

Resonant continuum in the Hartree-Fock+BCS approximation

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A method for incorporating the effect of the resonant continuum into Hartree-Fock+BCS equations is proposed. The method is applied for the case of a neutron-rich nucleus calculated with a Skyrme-type force plus a zero-range pairing interaction and the results are compared with Hartree-Fock-Bogoliubov calculations. It is shown that the widths of resonant states have an important effect on the pairing properties of nuclei close to the drip line.

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In nuclei far from the β -stability line there are circumstances in which the resonant part of the particle continuum plays an important role. One of the first examples was given by Migdal [1], who anticipated the existence of halo nuclei such as ^{11}Li by showing that two neutrons in a potential well can form a dineutron state in the region of the nuclear surface if the potential has a resonant level with energy close to zero. Here, the role of the resonance is to enhance the pairing correlations of the two neutrons whose attraction is otherwise too weak to bind the system. The interplay between the resonant continuum and pairing correlations can also be important for the estimation of unbound processes such as single-particle excitations lying above the particle emission threshold, which may be found especially in nuclei close to the drip line. Thus, if the excitation energy is close to the energy of a narrow resonance then one expects an excitation of one-quasiparticle type, in which the excited nucleon stays a finite time before decaying. Besides the unbound processes mentioned above, resonant states are important for determining the pairing properties of the ground state of bound nuclei far from the β -stability line. Although in such calculations one should consider in principle the complete particle continuum, the largest contribution to the pairing correlations is expected to come from the resonant continuum part [2].

The aim of this Rapid Communication is to propose a method for incorporating the effect of the resonant continuum in the Hartree-Fock+BCS (HF+BCS) approximation. More precisely we investigate here the effect of the width of the resonances on the pairing properties of nuclei far from stability. As discussed below, this effect is difficult to estimate in self-consistent Hartree-Fock-Bogoliubov (HFB) calculations which are presently used for describing pairing correlations in nuclei close to the drip line.

In order to derive the BCS equations in the presence of the continuum we first discretize the single-particle continuum spectrum by enclosing the nucleus inside a box of a very large radius R_b . This is only a formal step, since it will be seen that the parameter R_b does not appear in the final results. Thus the genuine continuum is replaced by a set of discrete states with the level density given by [3]

$$g(\epsilon) = \sum_{\nu} \{g_{\nu}(\epsilon) + g_{\nu}^{free}(\epsilon)\} \equiv \sum_{\nu} \tilde{g}_{\nu}, \quad (1)$$

where $g_{\nu}(\epsilon) \equiv (1/\pi)(2j_{\nu}+1)(d\delta_{\nu}/d\epsilon)$ is the so-called continuum level density [4] and δ_{ν} is the phase shift of angular momentum $\nu \equiv (l_{\nu}, j_{\nu})$. The quantity $g_{\nu}^{free}(\epsilon)$ is the level density in the absence of the mean field and is given by $g_{\nu}^{free}(\epsilon) \equiv (1/\pi)(2j_{\nu}+1)(dk/d\epsilon)R_b$, where k is the momentum corresponding to the energy ϵ . The wave functions corresponding to the positive energy states and normalized within the box are defined by $\psi_{\nu}(\epsilon, r) \equiv N_{\nu}^{-1/2}(\epsilon)\varphi_{\nu}(\epsilon, r)$, where $N_{\nu}(\epsilon)$ is the norm of the scattering state $\varphi_{\nu}(\epsilon, r)$ in the box volume. It can be easily shown that for the scattering states selected by the box $N_{\nu}(\epsilon) = (2j_{\nu}+1)^{-1}\tilde{g}_{\nu}(\epsilon)$.

The gap equations for the states in the box can be written in terms of level density as follows:

$$\Delta_i = \sum_j V_{ii, jj} \tilde{g}_j v_j + \sum_{\nu} \int_{I_{\nu}} \tilde{g}_{\nu}(\epsilon) \tilde{V}_{ii, \nu\epsilon} \tilde{u}_{\nu}(\epsilon) v_{\nu}(\epsilon) d\epsilon, \quad (2)$$

$$\begin{aligned} \Delta_{\nu}(\epsilon) = & \sum_j \tilde{V}_{\nu\epsilon, jj} \tilde{g}_j v_j + \sum_{\nu'} \int_{I_{\nu'}} \tilde{g}_{\nu'}(\epsilon') \\ & \times \tilde{V}_{\nu\epsilon, \nu'\epsilon'} \tilde{u}_{\nu'}(\epsilon') v_{\nu'}(\epsilon') d\epsilon', \quad (3) \end{aligned}$$

where the indices i, j run over the bound states and I_{ν} is an energy interval associated with each partial wave (l_{ν}, j_{ν}) . The matrix elements of the interaction involving states in the continuum are given by $\tilde{V}_{ii, \nu\epsilon} \equiv \langle \psi_i \psi_{\bar{i}} | V | \psi_{\nu}(\epsilon) \psi_{\bar{\nu}}(\epsilon) \rangle$, $\tilde{V}_{\nu\epsilon, \nu'\epsilon'} \equiv \langle \psi_{\nu}(\epsilon) \psi_{\bar{\nu}}(\epsilon) | V | \psi_{\nu'}(\epsilon') \psi_{\bar{\nu}'}(\epsilon') \rangle$. The rest of the notations are standard [5]. It can be noticed that according to the BCS approach the generalized gap equations above take into account only pairing between time-reversed continuum states $\nu\epsilon$, $\bar{\nu}\epsilon$. A more general pairing between continuum states at neighboring energies is conceivable and this would just be taken care of by a continuum HFB approach. At the moment there exist only HFB calculations performed with a box boundary condition and we shall numerically compare their results with those obtained in the present approach.

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The largest contributions to the integrals above come from the regions where the wave functions $\psi_\nu(\epsilon)$ have a large localization inside the nucleus. This condition is fulfilled in energy regions where the S matrix has poles close to the real energy axis, i.e., near narrow single-particle resonances. The integrals can also have large contributions from energy intervals close to zero energy if the S matrix has poles corresponding to loosely bound states or virtual states near threshold [1,6]. In the I_ν intervals defined above the positive energy wave functions have the largest localization inside a sphere of radius D , where D is of the order of a few times the nuclear radius. Within D the positive energy wave functions can be related to the scattering wave function at resonant energy ϵ_ν through simple factorization formulas [1,6–8]. Following Refs. [7,8], the wave function $\psi_\nu(\epsilon)$ inside D can be approximated by

$$\psi_\nu(\epsilon, r) \approx g_\nu^{1/2}(\epsilon) \tilde{g}_\nu^{-1/2}(\epsilon) \phi_\nu(\epsilon_\nu, r) \equiv \tau_\nu^{1/2}(\epsilon) \phi_\nu(\epsilon_\nu, r), \quad (4)$$

where $\phi_\nu(\epsilon_\nu, r)$ is the scattering wave function calculated at the resonant energy ϵ_ν and normalized within a sphere of radius D . This factorization relation is very useful for evaluating matrix elements of finite range interactions for which it is sufficient to carry space integrals over the volume inside the radius D only. For instance, we will use $\tilde{V}_{i\bar{i}, \nu\bar{\nu}\epsilon} \approx \tau_\nu(\epsilon) V_{i\bar{i}, \nu\bar{\nu}\epsilon_\nu}$ and $\tilde{V}_{\nu\bar{\nu}\epsilon, \nu'\bar{\nu}'\epsilon'} \approx \tau_\nu(\epsilon) \tau_{\nu'}(\epsilon') V_{\nu\bar{\nu}\epsilon_\nu, \nu'\bar{\nu}'\epsilon'_{\nu'}}$, where on the right hand sides the matrix elements of the interaction are calculated using the wave functions $\phi_\nu(\epsilon_\nu, r)$. For a discussion of the accuracy of these approximations see Ref. [8].

With the help of this factorization the gap equations (2),(3) become

$$\Delta_i = \sum_j V_{i\bar{i}j\bar{j}} u_j v_j + \sum_\nu V_{i\bar{i}, \nu\bar{\nu}\epsilon_\nu} \int_{I_\nu} g_\nu(\epsilon) u_\nu(\epsilon) v_\nu(\epsilon) d\epsilon, \quad (5)$$

$$\begin{aligned} \Delta_\nu &\equiv \sum_j V_{\nu\bar{\nu}\epsilon_\nu, j\bar{j}} u_j v_j + \sum_{\nu'} V_{\nu\bar{\nu}\epsilon_\nu, \nu'\bar{\nu}'\epsilon'_{\nu'}} \\ &\times \int_{I_{\nu'}} g_{\nu'}(\epsilon') u_{\nu'}(\epsilon') v_{\nu'}(\epsilon') d\epsilon', \end{aligned} \quad (6)$$

with $\Delta_\nu(\epsilon) = \tau_\nu(\epsilon) \Delta_\nu$. The last expression can be written as $\tilde{g}_\nu(\epsilon) \Delta_\nu(\epsilon) = g_\nu(\epsilon) \Delta_\nu$ and gives the connection between the gaps calculated with the wave functions $\psi_\nu(\epsilon)$ and $\phi_\nu(\epsilon)$. One can get the same relation if one writes the gap equation (3) in terms of a local pairing field $\Delta(r)$ of finite range which cuts off the contributions of the tail of the wave function $\psi_\nu(\epsilon, r)$ beyond the radius D . Thus,

$$\begin{aligned} \Delta_\nu(\epsilon) &= \int_0^{R_b} |\psi_\nu(\epsilon, r)|^2 \Delta(r) dr \\ &\approx \tau_\nu(\epsilon) \int_0^D |\phi_\nu(\epsilon, r)|^2 \Delta(r) dr \\ &\equiv \tau_\nu(\epsilon) \Delta_\nu. \end{aligned} \quad (7)$$

A similar relation can be derived for the positive energy single-particle spectrum. By using these relations it can be seen that the gap equations (5),(6) are independent of the box radius. As shown above, this is a consequence of the finite range of the pairing interaction, which is sensitive only to the inner part of the resonant continuum wave functions.

In the BCS approximation the number of particles is fixed consistently with the gap equations by counting the particles distributed in the model space in which the pairing interaction is effective. Using the same approximations as for deriving the gap equations one gets

$$N = \sum_i v_i^2 + \sum_\nu \int_{I_\nu} g_\nu(\epsilon) v_\nu^2(\epsilon) d\epsilon. \quad (8)$$

This equation together with the gap equations (5),(6) are the extended BCS equations for a general (finite range) pairing interaction including the contribution of the resonant continuum. Each resonance is characterized by the quantity Δ_ν , which acts as the averaged gap of that resonance.

The above BCS equations are well suited to be specialized to the approximation of constant pairing interaction since the resonant states $\phi_\nu(\epsilon_\nu, r)$ and the bound states have rather similar localizations inside the nucleus. Then, one just has to replace in Eqs. (5),(6) all matrix elements by a constant value G . The corresponding BCS equations are the same as the ones of Ref. [9]. It is worthwhile to point out that in the constant pairing approximation as defined here one preserves the variation of the matrix elements of the pairing interaction over the resonance region. Consequently, as seen in Eq. (7), the gap also changes in the resonance region and, therefore, the corresponding pairing field is not constant in the whole space.

We can now extend the above treatment of the resonant continuum to HF+BCS. In the case of a Skyrme force this is done by including into the nucleon densities the contributions of the positive energy states with energies in the selected intervals I_ν and by using the factorization relation (4). Thus the resonant continuum contribution to the particle density inside the sphere of radius D reads

$$\begin{aligned} \rho_c(r) &\approx \sum_\nu |\phi_\nu(\epsilon_\nu, r)|^2 \int_{I_\nu} g_\nu(\epsilon) v_\nu^2(\epsilon) d\epsilon \\ &\equiv \sum_\nu |\phi_\nu(\epsilon_\nu, r)|^2 \langle v^2 \rangle_\nu. \end{aligned} \quad (9)$$

Similar expressions can be derived for the kinetic energy density $T(r)$ and spin density $J(r)$:

$$T(r) \approx \sum_i v_i^2 |\nabla \psi_i(r)|^2 + \sum_\nu \langle v^2 \rangle_\nu |\nabla \phi_\nu(\epsilon_\nu, r)|^2, \quad (10)$$

$$\begin{aligned} J(r) &\approx -i \sum_i v_i^2 \psi_i^*(r) [\nabla \psi_i(r) \times \sigma] \\ &\quad -i \sum_\nu \langle v^2 \rangle_\nu \phi_\nu^*(\epsilon_\nu, r) [\nabla \phi_\nu(\epsilon_\nu, r) \times \sigma], \end{aligned} \quad (11)$$

where the first sum represents the contribution of the bound states. The above densities define the mean field and the single-particle spectrum. They depend on the occupation probabilities and they are calculated iteratively with the BCS equations, as in the usual HF+BCS calculations [10].

At this point we would like to comment on the relation between the HF+BCS equations derived above and the HFB approach. The advantage of the HFB approach to treat processes that involve the continuum part of the nuclear spectrum is that the finite range of the pairing field is explicitly taken into account. Therefore, the particle and pairing densities automatically acquire a proper asymptotic behavior [11,12]. In order to preserve the same behavior in the HF+BCS limit one should keep the physical condition of a finite range pairing field, as it is also done in HFB calculations in which the pairing field is not calculated self-consistently [13]. As seen in Eq. (7), a finite range pairing field implies a cutoff in the tail of the positive energy wave functions. Without this cutoff the solution of a HF+BCS calculation with the positive energy states discretized in a box would correspond to a nucleus in dynamical equilibrium with a nucleonic gas and not to the nucleus itself [3]. Generally the cutoff radius may be ambiguous but if one restricts oneself to the resonant continuum, then there is a rather large region outside the nucleus where the resonant wave functions have values close to zero before they start oscillating. In this case the HF+BCS results do not depend sensitively on the cutoff radius chosen in such region.

We now apply the above resonant HF+BCS approach to a nucleus far from stability, namely ^{84}Ni for which HFB results can be found [14]. Here, we wish to compare the results of three types of calculations: (A) the resonant HF+BCS approach where the widths of single-particle resonances are taken into account; (B) a discrete version of the approach where the widths are set to zero; (C) the HFB approach of Ref. [14] where the coordinate space equations are solved with a box boundary condition and, therefore, the width effects would be missing. The HF field is calculated with the SIII interaction [15] whereas for the pairing channel a zero-range density-dependent interaction is used, $V(\vec{r}_1, \vec{r}_2) = V_0[1 - \rho(\vec{r}_1)/\rho_c]\delta(\vec{r}_1 - \vec{r}_2)$, where $\rho(\vec{r})$ is the total density, $V_0 = 1128.75 \text{ MeV fm}^3$, and $\rho_c = 0.134 \text{ fm}^{-3}$. All calculations are carried out up to a distance $D = 22.5 \text{ fm}$ [see Eq. (4)], but the numerical results discussed in the following do not depend sensitively on the precise choice of D in the range $(3-4)R$, where R is the nuclear radius. The resonant states included in the HF+BCS calculations, with energies smaller than 5 MeV (the energy cutoff used in Ref. [14]), together with the last bound state are listed in Table I. The energy ϵ_ν (width Γ_ν) of a given resonance is extracted from the energy where the derivative of the phase shift reaches its maximum (half of its maximum) value. The energy intervals I_ν are defined such that $|\epsilon - \epsilon_\nu| \leq 2\Gamma_\nu$.

Let us first look at the results of case A. The total averaged gap and the Fermi energy are $\langle \Delta \rangle = 0.51 \text{ MeV}$ and $\lambda = -0.874 \text{ MeV}$, respectively. The total binding energy and the pairing energy are $E = -652.7 \text{ MeV}$ and $E_p = 3.4 \text{ MeV}$. The corresponding pairing field is shown in Fig. 1 while the averaged occupation probabilities and the averaged gaps of

TABLE I. Results of HF+BCS calculations for the nucleus ^{84}Ni . Δ_n and v_n^2 are the averaged gap and averaged occupation probability of the single-particle state n of energy ϵ_n and width Γ_n . The notations $\tilde{\Delta}_n$, \tilde{v}_n^2 , $\tilde{\epsilon}_n$ and $\tilde{\Gamma}_n$ stand for the corresponding quantities calculated without including the effect of the widths of resonant states in HF+BCS equations. The single-particle energies, their widths and the pairing gaps are expressed in MeV.

n	ϵ_n	$\tilde{\epsilon}_n$	Γ_n	$\tilde{\Gamma}_n$	v_n^2	\tilde{v}_n^2	Δ_n	$\tilde{\Delta}_n$
$s_{1/2}$	-0.647	-0.644	—	—	0.295	0.294	0.505	0.674
$d_{3/2}$	0.441	0.417	0.077	0.068	0.041	0.075	0.630	0.847
$g_{7/2}$	1.604	1.587	0.009	0.008	0.029	0.055	0.966	1.306
$h_{11/2}$	3.309	3.302	0.017	0.016	0.017	0.034	1.227	1.658

resonant states and the last bound state $3s_{1/2}$ are given in Table I. The change of the particle density due to pairing correlations is shown in Fig. 2. It can be seen that in the tail region the contribution of the bound states to the total density, given mainly by the loosely bound state $3s_{1/2}$, is dominant. In order to see how the neutrons are distributed at large distances, we have calculated the number of neutrons outside a sphere of radius 12 fm. We find that the total numbers of neutrons distributed in bound and resonant states between 12 and 22 fm are 0.069 and 0.037, respectively.

A proper estimation of the particle distribution at large distances is difficult in HFB calculations based on a box boundary condition. Due to the box the wave functions which are spread far from the nucleus are generally pushed towards smaller distances. Thus, in the HFB calculations of Ref. [14] the occupancy of the loosely bound state $3s_{1/2}$, which gives the dominant contribution in the density tail region, depends strongly on the box radius and is generally underestimated. Consequently the HFB density is smaller in the tail region than the HF+BCS density. As seen in Fig. 2 the tail of the HFB density is actually even smaller than the HF density.

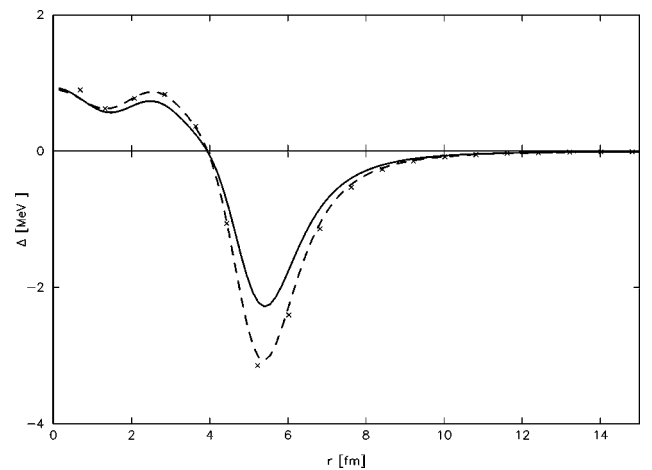


FIG. 1. Neutron pairing field as a function of the radius. The full (dashed) line shows the results of the HF+BCS calculations with (without) the effect of the width included. The line marked by crosses shows the HFB results of Ref. [14].

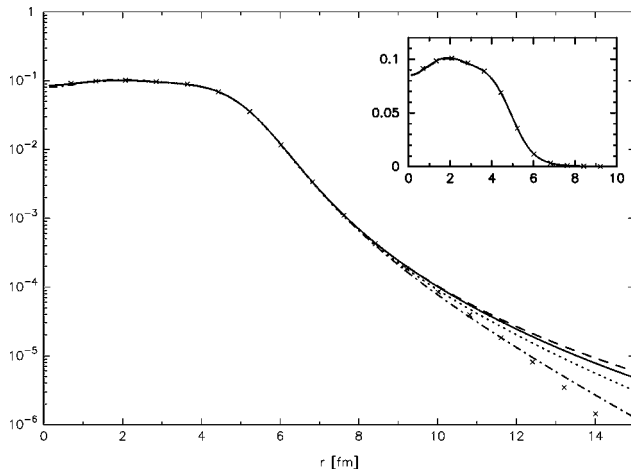


FIG. 2. Neutron density in ^{84}Ni , calculated in HF (long dashed line) and HF+BCS. In the order of decreasing tail the results of HF+BCS correspond to the following approximations: effect of the widths neglected; effect of the widths included; contribution of the bound states to the density. All densities are in fm^{-3} . The inset shows the corresponding densities in linear scale.

For case B the total averaged gap becomes $\langle\Delta\rangle=0.72$ MeV and the Fermi energy is $\lambda=-0.948$ MeV. The binding energy increases to the value $E=-653.1$ MeV while the pairing energy is equal to $E_p=6.2$ MeV. From Table I one can see that the occupancy of the resonant states is almost doubled compared to the case when the effect of the widths is taken into account. The corresponding changes in the pairing field and particle density are shown in Figs. 1,2. As seen in Fig. 2 the pairing field given by the HFB calculations based on a box boundary condition are quite similar to the HF+BCS pairing field of case B, i.e., calculated without taking into account the width effect. The same similarities are seen in the Fermi, binding, and pairing energies, which in the case of HFB are: $\lambda=-0.956$ MeV, $E=-653.7$ MeV, and $E_p=6.9$ MeV. These similarities show that in the HFB calculations with a box boundary condition the resonant continuum is actually described by quasibound states and, therefore, in such calculations the effect of the widths of resonant states upon pairing properties is not taken into account properly.

In conclusion one sees that in neglecting the contribution of the widths in HF+BCS calculations one enhances artificially the amount of pairing correlations. This enhancement is due to the fact that if the width is neglected then all the pairing strength is collected from the scattering state at the resonance energy. At this energy the scattering wave function has the highest spatial concentration (as compared with the nearby scattering functions) within the nuclear region. The effect of the width is to diminish the pairing strength because the pairs can now scatter also in the nearby states around the resonance energy which are less confined inside the nucleus. In a time dependent picture the dependence on the width seen above would correspond to the fact that a pair scattered to a resonance state has a finite lifetime, thus con-

tributing less to the pairing correlations as compared to the case of a very narrow (quasibound) state. In the HF+BCS approach presented here this effect is taken into account automatically through the continuum level density.

Formally, in a coordinate space HFB approach the contribution of the whole continuum is taken into account and, therefore, the effect of the resonant continuum discussed above should be also present. Furthermore, a HFB calculation also contains correlations from pairs in states which are not time-reversal partners. These correlations, which are absent in a HF+BCS approach, could be important for the scattering states with energies close to a resonance because their wave functions have similar localization properties [2]. However, the estimation of the effect of the resonance widths upon pairing correlations is still an open problem in the existing self-consistent HFB calculations. This is because the numerical methods used for solving the coordinate space HFB equations are based on discretizations of the continuous spectrum. With the currently used values of box radius ($R \approx 15-30$ fm) each resonance is represented by a single discrete state in the spherically symmetric case. To have a discrete level density high enough to properly describe the shape of the resonance would require an extremely large box radius, a condition which makes practical calculations untractable. This is the same difficulty one expects for HFB calculations in which the continuum is discretized by expanding the quasiparticle wave functions in a single particle basis [16]. In order to get, in these types of calculations, a proper level density in the region of a resonance one needs to use a basis of very large dimensions, larger than the dimensions commonly used for getting a correct asymptotic behavior of the weakly bound states. Thus, although the coordinate space HFB approach is in principle the appropriate tool for treating continuum effects, solving the HFB equations by imposing a box boundary condition to the solutions, or by using a single-particle basis expansion, does not guarantee that all effects of the continuum, particularly the effect of the widths of resonant states, are properly taken into account.

In summary, a method to include the resonant continuum in the HF+BCS approximation is presented. We have here concentrated on the regions of the continuous spectra which are close to single-particle resonances because they bring the most important contributions to pairing correlations. The method can be used to also take into account the effect of nonresonant continuum states close to the continuum threshold, which can be important in the presence of loosely bound states or virtual states. In the numerical example it has been shown that the widths of resonant states have an important effect on the pairing properties of nuclei close to the drip line. In order to describe this effect in a self-consistent HFB approach one needs to solve the HFB equations with proper boundary conditions. This work is in progress.

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