Quantum number projection at finite temperature via thermo field dynamics

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(Dated: March 30, 2022)

Abstract

Applying the thermo field dynamics, we reformulate exact quantum number projection in the finite-temperature Hartree-Fock-Bogoliubov theory. Explicit formulae are derived for the simultaneous projection of particle number and angular momentum, in parallel to the zero-temperature case. We also propose a practical method for the variation-after-projection calculation, by approximating entropy without conflict with the Peierls inequality. The quantum number projection in the finite-temperature mean-field theory will be useful to study effects of quantum fluctuations associated with the conservation laws on thermal properties of nuclei.

PACS numbers: 21.60.Jz, 21.10.-k, 21.90.+f, 05.30.Fk
I. INTRODUCTION

Transitions among different phases have been observed as temperature increases or decreases, in a wide variety of physical systems from elementary particles to condensed matters. They have attracted great interest both experimentally and theoretically, and profound physics content has been revealed particularly in infinite systems. Despite an isolated system, statistical properties of atomic nuclei have been investigated in terms of the so-called nuclear temperature [1], providing us with a ground to study phase transitions in nuclei. However, it is not straightforward to identify phase transitions in finite systems like nuclei, because the quantum fluctuations associated with finiteness of the system obscure the transitions [2, 3] so that even definition of ‘phases’ should depend on theoretical models to a considerable extent.

It will be natural, from theoretical points of view, to define phases in nuclei via the mean-field picture, since ‘phases’ in physical systems are more or less a semi-classical concept. Indeed, we discuss spherical/deformed and normal-fluid/superfluid phases in nuclei based on the mean-field approximation. Phase transitions are often connected to the spontaneous symmetry breaking, leading to violation of conservation laws. In the mean-field picture of nuclei, the rotational symmetry is broken in the deformed phase, and the particle number conservation is violated in the superfluid phase. However, the symmetry breaking in nuclei is a hypothetical effect due to the mean-field approximation. In practice, the conservation laws are restored via a sort of quantum fluctuations arising from correlations beyond the mean field. In studying statistical properties of finite systems, it will be significant to investigate effects of the symmetry restoration.

As the most general mean-field theory, we shall primarily consider the Hartree-Fock-Bogoliubov (HFB) approximation. To restore the symmetries, projection with respect to the quantum numbers should be applied [4]. The particle number projection as well as the angular momentum projection methods have been developed for zero-temperature cases; i.e. for the ground-state wave functions [5, 6], and also for the quantum-number-constrained HFB (CHFB) solutions along the yrast line [2, 8, 9]. For finite-temperature problems, projections with respect to the discrete symmetries such as the parity and the number-parity were explored more than two decades ago [10]. However, there is a certain complication in extending them to the continuous symmetries, arising from the non-commutability between the projection operator and the Boltzmann-Gibbs operator in the mean-field approximation. A way to overcome these problems has been found in Ref. [11] for the particle number projection within the Bardeen-Cooper-Schrieffer (BCS) approximation. General projection formalism in the variation-before-projection (VBP) scheme is developed in Ref. [12], and is extensively applied in the framework of the static-path approximation.

In this paper we reformulate the quantum number projection at finite temperature by employing the thermo field dynamics (TFD) [13, 14]. The TFD has been shown to be a powerful tool [15] to handle the thermal fluctuations within the mean-field theories. We
shall show that this is also true for the quantum-number-projected HFB theory at finite temperature. While the resultant formulae are equivalent to those in Ref. [12], the present formalism is advantageous in the following respects. In the TFD, the thermal expectation value of an observable is expressed in terms of a vacuum expectation value in an enlarged TFD space. Therefore explicit formulae are derived in a straightforward manner, keeping complete parallel to the zero-temperature formalism [16]. We demonstrate it for the simultaneous projection both of the particle number and the angular momentum. This leads to another advantage that variational parameters can be identified in an obvious manner and handled easily. While application of the present method to the VBP calculations is straightforward, further approximation is desired in order to carry out the variation-after-projection (VAP) calculations. We shall also discuss an approximation of the entropy, so as for the Peierls inequality [17] to hold which guarantees the variational principle for free energy. It is expected that this approximation scheme will make the VAP calculations practical.

In Sec. III, application of the thermo field dynamics (TFD) to the HFB theory at finite temperature is presented. In Sec. III, we formulate the TFD version of the quantum-number projection in the HFB at finite temperature. As well as general arguments, explicit formulae for the particle number and angular momentum projection are presented by taking specific basis-sets. Formulae in the BCS approximation are also given. In Sec. IV, we propose an approximation scheme for the entropy, which keeps the Peierls inequality. Finally, the paper is summarized in Sec. V.

II. FINITE-TEMPERATURE HFB THEORY AND THERMO FIELD DYNAMICS

A. HFB equation at finite temperature

In the variational derivation of the Hartree-Fock-Bogoliubov (HFB) equation at finite temperature [10, 18], a set of variational parameters \( \{ U_{k\mu}, V_{k\mu}, U^*_{k\mu}, V^*_{k\mu} \} \) is introduced through the generalized Bogoliubov transformation (GBT), which relates the original single-particle (s.p.) operators \( \{ c_k, c_k^\dagger \} \) to those in the quasiparticle (q.p.) picture \( \{ \alpha_\mu, \alpha_\mu^\dagger \} \),

\[
\begin{pmatrix}
  c_k \\
  c_k^\dagger
\end{pmatrix} = \sum_\mu W_{k\mu} \begin{pmatrix}
  \alpha_\mu \\
  \alpha_\mu^\dagger
\end{pmatrix}, \quad W_{k\mu} \equiv \begin{pmatrix}
  U_{k\mu} & V_{k\mu}^* \\
  V_{k\mu} & U_{k\mu}^*
\end{pmatrix}.
\]

(1)

The transformation matrix \( W \) obeys the unitarity relation \( W^\dagger W = WW^\dagger = 1 \). We express the original s.p. state as \( |i\rangle = c_i^\dagger |\text{vac.}\rangle \), with the vacuum \( |\text{vac.}\rangle \) satisfying \( c_i |\text{vac.}\rangle = 0 \). The q.p. vacuum \( |0\rangle \propto \Pi_{\mu} \alpha_\mu |\text{vac.}\rangle \) is annihilated by \( \alpha_\mu \), i.e. \( \alpha_\mu |0\rangle = 0 \). Note that \( \langle 0|0 \rangle = 1 \). An additional set of variational parameters \( \{ E_\mu \} \) comes into the problem through the trial
statistical operator
\[ \hat{w}_0 = \frac{e^{-\hat{H}_0/T}}{\text{Tr}(e^{-\hat{H}_0/T})}; \quad \hat{H}_0 = \sum_\mu E_\mu \alpha_\mu^\dagger \alpha_\mu, \quad (2) \]
where we put the Boltzmann constant \( k_B = 1 \). We denote the thermal average of an operator \( \hat{\mathcal{O}} \) by \( \langle \hat{\mathcal{O}} \rangle = \text{Tr}(\hat{w}_0 \hat{\mathcal{O}}) \), where the trace is taken over the grand canonical ensemble.

We consider the Hamiltonian comprised of up to two-body interactions,
\[ \hat{H} = \sum_i \varepsilon_i c_i^\dagger c_i + \frac{1}{4} \sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k, \quad (3) \]
where two kinds of nucleons are not discriminated to avoid unnecessary complication. The hermiticity of the Hamiltonian implies \( \varepsilon_i = \varepsilon_i^* \) and \( v_{ijkl} = -v_{jikl} = -v_{ijlk} = v_{klij}^* \). In the constrained HFB (CHFB) approximation at finite temperature, the grand potential is given by
\[ \Omega = \langle \hat{H}' \rangle - TS; \quad \hat{H}' \equiv \hat{H} - \lambda_p \hat{Z} - \lambda_n \hat{N} - \omega_{\text{rot}} \hat{J}_x, \quad (4) \]
where \( \lambda_p \) (\( \lambda_n \)) and \( \omega_{\text{rot}} \) are Lagrange multipliers, which are interpreted as proton (neutron) chemical potential and rotational frequency of the system, respectively. The proton-(neutron-) number operator \( \hat{Z} \) (\( \hat{N} \)) and the \( x \)-component of angular momentum operator \( \hat{J}_x \) are expressed in terms of the s.p. operators as
\[ \hat{Z} = \sum_{i \in p} c_i^\dagger c_i, \quad \hat{N} = \sum_{i \in n} c_i^\dagger c_i, \quad \hat{J}_x = \sum_{i j (\text{all})} \langle i | \hat{J}_x | j \rangle c_i^\dagger c_j, \quad (5) \]
where the sum \( \sum_{i \in p} \) (\( \sum_{i \in n} \)) extends over the proton (neutron) states, and \( \sum_{ij (\text{all})} \) over both proton and neutron states. In the CHFB the conservations of proton number, neutron number and angular momentum are taken into account in their averages,
\[ \langle \hat{Z} \rangle = Z, \quad \langle \hat{N} \rangle = N, \quad \langle \hat{J}_x \rangle = \sqrt{J(J+1)}, \quad (6) \]
which indicate constraints. In calculations without some of the constraints, the associated Lagrange multipliers are set to be zero in Eq. (4).

The auxiliary Hamiltonian in Eq. (4) is rewritten in terms of the q.p. operators by the GBT (1),
\[ \hat{H}' = U_0 + \hat{H}_{11} + \hat{H}_{20} + \hat{H}_{22} + \hat{H}_{31} + \hat{H}_{40}. \quad (7) \]
For later convenience, explicit forms in the above expression are presented in Appendix A.

Ensemble averages of the bilinear forms in the q.p. operators are given by
\[ \langle \alpha_\mu^\dagger \alpha_\nu \rangle = f_\mu \delta_{\mu\nu}; \quad f_\mu = \frac{1}{e^{E_\mu/T} + 1}, \quad (8a) \]
\[ \langle \alpha_\mu \alpha_\nu \rangle = \langle \alpha_\mu^\dagger \alpha_\nu^\dagger \rangle = 0, \quad (8b) \]
where $f_\mu$ is the occupation number of the $\mu$-th q.p. level. Thus, the variation of the parameter $\delta E_\mu$ is converted to $\delta f_\mu = -f_\mu (1 - f_\mu) \delta E_\mu / T$. The approximate entropy $S$ in Eq. (1) is expressed as

$$S = -\text{Tr}(\hat{\omega}_0 \ln \hat{\omega}_0) = -\sum_\mu [f_\mu \ln f_\mu + (1 - f_\mu) \ln (1 - f_\mu)].$$

(9)

The s.p. density $\rho$ and the pair tensor $\kappa$ are defined by

$$\rho_{ij} = \langle c_j^\dagger c_i \rangle = [V^*(1 - f)V + U f^\dagger]_{ij},$$

(10a)

$$\kappa_{ij} = \langle c_j c_i \rangle = [V^*(1 - f)U^\dagger + U f]_{ij}.$$  

(10b)

The ensemble average of $\hat{H}'$ becomes

$$\langle \hat{H}' \rangle = \text{Tr}_{s.p.} \left( \xi \rho + \frac{1}{2} \Gamma \rho + \frac{1}{2} \Delta \kappa^\dagger \right) = U_0 + \sum_\mu (H_{11})_{\mu \mu} f_\mu + 2 \sum_{\mu \nu} (H_{22})_{\mu \nu \mu \nu} f_\mu f_\nu,$$

(11)

where $\text{Tr}_{s.p.}$ stands for the trace over the s.p. space,

$$\xi_{ij} = (\varepsilon_i - \lambda_\tau) \delta_{ij} - \omega_{\text{rot}} \langle i | \hat{J}_x | j \rangle$$

(12)

with $\tau = p$ (n) for proton (neutron), while the HF potential matrix $\Gamma$ and the pair potential matrix $\Delta$ are defined by

$$\Gamma_{ij} = (\Gamma^\dagger)_{ij} = \sum_{kl} v_{ijkl} \rho_{lk},$$

(13a)

$$\Delta_{ij} = -\Delta_{ji} = \frac{1}{2} \sum_{kl} v_{ijkl} \kappa_{kl}.$$  

(13b)

The variational principle $\delta \Omega = \delta (\langle \hat{H}' \rangle - TS) = 0$ yields

$$(H_{11}^{\text{eff}})_{\mu \nu} \equiv \left[ U^\dagger (\xi + \Gamma) U - V^\dagger (\xi + \Gamma)^* V + U^\dagger \Delta V - V^\dagger \Delta^* U \right]_{\mu \nu}$$

$$= (H_{11})_{\mu \nu} + 4 \sum_\rho (H_{22})_{\mu \rho \nu \rho} f_\rho$$

$$= T \frac{\partial S}{\partial f_\mu} \delta_{\mu \nu} = E_\mu \delta_{\mu \nu},$$

(14a)

$$(H_{20}^{\text{eff}})_{\mu \nu} \equiv \left[ U^\dagger (\xi + \Gamma)V^* - V^\dagger (\xi + \Gamma)^* U^* + U^\dagger \Delta U^* - V^\dagger \Delta^* V^* \right]_{\mu \nu}$$

$$= (H_{20})_{\mu \nu} + 6 \sum_\rho (H_{31})_{\mu \rho \rho \rho} f_\rho = 0.$$  

(14b)

These equations are summarized in the form of the HFB coupled equation at finite temperature,

$$\sum_l \left( \begin{array}{cc} \xi + \Gamma & \Delta \\ -\Delta^* & -(\xi + \Gamma)^* \end{array} \right)_{kl} \left( \begin{array}{c} U \\ V \end{array} \right)_{l\mu} = \left( \begin{array}{c} U \\ V \end{array} \right)_{k\mu} E_\mu.$$  

(15)

In the CHFB case this equation should be solved together with the constraints in Eq. (6), by which the Lagrange multipliers $\lambda_\rho$, $\lambda_n$ and $\omega_{\text{rot}}$, as well as self-consistent q.p. energies $E_\mu$, are determined as functions of quantum numbers and temperature.
B. Bogoliubov transformation extended by TFD

In the thermo field dynamics (TFD) [13, 14], the original q.p. operator space \{\alpha_\mu, \alpha_\mu^\dagger\} is enlarged by including newly introduced tilded operators; \{\alpha_\mu, \tilde{\alpha}_\mu, \alpha_\mu^\dagger, \tilde{\alpha}_\mu^\dagger\}. Correspondingly, the q.p. vacuum in the enlarged space is defined by \vert 0 \rangle \otimes \vert \tilde{0} \rangle, where \vert \tilde{0} \rangle is the tilded vacuum satisfying \tilde{\alpha}_\mu \vert \tilde{0} \rangle = 0. The TFD vacuum \vert 0 \rangle \otimes \vert \tilde{0} \rangle is hereafter denoted by \vert 0 \rangle for the sake of simplicity, i.e. \alpha_\mu \rangle 0 = \tilde{\alpha}_\mu \rangle 0 = 0. In order to handle ensemble averages in a thermal equilibrium at temperature \( T \), the TFD vacuum \vert 0 \rangle is transformed to the temperature-dependent vacuum by the following unitary transformation,

\[
\vert 0_T \rangle = e^{-\hat{G}} \vert 0 \rangle, \quad \hat{G} = -\sum_\mu \partial_\mu (\alpha_\mu^\dagger \tilde{\alpha}_\mu - \tilde{\alpha}_\mu \alpha_\mu),
\]

where

\[
\sin \partial_\mu = f_\mu^{1/2} \equiv g_\mu, \quad \cos \partial_\mu = (1 - f_\mu)^{1/2} \equiv \bar{g}_\mu.
\]

This unitary transformation relates the operator set \{\alpha_\mu, \tilde{\alpha}_\mu, \alpha_\mu^\dagger, \tilde{\alpha}_\mu^\dagger\} to new set of the temperature-dependent operators \{\beta_\mu, \bar{\beta}_\mu, \bar{\beta}_\mu^\dagger, \beta_\mu^\dagger\},

\[
\alpha_\mu = e^{\tilde{\beta}_\mu \bar{\beta}_\mu^\dagger} e^{-\tilde{\beta}_\mu \bar{\beta}_\mu} \equiv \bar{g}_\mu \beta_\mu + g_\mu \beta_\mu^\dagger,
\]

\[
\tilde{\alpha}_\mu = e^{\beta_\mu \bar{\beta}_\mu^\dagger} e^{-\beta_\mu \bar{\beta}_\mu} \equiv \bar{g}_\mu \bar{\beta}_\mu - g_\mu \beta_\mu^\dagger,
\]

so that the temperature-dependent vacuum should fulfill \beta_\mu \vert 0_T \rangle = \bar{\beta}_\mu \vert 0_T \rangle = 0. The temperature-dependent quasiparticles created by \beta^\dagger or \bar{\beta}^\dagger will hereafter be called TFD quasiparticles. The thermal average of an observable \hat{O} is then expressed by the vacuum expectation value at \vert 0_T \rangle,

\[
\langle \hat{O} \rangle = \text{Tr}(\hat{w}_0 \hat{O}) = \langle 0_T \vert \hat{O} \vert 0_T \rangle.
\]

Now we unify two unitary transformations [11] and [18] to compose an extended form of the GBT [15],

\[
\begin{pmatrix}
\hat{c} \\
\hat{\tilde{c}} \\
\hat{c}^\dagger
\end{pmatrix}_k = \sum_\mu \hat{W}_{k\mu} \begin{pmatrix}
\beta \\
\bar{\beta} \\
\beta^\dagger
\end{pmatrix}_\mu, \quad \hat{W}_{k\mu} = \begin{pmatrix}
\bar{U} & \bar{V}^* \\
V \bar{g} & U^* \bar{g}
\end{pmatrix}_{k\mu}, \quad \hat{U}_{k\mu} = \begin{pmatrix}
U \bar{g} & V^* \bar{g} \\
-V \bar{g} & U^* \bar{g}
\end{pmatrix}_{k\mu}, \quad \hat{V}_{k\mu} = \begin{pmatrix}
V \bar{g} & U^* \bar{g} \\
-U \bar{g} & V^* \bar{g}
\end{pmatrix}_{k\mu}.
\]

Because of the unitarity relation \hat{W} \hat{W}^\dagger = \hat{W}^\dagger \hat{W} = 1, the matrix inverse to \hat{W} is given by

\[
\hat{W}^{-1} = \hat{W}^\dagger = \begin{pmatrix}
\hat{U}^\dagger & \hat{V}^\dagger \\
\hat{V}^{\dagger \text{tr}} & \hat{U}^{\dagger \text{tr}}
\end{pmatrix}.
\]
III. QUANTUM NUMBER PROJECTION IN FINITE-TEMPERATURE HFB THEORY

A. Projection operators

1. General form

Since quantum numbers are usually associated with a certain group structure of the system, projection with respect to the quantum numbers is also introduced in connection to the group. In general, a projection operator $\hat{P}_{\mu\nu}^{(\alpha)}$ is defined as a subring basis corresponding to an irreducible representation (irrep.) $\rho^{(\alpha)}$ of a group $G$\,[19, 20],

$$\hat{P}_{\mu\nu}^{(\alpha)} = \frac{\dim(\rho^{(\alpha)})}{g} \sum_{x \in G} \rho^{(\alpha)}_{\nu\mu}(x^{-1}) x,$$  \hspace{1cm} (23)

where $x$ stands for an element of $G$, $\dim(\rho^{(\alpha)})$ is the dimension of the representation matrix $\rho^{(\alpha)}$, and $g$ the order of $G$. The property of group representation yields

$$\hat{P}_{\mu\nu}^{(\alpha)} \hat{P}_{\mu'\nu'}^{(\beta)} = \delta_{\alpha\beta} \delta_{\nu\mu'} \hat{P}_{\mu\nu}^{(\alpha)},$$ \hspace{1cm} (24)

justifying a convenient bracket representation of the projection operator, $\hat{P}_{\mu\nu}^{(\alpha)} = |\alpha\mu\rangle\langle \alpha\mu|$. The projection on the subspace corresponding to the irrep. $\rho^{(\alpha)}$, without referencing $\mu$, is obtained by

$$\hat{P}_{\alpha} = \sum_{\mu} \hat{P}_{\mu\mu}^{(\alpha)} = \sum_{\mu} |\alpha\mu\rangle\langle \alpha\mu|.$$ \hspace{1cm} (25)

It is obvious that $\hat{P}_{\alpha}$ is idempotent, i.e. $\hat{P}_{\alpha}^2 = \hat{P}_{\alpha}$.

When $G$ is not simple and is decomposed into a direct product of an invariant subgroup and the complementary quotient group as $G_1 \otimes G_2$, its irrep. $\rho^{(\alpha)}$ is also a product such as $\rho^{(\alpha_1)}_1 \otimes \rho^{(\alpha_2)}_2$, where $\rho^{(\alpha_i)}_i$ is an irrep. of $G_i$ ($i = 1, 2$). Denoting the projection operator on $\rho^{(\alpha_i)}_i$ by $\hat{P}_{\alpha_i}$, the projection operator on $\rho^{(\alpha)}$ is $\hat{P}_{\alpha} = \hat{P}_{\alpha_1} \hat{P}_{\alpha_2}$. Therefore, projection operators of simple groups are essential.

In the following we assume $G$ to be a compact simple group or a product of such groups, whose element $x$ is represented by an appropriate unitary operator $\hat{Q} = e^{-i\hat{S}}$. Here $\hat{S} = \hat{S}(\Theta)$ is a hermitian operator, which belongs to a Lie algebra associated with $G$ and is dependent on a set of parameters $\Theta$. The projection operator $\hat{P}_{\alpha}$ is represented in the integral form

$$\hat{P}_{\alpha} = \int d\Theta \zeta_{\alpha}(\Theta) \hat{Q},$$ \hspace{1cm} (26)

where $\zeta_{\alpha}(\Theta)$ is an appropriate function of $\Theta$ and is derived from Eq. (23).
For the angular momentum projection, the relevant group is $SU(2)$, which is denoted by $SU(2)_J$ in this paper. The group element is the rotation operator $\hat{R}$, whose parameters are represented by $\Phi$. In practice, we consider two alternative parameterizations. One is the Euler angles $\Phi = (\alpha, \beta, \gamma)$. The rotation is also represented by an angle $\omega$ ($0 \leq \omega < 2\pi$) around an axis indicated by a unit vector $\vec{n}$. Using the representation $n_x = \sin\theta\cos\phi, n_y = \sin\theta\sin\phi, n_z = \cos\theta$, we arrive at the other parameterization $\Phi = (\omega, \theta, \phi)$. Corresponding to these parameterizations, the rotation operator is expressed in two ways as

$$\hat{R}(\Phi) = e^{-i\alpha J_z}e^{-i\beta J_y}e^{-i\gamma J_z} = e^{-i\omega(n_xJ_x+n_yJ_y+n_zJ_z)}, \quad (27)$$

where the angular momentum operators are defined in terms of the s.p. operators as in Eq. (5), $\hat{J}_k = \sum_{ij}^{(\text{all})} \langle i|\hat{J}_k|j \rangle c^*_i c_j$ ($k = x, y, z$).

The angles $(\omega, \theta, \phi)$ are related to the Euler angles by

$$\cos\frac{\omega}{2} = \cos\frac{\beta}{2} \cos\frac{\alpha + \gamma}{2}, \quad \tan\theta = \tan\frac{\beta}{2} \csc\frac{\alpha + \gamma}{2}, \quad \phi = \pi + \alpha - \gamma. \quad (29)$$

The order of the group is determined by the volume of the parameter space,

$$g = \int_{0}^{2\pi} d\alpha \int_{0}^{\pi} \sin\beta d\beta \int_{0}^{4\pi} d\gamma = 4 \int_{0}^{2\pi} \sin^2\frac{\omega}{2} d\omega \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{2\pi} d\phi = 16\pi^2, \quad (30)$$

where the range of $\gamma$ is taken to be $0 \leq \gamma < 4\pi$ for the double-valued representation corresponding to half-odd-integer spin. The irrep. of $SU(2)_J$ is given by the Wigner $D$-function $[21,22]$,

$$D^J_{MK}(\Phi) \equiv \langle JM|\hat{R}(\Phi)|JK \rangle = e^{-i\alpha M}d^J_{MK}(\beta)e^{-i\gamma K}, \quad (31)$$

which is a unitary matrix of dimension $(2J+1)$. Then Eq. (23) yields the following projection operator,

$$\hat{P}^J_{MK} = \hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_{0}^{2\pi} d\alpha \int_{0}^{\pi} \sin\beta d\beta \int_{0}^{4\pi} d\gamma D^J_{MK}(\Phi)\hat{R}(\Phi). \quad (32)$$

For integer spin $J$, the integral $\int_{0}^{4\pi} d\gamma$ may be replaced by $2\int_{0}^{2\pi} d\gamma$. We express the character of the representation matrix $D^J_{MK}(\Phi)$ as

$$\chi_J(\omega) = \sum_{M=-J}^{J} D^J_{MM}(\Phi) = \frac{\sin[(J+1/2)\omega]}{\sin(\omega/2)}. \quad (33)$$

The real function $\chi_J(\omega)$ can be represented in many different ways as listed in Ref. [22]. If the magnitude of angular momentum $J$ is subject to the projection while its $z$-component in the laboratory frame $M$ is not referenced, the projection operator is given by

$$\hat{P}_J = \hat{P}^J_J = \frac{2J+1}{4\pi^2} \int_{0}^{2\pi} \sin^2\frac{\omega}{2} d\omega \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{2\pi} d\phi \chi_J(\omega)\hat{R}(\Phi). \quad (34)$$
3. Particle number projection operators

The relevant group to the particle number projection is the gauge group $U(1)$, whose group elements are parameterized by a single variable $\varphi$ for the particle number operator $\hat{N}$; \( \exp(-i\varphi \hat{N}) \). For neutrons, the group is denoted by $U(1)_N$, and the projection operator, which projects out states having the exact neutron number $N$, is given by,

\[
\hat{P}_N = \hat{P}_N^\dagger = \frac{1}{2\pi} \int_0^{2\pi} e^{-i\varphi_n(\hat{N}-N)} d\varphi_n.
\]

Likewise, the proton number projection is implemented by the operator,

\[
\hat{P}_Z = \hat{P}_Z^\dagger = \frac{1}{2\pi} \int_0^{2\pi} e^{-i\varphi_p(\hat{Z}-Z)} d\varphi_p,
\]

and the relevant group to $\hat{P}_Z$ is denoted by $U(1)_Z$. The product operator $\hat{P}_Z \hat{P}_N$ is employed for the $U(1)_Z \times U(1)_N$ projection, by which the canonical trace is calculable from the grand-canonical trace.

4. $SU(2)_J \times U(1)_Z \times U(1)_N$ projection operator

The projector of simultaneous projection of angular momentum $J$, proton number $Z$ and neutron number $N$ is $\hat{P}_{(J,Z,N)} = \hat{P}_J \hat{P}_Z \hat{P}_N$, which satisfies $\hat{P}_{(J,Z,N)}^2 = \hat{P}_{(J,Z,N)}$. This $\hat{P}_{(J,Z,N)}$ can be expressed in the form of Eq. (26), with $\Theta = (\Phi, \varphi_p, \varphi_n)$. The operator $\hat{Q}$ stands for

\[
\hat{Q} = \hat{R}(\Phi) e^{-i\varphi_p \hat{Z}} e^{-i\varphi_n \hat{N}} = e^{-i\hat{S}},
\]

where

\[
\hat{S} = \varphi_p \hat{Z} + \varphi_n \hat{N} + \omega \hat{n} \cdot \vec{J}; \quad \hat{n} \cdot \vec{J} \equiv n_x \hat{J}_x + n_y \hat{J}_y + n_z \hat{J}_z.
\]

Obviously $\hat{P}_{(J,Z,N)}$ commutes with the total nuclear Hamiltonian $\hat{H}$, which conserves angular momentum, nucleon number and charge. However, note that $[\hat{P}_{(J,Z,N)}, \hat{H}_0] \neq 0$.

5. Parity and number-parity projection operators

The space reflection forms the discrete group isomorphic to $S_2$. The projection operator with respect to the space parity can be expressed in the form similar to Eq. (26), with the integral converted to a discrete sum,

\[
\hat{P}_\pi = \frac{1}{2} \left[ 1 + \xi \exp \left(i\pi \sum_k c_k^\dagger c_k \right) \right].
\]
Here $\xi = +1$ ($\xi = -1$) for the projection of positive (negative) parity state, and $\sum_k^-$ denotes the sum extending only over the s.p. states of negative parity. As far as the parity is not mixed in the q.p. state $\mu$, the projection operator is also written as

$$\hat{P}_\pi = \frac{1}{2} \left[1 + \xi \exp \left(i\pi \sum_\mu \alpha_\mu^\dagger \alpha_\mu \right)\right],$$

as given in Ref. [10].

The number-parity is relevant to another $S_2$ group, which is a discrete subgroup of $U(1)_Z$ or of $U(1)_N$. Respective to protons and neutrons, the number-parity projection is carried out by the operator

$$\hat{P}_q = \frac{1}{2} \left[1 + \eta \exp \left(i\pi \sum_k c_k^\dagger c_k \right)\right],$$

where $\eta = +1$ ($\eta = -1$) for the projection of the state of even (odd) number-parity. Apart from the denominator, this is obtained by restricting $\phi_n$ in $\hat{P}_N$ (or $\phi_p$ in $\hat{P}_Z$) only to 0 and $\pi$. Since the GBT does not mix the number-parity, $\hat{P}_q$ is equivalently represented in terms of the q.p. operators [10],

$$\hat{P}_q = \frac{1}{2} \left[1 + \eta \exp \left(i\pi \sum_\mu \alpha_\mu^\dagger \alpha_\mu \right)\right].$$

### B. Extended form of linear transformation

We now consider the projected statistics. The projected ensemble average of an operator $\hat{O}$ is newly defined by

$$\langle \hat{O} \rangle_P \equiv \text{Tr}(\hat{w}_P \hat{O}) = \frac{\text{Tr}(\hat{P} e^{-\beta \hat{H}_0} \hat{O} \hat{P})}{\text{Tr}(\hat{P} e^{-\beta \hat{H}_0})} = \frac{\text{Tr}(e^{-\beta \hat{H}_0} \hat{P} \hat{O} \hat{P})}{\text{Tr}(e^{-\beta \hat{H}_0})},$$

where the statistical operator with projection is introduced as

$$\hat{w}_P \equiv \frac{\hat{P} e^{-\beta \hat{H}_0} \hat{P}}{\text{Tr}(e^{-\beta \hat{H}_0})}. $$

For an operator commutable with $\hat{P}$, $\langle \hat{O} \rangle_P$ is calculated in the TFD by

$$\langle \hat{O} \rangle_P = \frac{\text{Tr}(\hat{w}_0 \hat{P} \hat{O})}{\text{Tr}(\hat{w}_0 \hat{P})} = \frac{\langle 0_T | \hat{O} \hat{P} | 0_T \rangle}{\langle 0_T | \hat{P} | 0_T \rangle}. $$

Substituting the projector by the form of Eq. [26], we obtain

$$\langle \hat{O} \rangle_P = \frac{\int \zeta(\theta) \langle 0_T | \hat{Q} \hat{P} | 0_T \rangle d\theta}{\int \zeta(\theta) \langle 0_T | \hat{P} | 0_T \rangle d\theta}.$$
Thus, in course of projection calculations, we meet with the TFD vacuum expectation values of following types:

\[
\langle 0_T | \left\{ \frac{1}{\beta_1 \beta_2 \beta_3 \beta_4} \right\} | 0_T \rangle,
\]

(47)

where \( \beta \) represents any of the TFD q.p. operator of four types, \( \beta_\mu, \beta_\mu^\dagger, \tilde{\beta}_\mu, \tilde{\beta}_\mu^\dagger \). The operator \( \hat{Q} \) is given in Eqs. (37,38) for the \( SU(2)_T \times U(1)_Z \times U(1)_N \) projection.

We here define the transformation matrix of the s.p. operator with respect to the unitary transformation \( \hat{Q} \), assuming that \( \hat{Q} \) conserves the particle number,

\[
\hat{Q} c_k \hat{Q}^\dagger = \sum_{k'} Q_{kk'} c_{k'}.
\]

(48)

This linear transformation is extended to the TFD space by

\[
\hat{Q} \left( \begin{array}{c} \beta_\mu \\
\tilde{\beta}_\mu \\
\beta_\mu^\dagger \\
\tilde{\beta}_\mu^\dagger \end{array} \right) \hat{Q}^\dagger = \sum_{k,k'} \sum_\nu \left( \bar{W}^\dagger \right)_{\mu k} \left( \begin{array}{c} Q_{kk'} \\
0 \\
1 \\
0 \end{array} \right) _{\nu k'} \left( \begin{array}{c} \beta_\nu \\
\tilde{\beta}_\nu \\
\beta_\nu^\dagger \\
\tilde{\beta}_\nu^\dagger \end{array} \right)
\]

(49)

Applying the TFD-extension of the GBT in Eqs. (20,21,22), we convert the above transformation to the one among the TFD q.p. operators,

\[
\hat{Q} \left( \begin{array}{c} \beta_\mu \\
\tilde{\beta}_\mu \\
\beta_\mu^\dagger \\
\tilde{\beta}_\mu^\dagger \end{array} \right) \hat{Q}^\dagger = \sum_{k,k'} \sum_\nu (\bar{W})_{\mu k} \left( \begin{array}{c} Q_{kk'} \\
0 \\
1 \\
0 \end{array} \right) _{\nu k'} \left( \begin{array}{c} \beta_\nu \\
\tilde{\beta}_\nu \\
\beta_\nu^\dagger \\
\tilde{\beta}_\nu^\dagger \end{array} \right).
\]

\[
\equiv \sum_\nu \left( \begin{array}{c} K \\
M \\
L \end{array} \right) _{\mu \nu} \left( \begin{array}{c} \beta_\nu \\
\tilde{\beta}_\nu \\
\beta_\nu^\dagger \\
\tilde{\beta}_\nu^\dagger \end{array} \right).
\]

(50)

In the last expression, there appear four types of the matrices \( K, L, M \) and \( \bar{N} \), which play central roles in the projection calculation [3,16]. In the present formalism, these matrices, whose dimension is also doubled, are given by

\[
K_{\mu \nu} = L^*_{\mu \nu} = \left( \begin{array}{cc} \bar{g}(U^{\dagger}QU + V^{\dagger}Q^*V)\bar{g} + g^2 & \bar{g}(U^{\dagger}QV^* + V^{\dagger}Q^*U^*)g \\
g(V^{\dagger}QU + U^{\dagger}Q^*V)\bar{g} & g(V^{\dagger}QV^* + U^{\dagger}Q^*U^*)g + \bar{g}^2 \end{array} \right)_{\mu \nu},
\]

(51a)

\[
M_{\mu \nu} = \bar{N}^*_{\mu \nu} = \left( \begin{array}{cc} \bar{g}(V^{\dagger}QU + U^{\dagger}Q^*V)\bar{g} & \bar{g}(V^{\dagger}QV^* + U^{\dagger}Q^*U^*)g - \bar{g}g \\
g(U^{\dagger}QU + V^{\dagger}Q^*V)\bar{g} - \bar{g}g & g(U^{\dagger}QV^* + V^{\dagger}Q^*U^*)g \end{array} \right)_{\mu \nu},
\]

(51b)

where we have employed abbreviated notations, e.g.,

\[
[\bar{g}(U^{\dagger}QU + V^{\dagger}Q^*V)g + g^2]_{\mu \nu} = \sum_{k,k'} \bar{g}_\mu(U_{k\mu}^*Q_{kk'}U_{k'\nu} + V_{k\mu}^*Q_{kk'}^*V_{k'\nu})g_\nu + g^2_\delta_{\mu \nu}.
\]

(52)
C. Wick’s theorem and reduction formulae

Corresponding to Eq. (48), the operator \( \hat{S} \) in \( \hat{Q} = e^{-i\hat{S}} \) has the form
\[
\hat{S} = \sum_{k,k'} S_{kk'} c^\dagger_k c_{k'}.
\] (53)

According to the general prescription of projection calculation [16], we represent \( \hat{S} \) in terms of the TFD q.p. operators as
\[
\hat{S} = \bar{S}^{(0)} + \sum_{\mu,\nu(\text{all})} \bar{S}^{(1)}_{\mu\nu} \beta^\dagger_\mu \beta_\nu + \frac{1}{2} \sum_{\mu,\nu(\text{all})} (\bar{S}^{(2)}_{\mu\nu} \beta^\dagger_\mu \beta^\dagger_\nu + \text{h.c.}),
\] (54)

where the summation \( \sum_{\mu,\nu(\text{all})} \) extends over both the tilded and non-tilded q.p. states. On the other hand, the TFD-extension of the GBT derives an alternative form as
\[
\hat{S} = \sum_{\mu,\nu>0} \left( \beta^\dagger_\mu \tilde{\beta}^\dagger_\mu \beta_\nu \tilde{\beta}_\nu \right) \begin{pmatrix}
\bar{S}_{11} & \bar{S}_{12} \\
\bar{S}_{21} & \bar{S}_{22}
\end{pmatrix}_{\mu\nu} \begin{pmatrix}
\beta_\nu \\
\tilde{\beta}_\nu
\end{pmatrix}
\]
\[
= \text{Tr}(\bar{S}_{22}) + \sum_{\mu,\nu} \left\{ \left( \beta^\dagger_\mu \tilde{\beta}^\dagger_\mu \right) \left( \bar{S}_{11} - \bar{S}^{\text{tr}}_{22} \right)_{\mu\nu} \begin{pmatrix}
\beta_\nu \\
\tilde{\beta}_\nu
\end{pmatrix} + \left[ \left( \beta^\dagger_\mu \tilde{\beta}^\dagger_\mu \right) \left( \bar{S}_{12} \right)_{\mu\nu} \begin{pmatrix}
\beta^\dagger_\nu \\
\tilde{\beta}^\dagger_\nu
\end{pmatrix} + \text{h.c.} \right] \right\},
\] (55)

where \( \bar{S}_{11}, \bar{S}_{12}, \bar{S}_{21} \) and \( \bar{S}_{22} \) are calculated as
\[
(\bar{S}_{11})_{\mu\nu} = \begin{pmatrix}
(\bar{g}U^\dagger S \bar{g}g)_{\mu\nu} & (\bar{g}U^\dagger S V^* \bar{g}g)_{\mu\nu} \\
(g V^\text{tr} S \bar{g}g)_{\mu\nu} & (g V^\text{tr} S V^* \bar{g}g)_{\mu\nu}
\end{pmatrix},
\]
(56a)
\[
(\bar{S}_{22})_{\mu\nu} = \begin{pmatrix}
(g V^\text{tr} S V^* \bar{g}g)_{\mu\nu} & (g V^\text{tr} S U \bar{g}g)_{\mu\nu} \\
(g U^\dagger S V^* \bar{g}g)_{\mu\nu} & (g U^\dagger S U \bar{g}g)_{\mu\nu}
\end{pmatrix},
\]
(56b)
\[
(\bar{S}_{12})_{\mu\nu} = (\bar{S}^{\dagger}_{21})_{\mu\nu} = \begin{pmatrix}
(\bar{g}U^\dagger S V^* \bar{g}g)_{\mu\nu} & (\bar{g}U^\dagger S U \bar{g}g)_{\mu\nu} \\
(g V^\text{tr} S V^* \bar{g}g)_{\mu\nu} & (g V^\text{tr} S U \bar{g}g)_{\mu\nu}
\end{pmatrix}.
\]
(56c)

Comparing (54) with the last expression in (55), we obtain
\[
\bar{S}^{(0)} = \text{Tr}\bar{S}_{22}, \quad \bar{S}^{(1)} = \bar{S}_{11} - \bar{S}^{\text{tr}}_{22}, \quad \bar{S}^{(2)} = 2\bar{S}_{12} = 2\bar{S}^{\dagger}_{21}.
\] (57)

By applying the general formalism of projection [16], the TFD vacuum expectation value of the operator \( \hat{Q} \) is given by
\[
\langle 0_T|\hat{Q}|0_T \rangle = (\det \bar{K})^{1/2} \exp \left[ -i \left( \bar{S}^{(0)} + \frac{1}{2} \text{Tr}\bar{S}^{(1)} \right) \right] = (\det \bar{K})^{1/2} \exp \left[ -\frac{i}{2} \text{Tr}S \right].
\] (58)

It is noted that \( \text{Tr}S \) vanishes for the traceless algebra like that associated with \( SU(2)_J \), while gives dimension of the s.p. space for \( U(1)_Z \) and \( U(1)_N \).
In order to apply the generalized Wick’s theorem to reduce the quantities in (57), we introduce an operator symbol \([\hat{Q}] [16]\), and express the TFD vacuum expectation value of an operator \(\hat{O}\) as

\[
\langle 0_T | \hat{O} \hat{Q} | 0_T \rangle = \langle 0_T | \hat{Q} | 0_T \rangle \langle 0_T | \hat{O} | \hat{Q} | 0_T \rangle ; \quad [\hat{Q}] = \frac{\hat{Q}}{\langle 0_T | \hat{Q} | 0_T \rangle}.
\] (59)

Then, the basic matrix elements generalized by the TFD, which are building blocks for the quantum number projection at finite temperature, are provided by

\[
A_{\mu \nu} \equiv \langle 0_T | [\hat{Q}] \beta_\mu^\dagger \beta_\nu^\dagger | 0_T \rangle = [\hat{M} \hat{K}^{-1}]_{\mu \nu} = -[(\hat{K}^{tr})^{-1} \hat{M}^{tr}]_{\mu \nu},
\] (60a)

\[
B_{\mu \nu} \equiv \langle 0_T | \beta_\mu \beta_\nu | 0_T \rangle = [\hat{K}^{-1} \hat{N}]_{\mu \nu} = -[\hat{N}^{tr} (\hat{K}^{tr})^{-1}]_{\mu \nu},
\] (60b)

\[
C_{\mu \nu} \equiv \langle 0_T | \beta_\mu \beta_\nu^\dagger | 0_T \rangle = [\hat{K}^{-1}]_{\mu \nu},
\] (60c)

where the suffixes \(\mu\) and \(\nu\) represent all the possible q.p. states. The TFD version of the generalized Wick’s theorem [16] is exemplified by

\[
\langle 0_T | [\hat{Q}] \beta_\mu^\dagger \beta_\mu^\dagger \beta_\nu^\dagger \beta_\nu^\dagger | 0_T \rangle = A_{\mu \rho} A_{\rho \sigma} - A_{\mu \rho} A_{\nu \sigma} + A_{\mu \sigma} A_{\nu \rho},
\] (61a)

\[
\langle 0_T | \beta_\mu \beta_\nu | 0_T \rangle = C_{\mu \rho} C_{\rho \sigma} - C_{\mu \rho} C_{\nu \sigma} + C_{\mu \sigma} C_{\nu \rho},
\] (61b)

\[
\langle 0_T | \beta_\mu \beta_\nu \beta_\rho \beta_\sigma | 0_T \rangle = B_{\mu \rho} C_{\rho \sigma} - B_{\mu \rho} C_{\nu \sigma} + C_{\mu \sigma} B_{\nu \rho},
\] (61c)

\[
\langle 0_T | \beta_\mu \beta_\nu \beta_\rho \beta_\sigma | 0_T \rangle = B_{\mu \rho} B_{\nu \sigma} - B_{\mu \rho} B_{\nu \sigma} + B_{\mu \sigma} B_{\nu \rho}.
\] (61d)

For the SU\((2)_J \times U(1)_Z \times U(1)_N\) projection, we have

\[
\frac{1}{2} \text{Tr}S = \varphi_p \Omega_p + \varphi_n \Omega_n,
\] (62)

where the quantity \(\Omega_p = \sum_{j p} (j + 1/2) \quad (\Omega_n = \sum_{j n} (j + 1/2))\) represents a half-number of total s.p. levels in the model space. Hence, we obtain

\[
\langle 0_T | \hat{P}_{(J,Z,N)} | 0_T \rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{-i \varphi_p (\Omega_p - Z)} d\varphi_p \frac{1}{2\pi} \int_0^{2\pi} e^{-i \varphi_n (\Omega_n - N)} d\varphi_n
\]

\[
\times \frac{2J + 1}{4\pi^2} \int_0^{2\pi} \sin^2 \frac{\omega}{2} d\omega \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \chi_J(\omega) (\det \hat{K})^{1/2},
\] (63)

and

\[
\langle 0_T | \hat{H} \hat{P}_{(J,Z,N)} | 0_T \rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{-i \varphi_p (\Omega_p - Z)} d\varphi_p \frac{1}{2\pi} \int_0^{2\pi} e^{-i \varphi_n (\Omega_n - N)} d\varphi_n
\]

\[
\times \frac{2J + 1}{4\pi^2} \int_0^{2\pi} \sin^2 \frac{\omega}{2} d\omega \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \chi_J(\omega) (\det \hat{K})^{1/2} \langle 0_T | \hat{H} [\hat{Q}] | 0_T \rangle.
\] (64)
Applying Eq. (61) to \( \langle 0_T | \hat{H} | \hat{Q} | 0_T \rangle \), we can compute the Hamiltonian kernel in Eq. (64). The \( SU(2)_J \times U(1)_Z \times U(1)_N \) projected thermal energy is calculated from Eq. (65), by carrying out integrals in Eqs. (63, 64). It is pointed out that the method of integration, which has been demonstrated to be successful in the zero-temperature case [5, 9], is available also for the projected statistics. If we choose Euler angles \((\alpha, \beta, \gamma)\) rather than the variables \((\omega, \theta, \phi)\) for integral variables, the Gauss-Chebyshev quadrature formula will be useful for the \(\alpha\) and \(\gamma\) integrals as well as the \(\varphi_p\) and \(\varphi_n\) integrals, and the Gauss-Legendre quadrature formula for the \(\beta\) integral, since the function \(\chi_J(\omega)\) is nothing but a sum of the Wigner \(D\)-functions.

It should be noticed that the original q.p. occupation number is affected by the projection. Using the TFD transformation in (18), we get

\[
\alpha_\mu^\dagger \alpha_\mu = f_\mu + (1 - f_\mu) \beta_\mu^\dagger \beta_\mu - \sqrt{f_\mu (1 - f_\mu)} \beta_\mu \bar{\beta}_\mu + \sqrt{f_\mu (1 - f_\mu)} \beta_\mu^\dagger \bar{\beta}_\mu^\dagger. \tag{65}
\]

The first and third terms in the above expression contribute to the projected occupation number, when the projection operator is placed on the right of \(\alpha_\mu^\dagger \alpha_\mu\). For \(\hat{P}(J, Z, N)\), the projected q.p. occupation number is calculated by

\[
\langle 0_T | \alpha_\mu^\dagger \alpha_\mu \hat{P}(J, Z, N) | 0_T \rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{-i\varphi_p(\Omega_p-Z)} d\varphi_p \frac{1}{2\pi} \int_0^{2\pi} e^{-i\varphi_n(\Omega_n-N)} d\varphi_n \times \frac{2J + 1}{4\pi^2} \int_0^{2\pi} \sin^2 \frac{\omega}{2} d\omega \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \times \chi_J(\omega) (\det \bar{K})^{1/2} [f_\mu - \sqrt{f_\mu (1 - f_\mu)} (\bar{K}^{-1} \bar{N})_{\mu\mu}] \tag{66}
\]

The present formalism is summarized by Eqs. (46, 58, 59, 61) for general cases, with \(A_{\mu\nu}, B_{\mu\nu}, C_{\mu\nu}\) of Eq. (60), and \(\bar{K}_{\mu\nu} = \bar{L}_{\mu\nu}^*, \bar{M}_{\mu\nu} = \bar{N}_{\mu\nu}^*\) of Eq. (51), which are functions of the GBT coefficients \(\{U_{\mu\nu}, V_{\mu\nu}, U_{\mu\nu}^*, V_{\mu\nu}^*\}\) and the q.p. occupation numbers \(f_\mu\). The integral in Eq. (66) is exemplified by Eqs. (63, 64, 66) for the \(SU(2)_J \times U(1)_Z \times U(1)_N\) projection. The resultant formulae are equivalent to those derived in Ref. [12], despite the difference in appearance. It still deserves noting that the present formulae are straightforward extension of the zero-temperature formulae of Refs. [9, 16].

D. Representation in specific bases

For practical use, we here present explicit forms of the quantities relevant to the \(SU(2)_J \times U(1)_Z \times U(1)_N\) projection, taking specific s.p. bases.

1. Spherical bases

Each s.p. level \(|\tau nljm\rangle\) is specified by \(\tau (= p, n)\), radial quantum number \(n\), orbital angular momentum \(l\), total angular momentum \(j (= l \pm 1/2)\) and its projection to the \(z\)-axis
m. Here the s.p. state $k$ is regarded as an abbreviation of $(\tau nljm)$, namely, $|k\rangle \equiv |\tau nljm\rangle$. Analogously, $|k'\rangle \equiv |\tau 'n'j'm'\rangle$. For the projection $\hat{P}_{(J,Z,N)}$, we have $\hat{Q} = e^{-i\varphi_x} \hat{R}$, yielding the $Q$-matrix in Eq. (48) of

$$Q_{kk'} = Q_{\tau nljm, \tau n'l'j'm'} = \delta_{\tau\tau'}\delta_{\nu\nu'}\delta_{jj'} e^{i\varphi_x} D^{j\ast}_{m'm}.$$

(67)

The $\tilde{K}$, $\tilde{L}$, $\tilde{M}$ and $\tilde{N}$ matrices are explicitly written as

$$\tilde{K}_{\mu\nu} = \tilde{L}^*_{\mu\nu} = \left( \begin{array}{c} \bar{g}(U^\dagger e^{i\varphi} D^\dagger U + V^\dagger e^{-i\varphi} D^\dagger V)\bar{g} + g^2 \bar{g}(U^\dagger e^{i\varphi} D^\dagger V^\ast + V^\dagger e^{-i\varphi} D^\dagger U^\ast)g \\ g(V^\dagger e^{i\varphi} D^\dagger U + U^\dagger e^{-i\varphi} D^\dagger V)\bar{g} + g^2 \bar{g}(V^\dagger e^{i\varphi} D^\dagger V^\ast + U^\dagger e^{-i\varphi} D^\dagger U^\ast)g \end{array} \right)_{\mu\nu},$$

(68a)

$$\tilde{M}_{\mu\nu} = \tilde{N}^*_{\mu\nu} = \left( \begin{array}{c} \bar{g}(V^\dagger e^{i\varphi} D^\dagger U + U^\dagger e^{-i\varphi} D^\dagger V)\bar{g} - \bar{g}g \bar{g}(V^\dagger e^{i\varphi} D^\dagger V^\ast + U^\dagger e^{-i\varphi} D^\dagger U^\ast)g \\ g(U^\dagger e^{i\varphi} D^\dagger U + V^\dagger e^{-i\varphi} D^\dagger V)\bar{g} - \bar{g}g \bar{g}(U^\dagger e^{i\varphi} D^\dagger V^\ast + V^\dagger e^{-i\varphi} D^\dagger U^\ast)g \end{array} \right)_{\mu\nu},$$

(68b)

where, e.g.,

$$[\bar{g}(U^\dagger e^{i\varphi} D^\dagger U + V^\dagger e^{-i\varphi} D^\dagger V)g + g^2]_{\mu\nu} = \sum_{k,k'} \delta_{\tau\tau'}\delta_{\nu\nu'}\delta_{jj'} \bar{g}_u(U^\dagger_{k\mu} e^{i\varphi} D_{m'm}^j U^\ast_{k'\nu} + V^\dagger_{k\mu} e^{-i\varphi} D_{m'm}^j V^\ast_{k'\nu})g_{\nu'} + g^2_{\mu}\delta_{\mu\nu}. \quad (69)$$

When we take only the particle number projection, all $D_{m'm}^j$ should be replaced by $\delta_{mm'}$.

2. Goodman’s bases

Whole spherical basis states for a given set of quantum numbers $(\tau nlj)$ can be separated into two sets $\{|\tau nljm\rangle\}$ and $\{|\tau nljm\rangle\}$. The first set $\{|\tau nljm\rangle\}$ consists of the states having $(m - 1/2)$ equal to even integers, while the second set $\{|\tau nljm\rangle \equiv \hat{T}|\tau nljm\rangle\}$ having $(m - 1/2)$ equal to odd integers, where $\hat{T}$ is the time-reversal transformation. The phase convention is assumed to be

$$|\tau nljm\rangle \equiv \hat{T}|\tau nljm\rangle = (-1)^{j-m+1}|\tau nlj-m\rangle, \quad \hat{T}^2|\tau nljm\rangle = -|\tau nljm\rangle. \quad (70)$$

Since the auxiliary Hamiltonian in Eq. (44) is invariant under the rotation about the $x$-axis by angle $\pi$, i.e. $\hat{R}_x = e^{-i\pi j_x}$, the solution of the CHFB equation usually becomes eigenstates of $\hat{R}_x$. Therefore, a convenient choice is to employ the set of eigenstates of $\hat{R}_x$ for s.p. basis.

From the relations as

$$\hat{R}_x c^\dagger_{\tau nljm} \hat{R}_x^\dagger = e^{-i\pi j} c^\dagger_{\tau nlj-m}, \quad (\hat{R}_x)^2 c^\dagger_{\tau nljm} (\hat{R}_x^\dagger)^2 = -c^\dagger_{\tau nljm},$$

(71)

we find that the eigenvalues of $\hat{R}_x$ are $\pm i$,

$$\hat{R}_x c^\dagger_k \hat{R}_x^\dagger = -ic^\dagger_k, \quad \hat{R}_x c^\dagger_k \hat{R}_x^\dagger = +ic^\dagger_k.$$

(72)
where the corresponding eigenoperators are given by

\[
c_k^\dagger = \frac{1}{\sqrt{2}} [c_{\tau n lj m}^\dagger + (-1)^{j-1/2}c_{\tau n lj m-1}^\dagger], \quad c_k^\dagger = \frac{(-1)^{l+m+1/2}}{\sqrt{2}} [c_{\tau n lj m}^\dagger - (-1)^{j-1/2}c_{\tau n lj m-1}^\dagger]. \tag{73}
\]

The operator \( \hat{R}_x \) is called signature operator, and the bases \((k \bar{k})\) are called Goodman's bases. It is sufficient to adopt the bases of Eq. (73) only for even \((m - 1/2)\) to avoid repetition, which will symbolically be indicated by \(k > 0\). Using the relations in Eq. (71), we can confirm that \(c_k^\dagger\) and \(c_k^\dagger\) are related to each other by the time-reversal transformation,

\[
\hat{T} c_k^\dagger \hat{T}^{-1} = c_{k'}^\dagger, \quad \hat{T} c_k^\dagger \hat{T}^{-1} = -c_{k'}^\dagger.
\tag{74}
\]

Accordingly matrix forms for expectation values of relevant quantities are also simplified. As an example, we here present the angular momentum components,

\[
(\hat{J}_x)_{(k \bar{k}), (k' \bar{k}')} = \begin{pmatrix} \langle k|\hat{J}_x|k'\rangle & 0 \\ 0 & \langle k|\hat{J}_x|k'\rangle \end{pmatrix}, \quad (\hat{J}_y)_{(k \bar{k}), (k' \bar{k}')} = \begin{pmatrix} 0 & \langle k|\hat{J}_y|k'\rangle \\ \langle k|\hat{J}_y|k'\rangle & 0 \end{pmatrix},
\]

\[
(\hat{J}_z)_{(k \bar{k}), (k' \bar{k}')} = \begin{pmatrix} 0 & \langle k|\hat{J}_z|k'\rangle \\ \langle k|\hat{J}_z|k'\rangle & 0 \end{pmatrix}.
\tag{75}
\]

Due to time-reversal properties, we have the following relations,

\[
\langle k|\hat{J}_x|k'\rangle = -\langle k'|\hat{J}_x|k\rangle, \quad \langle k|\hat{J}_y|k'\rangle = \langle k'|\hat{J}_y|k\rangle, \quad \langle k|\hat{J}_z|k'\rangle = \langle k'|\hat{J}_z|k\rangle.
\tag{76}
\]

Unless the signature is spontaneously violated, the q.p. operators \(\alpha_\mu^\dagger\) and \(\alpha_\mu\) belonging to the HFB eigenvalues \(E_\mu\) and \(E_{\bar{\mu}}\), respectively, are classified in a similar manner,

\[
\hat{R}_x \alpha_\mu^\dagger \hat{R}_x^\dagger = -i \alpha_\mu^\dagger, \quad \hat{R}_x \alpha_\mu^\dagger \hat{R}_x^\dagger = +i \alpha_\mu^\dagger \quad \text{and} \quad \hat{T} \alpha_\mu^\dagger \hat{T}^{-1} = \alpha_\mu^\dagger, \quad \hat{T} \alpha_{\bar{\mu}}^\dagger \hat{T}^{-1} = -\alpha_{\bar{\mu}}^\dagger.
\tag{77}
\]

The conservation of the signature simplifies the structure of the GBT matrix as

\[
\begin{pmatrix} c_k \\ c_k^\dagger \\ c_k^\dagger \\ c_k^\dagger \end{pmatrix} = \sum_{\mu > 0} \begin{pmatrix} U_{k\mu} & 0 & 0 & V^*_k \bar{\mu} \\ 0 & U_{k\bar{\mu}} & V^*_k \mu & 0 \\ 0 & V_{k\mu} & U^*_k \bar{\mu} & 0 \\ V_{k\bar{\mu}} & 0 & 0 & U^*_k \mu \end{pmatrix} \begin{pmatrix} \alpha_\mu \\ \alpha_{\bar{\mu}} \\ \alpha_{\mu}^\dagger \\ \alpha_{\bar{\mu}}^\dagger \end{pmatrix}.
\tag{78}
\]

Therefore, the TFD-extension of the GBT is represented as

\[
\begin{pmatrix} C_{(k \bar{k})} \\ C_{(k \bar{k})}^\dagger \end{pmatrix} = \sum_{\mu > 0} \bar{W}_{(k \bar{k}), (\mu \bar{\mu})} \begin{pmatrix} B_{(\mu \bar{\mu})} \\ B_{(\mu \bar{\mu})}^\dagger \end{pmatrix}; \quad C_{(k \bar{k})} = \begin{pmatrix} c_k \\ c_k^\dagger \\ c_k^\dagger \\ c_k^\dagger \end{pmatrix}, \quad B_{(\mu \bar{\mu})} = \begin{pmatrix} \beta_\mu \\ \beta_{\bar{\mu}} \\ \bar{\beta}_\mu \\ \bar{\beta}_{\bar{\mu}} \end{pmatrix}.
\tag{79}
\]
The transformation matrix \( W \) is given by
\[
W_{(k\bar{k}),(\mu\bar{\mu})} = 
\begin{pmatrix}
\bar{U}_{(k\bar{k}),(\mu\bar{\mu})} & \bar{V}_{(k\bar{k}),(\mu\bar{\mu})} \\
\bar{V}_{(k\bar{k}),(\mu\bar{\mu})} & \bar{U}_{(k\bar{k}),(\mu\bar{\mu})}
\end{pmatrix}
\] (80a)
\[
\bar{U}_{(k\bar{k}),(\mu\bar{\mu})} = 
\begin{pmatrix}
U_{k\mu}g_\mu & 0 & 0 & V_{k\mu}^*g_\mu \\
0 & U_{k\mu}^*g_\mu & V_{k\mu}^*g_\mu & 0 \\
0 & -V_{k\mu}^*g_\mu & U_{k\mu}^*g_\mu & 0 \\
-V_{k\mu}^*g_\mu & 0 & 0 & U_{k\mu}^*g_\mu
\end{pmatrix}
\] (80b)
\[
\bar{V}_{(k\bar{k}),(\mu\bar{\mu})} = 
\begin{pmatrix}
0 & V_{k\mu}^*g_\mu & U_{k\mu}^*g_\mu & 0 \\
0 & -U_{k\mu}^*g_\mu & V_{k\mu}^*g_\mu & 0 \\
0 & -U_{k\mu}^*g_\mu & V_{k\mu}^*g_\mu & 0
\end{pmatrix}
\]

We now consider the \( SU(2)_J \times U(1)_Z \times U(1)_N \) projection. The operator \( \hat{Q} = e^{-i\varphi}\hat{R} \) gives the transformation rules for the s.p. operators \( \hat{Q} \),
\[
\hat{Q}c_k\hat{Q}^\dagger = e^{i\varphi_r} \sum_{k'>0} \left( F_{kk'}c_{k'} + G_{kk'}^*c_{k'}^* \right),
\hat{Q}c_k\hat{Q}^\dagger = e^{i\varphi_r} \sum_{k'>0} \left( G_{kk'}c_{k'} + F_{kk'}^*c_{k'}^* \right),
\]
where the coefficients \( F \) and \( G \) are defined by
\[
F_{kk'} = F_{k\bar{k}'} = \delta_{rr} \delta_{nn'} \delta_{ll'} \delta_{jj'} \frac{1}{2} \left[ D_{m',m}^j + D_{-m',-m}^j + (-1)^{j-1/2} (D_{m',-m}^j + D_{-m',m}^j) \right],
\]
\[
G_{kk'} = -G_{k\bar{k}'} = \delta_{rr} \delta_{nn'} \delta_{ll'} \delta_{jj'} \frac{(-1)^{l+m'+1/2}}{2} \left[ D_{m',m}^j - D_{-m',-m}^j + (-1)^{j-1/2} (D_{m',-m}^j - D_{-m',m}^j) \right].
\]

The transformation is converted to the one among the TFD q.p. operators via Eqs. (70),
\[
\hat{Q} \left( \begin{pmatrix} B_{(\mu\bar{\mu})} \\ B_{(\mu\bar{\mu})}^\dagger \end{pmatrix} \right) \hat{Q}^\dagger = \sum_{\nu>0} \left( \begin{pmatrix} \bar{K}^{(\mu\bar{\mu})},(\nu\bar{\nu}) \\ \bar{M}^{(\mu\bar{\mu})},(\nu\bar{\nu}) \end{pmatrix} \begin{pmatrix} \bar{N}^{(\mu\bar{\mu})},(\nu\bar{\nu}) \\ \bar{L}^{(\mu\bar{\mu})},(\nu\bar{\nu}) \end{pmatrix} \left( \begin{pmatrix} B_{(\nu\bar{\nu})} \\ B_{(\nu\bar{\nu})}^\dagger \end{pmatrix} \right) \right),
\]

\[
(83)
\]
where the submatrices $K$, $L$, $M$ and $N$ are provided by

$$
\tilde{K}_{(\mu\bar{\mu}), (\nu\bar{\nu})} = \tilde{L}_{(\mu\bar{\mu}), (\nu\bar{\nu})} = \\
\left( \begin{array}{ccc}
\bar{g}_\mu (U^\dagger e^{i\varphi_r} F^* U + V^\dagger e^{-i\varphi_r} F^* V)_{\mu\nu} \bar{g}_\nu \\
g_\mu (U^\dagger e^{i\varphi_r} G^* U + V^\dagger e^{-i\varphi_r} G^* V)_{\mu\nu} \\
g_\mu (V^\dagger e^{i\varphi_r} G^* U + U^\dagger e^{-i\varphi_r} F^* V)_{\mu\nu} \\
g_\mu (V^\dagger e^{i\varphi_r} F^* U + U^\dagger e^{-i\varphi_r} G^* V)_{\mu\nu}
\end{array} \right) \\
\pm \delta_{\mu\nu} \left( \begin{array}{ccc}
g_\mu^2 & 0 & 0 \\
0 & g_\mu^2 & 0 \\
0 & 0 & g_\mu^2
\end{array} \right), \quad (84a)
$$

$$
\tilde{M}_{(\mu\bar{\mu}), (\nu\bar{\nu})} = \tilde{N}_{(\mu\bar{\mu}), (\nu\bar{\nu})} = \\
\left( \begin{array}{ccc}
\bar{g}_\mu (V^\dagger e^{i\varphi_r} G^* U + U^\dagger e^{-i\varphi_r} F^* V)_{\mu\nu} \\
g_\mu (V^\dagger e^{i\varphi_r} F^* U + U^\dagger e^{-i\varphi_r} G^* V)_{\mu\nu} \\
g_\mu (U^\dagger e^{i\varphi_r} G^* U + V^\dagger e^{-i\varphi_r} G^* V)_{\mu\nu} \\
g_\mu (U^\dagger e^{i\varphi_r} F^* U + V^\dagger e^{-i\varphi_r} F^* V)_{\mu\nu}
\end{array} \right) \\
- \delta_{\mu\nu} \left( \begin{array}{ccc}
0 & g_\mu \bar{g}_\mu & 0 \\
0 & 0 & g_\mu \bar{g}_\mu \\
\bar{g}_\mu g_\mu & 0 & 0
\end{array} \right), \quad (84b)
$$

Note that, for the case of particle number projection only, all the matrices $F$ should be replace by an identity, and $G$ by zero.

### E. Formulae in BCS approximation

We continue to work with the Goodman's bases. The HFB approximation is reduced to the BCS approximation by the replacements

$$
U_{k\mu} = U_{k\bar{\mu}} = u_k \delta_{k\mu}, \quad V_{k\bar{\mu}} = -V_{k\mu} = v_k \delta_{k\mu}.
$$

(85)
We here assume $u_k$ and $v_k$ to be real. Thereby the BCS transformation is expressed as

$$
\begin{pmatrix}
  c_k \\
c_k^\dagger \\
  \bar{c}_k \\
  \bar{c}_k^\dagger
\end{pmatrix}
= \begin{pmatrix}
  u_k & 0 & 0 & v_k \\
  0 & u_k & -v_k & 0 \\
  0 & v_k & u_k & 0 \\
  -v_k & 0 & 0 & u_k
\end{pmatrix}
\begin{pmatrix}
  \alpha_k \\
  \alpha_k^\dagger \\
  \overline{\alpha}_k \\
  \overline{\alpha}_k^\dagger
\end{pmatrix}.
$$

(86)

Accordingly, the quantum number projection is somewhat simplified in the BCS approximation. By using the notations

$$
\begin{align*}
\xi_{kk'} &= u_k u_{k'} e^{i\phi} + v_k v_{k'} e^{-i\phi} = (u_k u_{k'} + v_k v_{k'}) \cos \varphi + i (u_k u_{k'} - v_k v_{k'}) \sin \varphi, \\
\eta_{kk'} &= u_k v_{k'} e^{i\phi} - v_k u_{k'} e^{-i\phi} = (u_k v_{k'} - v_k u_{k'}) \cos \varphi + i (u_k v_{k'} + v_k u_{k'}) \sin \varphi,
\end{align*}
$$

(87)

the matrices $\bar{K}, \bar{L}, \bar{M}$ and $\bar{N}$ for the $SU(2)_J \times U(1)_Z \times U(1)_N$ projection are obtained by

$$
\bar{K}_{(kk'),(k'k')} = \bar{L}_{(kk'),(k'k')}^* =
\begin{pmatrix}
  \bar{g}_k \xi_{kk'} F_{kk'}^* g_{k'} \\
  -\bar{g}_k \eta_{kk'} G_{kk'}^* g_{k'} \\
  -\bar{g}_k \eta_{kk'} F_{kk'}^* g_{k'} \\
  -\bar{g}_k \eta_{kk'} G_{kk'}^* g_{k'}
\end{pmatrix}
- \delta_{kk'}
\begin{pmatrix}
  0 & 0 & 0 & 0 \\
  0 & \bar{g}_k^2 & 0 & 0 \\
  0 & 0 & \bar{g}_k^2 & 0 \\
  0 & 0 & 0 & \bar{g}_k^2
\end{pmatrix},
$$

(88a)

$$
\bar{M}_{(kk'),(k'k')} = \bar{N}_{(kk'),(k'k')}^* =
\begin{pmatrix}
  -\bar{g}_k \eta_{kk'} F_{kk'}^* g_{k'} \\
  -\bar{g}_k \eta_{kk'} G_{kk'}^* g_{k'} \\
  -\bar{g}_k \eta_{kk'} F_{kk'}^* g_{k'} \\
  -\bar{g}_k \eta_{kk'} G_{kk'}^* g_{k'}
\end{pmatrix}
- \delta_{kk'}
\begin{pmatrix}
  0 & 0 & g_k \bar{g}_k & 0 \\
  0 & 0 & 0 & g_k \bar{g}_k \\
  g_k \bar{g}_k & 0 & 0 & 0 \\
  \bar{g}_k g_k & 0 & 0 & 0
\end{pmatrix}.
$$

(88b)
For the case of the number projection only, putting \( F = 1 \) and \( G = 0 \) in the above expression and employing \( \xi_{kk} = \cos \varphi + i(u_k^2 - v_k^2) \sin \varphi, \eta_{kk} = -\eta_{kk}^* = 2iu_kv_k \sin \varphi \), we get

\[
\begin{align*}
\tilde{K}_{(kk), (k'k')} &= \tilde{L}_{(kk), (k'k')}^* = \delta_{kk'} \begin{pmatrix}
\tilde{g}_k^2 \xi_{kk} + g_k^2 & 0 & 0 & \tilde{g}_k g_k \eta_{kk} \\
0 & \tilde{g}_k^2 \xi_{kk} + g_k^2 & -\tilde{g}_k g_k \eta_{kk} & 0 \\
0 & -\tilde{g}_k g_k \eta_{kk} & \tilde{g}_k^2 \xi_{kk}^* + g_k^2 & 0 \\
g_k \tilde{g}_k \eta_{kk} & 0 & 0 & \tilde{g}_k^2 \xi_{kk}^* + g_k^2
\end{pmatrix}, \\
\tilde{M}_{(kk), (k'k')} &= \tilde{N}_{(kk), (k'k')}^* = \delta_{kk'} \begin{pmatrix}
0 & -\tilde{g}_k \tilde{g}_k \eta_{kk} & \tilde{g}_k \eta_{kk} (\xi_{kk}^* - 1) & 0 \\
\tilde{g}_k \tilde{g}_k \eta_{kk} & 0 & 0 & \tilde{g}_k g_k (\xi_{kk}^* - 1) \\
g_k \tilde{g}_k (\xi_{kk} - 1) & 0 & 0 & g_k \tilde{g}_k \eta_{kk} \\
0 & g_k \tilde{g}_k (\xi_{kk} - 1) & -g_k g_k \eta_{kk} & 0
\end{pmatrix}.
\end{align*}
\]

Eq. (89a) yields

\[
(\det \tilde{K})^{1/2} = \prod_{k > 0} [f_k (1 - f_k) + (1 - f_k)f_k + (1 - f_k)(1 - f_k)\xi_{kk} + f_k f_k \xi_{kk}^*].
\]

Eqs. (89,90) give the formulae equivalent to those in Ref. [11].

### IV. APPROXIMATION OF ENTROPY

Once the original Bogoliubov transformation (11) and the q.p. energy in Eq. (2) are determined, the projection method discussed in Sec. III is straightforwardly applicable. This indicates the variation-before-projection (VBP) calculations. However, there still remains a serious problem in formulating the variation-after-projection (VAP) calculations [12].

Between the exact free energy \( F^{\text{exact}} \), which is generated by the exact Boltzmann-Gibbs operator \( \exp(-\tilde{H}/T) \), and an approximate one \( F_P \), which is generated by \( \hat{P} \exp(-\tilde{H}/T) \hat{P} \) in our case, the Peierls inequality holds [10],

\[
F^{\text{exact}} = -T \ln[\text{Tr}(e^{-\tilde{H}/T} \hat{P})] \leq F_P = E_P - TS_P.
\]

This inequality vindicates the variational calculations minimizing \( F_P \). The approximate energy \( E_P \) is expressed in terms of the TFD vacuum expectation value by

\[
E_P = \text{Tr}(\hat{w}_P \tilde{H}) = \frac{\text{Tr}(w_0 \tilde{H} \hat{P})}{\text{Tr}(w_0 \hat{P})} = \frac{\langle 0_T | \tilde{H} \hat{P} | 0_T \rangle}{\langle 0_T | \hat{P} | 0_T \rangle}.
\]

The entropy is given by

\[
S_P = -\text{Tr}(\hat{w}_P \ln \hat{w}_P) = -\text{Tr} \left[ \frac{e^{-\tilde{H}_0/T} \hat{P}}{\text{Tr}(e^{-\tilde{H}_0/T} \hat{P})} \ln \left( \frac{e^{-\tilde{H}_0/T} \hat{P}}{\text{Tr}(e^{-\tilde{H}_0/T} \hat{P})} \right) \right],
\]

\[20\]
where a relation \( \hat{P} \ln(\hat{P} \hat{A} \hat{P}) = \hat{P} \ln(\hat{A} \hat{P}) \) for any operator \( \hat{A} \) is applied. However, no further reduction is allowed because \( [\hat{P}, \hat{H}_0] \neq 0 \). Since the projection operator remains in the logarithmic function, it is prohibitively difficult to deal with the entropy in Eq. (93) without further approximation.

In order to make the VAP calculations practical, we here discuss an additional approximation on the entropy. The VAP scheme is based on the fact that an approximate entropy does not exceed the exact one, or the Peierls inequality \( (91) \). Therefore, any approximation method adopted in the VAP scheme should not conflict with those inequalities.

We now introduce a projected space \( \mathcal{P} \) and denote its complementary space by \( \mathcal{Q} \). The operator \( \hat{P} e^{-\hat{H}_0/T} \hat{P} \) is hermitian and non-negative. We here denote eigenstates of \( \hat{P} e^{-\hat{H}_0/T} \hat{P} \) by \( |K\rangle \) and its eigenvalue by \( \omega_K(\geq 0) \),

\[
\hat{P} e^{-\hat{H}_0/T} \hat{P} |K\rangle = |K\rangle \omega_K.
\]

Any states in the \( \mathcal{Q} \) are eigenstates of \( \hat{P} e^{-\hat{H}_0/T} \hat{P} \) with the null eigenvalue. The \( \mathcal{P} \) space is also spanned by eigenstates of \( \hat{P} e^{-\hat{H}_0/T} \hat{P} \). For \( |K\rangle \in \mathcal{P} \), \( \hat{P}|K\rangle = |K\rangle \) leads to

\[
\omega_K = (K|\hat{P} e^{-\hat{H}_0/T} \hat{P}|K) = (K|e^{-\hat{H}_0/T}|K).
\]

Therefore, an essential part of the entropy is expressed as

\[
\text{Tr}[\hat{P} e^{-\hat{H}_0/T} \hat{P} \ln(\hat{P} e^{-\hat{H}_0/T} \hat{P})] = \sum_{K\in\mathcal{P}} \omega_K \ln \omega_K = \sum_{K\in\mathcal{P}} (K|e^{-\hat{H}_0/T}|K) \ln(K|e^{-\hat{H}_0/T}|K).
\]

Observing that the functional form of the above expression is the convex function \( F(x) = x \ln x \) with \( x = (K|e^{-\hat{H}_0/T}|K) \), we apply the inequality \( (12) \) in Appendix B to derive a useful inequality as follows,

\[
\text{Tr}[\hat{P} e^{-\hat{H}_0/T} \hat{P} \ln(\hat{P} e^{-\hat{H}_0/T} \hat{P})] \leq \sum_{K\in\mathcal{P}} (K|e^{-\hat{H}_0/T} \ln e^{-\hat{H}_0/T}|K)
\]

\[
= -\frac{1}{T} \sum_{K\in\mathcal{P}} (K|e^{-\hat{H}_0/T} \hat{\mathcal{H}}_0|K)
\]

\[
= -\frac{1}{T} \sum_{K\in\mathcal{P}+\mathcal{Q}} (K|\hat{P} e^{-\hat{H}_0/T} \hat{H}_0|K) = -\frac{1}{T} \text{Tr}(e^{-\hat{H}_0/T} \hat{H}_0 \hat{P}).
\]

Thus, we obtain an inequality between two approximate entropies \( S_{\mathcal{P}} \) and \( S_{\mathcal{P}}' \), which is defined below,

\[
S_{\mathcal{P}} = -\text{Tr} \left[ \frac{\hat{P} e^{-\hat{H}_0/T} \hat{P}}{\text{Tr} e^{-\hat{H}_0/T} \hat{P}} \ln \left( \frac{\hat{P} e^{-\hat{H}_0/T} \hat{P}}{\text{Tr} e^{-\hat{H}_0/T} \hat{P}} \right) \right]
\]

\[
\geq \frac{1}{T} \frac{\text{Tr}(e^{-\hat{H}_0/T} \hat{H}_0 \hat{P})}{\text{Tr}(e^{-\hat{H}_0/T} \hat{P})} + \ln \text{Tr}(e^{-\hat{H}_0/T} \hat{P}) \equiv S_{\mathcal{P}}'.
\]

21
The approximate free energy defined by $S'_p$ satisfies the Peierls inequality,

$$F'_p \equiv E_p - TS'_p \geq F_p = E_p - TS_p \geq F^{\text{exact}}.$$  \hspace{1cm} (99)

It is noted that this approximate entropy $S'_p$ can also be obtained by dealing with the logarithmic function in Eq. (93) by $\hat{P} \ln(e^{-\hat{H}_0/T\hat{P}}) \approx -\hat{P}\hat{H}_0\hat{P}/T$, as if $\hat{H}_0$ and $\hat{P}$ were commutable, though such an ansatz is not adopted in the present argument. An crucial point is that this approximation preserves the Peierls inequality (99), which gives a ground for the variational calculations. Therefore, $F'_p$ will be available for the VAP calculation, since the smaller $F'_p$ gives the better approximation to $F^{\text{exact}}$. The TFD expression of $F'_p$ is given by

$$F'_p = \frac{\langle 0_T| (\hat{H} - \hat{H}_0)\hat{P}|0_T \rangle}{\langle 0_T|\hat{P}|0_T \rangle} - T \ln\langle 0_T|\hat{P}|0_T \rangle + T \sum_{\mu(\text{all})} \ln(1 - f_\mu).$$  \hspace{1cm} (100)

In $F'_p$, all the quantities can be calculated in the formalism presented in Sec. III. For the $SU(2)J \times U(1)Z \times U(1)N$ projection, $\langle 0_T|\hat{P}|0_T \rangle$ and $\langle 0_T|\hat{H}\hat{P}|0_T \rangle$ are given by Eq. (63) and Eq. (64), respectively. Moreover, $\langle 0_T|\hat{H}_0\hat{P}|0_T \rangle$ is immediately obtained from Eq. (66). Since these elements are expressed as functions of the GBT coefficients $U_{k\mu}$, $V_{k\mu}$, $U^{*}_{k\mu}$, $V^{*}_{k\mu}$ and $f_\mu = \sin^2 \vartheta_\mu$ (i.e. coefficients of the TFD-extended GBT), the variation of $F'_p$ with respect to these variables produces a closed set of independent VAP equations.

V. SUMMARY AND DISCUSSIONS

Although the mean-field theories play an important role in nuclear physics at finite temperature as well as at zero temperature, the mean-field solutions often violate conservation laws. In order to restore desired quantum numbers for thermally equilibrated many-body states of an isolated finite system like a nucleus, we have applied the thermo field dynamics (TFD) to construct a transparent and practical formalism of the quantum-number-projected statistics. In the TFD, an ensemble average of an observable is expressed by a TFD vacuum expectation value, whereas the single-particle operator space is doubled by introducing tilded operators. Making use of this method, we have derived formulae for the projected statistics at finite temperature. As an example, we have shown explicit representations for the projection of angular momentum as well as that of particle numbers. A significant advantage of this formalism is to keep a complete parallel with the zero-temperature case, so that the projection method and the corresponding computer code, which have been demonstrated to be successful, could be directly translated to the projection at finite temperature, apart from the variation.

Our formalism presented in Sec. III is, in principle, applicable to both the variation-before-projection (VBP) and the variation-after-projection (VAP) schemes. In the mean-field calculations without the projections, sharp phase transitions appear; for instance, there could be a discontinuity in heat capacity at the critical temperature. This is not realistic.
for finite systems, in which quantum fluctuations of the fields often wash out the distinct signature of transitions. While such unrealistic signature remains by the VBP calculations, the VAP scheme is expected to smooth it out, including a significant portion of the fluctuations. However, the VAP calculations minimizing the projected free energy are impractical without further approximation, since the entropy does not take a simple form because of the non-commutability of $\hat{P}$ with $\hat{H}_0$. Thus, in Sec. IV, we have discussed an additional approximation for the entropy, which is expected to resolve this problem. It should be emphasized that the Peierls inequality, which is an important requisite justifying the variation, is proven to be satisfied in this approximation.

We have adopted the HFB or constrained HFB (CHFB) self-consistent solution at finite temperature for the basic quasiparticle picture, and have developed the TFD formalism on it. The CHFB approximation is the most effective mean-field theory in describing nuclear structure at low temperature or along the yrast. It is commented here that, whereas the constraints might not look important when the projection is implemented, it can still be useful. In the VBP calculation, it could be essentially important to obtain a mean-field solution well connected to the true many-body solution. Also in the VAP calculations, the CHFB solution may be used to obtain good initial configurations. Furthermore, if there remain some quantum numbers unprojected, $\hat{C}_j$ ($j = 1, 2, \cdots, N_c$), they could be handled in the CHFB scheme in the projected statistics for other quantum numbers, by replacing the Hamiltonian $\hat{H}$ by the auxiliary one $\hat{H}' = \hat{H} - \sum_{j=1}^{N_c} \lambda_j \hat{C}_j$ in the free energy in Eqs. (91, 92, 100).

The present formalism will be useful in investigating effects of quantum fluctuations connected to the conservation laws on thermal properties of nuclei. A topical example is the pairing correlations at finite temperature. Although the superfluid-to-normal phase transition has been predicted to occur at relatively low temperature ($0.5 \lesssim T_c \lesssim 1$ MeV) [18, 24, 25], it is not yet well established in nuclei. Based on a precise measurement of nuclear level densities, the superfluid-to-normal transition in nuclei has been discussed recently [26]. While there is no sharp discontinuity as in infinite systems, the $S$-shape behavior in the graph of heat capacity vs. temperature, $C(T)$, has been argued to be a signature of the transition [26, 27]. For proper understanding of the phase transition and its relation to the $S$-shape, it is important to investigate effect of the quantum fluctuations in connection with the conservation laws, although the other quantum fluctuations cannot be neglected in quantitative description [28], particularly around the critical temperature. This situation holds also for the deformed-to-spherical shape phase transition.

Several theoretical frameworks have been invented to take into account the quantum fluctuations not restricted to those connected to the conservation laws; for instance, the static-path approximation (SPA) [2, 29, 30] and the shell-model Monte Carlo (SMMC) approach [31]. Whereas we have mainly focused our discussion on the projections in the mean-field approximations, it will be straightforward to incorporate the projections into the above extensive methods, in which the wave functions are represented by a superposition of
those in the mean-field theories. In practice, the SPA calculations with the particle-number and angular momentum projections have been carried out \[12, 32\], based on the conventional thermal formalism. With its simplicity the present TFD formulation of projections will be useful also in this course. The projections combined with the SMMC have been restricted to relatively simple cases \[3, 31\], in which \(\hat{P}, \hat{H}_0 = 0\) holds. The present formulation may help applying more general projections to the SMMC implementation; e.g. the angular momentum projection, and the particle-number projection in the pairing decomposition.

Acknowledgments

One of the authors (H. N.) acknowledge the financial support of the Grant-in-Aid for Scientific Research (B), No. 15340070, by the Ministry of Education, Culture, Sports, Science and Technology, Japan.

APPENDIX A: QUASIPARTICLE REPRESENTATION OF HAMILTONIAN

We here present the quasiparticle representation of the Hamiltonian \(\hat{H}'\) given in Eq. \(\text{[1]}\). The Hamiltonian is assumed to consist of up to the two-body interactions as in Eq. \(\text{[3]}\). Applying the Bogoliubov transformation in Eq. \(\text{[1]}\), we rewrite \(\hat{H}'\) in terms of quasiparticle operators,

\[
U_0 = \langle \text{vac.}|\hat{H}'|\text{vac.}\rangle - \lambda_p Z - \lambda_n N - \omega_{\text{rot}} \sqrt{J(J+1)}
= \text{Tr}_{s.p.} \left( \xi \rho^{(0)} + \frac{1}{2} \Gamma^{(0)} \rho^{(0)} + \frac{1}{2} \Delta^{(0)} K^{(0)} \right), \tag{A1a}
\]

\[
\hat{H}_{11} = \sum_{\mu \nu} (H_{11})_{\mu \nu} \alpha_\mu^\dagger \alpha_\nu, \tag{A1b}
\]

\[
\hat{H}_{20} = \frac{1}{2} \sum_{\mu \nu} \left[ (H_{20})_{\mu \nu} \alpha_\mu^\dagger \alpha_\nu^\dagger + (H_{20})^*_{\mu \nu} \alpha_\nu \alpha_\mu \right], \tag{A1c}
\]

\[
\hat{H}_{22} = \sum_{\mu \nu \rho \sigma} (H_{22})_{\mu \nu \rho \sigma} \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\rho \alpha_\sigma, \tag{A1d}
\]

\[
\hat{H}_{31} = \sum_{\mu \nu \rho \sigma} \left[ (H_{31})_{\mu \nu \rho \sigma} \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\sigma^\dagger \alpha_\rho + (H_{31})^*_{\mu \nu \rho \sigma} \alpha_\rho \alpha_\sigma \alpha_\nu \alpha_\mu \right], \tag{A1e}
\]

\[
\hat{H}_{40} = \sum_{\mu \nu \rho \sigma} \left[ (H_{40})_{\mu \nu \rho \sigma} \alpha_\mu^\dagger \alpha_\nu^\dagger \alpha_\sigma \alpha_\rho + (H_{40})^*_{\mu \nu \rho \sigma} \alpha_\rho \alpha_\sigma \alpha_\nu \alpha_\mu \right], \tag{A1f}
\]
where

\[
(H_{11})_{\mu\nu} = \bigg[ U^\dagger(\xi + \Gamma^{(0)}\Delta^{(0)}\Delta^{(0)*}U - V^\dagger(\xi + \Gamma^{(0)})^*V + U^\dagger\Delta^{(0)}V - V^\dagger\Delta^{(0)*}V\bigg]_{\mu\nu},
\]

\[
(H_{20})_{\mu\nu} = \bigg[ U^\dagger(\xi + \Gamma^{(0)}V^* - V^\dagger(\xi + \Gamma^{(0)})^*U^* + U^\dagger\Delta^{(0)}U^* - V^\dagger\Delta^{(0)*}V^*\bigg]_{\mu\nu},
\]

\[
(H_{22})_{\mu\nu\rho\sigma} = \frac{1}{4} \sum_{ijkl} v_{ijkl} \bigg[ U_{i\mu}^*U_{j\nu}U_{k\sigma}U_{l\rho} + V_{k\mu}^*V_{l\nu}V_{j\sigma}V_{i\rho} - U_{i\mu}^*V_{j\nu}U_{k\rho}U_{l\sigma} + U_{i\mu}^*V_{j\nu}U_{k\rho}V_{l\sigma} + U_{i\mu}^*V_{j\nu}U_{k\rho}U_{l\sigma} - U_{i\mu}^*V_{j\nu}V_{k\rho}V_{l\sigma}\bigg],
\]

\[
(H_{31})_{\mu\rho\sigma} = \frac{1}{6} \sum_{ijkl} v_{ijkl} \bigg[ U_{i\mu}^*U_{j\nu}U_{k\sigma}V_{l\rho} + U_{i\mu}^*V_{j\nu}V_{k\sigma}V_{l\rho} + U_{i\mu}^*U_{j\nu}U_{k\sigma}V_{l\rho}^* + U_{i\mu}^*U_{j\nu}V_{k\sigma}V_{l\rho}^* + U_{i\mu}^*U_{j\nu}U_{k\sigma}V_{l\rho}^* + U_{i\mu}^*U_{j\nu}V_{k\sigma}V_{l\rho}^*\bigg],
\]

\[
(H_{40})_{\mu\rho\sigma} = \frac{1}{24} \sum_{ijkl} v_{ijkl} \bigg[ U_{i\mu}^*U_{j\nu}U_{k\sigma}V_{l\rho}V_{l\sigma}^* - U_{i\mu}^*U_{j\nu}V_{k\rho}V_{l\sigma}^* - U_{i\mu}^*U_{j\nu}V_{k\rho}V_{l\sigma}^* - U_{i\mu}^*U_{j\nu}V_{k\rho}V_{l\sigma}^* - U_{i\mu}^*U_{j\nu}V_{k\rho}V_{l\sigma}^* - U_{i\mu}^*U_{j\nu}V_{k\rho}V_{l\sigma}^*\bigg].
\]

Definition of \( \xi \) is the same as given in Eq. (12). \( \Gamma^{(0)} \) and \( \Delta^{(0)} \) are defined in an analogous manner to Eq. (13), with the single-particle density \( \rho^{(0)} \) and the pair tensor \( \kappa^{(0)} \) defined by

\[
\rho_{ij}^{(0)} = \langle \text{vac}|c_j^\dagger c_i|\text{vac}\rangle = (V^*V^{tr})_{ij},
\]

\[
\kappa_{ij}^{(0)} = -\kappa_{ji}^{(0)} = \langle \text{vac}|c_j c_i|\text{vac}\rangle = (V^*U^{tr})_{ij}.
\]

**APPENDIX B: PROOF OF INEQUALITY USED IN SECTION IV**

Let \( F(x) \) be a real function, which is convex downwards (or concave upwards) in a simply connected domain of the variable \( x > 0 \), and \( x_0 \) belongs to the same domain. This leads to the inequality

\[
F(x) \geq F(x_0) + F'(x_0)(x - x_0).
\]

As far as \( F''(x) > 0 \), the the left-hand side (lhs) and the right-hand side (rhs) of Eq. (B1) become equal only at \( x = x_0 \). For a hermitian and non-negative operator \( \hat{O} \) and a given physical state \( |i\rangle \), the following relation turns out,

\[
\langle i|F(\hat{O})|i\rangle \geq F(\langle i|\hat{O}|i\rangle).
\]

This inequality is proven as follows.

First, we introduce a complete set of the eigenstates of the operator \( \hat{O} \), denoted by \( \{|k\}\} \). Each eigenstate \( |k\rangle \) satisfies

\[
\hat{O}|k\rangle = \langle k|\omega_k\rangle.
\]

Then, the state \( |i\rangle \) is expanded by \( \{|k\}\}

\[
|i\rangle = \sum_{k} |k\rangle u_{ki}.
\]
which is a unitary transformation. Using Eqs. (B1, B4), we obtain
\[
\langle i| F(\hat{O})| i \rangle = \sum_k |u_{ki}|^2 F(\omega_k) \\
\geq \sum_k |u_{ki}|^2 \left[ F(\langle i|\hat{O}|i \rangle) + F'(\langle i|\hat{O}|i \rangle)(\omega_k - \langle i|\hat{O}|i \rangle) \right] = F(\langle i|\hat{O}|i \rangle),
\]
by applying Eq. (B1) with setting \( x = \omega_k \) and \( x_0 = \langle i|\hat{O}|i \rangle \), and using \( \sum_k |u_{ki}|^2 = 1 \) and \( \sum_k |u_{ki}|^2 \omega_k = \langle i|\hat{O}|i \rangle \). It is now obvious that the lhs and the rhs of Eq. (B2) are equal only if \( |i\rangle \) is an eigenstate of \( \hat{O} \).

It has been verified \[17\] that, if \( F'(x) < 0 \) and \( F''(x) > 0 \), we have
\[
\sum_i \langle i| F(\hat{O})| i \rangle \geq \sum_i F(\langle i|\hat{O}|i \rangle).
\]
We have here derived the inequality (B2) in more general manner, by lifting the sum over \( i \) and the condition \( F'(x) < 0 \), besides that truncation scheme is also discussed in Ref. \[17\].

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