Continuum effects on the pairing in neutron drip-line nuclei studied with the canonical-basis HFB method

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Abstract

The canonical-basis HFB method provides an efficient way to describe pairing correlations involving the continuum part of the single-particle spectrum in coordinate-space representations. It can be applied to superconducting deformed drip-line nuclei as easily as to stable or spherical nuclei. This method is applied to a simulation of the approach to the neutron drip line. It turns out that the HFB solution has a stronger pairing and a smaller deformation as the Fermi level is raised. However, such changes are smooth and finite. No divergences or discontinuities of the radius or other quantities are found in the limit of zero Fermi energy. The nuclear density continues to be localized even a little beyond the drip line.

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In nuclei near the neutron drip line, the pairing correlation among the neutrons involves significantly the continuum (positive-energy) part of the Hartree-Fock (HF) single-particle states. In principle, there is no difficulty to treat such nuclei with the Hartree-Fock-Bogoliubov (HFB) method, which is the framework to incorporate the pairing correlation into mean-field approximations. Indeed, there is no practical problem concerning spherical nuclei [1, 2]. However, deformed nuclei are not so easy to treat. The difficulty originates in the huge number of quasiparticle states, most of which are spatially dislocalized continuum-spectrum states. In the quasi-particle formalism, two methods have been used to overcome the difficulty, one using transformed oscillator basis [3] and the other using a coordinate mesh but only for axially symmetric nuclei [4].

Mathematically, HFB ground states can be expressed in the form of the BCS variational function. The single-particle states in this expression are localized. They are called the HFB canonical basis. This localization makes the level density of the canonical basis by far smaller than that of the quasiparticle states because the former is proportional to the volume of the nucleus while the latter to the volume of the cavity to discretize the positive energy orbitals. The canonical-basis HFB method enables one to obtain the canonical orbitals without knowing anything about the huge number of quasiparticle states. It can be applied to deformed neutron-rich nuclei without difficulties.
The canonical-basis HFB method was originally introduced for spherical nuclei in Ref. [5]. I improved the method and implemented it for deformed nuclei [6, 7]. I also found the necessity of momentum dependence for the contact pairing interactions if one employs completely coordinate-space representations (like three-dimensional Cartesian mesh, unlike the radial mesh).

In quasiparticle HFB method, the canonical orbitals are obtained from the one-body density matrix and thus people have not noticed the existence of a more direct relation to the Hamiltonian. The canonical-basis formalism discloses this relation. Namely, canonical orbitals above the Fermi level are roughly the bound eigenstates of the pairing Hamiltonian. It is not the HF Hamiltonian which generates them. This finding is helpful to understand the shell structure in the continuum part of the spectrum [7].

Now, let me show a result of a calculation performed with the canonical-basis method. It is a simulation of the approach to the neutron drip line. The system is the $N = Z = 14$ nucleus. Instead of increasing the difference $N - Z$, I modify the parameters of the mean-field interaction. Namely, $t_0$ of the Skyrme force is increased (toward zero from below) to raise the Fermi level while $t_3 (> 0)$ is decreased so that the saturation density of the symmetric nuclear matter is unchanged. This approach is taken only because the present version of my computer program is designed for $N = Z$ systems. I will examine the adequacy of this approach in future.

The interaction in the mean-field channel is the Skyrme SIII force [8] without the spin-orbit term. The coulomb force is also turned off. Owing to the omission of these two interactions, the single-particle states are four-fold degenerated. I take into account 70 canonical basis states in each of the four spin-isospin sectors. The parameters of the pairing interaction [7] are $v_p = -880$ MeV fm$^3$, $k_c = 2$ fm$^{-1}$, and $\rho_c = 0.32$ fm$^{-3}$, and $\tilde{\rho}_c = \infty$.

A three-dimensional Cartesian mesh representation is employed to express the single-particle wavefunctions without assuming any spatial symmetries. The mesh spacing is 0.8 fm while the edge of the cubic cavity is 40 fm.

Fig. 1 shows how the HFB ground state changes as the Fermi level ($\lambda$) rises. The pairing gap is enhanced almost by a factor of two at the drip line (where $\lambda = 0$ MeV) compared with the solution for the original SIII force ($\lambda = -11.7$ MeV). The quadrupole deformation $\beta$ is decreased by the enhanced pairing. The nucleus has a large prolate deformation at $\lambda = -11.7$ MeV but becomes spherical for $\lambda > -5.5$ MeV. On the other hand, the r.m.s. radius does not change so much. Its increase is only 35 % even at the drip line. Dislocalization of the density occurs not at $\lambda = 0$ MeV but at higher $\lambda$ (0.8 MeV). One can see only smooth changes at $\lambda \sim 0$ MeV.

Fig. 2 shows the energies (expectation value of the HF Hamiltonian) of canonical-basis states. One can see that discrete bound states are obtained for both negative and positive energies. For $\lambda > -5.5$ MeV, the nucleus becomes spherical and the levels are degenerated. At $\lambda \sim -3$ MeV, the orbitals are (from the bottom) s, p, s, d, p, f, s, d,
Figure 1: The average pairing gap (top), the quadrupole deformation parameter $\beta$ (middle), and the root-mean-square radius (bottom) plotted versus the Fermi level.
g, etc. Here again, there seems to be no violent changes at $\lambda \sim 0$ MeV. Positive-energy localized $s$ orbitals begin to spread over the cavity only for $\lambda > 300$ keV.

Considering general properties of HFB solutions\cite{1}, the true ground state must be a dislocalized state. The reason for the appearance of a localized solution seems to be as follows. The dislocalization of an orbital requires the increase of $v^2$ toward 1 because otherwise the orbital is confined in the pairing potential, which is usually very deep compared with the size of the kinetic energy term of the pairing Hamiltonian. However, since $v^2 = 1$ corresponds to weaker pairing correlation and larger total energy, a dislocalized solution is not necessarily reached in the iteration process of the gradient method in certain circumstances like when the Fermi level is positive but low. In contrast, with methods based on the diagonalization of the quasi-particle Hamiltonian, a direct jump to $v^2 = 1$ can take place and it results in the dislocalization of the corresponding orbital as soon as it becomes energetically favorable.

The localized HFB solutions for positive Fermi energies obtained in the canonical-basis formalism may be used as rough approximations to the nuclei just beyond the neutron drip line.

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Figure 2: Expectation value of the HF Hamiltonian for each canonical-basis state plotted versus the Fermi level.