Canonical-basis HFB method

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Advantages of a new method to obtain solutions of the Hartree-Fock-Bogoliubov (HFB) equation directory in the HFB canonical form are discussed in comparison with the ordinary method in which the solutions are expressed as the vacuum of Bogoliubov quasiparticles. A byproduct and necessary special cares are also described.

In order to treat the neutron-rich side of the nuclear chart, one has to take into account the pairing correlation in the continuum part (= positive-energy part) of the single-particle spectrum. One has to do so not only for nuclei very close to the neutron drip line because, for a reliable treatment of the pairing correlation in the presence of shell fluctuations, one has to consider explicitly at least (empirically speaking) half of a major shell above the Fermi level in BCS calculations. Namely, one has to treat the positive energy states explicitly if $\epsilon_{\rm F} > -\frac{1}{2}\hbar\omega_{\rm osc}$. This condition applies to roughly half of the nuclei in the nuclear chart and the number of such nuclei is about $\frac{10^4}{2}$.

One also has to consider the long tail for large r for neutron-rich nuclei. The large-r asymptotic form of the density looks like $\rho(r) \sim \left(e^{-\kappa r}/r\right)^2$, $\kappa = \sqrt{-2m\epsilon_{\rm F}}/\hbar$, where $\epsilon_{\rm F}$ is the energy of the last occupied Hartree-Fock (HF) orbital. In the presence of the pairing correlation, $\epsilon_{\rm F}$ is replaced with $\epsilon_{\rm F} - E_{\rm qp}^{(\rm min)}$, where $E_{\rm qp}^{(\rm min)}$ is the smallest quasiparticle excitation energy and is roughly equal to the pairing gap. This means that the tail is shortened by the pairing correlation. Therefore calculations of the density tail require a reliable treatment of the pairing.

In order to treat pairing correlations in the continuum and long density tails simultaneously, one has to employ the coordinate-space HFB method. Here, not a radial grid but a three-dimensional mesh representation is preferable because all the nuclei except near spherical magics are deformed. The three-dimensional mesh is, however, feasible only for Skyrme forces, for which the mean field becomes local. The canonical-basis HFB method [1, 2, 3, 4, 5] is a new method to obtain HFB solutions for Skyrme forces in three-dimensional Cartesian mesh representation with positive-energy states explicitly considered.

In the ordinary method to solve the HFB[6, 7, 8], the solutions are expressed as the vacuum of the Bogoliubov quasiparticles.

$$|\psi\rangle = \prod_{i=1}^{\#\rm basis} b_i|0\rangle, \qquad b_i = \sum_s \int d^3r \left\{\phi_i^*(\vec{r},s)\, a(\vec{r},s) + \psi_i(\vec{r},s)\, a^\dagger(\vec{r},s)\right\}, \tag{1}$$

where $b_i^\dagger$ are the creation operators of quasiparticles. The two kinds of amplitudes can be

obtained as the eigenvectors of the HFB super matrix,

$$\begin{pmatrix} -h & \tilde{h} \\ \tilde{h} & h \end{pmatrix} \begin{pmatrix} \phi_i \\ \psi_i \end{pmatrix} = \epsilon_i \begin{pmatrix} \phi_i \\ \psi_i \end{pmatrix}. \tag{2}$$

This method is not very efficient because the quasiparticle wavefunctions contain by far more information than is necessary to describe the ground state. Most of their information concerns particle or hole excitations.

HFB solutions can be expressed in the BCS form as

$$|\Psi\rangle = \prod_{i=1}^{i_{\max}} \left(u_i + v_i\, a_i^\dagger\, a_{\bar{i}}^\dagger\right)|0\rangle, \qquad a_i^\dagger = \sum_s \int d^3r\; \psi_i(\vec{r},s)\; a^\dagger(\vec{r},s), \tag{3}$$

where $a_i^\dagger$ is the creation operator of a nucleon in the ith HFB canonical basis state. This expression is exact when $i_{\max} = \frac{1}{2}\#\text{basis}$ according to the Bloch Messiah theorem. The essential advantage of this expression is that one may neglect $v^2 \ll 1$ states as far as the ground state is concerned. One can truncate the number of canonical basis by $i_{\max} = \mathcal{O}(A) \ll \#\text{basis}$ to a good approximation. The canonical-basis HFB method is a much more economical way to express HFB ground states of neutron rich nuclei than expressing them as quasiparticle vacua.

The canonical-basis method determines the canonical basis and the uv factors without the full knowledge of the quasiparticle states. This can be pursued in the gradient method under constraint of orthonormality among the canonical basis.

$$\frac{\delta E}{\delta \psi_i^*} = \mathcal{H}_i \psi_i = \sum_j \lambda_{ij} \psi_j, \qquad \mathcal{H}_i = v_i^2 h + u_i v_i \tilde{h}, \tag{4}$$

where h is the HF Hamiltonian and $\tilde{h}$ is the pairing Hamiltonian. This expression of $\mathcal{H}_i$ gives a new insight: The positive energy canonical basis are the bound states of the pairing Hamiltonian. Consequently, they are guaranteed to be spatially localized (by $\tilde{h}$, not by h) and form a discrete spectrum. See Ref.[4] for explanations.

The following table is a summary of the comparison between the two methods.

method	#basis	orthogonality condition	pairing force
quasi particle	$\propto$ box volume	redundant	δ-func, + dens. dep.
canonical basis	$\propto$ nuclear volume	essential	+ mom. dep.

In the canonical basis method, the Hamiltonian becomes state-dependent and thus the orthogonality among the canonical basis states should be explicitly taken care of. See Ref.[4] for how it can be made possible.

The canonical-basis method needs momentum-dependent (or finite-range) pairing interaction in order to circumvent the point collapse problem, which is peculiar to this method. It is depicted in Fig. 1. I have tried several ways to avoid the collapse to find unwanted side effects for many of them. See Ref. [4] for a detailed discussion.

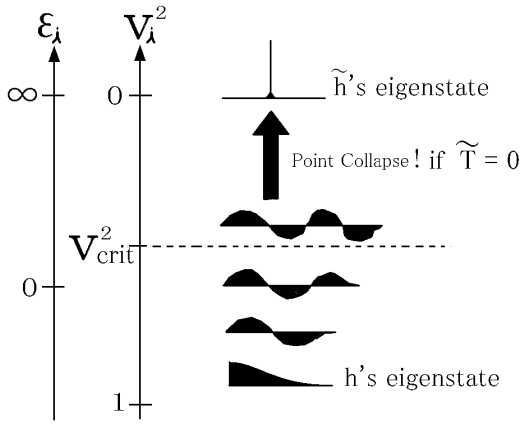

Fig. 1: Point collapse of a high-lying canonical orbital. The canonical orbital whose occupation probability is smaller than some critical value shrinks into a point unless the pairing Hamiltonian has a kinetic term.

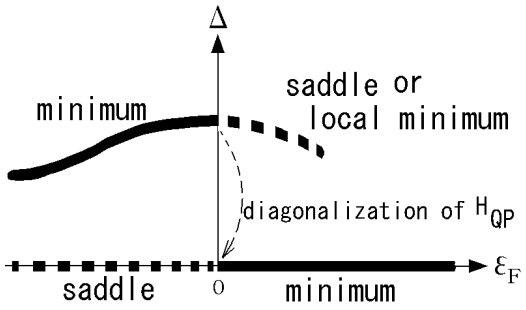

Fig. 2: The pairing gap Δ versus the Fermi level $\epsilon_{\rm F}$ for the global-minimum HFB solution (thick bold line) and possible local-minimum solutions (thick dash line).

In my talk I have shown the result of a simulation of the approach to the neutron drip line as a demonstration of the method and suggested a possibility to obtain approximate localized solutions for nearly bound systems (Fig. 2). Details can be found in Ref. [5].

I have also discussed on the extension of the method to the full Skyrme interaction with time-reversal symmetry imposed, which will be published in future.

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