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CORRELATED BCS OCCUPATION PROBABILITIES IN PROTON-NEUTRON SYSTEMS

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Abstract

The correlated BCS (CBCS) for **a** proton-neutron system is introduced by first-order perturbation theory, in which the quasiparticle interactions dropped in the BCS are approximately taken into account. The formulation of the occupation probabilities in the CBCS is derived in the angular momentumcoupling J-scheme. The applications of the CBCS for ^{46}Ti show some improvements compared to the standard BCS theory.

1 Introduction

The BCS theory developed by Bardeen, Cooper and Schrieffer [1] has successfully explained the superconductivity of the superconducting metals at very low temperature. The adoption of the BCS theory into nuclear physics followed the suggestions of Bohr, Mottelson and Pines and the exploratory work of Belyaev [2, 3]. The first application is to even number semi-magic nuclei, where the ground states are considered to be constructed by pairing configurations. This model is a useful tool to explain a large variety of nuclear properties [4, 5]. The best known form of this theory is obtained by means of the Bogoliubov transformation and Ritz variational principle [4, 5, 6, 7]. The BCS is an independent quasiparticle theory and its ground state is the quasiparticle vacuum. The disadvantage of BCS is that particle number is not conserved.

The application of the BCS theory to a proton-neutron (pn) system, i.e., open proton and neutron shells, is more complicated because we have two types of interacting particles. Of course, these particles can been rewritten as the identical particles if another quantum number–isospin– is introduced. But we will not use isospin formalism here because it is usually applied in heavy nuclei with a large neutron excess where the pn formalism is more appropriate.

Several theories were suggested in order to describe pn system. The simplest method provides separate Bogoliubov transformations for protons and neutrons, respectively. Thus the quasiprotons and quasineutrons are well defined, and the ground state is the vacuum corresponding to both types of quasiparticles. In this formalism, the BCS equations for protons and neutrons retain the same form as those obtained from the semi-magic nuclei case, and they are just coupled through the mean field [7, 17]. In this model, only $pp-$ and $nn-$ pairing are taken into account. Another formulation that has been proposed by Lane [6] and considered by a number of authors[7, 12, 13] is to give up the distinction between the protons and neutrons by using a generalized Bogoliubov transformation that mixes protons and neutrons to obtain two kinds of new mixed quasiparticles. The BCS types of equations can be derived. They include all kinds of pairing, i.e. $pp-$, $nn-$ and $pn-$ pairing, where complex mean field and potentials are required [13].

In this paper, we concentrate on the first method because well defined quasiprotons and quasineutrons are necessary when one develops proton-neutron QRPA theory [8, 9, 10, 11]. In section 2, we re-derive the BCS equation in angular momentum coupling space for the proton-neutron system. The correlated BCS wave function is introduced through perturbation theory in section 3. The summary is given in section 4.

2 BCS Theory for Proton-Neutron System

2.1 Nuclear Hamiltonian in quasiparticle space

In the shell-model basis, the nuclear Hamiltonian can be written in the J-scheme coupling proton-neutron formalism, which is given by [14]

$$
\begin{aligned}
H &= \sum_p \varepsilon_p^0 \sqrt{2j_p+1}(a_p^+ \otimes \tilde{a}_p)^{J=0,M=0} + \sum_n \varepsilon_n^0 \sqrt{2j_n+1}(a_n^+ \otimes \tilde{a}_n)^{J=0,M=0} \\
&+\frac{1}{4}\sum_{\substack{p_1\cdots p_4\\ JM}} (1+\delta_{p_1p_2})(1+\delta_{p_3p_4}) V^J_{p_1p_2p_3p_4} A^\dagger_{\rm pp}(p_1p_2,JM)A_{\rm pp}(p_3p_4,JM) \\
&+\frac{1}{4}\sum_{\substack{n_1,\cdots n_4\\ JM}} (1+\delta_{n_1n_2})(1+\delta_{n_3n_4}) V^J_{n_1n_2n_3n_4} A^\dagger_{\rm nn}(n_1n_2,JM)A_{\rm nn}(n_3n_4,JM) \\
&+\sum_{\substack{p_1n_1p_2n_2\\ JM}} V^J_{p_1n_1p_2n_2} A^\dagger_{\rm pn}(p_1n_1,JM)A_{\rm pn}(p_2n_2,JM), \qquad (1)
\end{aligned}
$$

where the labels p/n stand for the proton/neutron single-particle state (nlj). ε_p^0 (ε_n^0) is the single-proton (neutron) energy. $V^J_{p_1p_2p_3p_4}$, $V^J_{n_1n_2n_3n_4}$ and $V^J_{p_1n_1p_2n_2}$ are the matrix elements of two-proton, two-neutron and proton-neutron interaction, respectively. The two-proton, two-neutron and proton-neutron creation operators are defined by

$$A^\dagger_{\mathrm{pp}}(p_1p_2,JM) = \sum_{m_{p_1}m_{p_2}} \frac{< j_{p_1}m_{p_1}j_{p_2}m_{p_2}|JM >}{\sqrt{1+\delta_{p_1p_2}}} a^\dagger_{p_1m_{p_1}} a_{p_2m_{p_2}} \tag{2}$$

$$A^\dagger_{\mathrm{nn}}(n_1n_2,JM) = \sum_{m_{n_1}m_{n_2}} \frac{< n_1m_{n_1}n_2m_{n_2}|JM >}{\sqrt{1+\delta_{n_1n_2}}} a^\dagger_{n_1m_{n_1}} a_{n_2m_{n_2}} \tag{3}$$

$$A^\dagger_{\mathrm{pn}}(p_1n_1,JM) = \sum_{m_{p_1}m_{n_1}} < j_{p_1}m_{p_1}j_{n_1}m_{n_1}|JM > a^\dagger_{p_1m_{p_1}} a_{n_1m_{n_1}}, \tag{4}$$

where $a^\dagger$ is the particle creation operator.

The quasiprotons and quasineutrons are introduced by the Bogoliubov transformations, in the spherical shell-model basis,

$$c^+_{pm_p} = u_p a^+_{pm_p} + (-1)^{j_p+m_p} v_p a_{p-m_p}, \tag{5}$$

$$c^+_{nm_n} = u_n a^+_{nm_n} + (-1)^{j_n+m_n} v_n a_{n-m_n}, \tag{6}$$

with

$$u_p^2 + v_p^2 = u_n^2 + v_n^2 = 1. \tag{7}$$

Eq. (7) is required if the quasiparticles are assumed to be fermions[7, 4, 5].

In order to derive the BCS equation, we relax the fixed proton and neutron number restriction and introduce the extra terms to the Hamiltonian.

$$\tilde{H} = H - \lambda_\pi \hat{N}_\pi - \lambda_\nu \hat{N}_\nu, \tag{8}$$

where $\hat{N}_\pi$ and $\hat{N}_\nu$ are proton and neutron number operators. The Lagrange multipliers λ_π and λ_ν turn out to have the physical interpretation of proton and neutron Fermi energies. They are chosen to ensure that mean proton and neutron numbers are correct.

After carrying out the Bogoliubov transformation, the Hamiltonian can be rewritten as

$$\tilde{H} = H_{\mathrm{BCS}} + H_{\mathrm{int}}, \tag{9}$$

where

$$\begin{aligned} H_{\mathrm{BCS}} &= H_0 + H_{11}^{\mathrm{pp}} + H_{11}^{\mathrm{nn}} + (H_{20}^{\mathrm{pp}} + h.c) + (H_{20}^{\mathrm{nn}} + h.c), & (10) \\ H_{\mathrm{int}} &= H_{\mathrm{int}}^{\mathrm{pp}} + H_{\mathrm{int}}^{\mathrm{nn}} + H_{\mathrm{int}}^{\mathrm{pn}}, & (11) \end{aligned}$$

where the numerical subscripts indicate the number of quasiparticle creation and annihilation operators in each piece of the Hamiltonian. We also require that the above equations should be *normal ordered*, that is, destruction operators c stand to the right of creation operators $c^\dagger$.

2.2 BCS equations (independent quasiparticle)

The BCS equations only depend on H_{BCS} in Eq. (10). The terms in H_{BCS} are given by

$$\begin{aligned} H_0 &= \sum_p (2j_p+1)(\varepsilon_p - \lambda_\pi - \frac{1}{2}\Gamma_p)v_p^2 + \sum_n (2j_n+1)(\varepsilon_n - \lambda_\nu - \frac{1}{2}\Gamma_n)v_n^2 \\ &\quad -\frac{1}{2}\sum_p (2j_p+1)\Delta_p u_p v_p - \frac{1}{2}\sum_n (2j_n+1)\Delta_n u_n v_n, & (12) \\ H_{11}^{\mathrm{pp}} &= \sum_{p,m_p} \{(\varepsilon_p - \lambda_\pi)(u_p^2 - v_p^2) + 2u_p v_p \Delta_p\} c_{pm_p}^\dagger c_{pm_p}, & (13) \\ H_{11}^{\mathrm{nn}} &= \sum_{n,m_n} \{(\varepsilon_n - \lambda_\nu)(u_n^2 - v_n^2) + 2u_n v_n \Delta_n\} c_{nm_n}^\dagger c_{nm_n}, & (14) \\ H_{20}^{\mathrm{pp}} &= \sum_p (-1)^{j_p+m_p} \{(\varepsilon_p - \lambda_\pi)u_p v_p - \frac{1}{2}(u_p^2 - v_p^2)\Delta_p\} c_{pm_p}^\dagger c_{p-m_p}^\dagger, & (15) \end{aligned}$$

$$H_{20}^{\rm nn} = \sum_n (-1)^{j_n+m_n}\{(\varepsilon_n-\lambda_\nu)u_n v_n - \frac{1}{2}(u_n^2-v_n^2)\Delta_n\}c^\dagger_{nm_n}c^\dagger_{n-m_n}, \quad (16)$$

with

$$\varepsilon_p = \varepsilon_p^0 + \Gamma_p, \quad (17)$$

$$\varepsilon_n = \varepsilon_n^0 + \Gamma_n, \quad (18)$$

$$\Gamma_p = \frac{1}{2j_p+1}[\sum_{p',J}(1+\delta_{pp'})(2J+1)v_{p'}^2 V^J_{pp'pp'} + \sum_{n',J}(2J+1)v_{n'}^2 V^J_{pn'pn'}], \quad (19)$$

$$\Gamma_n = \frac{1}{2j_n+1}[\sum_{n',J}(1+\delta_{nn'})(2J+1)v_{n'}^2 V^J_{nn'nn'} + \sum_{p',J}(2J+1)v_{p'}^2 V^J_{p'np'n}], \quad (20)$$

$$\Delta_p = -\sum_{p'}\sqrt{\frac{2j'_p+1}{2j_p+1}}u_{p'}v_{p'}V^{J=0}_{ppp'p'}, \quad (21)$$

$$\Delta_n = -\sum_{n'}\sqrt{\frac{2j'_n+1}{2j_n+1}}u_{n'}v_{n'}V^{J=0}_{nnn'n'}, \quad (22)$$

Γ_p and Γ_n the are proton and neutron single-particle energy rearrangements. Δ_p and Δ_n are proton and neutron gaps. The r.h.s. of the gap equations (Eq. (21,22)) only depend on J=0 interaction matrix elements. The $J \neq 0$ terms are automatically equal to zero due to Clebsch-Gordan coefficient coupling. So the BCS is an S-pair theory. Also one finds only $pp-$ or $nn-$ paring is involved in the proton or neutron gap equation.

In order to derive the BCS equations, we will drop quasiparticle interaction terms $H_{\rm int}$, and let the BCS ground state be the vacuum corresponding to quasiprotons and quasineutrons introduced in Eqs. (5,6), i.e.,

$$c_{pm_p}|{\rm BCS}> = 0, \quad (23)$$

$$c_{nm_n}|{\rm BCS}> = 0, \quad (24)$$

where $|{\rm BCS}>$ is the BCS ground state.

The BCS equations can be obtained from the Ritz variation principle, in which the expectation value of $\tilde{H}$ is minimized [7, 5, 17]. It requires the coefficients of $H_{20}^{\rm pp}$ and $H_{20}^{\rm nn}$ in Eqs. (15,16) to be equal to zero, i.e.,

$$(\varepsilon_p - \lambda_\pi)u_p v_p - \frac{1}{2}(u_p^2 - v_p^2)\Delta_p = 0, \tag{25}$$

$$(\varepsilon_n - \lambda_\nu)u_n v_n - \frac{1}{2}(u_n^2 - v_n^2)\Delta_n = 0. \tag{26}$$

We introduce the quasiproton and quasineutron energies defined by

$$E_p = \sqrt{(\varepsilon_p - \lambda_\pi)^2 + \Delta_p^2}, \tag{27}$$

$$E_n = \sqrt{(\varepsilon_n - \lambda_\nu)^2 + \Delta_n^2}. \tag{28}$$

Then one solves Eqs. (25,26,7) and obtains

$$v_p^2 = \frac{1}{2}(1 - \frac{\varepsilon_p - \lambda_\pi}{E_p}), \tag{29}$$

$$v_n^2 = \frac{1}{2}(1 - \frac{\varepsilon_n - \lambda_\nu}{E_n}). \tag{30}$$

We reiterate that the BCS theory ceases to conserve particle numbers. The BCS wave function is required to have correct mean particle numbers. Thus the proton and neutron Fermi energies λ_π and λ_ν are chosen so that the mean proton and neutron numbers in the BCS satisfy

$$<\mathrm{BCS}|\hat{N}_\pi|\mathrm{BCS}> = \sum_p (2j_p + 1)v_p^2 = N_\pi, \tag{31}$$

$$<\mathrm{BCS}|\hat{N}_\nu|\mathrm{BCS}> = \sum_n (2j_n + 1)v_n^2 = N_\nu, \tag{32}$$

where N_π and N_ν are the proton and neutron numbers in the nuclear system. At this stage, the parameters v_p^2 and v_n^2 introduced in Bogoliubov transformations turn out to have the physical meaning of proton and neutron occupation probabilities.

Eqs. (17-22,27-30,31,32) are called the BCS equations. They can be solved iteratively. In the BCS equations, we find that the equations for protons and neutrons are coupled only through the proton-neutron interaction terms in the rearrangement Γ_p and Γ_n. Since the BCS equation is obtained by dropping quasiparticle interaction $H_{\rm int}$ terms, the BCS is an independent quasiparticle theory.

When v_p^2 and v_n^2 satisfy Eqs. (29,30), the BCS Hamiltonian in Eq. (10) becomes

$$H_{\rm BCS} = H_0 + \sum_{p,m_p} E_p c^\dagger_{pm_p} c_{pm_p} + \sum_{n,m_n} E_n c^\dagger_{nm_n} c_{nm_n}. \tag{33}$$

The BCS ground state energy is given by

$$\begin{aligned} E_{\rm BCS} &= <\mathrm{BCS}|H_{\rm BCS} + \lambda_\pi \hat{N}_\pi + \lambda_\nu \hat{N}_\nu|\mathrm{BCS}> \\ &= H_0 + \lambda_\pi N_\pi + \lambda_\nu N_\nu \\ &= \sum_p (2j_p+1)(\varepsilon_p - \frac{1}{2}\Gamma_p)v_p^2 + \sum_n (2j_n+1)(\varepsilon_n - \frac{1}{2}\Gamma_n)v_n^2 \\ & \quad -\frac{1}{2}\sum_p (2j_p+1)\Delta_p u_p v_p - \frac{1}{2}\sum_n (2j_n+1)\Delta_n u_n v_n. \end{aligned} \tag{34}$$

The BCS excitations are constructed by

$$|h\mathrm{qp}l\mathrm{qn}> = \prod_i^h \prod_j^l c^\dagger_{p_i m_{p_i}} c^\dagger_{n_j m_{n_j}} |\mathrm{BCS}> . \tag{35}$$

The excitation energy is

$$E_{h\mathrm{qp}l\mathrm{qn}} = E_{\rm BCS} + \sum_i^h E_{p_i} + \sum_j^l E_{n_j}. \tag{36}$$

The configuration corresponding to this excitation is obtained by creating h quasiprotons and l quasineutrons with respect to the ground state $|\mathrm{BCS}>$.

3 Correlated BCS Theory

3.1 Interactions between quasiparticles

As we mentioned before, the $H_{\rm int}$ term describes the interactions between the quasiparticles, consisting of like particle interaction $H_{\rm int}^{\rm pp}$ and $H_{\rm int}^{\rm nn}$ and unlike particle interaction $H_{\rm int}^{\rm pn}$. Since $H_{\rm int}^{\rm nn}$ is identical with $H_{\rm int}^{\rm pp}$ if p/n labels are interchanged, we will give $H_{\rm int}^{\rm pp}$ here. Now the expressions of each term in $H_{\rm int}$ are given by

$$
\begin{aligned}
H_{\rm int}^{\rm pp} &= H_{22}^{\rm pp} + (H_{31}^{\rm pp} + h.c) + (H_{40}^{\rm pp} + h.c) && (37)\\
H_{\rm int}^{\rm pn} &= H_{22}^{\rm pn} + (H_{40}^{\rm pn} + h.c) + (P_{31}^{\rm pn} + h.c)\\
&\quad +(N_{31}^{\rm pn} + h.c) + P_{22}^{\rm pn} + N_{22}^{\rm pn}, && (38)
\end{aligned}
$$

where the numerical subscripts again indicate the number of quasiparticle creation and annihilation operators in each piece of $H_{\rm int}$.

$$
\begin{aligned}
H_{40}^{\rm pp} &= -\frac{1}{4}\sum_{\substack{p_1\cdots p_4,\\ JM}} (1+\delta_{p_1p_2})(1+\delta_{p_3p_4}) u_{p_1}u_{p_2}v_{p_3}v_{p_4} V^J_{p_1p_2p_3p_4}\\
&\quad \mathcal{A}^\dagger_{\rm pp}(p_1p_2, JM)\tilde{\mathcal{A}}^\dagger_{\rm pp}(p_3p_4, JM), && (39)\\
H_{31}^{\rm pp} &= -\frac{1}{2}\sum_{\substack{p_1\cdots p_4,\\ JM}} (1+\delta_{p_1p_2})(1+\delta_{p_3p_4}) V^J_{p_1p_2p_3p_4}\\
&\quad (u_{p_1}u_{p_2}u_{p_3}v_{p_4} - v_{p_1}v_{p_2}v_{p_3}u_{p_4})\mathcal{A}^\dagger_{\rm pp}(p_1p_2, JM)\tilde{\mathcal{D}}^\dagger_{\rm pp}(p_3p_4, JM), && (40)\\
H_{22}^{\rm pp} &= \frac{1}{4}\sum_{\substack{p_1\cdots p_4,\\ JM}} \{(1+\delta_{p_1p_2})(1+\delta_{p_3p_4})(u_{p_1}u_{p_2}u_{p_3}u_{p_4} + v_{p_1}v_{p_2}v_{p_3}v_{p_4}) V^J_{p_1p_2p_3p_4}\\
&\quad +4u_{p_1}v_{p_2}u_{p_3}v_{p_4} W^J_{p_1p_2p_3p_4}\sqrt{(1+\delta_{p_1p_2})(1+\delta_{p_3p_4})(1+\delta_{p_1p_3})(1+\delta_{p_2p_4})}\}\\
&\quad \mathcal{A}^\dagger_{\rm pp}(p_1p_2, JM)\mathcal{A}^\dagger_{\rm pp}(p_3p_4, JM), && (41)\\
H_{40}^{\rm pn} &= -\sum_{\substack{p_1n_1p_2n_2,\\ JM}} V^J_{p_1n_1p_2n_2} u_{p_1}u_{n_1}v_{p_2}v_{n_2}\mathcal{A}^\dagger_{\rm pn}(p_1n_1, JM)\tilde{\mathcal{A}}^\dagger_{\rm pn}(p_2n_2, JM), && (42)
\end{aligned}
$$

$$
\begin{aligned}
P_{31}^{\rm pn} &= -\sum_{\substack{p_1n_1p_2n_2,\\ JM}} V^J_{p_1n_1p_2n_2}\{u_{p_1}u_{n_1}v_{p_2}u_{n_2}\mathcal{A}^\dagger_{\rm pn}(p_1n_1,JM)\mathcal{P}^\dagger_{\rm pn}(p_2n_2,JM) \\
&\quad + v_{p_1}v_{n_1}u_{p_2}v_{n_2}\tilde{\mathcal{A}}^\dagger_{\rm pn}(p_1n_1,JM)\tilde{\mathcal{P}}^\dagger_{\rm pn}(p_2n_2,JM)\}, \qquad (43) \\
N_{31}^{\rm pn} &= -\sum_{\substack{p_1n_1p_2n_2,\\ JM}} V^J_{p_1n_1p_2n_2}\{u_{p_1}u_{n_1}u_{p_2}v_{n_2}\mathcal{A}^\dagger_{\rm pn}(p_1n_1,JM)\mathcal{N}^\dagger_{\rm pn}(p_2n_2,JM) \\
&\quad + v_{p_1}v_{n_1}u_{p_2}u_{n_2}\tilde{\mathcal{A}}^\dagger_{\rm pn}(p_1n_1,JM)\tilde{\mathcal{N}}^\dagger_{\rm pn}(p_2n_2,JM)\}, \qquad (44) \\
H_{22}^{\rm pn} &= \sum_{\substack{p_1n_1p_2n_2,\\ JM}} \{(u_{p_1}u_{n_1}u_{p_2}u_{n_2}+v_{p_1}v_{n_1}v_{p_2}v_{n_2})V^J_{p_1n_1p_2n_2} \\
&\quad +(u_{p_1}v_{n_1}u_{p_2}v_{n_2}+v_{p_1}u_{n_1}v_{p_2}u_{n_2})W^J_{p_1n_1p_2n_2}\} \\
&\quad \mathcal{A}^\dagger_{\rm pn}(p_1n_1,JM)\mathcal{A}_{\rm pn}(p_2n_2,JM), \qquad (45) \\
P_{22}^{\rm pn} &= -\sum_{\substack{p_1n_1p_2n_2,\\ JM}} V^J_{p_1n_1p_2n_2}u_{p_1}v_{n_1}v_{p_2}u_{n_2}\tilde{\mathcal{P}}^\dagger_{\rm pn}(p_1n_1,JM)\mathcal{P}^\dagger_{\rm pn}(p_2n_2,JM), \qquad (46) \\
N_{22}^{\rm pn} &= -\sum_{\substack{p_1n_1p_2n_2,\\ JM}} V^J_{p_1n_1p_2n_2}v_{p_1}u_{n_1}u_{p_2}v_{n_2}\tilde{\mathcal{N}}^\dagger_{\rm pn}(p_1n_1,JM)\mathcal{N}^\dagger_{\rm pn}(p_2n_2,JM). \qquad (47)
\end{aligned}
$$

The notations used in the above equations are defined by

$$
\begin{aligned}
\mathcal{A}^\dagger{}_{\rm pp}(p_1p_2,JM) &= \sum_{m_{p_1}m_{p_2}} \frac{<j_{p_1}m_{p_1}j_{p_2}m_{p_2}|JM>}{\sqrt{1+\delta_{p_1p_2}}}c^\dagger_{p_1m_{p_1}}c^\dagger_{p_2m_{p_2}}, \qquad (48) \\
\mathcal{D}_{\rm pp}(p_1p_2,JM) &= \sum_{m_{p_1}m_{p_2}} <j_{p_1}m_{p_1}j_{p_2}m_{p_2}|JM> c^\dagger_{p_1m_{p_1}}\tilde{c}_{p_2m_{p_2}}, \qquad (49) \\
\mathcal{A}^\dagger_{\rm pn}(p_1n_1,JM) &= \sum_{m_{p_1}m_{n_1}} <j_{p_1}m_{p_1}j_{n_1}m_{n_1}|JM> c^\dagger_{p_1m_{p_1}}c^\dagger_{n_1m_{n_1}}, \qquad (50) \\
\mathcal{P}_{\rm pn}(p_1n_1,JM) &= \sum_{m_{p_1}m_{n_1}} <j_{p_1}m_{p_1}j_{n_1}m_{n_1}|JM> \tilde{c}^\dagger_{p_1m_{p_1}}c_{n_1m_{n_1}}, \qquad (51) \\
\mathcal{N}_{\rm pn}(p_1n_1,JM) &= \sum_{m_{p_1}m_{n_1}} <j_{p_1}m_{p_1}j_{n_1}m_{n_1}|JM> \tilde{c}^\dagger_{n_1m_{n_1}}c_{p_1m_{p_1}}, \qquad (52)
\end{aligned}
$$

with

$$
\mathcal{A}(j_1j_2,JM) = (\mathcal{A}^\dagger(j_1j_2,JM))^\dagger, \qquad (53)
$$

$$\tilde{A}(j_1j_2,JM) \;=\; (-1)^{J+M}A(j_1j_2,J-M), \tag{54}$$

W^J is particle-hole interaction defined by the Pandya transformation,

$$W^J_{pn,p'n'} = -(-1)^{j_p+j_n+j_{p'}+j_{n'}}\sum_{J'}(2J'+1)\begin{Bmatrix} j_p & j_n & J \\ j_p' & j_n' & J' \end{Bmatrix} V^{J'}_{pn',p'n}. \tag{55}$$

3.2 Correlated BCS wave function

Since the quasiparticle interaction term $H_{\rm int}$ is dropped in the BCS, we can incorporate its effects approximately by using it to improve our lowest-order results with the Rayleigh-Schrödinger perturbation theory [15, 16]. The first-order correction terms are rather easily evaluated if we are only interested in the BCS ground state. H_{31} and H_{22} both contain an annihilation operator c as the rightmost operator and hence give zero when operating on the BCS ground state (quasiparticle vacuum). This means that, in this order, the corrections mix the four quasiparticle excitations with the quasiparticle vacuum via H_{40}.

Since H_{40} consists of three terms $H_{40}^{\rm pp}$, $H_{40}^{\rm nn}$ and $H_{40}^{\rm pn}$, the quasiparticle excitations connected to the ground state corrections contains three kinds of configuration, four-quasiproton, four-quasineutron and two-quasiproton two-quasineutron excitations. They are denoted as $|4{\rm qp}>$, $|4{\rm qn}>$ and $|2{\rm qpn}>$, and corresponding to $(h=4,\, l=0)$, $(h=0,\, l=4)$ and $(h=2,\, l=2)$ in Eq. (35), respectively. Therefore excitation energies are given by Eq. (36). The correlated BCS ground state wave function can be represented as

$$\begin{aligned}|{\rm CBCS}> \;&=\; \mathcal{N}(|{\rm BCS}> + \sum_k \frac{<k|H_{\rm int}|{\rm BCS}>}{E_{\rm BCS}-E_k}|k>) \\ &=\; \mathcal{N}(|{\rm BCS}> + \sum_{4{\rm qp}} \frac{<4{\rm qp}|H_{40}^{\rm pp}|{\rm BCS}>}{E_{\rm BCS}-E_{4{\rm qp}}}|4{\rm qp}>\end{aligned}$$

$$+\sum_{4\text{qn}} \frac{<4\text{qn}|H_{40}^{\text{nn}}|\text{BCS}>}{E_{\text{BCS}}-E_{4\text{qn}}}|4\text{qn}>$$

$$+\sum_{2\text{qpn}} \frac{<2\text{qpn}|H_{40}^{\text{pn}}|\text{BCS}>}{E_{\text{BCS}}-E_{2\text{qpn}}}|2\text{qpn}>), \tag{56}$$

where $\mathcal{N}$ is the normalization factor, and $|k>$ denotes any excitations. However, this correction is expected to be small so that the gap properties of the pairing solution are not destroyed.

In order to simplify our calculation, the interactions between like particle are assumed to be relatively small and dropped. Thus Eq. (56) becomes

$$|\text{CBCS}>\approx \mathcal{N}(|\text{BCS}> + \sum_{2\text{qpn}} \frac{<2\text{qpn}|H_{40}^{\text{pn}}|\text{BCS}>}{E_{\text{BCS}}-E_{2\text{qpn}}}|2\text{qpn}>). \tag{57}$$

The word *correlated* implies including the quasiparticle correlation terms in Eqs. (56,57).

3.3 Construction of two-quasiproton two-quasineutron excitations in the J-scheme

The two-proton and two-neutron doublet excitations $|2\text{qpn}>$ are simply obtained by choosing $h = l = 2$ in Eq. (35) in the m-scheme, where one normalized factor may be introduced. But if we are only interested in some special J values, the J-scheme representation is useful because of rather smaller dimensions involved. For example, only J=1 excitations are needed in Gamow-Teller transitions. Thus we define a two-quasiproton two-quasineutron doublet creation operator in the J-scheme,

$$\begin{aligned} B^{\dagger}_{J'J''}(p_1n_1p_2n_2, JM) &= N_B(\mathcal{A}^{\dagger}(p_1n_1, J'M') \otimes \mathcal{A}^{\dagger}(p_2n_2, J''M''))^{JM} \\ &= N_B \sum_{M'M''} < J'M'J''M''|JM > \\ &\quad \times \mathcal{A}^{\dagger}(p_1n_1, J'M')\mathcal{A}^{\dagger}(p_2n_2, J''M''), \end{aligned} \tag{58}$$

where N_B is the normalization factor of B^+. The two-quasiproton two-quasineutron excitations are given by

$$|2\text{qpn}> = B^{\dagger}_{J'J''}(p_1n_1p_2n_2, JM)|\text{BCS}> . \tag{59}$$

However, when one constructs the $|2\text{qpn}>$ excitations, identical states must be excluded in order to avoid double counting.

The normalization factor N_B is determined by

$$\begin{aligned} <2\text{qpn}|2\text{qpn}> &= <\text{BCS}|B_{J'J''}(p_1n_1p_2n_2, JM)B^{\dagger}_{J'J''}(p_1n_1p_2n_2, JM)|\text{BCS}> \\ &= 1. \end{aligned} \tag{60}$$

Then we obtain,

$$\begin{aligned} N_B^{-2} &= 1 + (-1)^{j_{n_1}+j_{n_2}+J}(2J+1)(2J'+1)(2J''+1)\delta_{p_1p_2}\left\{\begin{array}{ccc} j_{p_1} & j_{n_1} & J' \\ j_{n_2} & j_{p_2} & J'' \\ J'' & J' & J \end{array}\right\} \\ &+(-1)^{j_{p_1}+j_{p_2}+J}(2J+1)(2J'+1)(2J''+1)\delta_{n_1n_2}\left\{\begin{array}{ccc} j_{n_1} & j_{p_1} & J' \\ j_{p_2} & j_{n_2} & J'' \\ J'' & J' & J \end{array}\right\} \\ &+\delta_{J'J''}\delta_{p_1p_2}\delta_{n_1n_2}. \end{aligned} \tag{61}$$

Since the BCS ground state has spin $J = 0$, only $J = 0$ two-quasiproton two-quasineutron excitations in Eq. (59) contribute to the ground state correction. Therefore we have $J' = J''$ and $M' = -M''$. Then two-quasiproton two-quasineutron excitations used in the correlated BCS wave function are restricted to

$$\begin{aligned} |2\text{qpn}> &= N_B B^{\dagger}_{J'J'}(p_1n_1p_2n_2, 00)|\text{BCS}> \\ &= |(p_1n_1)^{J'}(p_2n_2)^{J'}> . \end{aligned} \tag{62}$$

The last notation will be frequently used in later discussions.

According to perturbation theory, all unperburbed states involved in Eq. (57) must form an orthogonal basis. But the excitations created by Eq. (59) or (62) are not orthogonal each other. Let's consider any two states,

$$|k> \;=\; |2\mathrm{qpn}>= N_B B^{\dagger}_{JJ}(p_1n_1p_2n_2,00)|\mathrm{BCS}>\,, \tag{63}$$

$$|k'> \;=\; |2\mathrm{qpn}'>= N_{B'} B^{\dagger}_{J'J'}(p'_1n'_1p'_2n'_2,00)|\mathrm{BCS}>\,. \tag{64}$$

The orthogonal condition requires $<k|k'>=\delta_{kk'}$. But the overlap between them is

$$\begin{aligned}
\chi_{kk'} &= <\mathrm{BCS}|B_{JJ}(p_1n_1p_2n_2,00)B^{\dagger}_{J'J'}(p'_1n'_1p'_2n'_2,00)|\mathrm{BCS}> \\
&= N_BN_{B'}\{\delta_{p_1p'_1}\delta_{n_1n'_1}\delta_{p_2p'_2}\delta_{n_2n'_2}\delta_{JJ'} \\
&\quad +(-1)^{j_{n_1}+j_{n_2}+J+J'}(2J+1)(2J'+1)\left\{\begin{array}{ccc} j_{p_1} & j_{n_1} & J \\ j_{n_2} & j_{p_2} & J \\ J' & J' & 0 \end{array}\right\}\delta_{p_1p'_2}\delta_{n_1n'_1}\delta_{p_2p'_1}\delta_{n_2n'_2} \\
&\quad +(-1)^{j_{p_1}+j_{p_2}+J+J'}(2J+1)(2J'+1)\left\{\begin{array}{ccc} j_{n_1} & j_{p_1} & J \\ j_{p_2} & j_{n_2} & J \\ J' & J' & 0 \end{array}\right\}\delta_{p_1p'_1}\delta_{n_1n'_2}\delta_{p_2p'_2}\delta_{n_2n'_1} \\
&\quad +\delta_{p_1p'_2}\delta_{n_1n'_2}\delta_{p_2p'_1}\delta_{n_2n'_1}\delta_{JJ'}\},
\end{aligned} \tag{65}$$

where N_B and $N_{B'}$ are the normalization factors for states $|2\mathrm{qpn}>$ and $|2\mathrm{qpn}'>$.

The $\chi_{kk'}$ is nonzero only for the following cases,

(A) $p_1 = p'_1$ $n_1 = n'_1$ $p_2 = p'_2$ $n_2 = n'_2$ $J = J'$

(B) $p_1 = p'_2$ $n_1 = n'_2$ $p_2 = p'_1$ $n_2 = n'_1$ $J = J'$

(C) $p_1 = p'_2$ $n_1 = n'_1$ $p_2 = p'_1$ $n_2 = n'_2$ $J,\ J'$

(D) $p_1 = p'_2$ $n_1 = n'_2$ $p_2 = p'_2$ $n_2 = n'_2$ $J,\ J'$.

For case (A) or (B), it is easy to obtain $\chi = 1$. It indicates that states $|2\mathrm{qpn}>$ and $|2\mathrm{qpn}'>$ are identical. On the other hand, we can exclude all double counted $|2\mathrm{qpn}>$

states through this overlap procedure. For cases (C) and (D), $0 < \chi < 1$ implies that two states are not orthogonal.

We have to use the Gram-Schmidt orthogonalization procedure to obtain normalized orthogonal states from the normalized nonorthogonal states $|2\text{qpn}>$ (in fact, they are not linearly independent). Finally, we obtain

$$|p_1 n_1 p_2 n_2, k >= \sum_i \alpha_{ik} |(p_1 n_1)^{J_i} (p_2 n_2)^{J_i} > . \tag{66}$$

The coefficients α are obtained from orthogonalization which relate to χ. For the new state $|p_1 n_1 p_2 n_2, k>$, we have

$$< p_1 n_1 p_2 n_2, k | p_1 n_1 p_2 n_2, k' >= \delta_{kk'}. \tag{67}$$

These states will be employed to calculate the first-order perturbation.

The excitation energy for state $|p_1 n_1 p_2 n_2, k>$ is given by

$$E_k = (E_{\text{BCS}} + E_{p_1} + E_{p_2} + E_{n_1} + E_{n_2}). \tag{68}$$

So the energy denominator in Eq. (57) is

$$E_{\text{BCS}} - E_k = -(E_{p_1} + E_{p_2} + E_{n_1} + E_{n_2}). \tag{69}$$

3.4 Occupations in the correlated BCS

Based on the discussions in the last subsection, we can start to derive a formalism for the occupation probabilities in the correlated BCS theory. In this subsection, we will derive the correlated BCS wave function expression and occupation probability. One inserts $|p_1 n_1 p_2 n_2, k>$ into Eq. (57) instead of $|2\text{qpn}>$, the correction terms become

$$\sum_{2\text{qpn}} \frac{< 2\text{qpn} | H_{40}^{\text{pn}} | \text{BCS} >}{E_{\text{BCS}} - E_{2\text{qpn}}} |2\text{qpn}>$$

$$= - \sum_{\substack{p_1 n_1 p_2 n_2 \\ k}} \frac{< p_1 n_1 p_2 n_2, k | H_{40}^{\mathrm{pn}} | \mathrm{BCS} >}{E_{p_1} + E_{n_1} + E_{p_2} + E_{n_2}} | p_1 n_1 p_2 n_2, k >$$

$$= - \sum_{\substack{p_1 n_1 p_2 n_2 \\ k}} \frac{\sum_i \alpha_{ki} < \mathrm{BCS} | B_{J_i J_i}(p_1 n_1 p_2 n_2, 00) H_{40}^{\mathrm{pn}} | \mathrm{BCS} >}{E_{p_1} + E_{n_1} + E_{p_2} + E_{n_2}}$$

$$\times \sum_j \alpha_{kj} B^{\dagger}_{J_j J_j}(p_1 n_1 p_2 n_2, 00) | \mathrm{BCS} >$$

$$= - \sum_{\substack{p_1 n_1 p_2 n_2 \\ j}} \frac{\sum_k \sum_i \alpha_{ki} \alpha_{kj} < \mathrm{BCS} | B_{J_i J_i}(p_1 n_1 p_2 n_2, 00) H_{40}^{\mathrm{pn}} | \mathrm{BCS} >}{E_{p_1} + E_{n_1} + E_{p_2} + E_{n_2}}$$

$$\times B^{\dagger}_{J_j J_j}(p_1 n_1 p_2 n_2, 00) | \mathrm{BCS} > , \tag{70}$$

where the matrix element in above equation is

$$< \mathrm{BCS} | B_{J_i J_i}(p_1 n_1 p_2 n_2, 00) H_{40}^{\mathrm{pn}} | \mathrm{BCS} > = - N_{Bi} \sqrt{2J_i + 1} G^{J_i}_{p_1 n_1 p_2 n_2}, \tag{71}$$

with

$$G^{J_i}_{p_1 n_1 p_2 n_2} = V^{J_i}_{p_1 n_1 p_2 n_2} (u_{p_1} u_{n_1} v_{p_2} v_{n_2} + v_{p_1} v_{n_1} u_{p_2} u_{n_2})$$
$$- W^{J_i}_{p_1 n_1 p_2 n_2} (v_{p_1} u_{n_1} u_{p_2} v_{n_2} + u_{p_1} v_{n_1} v_{p_2} u_{n_2}). \tag{72}$$

The matrix elements V and W are the particle-particle and particle-hole interaction, resepctively. Therefore the correlated BCS wave function in Eq. (57) is given by

$$| \mathrm{CBCS} > = \mathcal{N} \{ 1 + \sum_{\substack{p_1 n_1 p_2 n_2 \\ j}} \frac{F_{p_1 n_1 p_2 n_2}}{E_{p_1} + E_{n_1} + E_{p_2} + E_{n_2}} B^{\dagger}_{J_j J_j}(p_1 n_1 p_2 n_2, 00) \} | \mathrm{BCS} > , \tag{73}$$

where

$$F_{p_1 n_1 p_2 n_2} = \sum_k \sum_i N_{Bi} \alpha_{ki} \alpha_{kj} \sqrt{2J_i + 1} G^{J_i}_{p_1 n_1 p_2 n_2}. \tag{74}$$

One finds F is a function of j where k and i are already summed over.

The occupation probabilities for the protons and neutrons are given by

$$< \mathrm{CBCS} | a^{\dagger}_{pm_p} a_{pm_p} | \mathrm{CBCS} > = v_p^2 +$$

$$
\begin{aligned}
& \mathcal{N}^2 \ \frac{(u_p^2 - v_p^2)}{2j_p + 1} \sum_{p_1 n_1 n_2} (\frac{F_{p_1 n_1 p n_2}}{E_{p_1} + E_{n_1} + E_p + E_{n_2}})^2, (75) \\
< \mathrm{CBCS}|a^{\dagger}_{nm_n} a_{nm_n}|\mathrm{CBCS} > \ = \ & v_n^2 + \\
& \mathcal{N}^2 \ \frac{(u_n^2 - v_n^2)}{2j_n + 1} \sum_{p_1 p_2 n_1} (\frac{F_{p_1 n_1 p_2 n}}{E_{p_1} + E_{n_1} + E_{p_2} + E_n})^2, (76)
\end{aligned}
$$

where E, u^2 and v^2 are given in the last section.

The correlated BCS wave function is required to have correct mean proton and neutron numbers, and we have

$$
< \mathrm{CBCS}|\hat{N}_\pi|\mathrm{CBCS} > \ = \ N_\pi \quad (77)
$$

$$
< \mathrm{CBCS}|\hat{N}_\nu|\mathrm{CBCS} > \ = \ N_\nu \quad (78)
$$

Eqs. (17-22,27-30,75,76) are called the correlated BCS equations. They can be solved iteratively. We point out that parameters v_p^2 and v_n^2 have lost the physical interpretations of occupation probabilities, because of the existing additional terms in Eq. (75,76).

Since the BCS theory violates the particle number conservation, the constructed BCS excitations in Eq. (59) include some spurious states [11]. But they have not been projected out, because we believe that they are not very important in our calculations.

4 Applications

We apply the correlated BCS theory to study the ground state properties of ^{46}Ti in the full $0f1p$ shell, where there are two protons and four neutrons. The occupation probabilities and the quasiparticle energies are calculated from the correlated BCS equation Eqs. (17-22,27-30,75,76). They are solved iteratively by constraining the mean proton and neutron numbers to be 2 and 4, respectively. The effective twobody interaction used here is the MSOBEP [18], which is a recently derived effective interaction within the $0f1p$ shell in the range mass $40 \sim 50$.

The occupation probabilities obtained from the correlated BCS are given in Table 1 and compared to the BCS and the large-basis shell-model calculations. The shell-model calculations are carried out by OXBASH code [19]. We find the correlated BCS calculation improves upon the BCS occupation numbers, bring them more in line with the large-basis shell-model result, but there are still some differences in these models. The disagreements may be from the some perturbation terms which are not included in our calculation, or from the BCS approximation itself which may not be very good basis. For example, d-pairs ($J^\pi = 2^+$) which play an important role in nuclear structure have not been taken into account in the BCS.

The correlated BCS parameters are presented in Table 2. We find that v^2 are not equal to the relevant occupation probabilities given in Table 1. In the correlated BCS, the Fermi level of proton and neutron are -13.216 MeV and -10.942 MeV, comparing to -12.968 MeV and -10.868 MeV in the BCS.

5 Summary

In this paper, we re-derived the BCS equations for proton-neutron systems in an angular momentum coupling space. The correlated BCS (CBCS) wave function is introduced through the first-order perturbation theory. The quasiparticle interactions H_{int} dropped in the BCS theory are considered as the perturbation Hamiltonian and incorporated approximately. In order to simplify our calculations, we only consider the proton-neutron interaction term in H_{int} which is believed to be more important than the like particle interactions. The formalism for the occupation probabilities

Table 1: ^{46}Ti: The occupation probabilities $< |a^\dagger_{jm} a_{jm}| >$ for protons and neutrons obtained from the BCS, correlated BCS (CBCS) and shell-model calculations, respectively.

level	BCS	CBCS	Shell model
$\pi f_{7/2}$	0.239	0.222	0.187
$\pi p_{3/2}$	0.009	0.022	0.078
$\pi f_{5/2}$	0.008	0.020	0.022
$\pi p_{1/2}$	0.004	0.008	0.031
$\nu f_{7/2}$	0.480	0.459	0.404
$\nu p_{3/2}$	0.018	0.036	0.092
$\nu f_{5/2}$	0.013	0.027	0.054
$\nu p_{1/2}$	0.007	0.011	0.040

Table 2: The correlated BCS parameters, u_i^2, v_i^2, gap parameters Δ_i (MeV) and quasiparticle energies E_i (MeV) for ^{46}Ti

level	u_i^2	v_i^2	Δ_i	E_i
$\pi f_{7/2}$	0.817	0.183	1.203	1.556
$\pi p_{3/2}$	0.992	0.008	0.911	5.105
$\pi f_{5/2}$	0.993	0.007	1.314	7.592
$\pi p_{1/2}$	0.996	0.004	0.874	7.275
$\nu f_{7/2}$	0.546	0.454	1.447	1.453
$\nu p_{3/2}$	0.983	0.017	1.104	4.236
$\nu f_{5/2}$	0.987	0.013	1.574	7.076
$\nu p_{1/2}$	0.993	0.007	1.069	6.478

in the CBCS is derived. The two-quasiproton two-quasineutron doublet excitations in the CBCS are introduced and discussed in the J-scheme. Since the excitations may be not orthogonal to each other, the Gram-Schmidt orthogonalization method is employed to obtain a new orthogonal basis.

We applied the CBCS theory to the study of the ground state properties of ^{46}Ti within the $0f1p$ shell and found that the the occupation probabilities have been improved compared to the standard BCS, but not enough to reproduce the shell-model results.

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