a system of non-linear equations of two or three dimensions. Consequently, it has to be solved with multi-dimensional Newton method. The only problem therein is to find a good starting point from where one can attain fast convergence to the exact solution in a stable way.

B. Determination of quasiparticle energy and integration constants

Following Ref. [26], it is convenient to introduce linearly independent solutions of Eq. (2) in order to determine the constants defined in Eqs. (9), (10), and (11):

$$\begin{pmatrix} u \\ v \end{pmatrix} = C_u^0 \begin{pmatrix} f_{u0} \\ g_{u0} \end{pmatrix} + C_v^0 \begin{pmatrix} f_{v0} \\ g_{v0} \end{pmatrix}, \quad (24)$$

$$\begin{pmatrix} u \\ v \end{pmatrix} = C_u^+ \begin{pmatrix} f_{u^+} \\ g_{u^+} \end{pmatrix} + C_u^- \begin{pmatrix} f_{u^-} \\ g_{u^-} \end{pmatrix} + C_v^+ \begin{pmatrix} f_{v^+} \\ g_{v^+} \end{pmatrix}, \quad (25)$$

where the introduced basis functions verify

$$\begin{aligned} f_{u0}(r) &\sim r^{\ell+1}, & g_{v0}(r) &\sim r^{\ell+1}, & f_{v0}(r) &\sim D_0 r^{\ell+3}, \\ g_{u0}(r) &\sim -D_0 r^{\ell+3}, & r \rightarrow 0, & & f_{u^\pm}(r) &\sim H_{\ell\eta_u}^\pm(k_u r), \\ g_{v^+}(r) &\sim H_{\ell\eta_v}^+(k_v r), & f_{v^+}(r) &\rightarrow 0, & g_{u^\pm}(r) &\rightarrow 0, \\ & & r \rightarrow +\infty, & & & \end{aligned} \quad (26)$$

with

$$D_0 = \frac{m^*(0)W(0)}{(2\ell+3)\hbar^2}. \quad (27)$$

Equation (27) is obtained inserting $u(r) = r^{\ell+1}$ and $v(r) = -D_0 r^{\ell+3}$ in the second equality of Eq. (2) and solving the equation keeping only dominant terms.

As the basis functions of Eqs. (24) and (25) depend only on k of the quasiparticle state, they can be calculated with direct integration, in a forward direction for Eq. (24) and in a backward direction for Eq. (25). Used methods to determine quasiparticle wave function differ according to their characters; S-matrix poles or scattering states, as discussed below.

C. Bound and resonant quasiparticle states

To find S-matrix poles, it is first necessary to start with a good approximation of k , denoted k_{app} . For that, a no-pairing approximation is firstly performed. Neglecting \hbar in Eq. (1), the Gamow-HFB equations reduce to the GHF equations:

$$h|\phi_i\rangle = e_i|\phi_i\rangle, \quad (28)$$

where e_i are complex (real) for resonant (bound) states. Equation (28) provides bound and narrow resonant single-particle

states of interest, which will be in finite number. As pairing potential \tilde{h} is weak compared to h , there will always be unique correspondence between the GHF single-particle S-matrix poles and the HFB quasiparticle S-matrix poles. Unless the quasiparticle S-matrix poles lie close to the Fermi energy, their lower (upper) components will be very close to $\phi_i(r)$ if $|\phi_i\rangle$ are (un)occupied at the HF level, so that the auxiliary energies \bar{e}_i , defined in Eq. (7), will be very close to the real parts of e_i . Secondly, the HFB matrix in Eq. (1) is diagonalized. It has been found that the use of a Pöschl-Teller-Ginocchio (PTG) basis provides sufficiently precise results [19]. Therefore, for E_i in Eq. (7) we use the quasiparticle energies obtained by diagonalizing the HFB matrix in the PTG basis. For a given GHF state of energy e_i , the starting quasiparticle energy E_{app} (from which k_{app} is immediately deduced), is then the HFB quasiparticle energy whose \bar{e}_i is closest to the real part of e_i . If the HFB quasiparticle S-matrix pole is far from the Fermi energy, E_{app} is very close to the exact energy. Otherwise, it will still provide a good starting point, as, in practice, one can have only one quasiparticle state close to the Fermi energy for a given (ℓ, j) -partial wave.

Furthermore, one demands $C_u^- = 0$, which translates into a linear eigenvalue problem of dimension equal to four, deduced from Eqs. (24) and (25), which one matches at $r = R_0$:

$$\begin{pmatrix} f_{u_0} & f_{v_0} & -f_{u^+} & -f_{v^+} \\ g_{u_0} & g_{v_0} & -g_{u^+} & -g_{v^+} \\ f'_{u_0} & f'_{v_0} & -f'_{u^+} & -f'_{v^+} \\ g'_{u_0} & g'_{v_0} & -g'_{u^+} & -g'_{v^+} \end{pmatrix} \begin{pmatrix} C_u^0 \\ C_v^0 \\ C_u^+ \\ C_v^+ \end{pmatrix} = 0, \quad (29)$$

where all matrix functions have been evaluated at $r = R_0$ by way of backward or forward integration. As the integration constants are not simultaneously equal to zero, they have to form an eigenvector of the matching matrix of Eq. (29), which we denote M hereafter, of eigenvalue equal to zero. However, the determinant of the 4×4 matrix M is zero uniquely for the exact value of k . Thus, the set of approximate constants to use as a starting point for Newton method is chosen as the eigenvector of ${}^t M M$ whose associated eigenvalue is the smallest in modulus (${}^t M M$ is used instead of M because it is symmetric). The constant ratios C_v^0/C_u^0 and C_v^+/C_u^+ used in Eq. (22) follow, as they are independent of the norm of the considered eigenvector. Exact determination of k , C_v^0/C_u^0 and C_v^+/C_u^+ can then be worked out via three-dimensional Newton method.

D. Scattering quasiparticle state

If one considers a scattering state, it is convenient to define a^+ , a^- , b^+ , b^- so that $C_u^\pm = a^\pm C_u^0 + b^\pm C_v^0$. Moreover, as all constants are calculated up to a normalization factor, one can impose $C_u^0 = 1$. Upper components of Eqs. (24) and (25) matched at $r = R$ and Eq. (26) provide linear equations for a^\pm and b^\pm :

$$\begin{aligned} a^+ f_{u^+}(R) + a^- f_{u^-}(R) &= f_{u_0}(R), & b^+ f_{u^+}(R) + b^- f_{u^-}(R) \\ &= f_{v_0}(R), \\ a^+ f'_{u^+}(R) + a^- f'_{u^-}(R) &= f'_{u_0}(R), & b^+ f'_{u^+}(R) + b^- f'_{u^-}(R) \\ &= f'_{v_0}(R). \end{aligned} \quad (30)$$

From the knowledge of a^\pm and b^\pm , matching lower components in Eqs. (24) and (25) at $r = R_0$ determines C_v^0 and C_v^+ via linear equations as well:

$$\begin{aligned} C_v^0 [g_{v_0}(R_0) - b^+ g_{u^+}(R_0) - b^- g_{u^-}(R_0)] - C_v^+ g_{v^+}(R_0) \\ = a^+ g_{u^+}(R_0) + a^- g_{u^-}(R_0) - g_{u_0}(R_0), \\ C_v^0 [g'_{v_0}(R_0) - b^+ g'_{u^+}(R_0) - b^- g'_{u^-}(R_0)] - C_v^+ g'_{v^+}(R_0) \\ = a^+ g'_{u^+}(R_0) + a^- g'_{u^-}(R_0) - g'_{u_0}(R_0). \end{aligned} \quad (31)$$

As $C_u^\pm = a^\pm + b^\pm C_v^0$, all constants are determined with simple two-dimensional linear systems. Newton method applied to Eq. (23) converges very quickly using the obtained set of constants as a starting point. Note that the use of $H_{\ell\eta_u}^\pm(k_u r)$ functions in Eqs. (25) and (26) can be sometimes unstable, especially for the proton case, where, for low scattering energies, they can be very large and cancel almost exactly in Eq. (10). In this case, it is better to use regular and irregular Coulomb wave functions, $F_{\ell\eta_u}(k_u r)$ and $G_{\ell\eta_u}(k_u r)$, as basis functions.

V. NORMAL AND PAIRING DENSITIES

As quasiparticle states of complex energy form a complete set [see Eq. (21)], one can directly express densities with upper and lower components of quasiparticle states:

$$\begin{aligned} \rho_{\ell j}(r) &= \sum_{n \in (b,d)} v^2(k_n, r) + \int_{L^+} v^2(k, r) dk, \\ \rho(r) &= \sum_{\ell j} \rho_{\ell j}(r), \\ \tilde{\rho}_{\ell j}(r) &= - \sum_{n \in (b,d)} u(k_n, r) v(k_n, r) - \int_{L^+} u(k, r) v(k, r) dk, \\ \tilde{\rho}(r) &= \sum_{\ell j} \tilde{\rho}_{\ell j}(r), \end{aligned} \quad (32)$$

where $\rho_{\ell j}(r)$ and $\tilde{\rho}_{\ell j}(r)$ are, respectively, partial normal and pairing densities related to a given partial wave with quantum numbers ℓ and j , and $\rho(r)$, $\tilde{\rho}(r)$ are respectively the normal and pairing densities of the HFB ground state. However, due to the zero-range character of Skyrme forces, it is necessary to introduce an energy cut in contour integrals, so that L^+ contour has to stop at finite energy E_{cut} (see Fig. 1). Note that, due to this requirement, it is necessary for L^+ complex contours to come back to the real axis. Even though quasiparticle wave functions are complex in Eq. (32), $\rho_{\ell j}(r)$ and $\tilde{\rho}_{\ell j}(r)$ are real because one is considering a HFB bound ground state, so that, due to Cauchy theorem, complex integration in Eq. (32) is equivalent to real integration in the standard case. As a consequence, the DFT can be applied also to the Gamow HFB formalism, i.e., potentials $V(r)$ and $W(r)$ in Eq. (2) are evaluated using the standard formulas of Ref. [14]. As shown in Fig. 1, the bound HF single-particle states can become resonant states when pairing correlations are added [37]. Thus, physical interpretation of a resonant quasiparticle is somewhat different from that of single-particle resonances: widths of the quasiparticle states associated with the HF

TABLE I. Bound and resonant neutron energies and widths for ^{90}Ni , calculated in the GHF approximation and in the GHFB/Coord. formalism. Single-particle energies (e_i) and quasiparticle energies (E_i) are given in MeV and widths (Γ) in keV. Note that the GHF $2s_{1/2}$ state dissolves into continuum quasiparticle states in the Gamow-HFB description.

States	GHF		GHFB/Coord.	
	e	Γ	E	Γ
$0s_{1/2}$	-52.618	0	51.573	$1.099 \cdot 10^{-3}$
$1s_{1/2}$	-24.630	0	24.348	46.006
$2s_{1/2}$	-1.196	0	-	-
$0p_{3/2}$	-41.655	0	40.796	27.282
$1p_{3/2}$	-12.986	0	12.658	490.565
$0p_{1/2}$	-42.881	0	38.870	27.138
$1p_{1/2}$	-11.189	0	10.816	404.299
$0d_{5/2}$	-29.921	0	29.141	0.780
$1d_{5/2}$	-2.592	0	3.181	194.181
$0d_{3/2}$	-30.657	0	25.095	22.567
$1d_{3/2}$	-0.349	0	2.173	560.608
$0f_{7/2}$	-18.177	0	17.654	397.374
$0f_{5/2}$	-11.331	0	11.065	645.638
$0g_{9/2}$	-6.770	0	6.570	0.807
$0g_{7/2}$	1.350	6.410	3.120	63.6131
$0h_{11/2}$	3.852	52.851	5.269	131.776

in this case assures convergence of numerical calculation. This concerns only for the neutron channel, as the pairing gap vanishes in the proton channel.

The result of calculation for normal and pairing densities are presented in Figs. 2 and 3. It is interesting to compare the

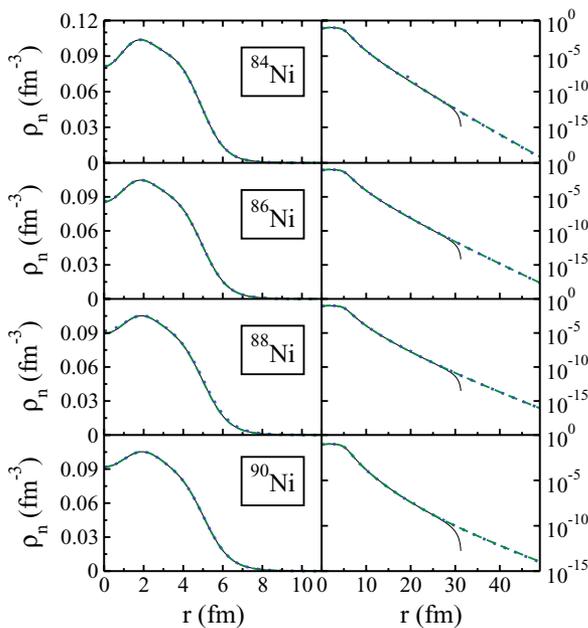


FIG. 2. (Color online) Neutron densities ρ_n both in normal (left-hand side) and logarithmic (right-hand side) scales. Results of the HFB/Box, GHFB/Coord., and GHFB/Config. calculations are displayed by solid, dashed, and dotted lines, respectively.

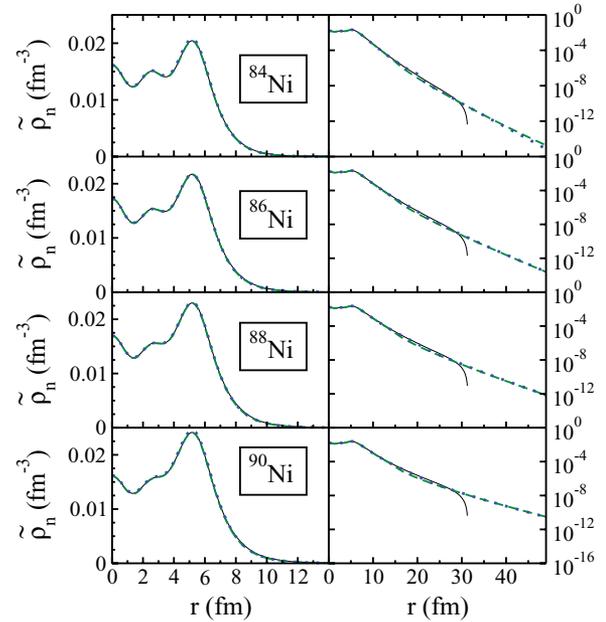


FIG. 3. (Color online) Same as Fig. 2 but for neutron pairing densities.

densities obtained by solving the Gamow-HFB equations in the coordinate or the GHF configurational space to those calculated by the standard coordinate space framework where the continuum is discretized with box boundary conditions. They are denoted GHFB/Coord., GHFB/Config., and HFB/Box., respectively. All results coincide in both normal and logarithmic scales for $r < 30$ fm. It was also checked that spurious imaginary parts of densities, caused by the discretization of the continuum of complex energy, were negligible, of the order of 10^{-6} [fm^{-3}] for GHFB/Coord. and 10^{-12} [fm^{-3}] for GHFB/Config., as the largest error values. In Table I, the bound and resonant single-particle states obtained by the GHF calculation are compared with the corresponding quasiparticle states calculated by the GHFB/Coord. method. It is obvious that bound HF states can give rise to unbound quasiparticle states carrying a sizable width when pairing correlations are switched on.

Physical observables associated with the HFB ground states are provided in Tables II and III. On the one hand, differences occur for neutron pairing energies, which are most sensitive to continuum effects [36]. While those of GHFB/Coord. compared to HFB/Box remain of the order of 500 keV, the difference between GHFB/Config. and HFB/Box pairing energies can be ~ 1.5 MeV. On the other hand, the rms radii and total energies are basically the same, with a discrepancy of at most ~ 300 keV for the latter. These results indicate that the GHFB/Coord., GHFB/Config., and HFB/Box treatments are all reliable methods to solve the HFB equations taking the continuum effects into account. As resonant states are explicitly treated in the Gamow HFB approach, this implies that the resonant effects can be well accounted for also by means of the HFB/Box method. This point is not necessarily widely accepted [37]. Even though the good agreements among the results of the GHFB/Coord., GHFB/Config., and

TABLE II. Gamow-HFB observables for ^{84}Ni and ^{86}Ni calculated with the GHFB/Coord., GHFB/Config., and HFB/Box methods. The rms radii are given in fm and other quantities in MeV. The proton chemical potential λ_p is not presented as there is no proton pairing gap.

	^{84}Ni			^{86}Ni		
	HFB/Box	GHFB/Coord.	GHFB/Config.	HFB/Box	GHFB/Coord.	GHFB/Config.
λ_n	-1.453	-1.430	-1.440	-1.037	-1.027	-1.029
r_n	4.451	4.450	4.450	4.528	4.526	4.526
r_p	3.980	3.982	3.982	4.001	4.001	4.001
Δ_n	1.481	1.535	1.564	1.667	1.658	1.669
E_n^{pair}	-30.70	-30.72	-31.85	-36.52	-35.85	-36.39
T_n	1084.53	1086.05	1086.46	1118.65	1118.68	1118.78
T_p	430.47	430.23	430.17	425.99	426.01	426.00
E_n^{so}	-63.379	-63.164	-63.01	-61.679	-61.712	-61.631
$E_{\text{dir}}^{\text{Coul}}$	132.94	132.89	132.88	132.26	132.25	132.25
$E_{\text{exc}}^{\text{Coul}}$	-10.138	-10.135	-10.135	-10.084	-10.085	-10.085
E_{tot}	-654.89	-654.89	-655.05	-656.933	-656.836	-656.971

HFB/Box calculations might be surprising, we see no reason to suspect that this is an exceptional case valid only for the Ni isotopes considered here. It will be interesting to examine this point further.

VIII. PERSPECTIVES FOR DESCRIBING DECAYING NUCLEI AND BEYOND-MEAN FIELD APPROACHES

The GHFB/Coord. method directly provides quasiparticle wave functions without using any intermediate basis states. Hence, it may be used also to describe decaying nuclear ground states in the HFB approximation. In fact, no HFB theory capable of describing decaying HFB ground states exists, even though an approximate scheme was proposed in Ref. [38]. The main difficulty is that it is not possible to construct the HFB ground state obeying the outgoing wave condition if one includes the full set of quasiparticle states of positive energy [38]. This arises from the fact that quasiparticles form a degenerate continuum of scattering states

for $E < |\lambda|$ if $\lambda > 0$, whereas they can only generate a discrete set of bound states in this region if $\lambda < 0$. It is impossible to remove quasiparticle states with $E < |\lambda|$ with the use of the GHFB/Config. method, because quasiparticle eigenenergies of the HFB matrix are complex. In contrast, the direct integration method (GHFB/Coord.) allows us to select which quasiparticle states are occupied in the HFB ground state. Hence, it may be possible to carefully study properties of decaying HFB states at least for the spherical case.

The GHF configurational approach (GHFB/Config.) may be more appropriate to study excited states in deformed nuclei by means of the QRPA. For deformed nuclei, basis expansion approaches may be easier compared to the calculation of deformed HFB ground states in coordinate space [16]. For calculating bound HFB ground states, we can use the PTG basis, which is more efficient than the GHF basis, considering the numerical cost of recalculating the GHF basis states inherent to the two-basis method (see Sec. VI). Once a HFB ground state is obtained in this way, one can readily calculate the GHF basis wave functions. The QRPA matrix would then

TABLE III. Same as in Table II but for ^{88}Ni and ^{90}Ni .

	^{88}Ni			^{90}Ni		
	HFB/Box	GHFB/Coord.	GHFB/Config.	HFB/Box	GHFB/Coord.	GHFB/Config.
λ_n	-0.671	-0.661	-0.665	-0.342	-0.330	-0.342
r_n	4.603	4.602	4.601	4.677	4.674	4.675
r_p	4.021	4.022	4.022	4.043	4.043	4.043
Δ_n	1.790	1.782	1.800	1.899	1.899	1.935
E_n^{pair}	-41.98	-41.26	-42.17	-47.158	-46.509	-48.449
T_n	1150.71	1150.74	1151.02	1182.52	1182.91	1183.79
T_p	421.71	421.71	421.70	417.38	417.35	417.31
E_n^{so}	-59.558	-59.559	-59.470	-56.898	-56.887	-56.822
$E_{\text{dir}}^{\text{Coul}}$	131.571	131.576	131.576	130.947	130.883	130.878
$E_{\text{exc}}^{\text{Coul}}$	-10.033	-10.033	-10.033	-9.980	-9.980	-9.980
E_{tot}	-658.167	-658.082	-658.272	-658.665	-658.635	-658.936

be represented afterward with respect to the quasiparticles wave functions expanded in the GHF basis, thus allowing the description of unbound QRPA excited states.

IX. CONCLUSION

The Berggren completeness relation, originally developed in the context of standard Schrödinger equation, has been extended to quasiparticles in the HFB formalism. It was shown that, as in the standard single-particle potential problem, bound, resonant and scattering quasiparticles are well defined and form a complete set, by which bound HFB ground states can be constructed. Both situations are very similar and can be treated by contour deformation of continuous real sets of states, even though physical interpretation of resonant quasiparticles is different from that of resonant single-particles. Numerical applications have been effected with neutron-rich nickel isotopes close to the drip line, for which continuum coupling is important. It was shown that the Gamow-HFB approach, both in coordinate and configurational space representations, properly describe densities and physical observables. Thus,

it provides us with an efficient tool to study ground states of medium and heavy nuclei close to the drip line. With these approaches, QRPA calculation fully taking into account continuum coupling may be efficiently carried out.

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