Thermal resonating Hartree-Bogoliubov theory based on the projection method*

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Dedicated to the Memory of Hideo Fukutome

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Abstract

We propose a rigorous thermal resonating mean-field theory (Res-MFT). A state
is approximated by superposition of multiple MF wavefunctions (WFs) composed of
non-orthogonal Hartree-Bogoliubov (HB) WFs. We adopt a Res-HB subspace spanned
by Res-HB ground and excited states. A partition function (PF) in a
$SO(2N)$ coherent state representation $|g\rangle$ ($N$:Number of single-particle states) is expressed as $\text{Tr}(e^{-\beta H}) = 2^{N-1}\int |g\rangle e^{-\beta H} |g\rangle dg$ ($\beta = 1/k_B T$). Introducing a projection operator $P$ to the Res-HB subspace, the PF in the Res-HB subspace is given as $\text{Tr}(Pe^{-\beta H})$, which is calculated within the Res-HB subspace by using the Laplace transform of $e^{-\beta H}$ and the projection method. The variation of the Res-HB free energy is made, which leads to a thermal HB density matrix $W^\text{thermal}_{\text{Res}}$ expressed in terms of a thermal Res-FB operator $F^\text{thermal}_{\text{Res}}$ as $W^\text{thermal}_{\text{Res}} = \{1_{2N} + \exp(\beta F^\text{thermal}_{\text{Res}})\}^{-1}$. A calculation of the PF by an infinite matrix continued fraction is cumbersome and a procedure of tractable optimization is too complicated. Instead, we seek for another possible and more practical way of computing the PF and the Res-HB free energy within the Res-MFT.

Keywords: Thermal resonating Hartree-Bogoliubov theory; Projection method

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1 Introduction

The strongly correlated fermion systems have been attracting much attention due to their abundant physical phenomenology such as, shape transition in nuclei, metal-insulator transition, high-$T_c$ superconductivity, magnetic substances with narrow $d$ bands. These latter electron systems show drastic electronic and magnetic changes by a slight environment modifications due to competitions of charge, magnetic and orbital orderings. All of the above systems are typical examples of the strongly correlated fermion systems. In the theoretical studies of such fermion systems, it is very important to treat fermion correlations and/or quantum fluctuations rigorously as far as possible. For this aim, several quantum many-body theories have been developed, such as Quantum Monte-Carlo simulation which provides a general technique to inspect numerically such systems \[1\], Real-Space Density Matrix Renomalization Group method \[2\] and Exact Diagonalization method \[3\]. There has been considerable progress both in a self-consistent mode-mode coupling theory for weak itinerant magnetism and a functional integral theory interpolating the extreme regimes of weak itinerant magnetism and localized spin moments \[4\]. The nature of electron correlation, particularly in a 2-D fermion system, has become an important problem in connection with high critical-temperature $T_c$ superconductivity. It is a new and hot unsolved problem. Twelve years have passed since Nagamatsu et al. discovered two-gap superconductivity (SC) of MgB$_2$ with $T_c=39K$ \[5\]. $T_c$ of conventional superconductors in the weak coupling regime has been described by the BCS theory \[6, 7\] and that of unconventional ones in the strong coupling has been done by the Eliashberg’s theory \[8\]. On the contrary, two gaps of MgB$_2$ have been predicted by Liu et al. \[9\], employing a weak-coupling two-gap model with the use of a $(\sigma, \pi)$ two-band model. Remember that the original idea of such a model was proposed long time ago by Suhl et al. and Kondo \[10, 11\]. On the other hand, employing the Eliashberg’s strong-coupling theory \[8\], Choi et al. \[12\] have also explained such properties of MgB$_2$. Further recent studies of new physics of high-$T_c$ superconductors have begun as viewed by Tohyama \[13\] in which hot topics in cuprate and iron-pnictide superconductors emerge. In cuprate ones, two-gap scenario is not necessarily inconsistent with the Anderson’s RVB theory \[14\]. While, according to Tohyama, it is natural to start with an itinerant model with a weak Coulomb interaction to describe electric structures of iron-pnictides. He and Kaneshita could explain a damping in high-energy spin excitation \[15\], using such an itinerant model and a theory based on an itinerant five-band Hubbard model and the random phase approximation \[16\]. These facts emphasize again an inevitable strict manipulation of the fermion correlations and/or quantum fluctuations mentioned above.

Now we are in a stage to study the above phenomena, particularly a currently topical high-$T_c$ problems such as $T_c$ itself and multi-gap standing on the spirit of the resonating mean-field. There exist many available theories for such problems. Among them, the resonating mean-field theory (Res-MFT) \[17, 18\] also may stand as a candidate for a possible and effective theory and is considered to be useful for such a theoretical approach. This is because the Res-MFT has a following characteristic feature: Fermion systems with large quantum fluctuations show serious difficulties in many-body problems at finite temperature. To approach such problems, Fukutome has developed the resonating Hartree-Fock theory (Res-HFT) \[17\] and Fukutome and one of the present authors (S.N.) have extended it directly to the resonating Hartree-Bogoliubov theory (Res-HBT) to include pair correlations \[18\] (referred to as I). This is our first motivation that we challenge such an exciting physics.
The Res-HBT is equivalent to the coupled Res-HB eigenvalue equations in which the orbital concept is still surviving though orbitals are resonating. This means that the band picture has a correspondence to the orbital concept in the Res-HB approximation though bands of different structures are resonating. The superposed HB wave functions (WFs) are the coherent state representations (CS reps). The Res-MFT was applied to describe a two-gap SC [19]. The Res-HFT has also been applied to the 1-D and 2-D Hubbard models [20] and has shown its own effectiveness by Fukutome and Tomita and their collaborators [21]. The applications of Res-HFT and Res-HBT have been, however, limited to the ground state property up to the present stage. To treat temperature-dependent phenomena such as high-$T_c$ superconductivity, an extension of the present theories to theories available for finite temperature case must be necessarily required. As the first trial, we have made an attempt at a Res-MFT description of thermal behavior of the two-gap SC [22] (referred to as II). The thermal variation has been made in a different way from the usual thermal-BCS theory [23, 24, 16] and got preliminary results. To improve solutions exactly, we construct a rigorous thermal Res-MFT basing on the projection-operator method and give another version of MF approximation describable a superconducting fermion system with $N$ single-particle states. A partition function in a $SO(2N)$ CS rep $|g⟩$ [25] is expressed as $\text{Tr}(e^{-\beta H})=2^{N-1}\int (⟨g|e^{-\beta H}|g⟩dg (\beta=1/k_BT)$ where integration is the group integration on the $SO(2N)$. Introducing a projection operator $P$ to the Res-HB subspace proposed in the Res-MFT [17, 18], the partition function in the Res-HB subspace is given as $\text{Tr}(Pe^{-\beta H})$. It is calculated within the Res-HB subspace by using the Laplace transform of $e^{-\beta H}$ and the projection operator method [26, 27, 28] which leads us to an infinite matrix continued fraction (IMCF).

The variation of the Res-HB free energy is executed parallel to the usual thermal BCS theory [6, 23, 24]. It induces a thermal HB density matrix $W_{\text{Res}}^\text{thermal}$ expressed in terms of a thermal Res-FB operator $F_{\text{Res}}^\text{thermal}$ as $W_{\text{Res}}^\text{thermal} = \{1_{2N} + \exp(\beta F_{\text{Res}}^\text{thermal})\}^{-1}$. The Res-HB coupled eigenvalue equation is extended to the thermal Res-HB coupled eigenvalue equation. A calculation of the partition function by the IMCF is very cumbersome and a procedure of tractable optimization is too complicated. Instead, we seek for another possible and more practical way of computing the Res-HB partition function and the Res-HB free energy within the framework of the Res-MFT.

In Sec. II we give a brief review of the Res-HBT. In Sec. III we derive an IMCF with the use of the projection operator. In Sec. IV, we give expressions for the thermal Res-HB density matrix and the thermal pair density matrix in term of the eigenvalues of the thermal Res-FB operator. We also propose tentative expressions for the thermal Res-HB interstate density matrix and overlap integral. In Sec. V, we introduce a quadratic Res-HB Hamiltonian and extend the HB free energy to the Res-HB free energy. In the occupation number space in a quasi-particle frame, we obtain explicit expressions for the approximately calculated Res-HB partition function and Res-HB free energy. Finally in Sec. VI, we give a summary and further perspectives. In Appendices, we provite a matrix element of the Laplace transform of $e^{-\beta H}$ and various types of matrix elements related to it. Further we give a proof of the commutability between thermal Res-FB operator and thermal HB density matrix and derive some equivalence relation.
2 Brief review of resonating Hartree-Bogoliubov theory

First, according to I let us briefly recapitulate the exact CS rep on a $SO(2N)$ group of a superconducting fermion system. We consider a fermion system with $N$ single-particle states. Let $c_\alpha$ and $c_\alpha^\dagger$, $\alpha = 1, \cdots, N$, be the annihilation and creation operators of the fermion. Owing to their anticommutation relation, the pair operators

\[
E_\alpha^\dagger = c_\alpha^\dagger c_\beta - \frac{1}{2}\delta_{\alpha\beta}, \quad E_\alpha = E_\alpha^\dagger, \\
E_{\alpha\beta} = c_\alpha c_\beta, \quad E^{\alpha\beta} = c_\alpha^\dagger c_\beta^\dagger, \quad E^{\alpha\overline{\beta}} = -E_{\alpha\overline{\beta}},
\]

(2.1)
satisfy the commutation relations of the $SO_z$ group on the Hilbert space of even fermion numbers. From this and the orthogonality of irrep matrices, a state vector is represented as

\[
\langle c \mid 0 \rangle = \frac{1}{\sqrt{2}} \int U(g) \Psi(g) dg,
\]

where the $(c, c^\dagger)$ is the $2N$-dimensional row vector $((c_\alpha), (c_\beta^\dagger))$ and the $a = (a_{\alpha\overline{\beta}})$ and $b = (b_{\alpha\beta})$ are $N \times N$ matrices, respectively. The $1_{2N}$ is the $2N$-dimensional unit matrix. $U(g)$ is an irreducible representation (irrep) of the $SO(2N)$ group on the Hilbert space of even fermion numbers. From this and the group integration on the $SO(2N)$, the $|0\rangle$ is a vacuum satisfying $c_\alpha |0\rangle = 0$. The $|g\rangle = U(g)|0\rangle$ is an HB WF and $\Psi(g) = \langle 0 | U^\dagger(g) | \Psi \rangle$. This is an exact $SO(2N)$ CS rep of a state vector $[29] [7]$. We define the overlap integral $\langle g | g' \rangle$ by

\[
\langle g | g' \rangle = \langle 0 | U^\dagger(g) U(g') | 0 \rangle = \langle 0 | U(g^\dagger g') | 0 \rangle.
\]

(2.5)

For the Hamiltonian $H$ of the fermion system, by using Eq. (2.4), the Schrödinger equation $(H - E) | \Psi \rangle = 0$ is converted to an integral equation on the $SO(2N)$ group

\[
\int \{ \langle g | H | g' \rangle - E \langle g | g' \rangle \} \Psi(g') dg' = 0, \quad \langle g | H | g' \rangle = \langle 0 | U^\dagger(g) H U(g') | 0 \rangle.
\]

(2.6)

From $\langle 0 | U(g) | 0 \rangle = [\det a]^\frac{1}{2}$, where det is determinant, and (2.3), we have an overlap integral

\[
\langle g | g' \rangle = [\det(a^\dagger a' + b^\dagger b')]^\frac{1}{2} = [\det z]^\frac{1}{2}, \quad z \equiv u^\dagger u', \quad z = (z_{ij}),
\]

(2.7)

where we introduce a $2N \times N$ isometric matrix $u$ by

\[
u = \begin{bmatrix} b \\ a \end{bmatrix}, \quad u^\dagger u = 1_N,
\]

(2.8)

so that $z$ is an $N \times N$ matrix.
The matrix elements of the pair operators (2.11) and a two-body operator between two HB WFs are calculated as follows:

\[ \langle g | E^\alpha_\beta + \frac{1}{2} \delta_{\alpha\beta} | g' \rangle = R_{\alpha\beta}(g, g') \cdot [\det z]^{1/2}, \quad R(g, g') = b' z^{-1} b', \]  

(2.9)

\[ \langle g | E_{\alpha|\beta} | g' \rangle = K_{\alpha\beta}(g, g') \cdot [\det z]^{1/2}, \quad K(g, g') = b' z^{-1} a^\dagger, \]  

(2.10)

\[ \langle g | E^{\alpha\gamma} E_{\delta\beta} | g' \rangle = \{ R_{\alpha\beta}(g, g') R_{\delta\gamma}(g, g') - R_{\delta\alpha}(g, g') R_{\beta\gamma}(g, g') - K^{*}_{\alpha\gamma}(g', g) K_{\delta\beta}(g, g') \} \cdot [\det z]^{1/2}. \]  

(2.11)

Let the Hamiltonian \( H \) of the system under consideration be

\[ H = h_{\alpha\beta} \left( E^\alpha_\beta + \frac{1}{2} \delta_{\alpha\beta} \right) + \frac{1}{4} [\alpha\beta][\gamma\delta] E^{\alpha\gamma} E_{\delta\beta}, \]  

(2.12)

in which the matrix \( h_{\alpha\beta} \) related to a single-particle Hamiltonian includes a chemical potential and the antisymmetrized matrix element of the interaction \( [\alpha\beta][\gamma\delta] \) satisfies the relations

\[ [\alpha\beta][\gamma\delta] = -[\alpha\delta][\gamma\beta] = [\gamma\delta][\alpha\beta] = [\beta\alpha][\delta\gamma]^*. \]  

(2.13)

Here we use the dummy index convention to take summation over the repeated indices.

Following I., we briefly recapitulate a new eigenvalue equation called the Res-HB eigenvalue equation. In quite a parallel manner to the Res-HF by Fukutome [17]. We approximate a low energy eigenstate \( |\Psi_{\text{Res}}\rangle \) of the Hamiltonian \( H \) by a discrete superposition of HB WFs which are denoted by \( |g_r\rangle, |g_s\rangle \cdots \). The \( |g_r\rangle \)'s are non-orthogonal and represent different collective correlation states. Then, the state \( |\Psi_{\text{Res}}\rangle \) is given as

\[ |\Psi_{\text{Res}}\rangle = \sum_{s=1}^{N} |g_s\rangle c_s. \]  

(2.14)

The general form of the \( N \times N \) matrix \( z \) and the \( 2N \times 2N \) HB interstate density matrix between \( |g_r\rangle \) and \( |g_s\rangle \) are, respectively, defined as

\[ z_{rs} = u_{s}^\dagger u_{r}, \quad W_{rs} = u_{s} z_{rs}^{-1} u_{r}^\dagger = W_{sr}^\dagger, \]  

(2.15)

whose matrix form is given as

\[ W_{rs} = \begin{bmatrix} R_{rs} & K_{rs} \\ -K^{*}_{sr} & 1_N - R^{*}_{sr} \end{bmatrix}, \quad W_{rs}^2 = W_{rs}, \]  

(2.16)

where \( R_{rs} \) and \( K_{rs} \) denote the densities and the pair densities and \( R_{sr} \) and \( K_{sr} \) mean the transition densities. The mixing coefficients \( c_s \) are normalized by the relation

\[ \langle \Psi_{\text{Res}} | \Psi_{\text{Res}} \rangle = \sum_{r,s=1}^{n} \langle g_r | g_s \rangle c_r^* c_s = \sum_{r,s=1}^{n} [\det z_{rs}]^{1/2} c_r^* c_s = 1. \]  

(2.17)

Using Eq. (2.16), the expectation value of the Hamiltonian \( H \) by the state \( |\Psi_{\text{Res}}\rangle \) is given as

\[ \langle \Psi_{\text{Res}} | H | \Psi_{\text{Res}} \rangle = \sum_{r,s=1}^{n} \langle g_r | H | g_s \rangle c_r^* c_s = \sum_{r,s=1}^{n} H[W_{rs}] \cdot [\det z_{rs}]^{1/2} c_r^* c_s. \]  

(2.18)

For our aim of further discussions, we adopt the following Lagrangian \( L_{\text{Res}}^{\text{HB}} \) with the Lagrange multiplier term to secure the normalization condition (2.17):

\[ L_{\text{Res}}^{\text{HB}} = \]
In the case of the temperature $T = 0$, the variation of $L_{\text{Res}}^\text{HB}$ with respect to $c_r^*$ leads to the Res-HB configuration interaction (CI) equation to determine the mixing coefficients $c_s$

$$\sum_{s=1}^n \{H[W_{rs}] - E\} \cdot [\det z_{rs}]^{\frac{1}{2}} c_s^* c_s = 0.$$  (2.20)

By the variations with respect to the HB interstate density matrix $W$ and the overlap integral $[\det z]^\frac{1}{2}$, we obtain the Res-HB equation to determine the $u_r$'s as

$$\sum_{s=1}^n \mathcal{K}_{rs} c_s^* c_s = 0,$$

$$\mathcal{K}_{rs} \equiv \{(1_{2N} - W_{rs}) F[W_{rs}] + H[W_{rs}] - E\} \cdot W_{rs} \cdot [\det z_{rs}]^{\frac{1}{2}},$$  (2.21)

in which the Fock-Bogoliubov (FB) operator is introduced as

$$F[W_{rs}] = \begin{bmatrix} F_{rs} & D_{rs} \\ -D_{sr}^* & -F_{sr}^* \end{bmatrix},$$  (2.22)

where the $N \times N$ matrices $F_{rs}$ and $D_{rs}$ are the functional derivatives of the $H[W_{rs}]$ with respect to the $W_{rs}^T$ in which $r$ stands for the transposition of a matrix. They are defined as

$$F_{rs;\alpha\beta} \equiv \frac{\delta H[W_{rs}]}{\delta R_{rs;\alpha\beta}} = h_{\alpha\beta} + [\alpha \beta | \gamma \delta] R_{rs;\gamma\delta},$$

$$D_{rs;\alpha\beta} \equiv \frac{\delta H[W_{rs}]}{\delta K_{sr;\alpha\beta}^*} = -\frac{1}{2} [\alpha \gamma | \beta \delta] K_{rs;\gamma\delta}.$$

It has already been shown in I that equation (2.21) is equivalent to the following Res-HB coupled eigenvalue equations:

$$[\mathcal{F}_r u_r]_i = \epsilon_{ri} u_{ri}, \quad \epsilon_{ri} \equiv \bar{\epsilon}_{ri} - \{H[W_{rr}] - E\} |c_r|^2,$$

$$\mathcal{F}_r \equiv \mathcal{F}[W_{rr}] |c_r|^2 + \sum_{s=1}^n (\mathcal{K}_{rs} c_s^* c_s + \mathcal{K}_{sr}^* c_r^* c_s) = \mathcal{F}_r^2,$$  (2.24)

where the primed summation is made under the restriction $s \neq r$ and the quasi-particle energy $\bar{\epsilon}_r = u_r^2 \mathcal{F}[W_{rr}] |c_r|^2 u_r = \delta_{ij} \bar{\epsilon}_{ri}$ satisfies the property of the usual HB orbital energy:

$$\bar{\epsilon}_r = \begin{bmatrix} \bar{\epsilon}_{r1} & \cdots & 0 \\ 0 & -\bar{\epsilon}_{r1} & \cdots \\ \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & -\bar{\epsilon}_{rN} \end{bmatrix}.$$  (2.25)

The $2N \times 2N$ matrix $\mathcal{F}_r$ is called the Res-Fock-Bogoliubov (Res-FB) operator. The Res-HB eigenvalue equation (2.21) means that every HB eigenfunction in a HB resonating state has its own orbital energies $\epsilon_r$, which declares the survival of the orbital concept in the Res-HB theory, though orbitals of different structures are resonating. The Res-HB CI equation (2.20) and the Res-HB eigenvalue equation (2.24) is solved iteratively if we start from suitable trial $u_r$'s. Once the HB WFs $|g_{fr}\rangle$ in the Res-HB ground state are determined, then the other solutions of the Res-HB CI equation give a series of the Res-HB excited states called resonon excitations. To show the usefulness of the Res-HBT without unnecessary complications, we have first applied it to a problem of describing the coexistence phenomenon of two deformed-shapes occurred in a simple and schematic model of nuclei [30], using the Bogoliubov-Valatin transformation [31]. The Res-HFT with the usual S-det has been applied to a simple LMG model of nuclei [32, 33], a NJL model of hadron [34, 35, 36] and that with spin-projected S-det is applied to a 1-D half-filled Hubbard model [37, 20, 21].
3 Derivation of infinite matrix continued fraction with the use of projection operator

As proved in II, the explicit form of partition function in the Res-HB subspace is given as

$$\text{Tr}(P e^{-\beta H}) = \sum_{r,s=1}^{n} \langle g_r | e^{-\beta H} | g_s \rangle (S^{-1})_{sr}, \quad (P \equiv \sum_{r,s=1}^{n} | g_r \rangle \langle S^{-1} | g_s \rangle,$$  \hspace{1cm} (3.1)

the R.H.S. of which is brought into a form suitable for applying the projection method by Fulde [38]. For this purpose we introduce the Laplace transform of \( f(\beta) = e^{-\beta H} \) and \( Q = 1 - P \),

$$\mathcal{L}\{f(\beta)\} = \tilde{f}(\tau) \equiv \int_{0}^{\infty} e^{-\tau \beta} e^{-\beta H} d\beta = \frac{1}{\tau + H} = \frac{1}{\tau + HQ} - \frac{1}{\tau + HQ} HP \frac{1}{\tau + H}, \quad (\text{Re}\{\tau\} > 0),$$  \hspace{1cm} (3.2)

We aim at evaluating the matrix \( \tilde{\mathcal{R}}(\tau) \) whose matrix elements are given by

$$\tilde{\mathcal{R}}_{uv}(\tau) = \langle g_u | \frac{1}{\tau + H} | g_v \rangle \equiv \tilde{\mathcal{R}}^{(0)}_{uv}(\tau). \quad (u, v = 1, \ldots, n)$$  \hspace{1cm} (3.3)

Let us denote \( H, \ | g_v \rangle, \ P, \ Q \) and \( S \) as \( H^{(0)}, \ | g_v^{(0)} \rangle, \ P^{(0)}, \ Q^{(0)} \) and \( S^{(0)} \), respectively. Using (3.2) we can express \( \tilde{\mathcal{R}}^{(0)}_{uv}(\tau) \) in the following form:

$$\tilde{\mathcal{R}}^{(0)}_{uv}(\tau) = \langle g_u | \frac{1}{\tau + H^{(0)}Q^{(0)}} | g_v^{(0)} \rangle - \langle g_u | \frac{1}{\tau + H^{(0)}Q^{(0)}} | g_v^{(0)} \rangle H^{(0)}P^{(0)} \frac{1}{\tau + H^{(0)}} | g_v^{(0)} \rangle.$$  \hspace{1cm} (3.4)

The first term is simply calculated as

$$\langle g_u | \frac{1}{\tau + H^{(0)}Q^{(0)}} | g_v^{(0)} \rangle = \frac{1}{\tau} \sum_{k=0}^{\infty} \langle g_u | \left( -\frac{H^{(0)}Q^{(0)}}{\tau} \right)^k | g_v^{(0)} \rangle = \frac{1}{\tau} \tilde{S}^{(0)}_{uv},$$  \hspace{1cm} (3.5)

where we have used \( Q^{(0)} | g_v^{(0)} \rangle = (1 - P^{(0)}) | g_v^{(0)} \rangle = 0 \) which is easily proved. Inserting the projection operator \( P^{(0)} \) into the second term in the second line of (3.4), it is rewritten as

$$- \langle g_u | \frac{1}{\tau + H^{(0)}Q^{(0)}} | H^{(0)}P^{(0)} \frac{1}{\tau + H^{(0)}} | g_v^{(0)} \rangle$$

$$= - \frac{1}{\tau} \sum_{r,s=1}^{n} \langle g_u | \frac{\tau + H^{(0)}Q^{(0)} - H^{(0)}Q^{(0)}H^{(0)} | g_r^{(0)} \rangle (S^{(0)-1})_{rs} \tilde{\mathcal{R}}^{(0)}_{uv}(\tau)$$

$$= \frac{1}{\tau} \sum_{r,s=1}^{n} \left[ L^{(0)}_{ur} + M^{(0)}_{ur}(\tau) \right] (S^{(0)-1})_{rs} \tilde{\mathcal{R}}^{(0)}_{uv}(\tau),$$  \hspace{1cm} (3.6)

where \( L^{(0)}_{ur} \) and \( M^{(0)}_{ur}(\tau) \) are defined as

$$L^{(0)}_{ur} \equiv - \langle g_u^{(0)} | H^{(0)} | g_r^{(0)} \rangle, \quad M^{(0)}_{ur}(\tau) \equiv \langle g_u^{(0)} | H^{(0)}Q^{(0)} \frac{1}{\tau + Q^{(0)}H^{(0)}Q^{(0)}} Q^{(0)}H^{(0)} | g_v^{(0)} \rangle.$$  \hspace{1cm} (3.7)

In expressing the \( M^{(0)}_{ur}(\tau) \), second equation of (3.7), we have used the idempotency relation \( Q^{(0)2} = Q^{(0)} \). Finally, substituting (3.5) and (3.6) into (3.4) and solving \( \tilde{\mathcal{R}}^{(0)}_{uv}(\tau) \) in a matrix notation, we have

$$\tilde{\mathcal{R}}^{(0)}(\tau) = \frac{1}{\tau I - [L^{(0)} + M^{(0)}(\tau)] S^{(0)-1} S^{(0)}}.$$  \hspace{1cm} (3.8)

In the above, different from the projection method by Fulde [38], we do not introduce the Liouville operator \( LA \equiv [H, A] \) for any operator \( A \) but use the original Hamiltonian \( H \). Further, to calculate the elements of the so-called memory matrix \( M^{(0)}_{ur}(\tau) \), we introduce the state \( | g_r^{(1)} \rangle \equiv Q^{(0)}H^{(0)} | g_r^{(0)} \rangle \) and the projection operator as
\[
P^{(1)} = \sum_{r,s=1}^{n} |g_{r}^{(1)}\rangle \langle S_{r}^{(1)-1}g_{s}^{(1)}| = P^{(1)\dagger}, \quad Q^{(1)} = 1 - P^{(1)},
\]
\[
P^{(1)2} = P^{(1)}, \quad Q^{(1)2} = Q^{(1)}, \quad P^{(1)}Q^{(1)} = Q^{(1)}P^{(1)} = 0,
\]

where \(S^{(1)} = (S_{rs}^{(1)}) = (g_{r}^{(1)}|g_{s}^{(1)}\rangle = \langle g_{0}^{(0)}|H^{(0)\dagger}H^{(0)}|g_{0}^{(0)}\rangle\) is an \(n \times n\) matrix and \(S^{(1)\dagger} = S^{(1)}\).

Using \(H^{(1)} \equiv Q^{(0)\dagger}H^{(0)\dagger}Q^{(0)}\) and the second equation of (3.7) we can express \(M_{uv}^{(0)}(\tau)\) as
\[
M_{uv}^{(0)}(\tau) = \langle g_{u}^{(1)}| \frac{1}{\tau + H^{(1)}} (Q^{(1)} + P^{(1)}) |g_{v}^{(1)}\rangle = \tilde{R}_{uv}^{(1)}(\tau)
\]
\[
= \langle g_{u}^{(1)}| \frac{1}{\tau + H^{(1)}} |g_{v}^{(1)}\rangle - \langle g_{u}^{(1)}| \frac{1}{\tau + H^{(1)}} H^{(1)}P^{(1)} \frac{1}{\tau + H^{(1)}} |g_{v}^{(1)}\rangle.
\] (3.10)

The first term is simply calculated in the same way as (3.5). Inserting the projection operator \(P^{(1)}\), first equation of (3.9), into the second term in second line of (3.10), we have
\[
-\langle g_{u}^{(1)}| \frac{1}{\tau + H^{(1)}} H^{(1)}P^{(1)} \frac{1}{\tau + H^{(1)}} |g_{v}^{(1)}\rangle
\]
\[
= -\frac{1}{\tau} \sum_{r,s=1}^{n} \langle g_{u}^{(1)}| \frac{\tau + H^{(1)}}{\tau + H^{(1)}Q^{(1)}} H^{(1)} |g_{r}^{(1)}\rangle (S_{r}^{(1)-1})_{rs} \tilde{R}_{sv}^{(1)}(\tau)
\]
\[
= \frac{1}{\tau} \sum_{r,s=1}^{n} \left[ L_{ur}^{(1)} + M_{uv}^{(1)}(\tau) \right] (S^{(1)-1})_{rs} \tilde{R}_{sv}^{(1)}(\tau),
\] (3.11)

\[
L_{ur}^{(1)} \equiv -\langle g_{u}^{(1)}|H^{(1)}|g_{r}^{(1)}\rangle, \quad M_{uv}^{(1)}(\tau) \equiv \langle g_{u}^{(1)}|H^{(1)}Q^{(1)} \frac{1}{\tau + Q^{(1)\dagger}H^{(1)}Q^{(1)}} Q^{(1)}H^{(1)}|g_{r}^{(1)}\rangle.
\] (3.12)

Solving \(\tilde{R}_{r}^{(1)}(\tau)\) of (3.10) in a matrix form, we have
\[
\tilde{R}_{r}^{(1)}(\tau) = \frac{1}{\tau \Pi - [L^{(1)} + M^{(1)}(\tau)] S^{(1)-1} S^{(1)}} S^{(1)}, \quad M^{(1)}(\tau) = \tilde{R}_{r}^{(2)}(\tau).
\] (3.13)

Substituting (3.13) into (3.8) and repeating the above procedure, ultimately we can get the final expression for \(\tilde{R}_{r}^{(0)}(\tau)\) in terms of IMCFs \(39 \ 40 \ 41 \) and \(42 \ 43 \ 44 \ 45 \ 46 \ 47\):
\[
\tilde{R}_{r}^{(0)}(\tau) = \frac{1}{\tau \Pi - [L^{(0)} + \frac{1}{\tau \Pi - [L^{(2)} + \cdots] S^{(2)-1} S^{(1)-1}]} S^{(0)-1} S^{(1)}} S^{(0)},
\] (3.14)

where we have introduced the following state and projection operator
\[
|g_{r}^{(l)}\rangle \equiv Q^{(l-1)\dagger}H^{(l-1)\dagger} |g_{r}^{(l-1)}\rangle = Q^{(l-1)\dagger}H^{(l-1)\dagger} Q^{(l-2)\dagger}H^{(l-2)\dagger} \cdots Q^{(0)\dagger}H^{(0)\dagger} |g_{0}^{(0)}\rangle,
\]
\[
Q^{(l)} \equiv 1 - \sum_{r,s=1}^{n} \langle g_{r}^{(l)}| S_{r}^{(1)-1} g_{s}^{(l)}\rangle, \quad Q^{(l)2} = Q^{(l)}, \quad S_{rs}^{(l)} \equiv \langle g_{r}^{(l)}| g_{s}^{(l)}\rangle, \quad (l \geq 2)
\] (3.15)

and \(\tau\)-independent matrix element \(L_{ur}^{(l)} \equiv -\langle g_{r}^{(l)}|H^{(l)}|g_{r}^{(l)}\rangle\) where \(H^{(l)} \equiv Q^{(l-1)\dagger}H^{(l-1)\dagger}Q^{(l-1)}\).

The first few matrices \(S_{rs}^{(l)}\) and \(L_{ur}^{(l)}\) are given in Appendix A. Finally, going back to the
of the original expression $\tilde{R}_{rs}(=\tilde{R}_{rs}(0))$ and making the inverse Laplace transform $\mathcal{L}^{-1}$, we can reach the desired partition function in the Res-HB subspace as

$$\text{Tr}(Pe^{-\beta H}) = \sum_{r,s=1}^{n} \mathcal{L}^{-1} \left\{ \tilde{R}_{rs}(\tau) \right\} = \sum_{r,s=1}^{n} \tilde{R}_{rs}(\beta) (S^{-1})_{sr}. \quad (3.16)$$

The form of IMCF (3.14) is also derived from the so-called tridiagonal vector recurrence relation for a first-order time derivative of $c$ which is quite similar to the form of (3.14). In the above if we choose $c_{n}$ and constant (p.p. 217-219), let us introduce a Green’s function matrix for $c$ of (3.17) is expressed in terms of the Green’s function matrix with an initial condition as

$$c_m(t) = \sum_{m=0}^{\infty} G_{m,m'}(t)c_m(0), \quad G_{m,m'}(0) = \mathbb{I}\delta_{m,m'}. \quad (3.18)$$

Substituting (3.18) into (3.17) and making a Laplace transform we obtain the following relation as a sufficient condition for the solution of (3.17):

$$Q_{m}^{-} \tilde{G}_{m-1,m'}(\tau) + (Q_{m} - \tau \mathbb{I}) \tilde{G}_{mm'}(\tau) + Q_{m}^{+} \tilde{G}_{m+1,m'}(\tau) = -\mathbb{I}\delta_{m,m'}. \quad (3.19)$$

Further introduce a matrix $\tilde{S}_{m}^{+}(\tau)$ which raises the number of the left index of the Laplace transformed Green’s function matrix through the relation

$$\tilde{G}_{m+1,m'}(\tau) = \tilde{S}_{m}^{+}(\tau) \tilde{G}_{m,m'}(\tau). \quad (3.20)$$

For the moment neglecting the inhomogeneous term in (3.19), we have

$$Q_{m}^{-} \tilde{G}_{m-1,m'}(\tau) + \left[ Q_{m} - \tau \mathbb{I} + Q_{m}^{+} \tilde{S}_{m}^{+}(\tau) \right] \tilde{G}_{m,m'}(\tau) = 0. \quad (3.21)$$

By multiplying (3.21) with the inverse of the matrix in the parenthesis and by comparing the result with the relation $\tilde{G}_{m,m'}(\tau) = \tilde{S}_{m-1}^{+}(\tau) \tilde{G}_{m-1,m'}(\tau)$, which is derived from (3.20), we can immediately obtain $\tilde{S}_{m-1}^{+}(\tau) = \left[\tau \mathbb{I} - Q_{m} - Q_{m}^{+} \tilde{S}_{m}^{+}(\tau)\right]^{-1} Q_{m}^{-}$. By the iteration we get the following relation in terms of IMCFs:

$$\tilde{S}_{m}^{+}(\tau) = \left[\tau \mathbb{I} - Q_{m+1} - Q_{m+1}^{+} \left[\tau \mathbb{I} - Q_{m+2} - Q_{m+2}^{+} \left[\tau \mathbb{I} - Q_{m+3} - \cdots \right]^{-1} Q_{m+3}^{-}\right]^{-1} Q_{m+2}^{-}\right]^{-1} Q_{m+1}^{-}. \quad (3.22)$$

Putting $m=0$, we can obtain the final expression for $\tilde{S}_{0}^{+}(\tau)$ as

$$\tilde{S}_{0}^{+}(\tau) = \frac{1}{\tau \mathbb{I} - Q_{1} - Q_{1}^{+}} \frac{1}{\tau \mathbb{I} - Q_{2} - Q_{2}^{+}} \frac{1}{\tau \mathbb{I} - Q_{3} - \cdots} \frac{1}{Q_{1}^{-}}, \quad (3.23)$$

which is quite similar to the form of (3.14). In the above if we choose $\tilde{S}_{0}^{+}(\tau)$, $Q_{m}$, $Q_{m}^{+}$ and $Q_{m}^{-}$ as

$$\tilde{S}_{0}^{+}(\tau) = \tilde{R}_{0}(\tau), \quad S^{[-1]} = \mathbb{I},$$

$$Q_{m} = \mathbb{I}(m-1)S^{[-1]}(m-1), \quad Q_{m}^{+} = \mathbb{I}, \quad Q_{m}^{-} = S^{[-1]}(m-2), \quad (3.24)$$

for $m=1, 2, \cdots$, respectively, the IMCF (3.23) just coincides with the previous IMCF (3.14).
4 Expression for thermal HB density matrix in terms of eigenvalues of thermal Res-FB operator

First we give the commutability relation and the equivalence relation

\[ [F_{\text{Res:F}}^{\text{thermal}}, W_{\text{Res:F}}^{\text{thermal}}] = 0, \] (4.1)

\[ \sum_{k=1}^{n} \sum_{s=1}^{n} \mathcal{K}_{\text{Res:F}}^{\text{thermal}}(k) c_{r}^{(k)} c_{s}^{(k)} = F_{\text{Res:F}}^{\text{thermal}} W_{\text{Res:F}}^{\text{thermal}} - W_{\text{Res:F}}^{\text{thermal}} F_{\text{Res:F}}^{\text{thermal}} W_{\text{Res:F}}^{\text{thermal}}. \] (4.2)

where \( \mathcal{K}_{\text{Res:F}}^{\text{thermal}}(k) \) is defined as

\[ \mathcal{K}_{\text{Res:F}}^{\text{thermal}}(k) = \{(1_{2N} - W_{\text{Res:F}}^{\text{thermal}}) F_{\text{Res:F}}^{\text{thermal}} W_{\text{Res:F}}^{\text{thermal}} + H W_{\text{Res:F}}^{\text{thermal}} - E_{r}^{(k)}\} \cdot W_{\text{Res:F}}^{\text{thermal}} \cdot [\det z_{\text{Res:F}}^{\text{thermal}}]^{\frac{1}{2}}. \] (4.3)

Both the relations (4.1) and (4.2) are proved in Appendix B. As shown in II, using (4.2), the direct variation of the Res-HB free energy leads us to the \( n^{\text{th}} \) thermal HB density matrix \( W_{\text{Res:F}}^{\text{thermal}} \), which is expressed in terms of the \( n^{\text{th}} \) thermal Res-FB operator \( F_{\text{Res:F}}^{\text{thermal}} \), as

\[ W_{\text{Res:F}}^{\text{thermal}} = \frac{1}{1_{2N} + \exp\{\beta F_{\text{Res:F}}^{\text{thermal}}\}}, \quad (r = 1, \cdots, n), \] (4.4)

where we have used again the relation \([F_{\text{Res:F}}^{\text{thermal}}, W_{\text{Res:F}}^{\text{thermal}}] = 0\). We rewrite \( W_{\text{Res:F}}^{\text{thermal}} \) as \( W_{\text{Res:F}}^{\text{thermal}} \) for later convenience. By using a Bogoliubov transformation \( g_{r} \), the \( W_{\text{Res:F}}^{\text{thermal}} \) is diagonalized as follows:

\[ \tilde{W}_{r} = g_{r} W_{\text{Res:F}}^{\text{thermal}} g_{r}^{\dag} \]

\[ = \begin{bmatrix} \tilde{w}_{r1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 - \tilde{w}_{rN} \end{bmatrix} = \begin{bmatrix} \tilde{w}_{r} & 0 \\ 0 & 1 - \tilde{w}_{r} \end{bmatrix}, \] (4.5)

where

\[ \tilde{w}_{r} = \frac{1}{1 + \exp\{\beta \epsilon_{r}^{\text{thermal}}\}}, \quad 1 - \tilde{w}_{r} = \frac{1}{1 + \exp\{-\beta \epsilon_{r}^{\text{thermal}}\}}, \quad (r = 1, \cdots, n) \] (4.6)

The diagonalization of the \( r^{\text{th}} \) thermal Res-FB operator \( F_{\text{Res:F}}^{\text{thermal}} \) by the same Bogoliubov transformation \( g_{r} \) leads to the eigenvalue \( \epsilon_{r}^{\text{thermal}} \). To this eigenvalue by adding a term \( \sum_{k=1}^{n} \{H W_{\text{Res:F}}^{\text{thermal}} - E_{r}^{(k)}\} |c_{r}^{(k)}|^{2} \cdot 1_{2N} \), the usual HB type of the eigenvalue \( \epsilon_{r}^{\text{thermal}} \) is realized. Using (4.5) we can derive the inverse transformation of (4.5) in the form

\[ g_{r} W_{\text{Res:F}}^{\text{thermal}} g_{r}^{\dag} = g_{r} W_{\text{Res:F}}^{\text{thermal}} g_{r}^{\dag} = \frac{1}{1_{2N} + \exp\{\beta F_{\text{Res:F}}^{\text{thermal}} + \sum_{k=1}^{n} \{H W_{\text{Res:F}}^{\text{thermal}} - E_{r}^{(k)}\} |c_{r}^{(k)}|^{2} \cdot 1_{2N}\}} g_{r} \]

\[ = \tilde{W}_{r} = \begin{bmatrix} \tilde{w}_{r} & 0 \\ 0 & 1_{N} - \tilde{w}_{r} \end{bmatrix} \] (4.7)

\[ \text{10} \]
Inversely transforming again, the desired \( r \)th thermal HB density matrix is obtained as

\[
W_{\text{Res}:rr}^{\text{thermal}} = g_r^* \tilde{W}_r g_r^T = \begin{bmatrix} a_r^* & b_r \\ b_r^* & a_r \end{bmatrix} \begin{bmatrix} \tilde{w}_r & 0 \\ 0 & 1_N - \tilde{w}_r \end{bmatrix} \begin{bmatrix} a_r^T & b_r^T \\ b_r & a_r^* \end{bmatrix}
\]

(4.8)

from which and the thermal density matrix \( W_{\text{Res}:rr}^{\text{thermal}} \) defined by the second equation of (2.6) in II but with \( s = r \), we have

\[
\begin{align*}
R_{\text{Res}:rr}^{\text{thermal}} &= a_r^* \tilde{w}_r a_r^T + b_r (1_N - \tilde{w}_r) b_r^T, \\
K_{\text{Res}:rr}^{\text{thermal}} &= a_r^* \tilde{w}_r b_r^T + b_r (1_N - \tilde{w}_r) a_r^T.
\end{align*}
\]

(4.9)

Further substituting (4.9) into \( F \) and \( D \) matrices given by (2.23), we can obtain

\[
\begin{align*}
F_{\text{Res}:rr;\alpha\beta}^{\text{thermal}} &= h_{\alpha\beta} + [\alpha\beta|\gamma\delta] R_{\text{Res}:rr;\delta\gamma}^{\text{thermal}}, \\
D_{\text{Res}:rr;\alpha\beta}^{\text{thermal}} &= -\frac{1}{2} [\alpha\gamma|\beta\delta] K_{\text{Res}:rr;\delta\gamma}^{\text{thermal}}.
\end{align*}
\]

(4.10)

The above formulas are the direct extension of the result and the condition for the self-consistent field (SCF) given by the single HB WF \([48, 49]\) to those by the multiple HB WFs. The explicit temperature dependence of the thermal HB interstate density matrix \( W_{\text{Res}:rs}^{\text{thermal}} \), however, can not be determined directly within the framework of the present theory.

The whole Res-HB subspace and the thermal Res-FB operator are represented in the forms of the direct sum, respectively, as

\[
g = \begin{bmatrix} g_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & g_n \end{bmatrix} = \sum_{r=1}^n \oplus g_r, \quad g_r = \begin{bmatrix} a_r & b_r^* \\ b_r & a_r^* \end{bmatrix},
\]

(4.11)

\[
F_{\text{Res}}^{\text{thermal}} = \begin{bmatrix} F_{\text{Res}:1}^{\text{thermal}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & F_{\text{Res}:n}^{\text{thermal}} \end{bmatrix} = \sum_{r=1}^n \oplus F_{\text{Res}:r}^{\text{thermal}}.
\]

(4.12)

The HB density matrix in the whole Res-HB subspace \( W_{\text{Res}} \) is also given in the form of the direct sum \( \sum_{r=1}^n \oplus W_{\text{Res}:rr} \). On the other hand, the thermal HB density matrix in the whole Res-HB subspace is also given in the form of the direct sum

\[
W_{\text{Res}}^{\text{thermal}} = g^* \tilde{W}_g g^T = \sum_{r=1}^n \oplus W_{\text{Res}:rr}^{\text{thermal}}, \quad W_{\text{Res}:rr}^{\text{thermal}} = g_r^* \tilde{W}_r g_r^T,
\]

(4.13)
however, in which the idempotency relation $W^{\text{thermal}}_{\text{Res};rs}^2 = W^{\text{thermal}}_{\text{Res};rs}$ is no longer approved.

Up to the present stage, we have not any knowledge concerning the thermal HB interstate density matrix. Although it is not a strict manner, for the time being, the $rs$-component of the thermal HB interstate density matrix is reasonably approximated as

$$W^{\text{thermal}}_{\text{Res};rs} \approx g_s \sqrt{\tilde{W}_r \sqrt{\tilde{W}_s} g_s^T} = \begin{bmatrix} a_r & b_r^* \\ b_r & a_r^* \end{bmatrix} \begin{bmatrix} \sqrt{w_r} & 0 \\ 0 & \sqrt{1_N - w_r} \end{bmatrix} \begin{bmatrix} \sqrt{w_s} & 0 \\ 0 & \sqrt{1_N - w_s} \end{bmatrix} \begin{bmatrix} a_s^T & b_s^T \\ b_s & a_s^T \end{bmatrix}$$  \tag{4.14}

Further substituting (4.15) into $F$ and $D$ matrices given by (2.23), we can obtain the matrices $F^{\text{thermal}}_{\text{Res};rs;\alpha\beta}$ and $D^{\text{thermal}}_{\text{Res};rs;\alpha\beta}$ which have the same forms as those given by (4.10). Of course, the temperature-dependent overlap integral $z^{\text{thermal}}_{\text{Res};rs}$ cannot be sought in the same form as that given by the second equation of (2.15). Therefore, we are forced to take it in a suitable way as far as possible. For the moment, we assume it to be the form as

$$z^{\text{thermal}}_{\text{Res};rs} = \left[ \sqrt{w_r} b_r^* \right] \left[ \begin{array}{c} b_s \sqrt{w_s} \\ a_s \sqrt{w_s} \end{array} \right] + \left[ \sqrt{1_N - w_r} b_r^* \right] \left[ \begin{array}{c} b_s \sqrt{1_N - w_s} \\ a_s \sqrt{1_N - w_s} \end{array} \right]$$  \tag{4.16}

Equations (4.9), (4.10) and (4.15) yield the temperature dependence of the HB interstate density matrix, Hamiltonian element and FB operator and equation (4.16) gives approximately a temperature-dependent overlap integral. Then all of these determine the temperature dependence of the $K^{\text{thermal}(k)}_{\text{Res};rs}$ (4.3). Thus, the thermal Res-HB coupled eigenvalue equations together with the thermal Res-FB operator (5.34), which are given later, are naturally set out within the framework of the present formal theory.

However, a calculation of the partition function by the IMCF is very cumbersome and a method of solving the above equations is too complicated to execute. As suggested by Fukutome [17], we pay attention mainly to a contribution from a diagonal part in the formula $\text{Tr}(Pe^{-\beta H})$ (3.1). Then the partition function in the Res-HB subspace is approximately calculated as

$$\text{Tr}(Pe^{-\beta H}) \approx \sum_{r=1}^n \langle g_r | e^{-\beta H} W_{rr} | e^{-\beta H} g_r \rangle (S^{-1})_{rr}$$  \tag{4.17}

where $H[W_{rr}]$ corresponds to the $r$-th Res-HB energy functional and $< H > g_r$ is the quasi-particle Hamiltonian in the $g_r$ quasi-particle frame whose explicit expression is given later. The formula (4.17) shows that if the Res-HB energy functional has multiple low energy local minima then they give a large contribution to the partition function and the $\text{resonon}$ spectrum recovers the energy levels of the system in the previous section. Based on such a useful observation, we will seek for another possible and more practical way of approximating a partition function and a free energy within the Res-MFT. This is made in the next section.
5 Approximation of partition function and free energy

Here, a more practical way to the Res-HB theory is given. To calculate approximately
a partition function in the Res-HB subspace, consider a matrix-valued variable \( \mathcal{Z} \) with
the same form as the one of (2.22) and introduce a quadratic HB Hamiltonian

\[
H[\mathcal{Z}] = \frac{1}{2} \begin{bmatrix} F & D \\ -D^* & -F^* \end{bmatrix} \mathcal{Z} \begin{bmatrix} c_r^\dagger \\ c_r \end{bmatrix}, \quad \mathcal{Z}^\dagger = \mathcal{Z} = \begin{bmatrix} F & D \\ -D^* & -F^* \end{bmatrix}, \quad F = (F_{\alpha\beta}), \quad D = (D_{\alpha\beta}),
\]

(5.1)

though we use the same symbols, \( F \) and \( D \) are not identical with the \( F \) and \( D \) used in (2.22).

In the statistical density matrix \( \hat{\mathcal{W}}(=e^{-\beta H/\text{Tr}(e^{-\beta H}))} \), instead of the original Hamiltonian \( H \),
we adopt the above quadratic Hamiltonian \( F \). Then, the approximate free energy, i.e., the usual HB free energy \( F[\mathcal{Z}] \) is given in the following form [48]:

\[
F[\mathcal{Z}] = \langle H - H[\mathcal{Z}] \rangle_2 - \frac{1}{\beta} \ln \text{Tr}(e^{-\beta H[\mathcal{Z}]}) - \frac{\text{Tr}(e^{-\beta H[\mathcal{Z}]})^2}{\text{Tr}(e^{-\beta H[\mathcal{Z}]})}, \quad \langle H \rangle_2 \equiv \frac{\text{Tr}(e^{-\beta H[\mathcal{Z}]})^2}{\text{Tr}(e^{-\beta H[\mathcal{Z}]})}, \quad \langle H[\mathcal{Z}] \rangle_2 \equiv \frac{\text{Tr}(e^{-\beta H[\mathcal{Z}]})}{\text{Tr}(e^{-\beta H[\mathcal{Z}]})}. \quad (5.2)
\]

A natural extension of the HB free energy to the Res-HB free one is easily made. We strongly
assume \( \mathcal{Z} = \sum_{r=1}^n \oplus \mathcal{F}_r \) where \( \mathcal{F}_r \) is the already known Res-FB operator (2.24). It is a crucial
and essential point that instead of (5.1) we introduce a quadratic Res-HB Hamiltonian

\[
H[\mathcal{Z}]_{\text{Res}} \equiv \frac{1}{2} \begin{bmatrix} \mathcal{F}_1 & \cdots & \mathcal{F}_r & \cdots & \mathcal{F}_n \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & \cdots & 0 \\ \mathcal{F}_r & \cdots & \mathcal{F}_n & \cdots & \mathcal{F}_1 \end{bmatrix} \begin{bmatrix} c_r^\dagger \\ \cdots \\ c_r \end{bmatrix}, \quad \mathcal{F}_r \equiv \begin{bmatrix} c_r^\dagger \\ \cdots \\ c_r \end{bmatrix}, \quad r = 1, \ldots, n.
\]

(5.3)

We can extend the HB free energy to the Res-HB free energy in the form

\[
F_{\text{Res}} = \text{Tr}(\mathcal{W}_{\text{Res}} \mathcal{H}) + \frac{1}{\beta} \text{Tr} \left\{ \mathcal{W}_{\text{Res}} \ln \mathcal{W}_{\text{Res}} \right\}, \quad \mathcal{W}_{\text{Res}} \equiv \frac{\text{Pe}^{-\beta H}}{\text{Tr}(\text{Pe}^{-\beta H})}.
\]

(5.4)

According to (5.4), with use of (5.3) the Res-HB free energy is modified as follows:

\[
F[\mathcal{Z}]_{\text{Res}} = \text{Tr}(\mathcal{W}[\mathcal{Z}]_{\text{Res}} H) + \frac{1}{\beta} \text{Tr} \left\{ \mathcal{W}[\mathcal{Z}]_{\text{Res}} \ln(\mathcal{W}[\mathcal{Z}]_{\text{Res}}) \right\}, \quad \mathcal{W}[\mathcal{Z}]_{\text{Res}} \equiv \frac{\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}}}{\text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}})},
\]

(5.5)

in which, by making the Taylor expansion of \( \ln P = \ln \{1-(1-P)\} \) and using \( P^2 = P \), we obtain

\[
\frac{1}{\beta} \text{Tr} \left\{ \mathcal{W}[\mathcal{Z}]_{\text{Res}} \ln(\mathcal{W}[\mathcal{Z}]_{\text{Res}}) \right\} = -\langle H[\mathcal{Z}]_{\text{Res}} \rangle_{\mathcal{Z},\text{Res}} - \frac{1}{\beta} \ln \text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}}).
\]

(5.6)

Using (5.6), the Res-HB free energy is also rewritten as

\[
F[\mathcal{Z}]_{\text{Res}} = \langle H - H[\mathcal{Z}]_{\text{Res}} \rangle_{\mathcal{Z},\text{Res}} - \frac{1}{\beta} \ln \text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}}),
\]

(5.7)

\[
\langle H[\mathcal{Z}]_{\text{Res}} \rangle_{\mathcal{Z},\text{Res}} \equiv \frac{\text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}} PH[\mathcal{Z}]_{\text{Res}})}{\text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}})}, \quad \langle H \rangle_{\mathcal{Z},\text{Res}} \equiv \frac{\text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}} PH)}{\text{Tr}(\text{Pe}^{-\beta H[\mathcal{Z}]_{\text{Res}}})}.
\]

(5.8)

With the use of the solved set of the Res-HB eigenvalue equations \( [\mathcal{F}_r u_{r}] = e_{r} u_{r} (2.24) \),
the quadratic Hamiltonian \( H[\mathcal{Z}]_{\text{Res}} \) (5.3) is diagonalized in the \( g_i \) quasi-particle frame as

\[
H[\mathcal{Z}]_{\text{Res}} = -\frac{1}{2} \epsilon \sum_{t=1}^n \sum_{i=1}^N \epsilon_{i t} d_{g_{i t}}^\dagger d_{g_{i t}}, \quad [c_r, c_r^\dagger] g_{i t} = \epsilon \sum_{t=1}^n \sum_{i=1}^N \epsilon_{i t} g_{i t}.
\]

(5.9)

We introduce the trace manipulation \( \text{tr} \) in the occupation number space and consider eigenvalues of the occupation number operator \( n_{g_{i t}} (= d_{g_{i t}}^\dagger d_{g_{i t}}) \) are either 0 or 1. From (5.9),
using the formula (3.1), we can compute approximately the second of the R.H.S. of (5.6) as
The addition of (5.11) to (5.13) and the use of (4.5) and
arise due to the superposition of HB WFs.

Taking only a single HB WF, (5.14) reduces to the usual statistical expectation value

\[
\langle g_s | (S^{-1})_{sr} \rangle
\]

then, the logarithm of which divided by \( \beta \) is approximately calculated as

\[
\frac{1}{\beta} \ln \text{Tr}(P e^{-\beta H[Z]_{\text{Res}}}) \approx \frac{1}{2} \epsilon + \frac{1}{\beta} \sum_{r=1}^{N} \sum_{i=1}^{N} \epsilon_{ri} \frac{w_{ri} \cdot f_r}{f_r}
\]

Further, the quantity \( \langle H[Z]_{\text{Res}} \rangle_{Z;\text{Res}} \) defined by the first equation of (5.8) is computed as

\[
\langle H[Z]_{\text{Res}} \rangle_{Z;\text{Res}} = -\frac{1}{2} \epsilon + \frac{1}{\beta} \sum_{r=1}^{N} \sum_{i=1}^{N} \epsilon_{ri} \frac{w_{ri} \cdot f_r}{f_r}
\]

Substituting the last equation of (5.10) into the denominator, i.e., \( \text{Tr}(P e^{-\beta H[Z]_{\text{Res}}}) \) and taking only the term with \( t = s \) or \( t = s' \), the \( \langle H[Z]_{\text{Res}} \rangle_{Z;\text{Res}} \) can be changed to a more compact form

\[
\langle H[Z]_{\text{Res}} \rangle_{Z;\text{Res}} = -\frac{1}{2} \epsilon + \frac{1}{\beta} \sum_{r=1}^{N} \sum_{i=1}^{N} \epsilon_{ri} \frac{w_{ri} \cdot f_r}{f_r}
\]

The addition of (5.11) to (5.13) and the use of (4.5) and \( \epsilon_{ri} \approx \frac{1}{\beta} \ln \left( \left( 1 - \frac{w_{ri}}{f_r} \right) / \frac{w_{ri}}{f_r} \right) \) lead to

\[
-\langle H[Z]_{\text{Res}} \rangle_{Z;\text{Res}} = -\frac{1}{\beta} \ln \text{Tr}(P e^{-\beta H[Z]_{\text{Res}}}) \approx \frac{1}{\beta} \sum_{r=1}^{N} \sum_{i=1}^{N} \left( 1 - \frac{w_{ri}}{f_r} \right) \left( \frac{1 - \frac{w_{ri}}{f_r}}{f_r} + \ln \frac{w_{ri}}{f_r} \right)
\]

This is identical with the entropy \( S_{\text{thermal HB}} \) in II except the modification \( \tilde{W}_{ri} \rightarrow w_{ri} \rightarrow \frac{w_{ri}}{f_r} \) in (4.9). Taking only a single HB WF, (5.14) reduces to the usual statistical expectation value by HB WF. The summation with respect to \( r \) in R.H.S. in (5.14) and multiplication by \( \frac{1}{f_r} \) arise due to the superposition of HB WFs.

Finally, a computation of the quantity \( \langle H \rangle_{Z;\text{Res}} \) defined by the second of (5.8) is made through the following procedures: Let us define new fermion \( SO(2N) \) Lie operators as

\[
E_{gij}^{\alpha} \equiv d_{gij}^{\dagger} d_{gij}, \quad E_{gij}^{\alpha i} \equiv d_{gij}^{\dagger} c_i, \quad E_{gij}^{\alpha i} \equiv d_{gij} c_i, \quad [d_{gij}, d_{gij}^{\dagger}] \equiv [c, c^\dagger] g_{ij}.
\]

The original fermion \( SO(2N) \) Lie ones are expressed in terms of the quasi-particle expectation values \( \langle E_{\beta}^{\alpha} \rangle_{g_{ij}} \), \( \langle E_{\alpha}\beta \rangle_{g_{ij}} \) and \( \langle E_{\alpha\beta}^{\alpha} \rangle_{g_{ij}} \) (c-numbers) and of the new \( SO(2N) \) Lie ones (5.15) (quantum mechanical fluctuations) as follows:

\[
E_{\alpha}^{\alpha} = \langle E_{\beta}^{\alpha} \rangle_{g_{ij}} \quad E_{\beta}^{\alpha} = \langle E_{\beta}^{\alpha} \rangle_{g_{ij}} + \left( a_{\alpha i} b_{\beta j} - b_{\beta i} a_{\alpha j} \right) \left( E_{gij}^{\alpha i} \right)_{g_{ij}} + \frac{1}{2} \delta_{ij} \epsilon_{\alpha i} b_{\beta j} E_{gij}^{\alpha i} + b_{\alpha i} a_{\beta j} E_{gij}^{\alpha i} + a_{\alpha i} b_{\beta j} E_{gij}^{\alpha i} + b_{\alpha i} a_{\beta j} E_{gij}^{\alpha i} \quad E_{\alpha\beta}^{\alpha} = -E_{\alpha\beta}^{\alpha}.
\]
On the $g_t$ quasi-particle frame, using (5.16), the original Hamiltonian $H$ (2.12) is transformed into $H_{gt}$ expressed as

$$H_{gt} = <H>_{gt} + \left\{ \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) F_{\alpha i}^{g_t} + \frac{1}{4} \left( b_{\beta_i} b_{\alpha i}^{\beta_j} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) D_{\beta_i}^{g_t} + \frac{1}{2} \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j*} \right) D_{\alpha i}^{g_t} \right\} \left( E_{\alpha i}^{g_t} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$+ \frac{1}{2} \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) D_{\beta_i}^{g_t} + \frac{1}{2} \left( b_{\beta_i} b_{\alpha i}^{\beta_j} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) D_{\alpha i}^{g_t} + \frac{1}{4} \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j*} \right) D_{\alpha i}^{g_t}$$

$$+ \frac{1}{16} \left[ \alpha \beta \right] \delta \left[ \left( a_{\alpha i}^{\gamma_j*} - a_{\alpha i}^{\gamma_j} \right) \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) + \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) \left( b_{\delta_i} b_{\beta_i} - b_{\delta_i} b_{\beta_i} \right) \right] \left( E_{\alpha i}^{g_t*} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$+ \frac{1}{16} \left[ \alpha \beta \right] \delta \left[ \left( a_{\alpha i}^{\gamma_j*} - a_{\alpha i}^{\gamma_j} \right) \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) + \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) \left( b_{\delta_i} b_{\beta_i} - b_{\delta_i} b_{\beta_i} \right) \right] \left( E_{\alpha i}^{g_t*} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$+ \frac{1}{8} \left[ \alpha \beta \right] \delta \left[ \left( a_{\alpha i}^{\gamma_j*} - a_{\alpha i}^{\gamma_j} \right) \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) + \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) \left( b_{\delta_i} b_{\beta_i} - b_{\delta_i} b_{\beta_i} \right) \right] \left( E_{\alpha i}^{g_t*} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$= \frac{1}{2} \delta_{\alpha \beta} < H >_{gt} + \frac{1}{4} \left[ \alpha \beta \right] \delta < H >_{gt} + \frac{1}{8} \left[ \alpha \beta \right] \delta < H >_{gt}. \tag{5.17}$$

Here the $E_{\alpha \beta}^t$, $E_{\alpha \beta}$ and $E_{\alpha \beta}^t$ are generators of rotation in the $2N$-dimensional Euclidian space. The $< H >_{gt}$ means an energy of classical motion of $SO(2N)$ fermion top. Under a quasi anti-commutation-relation approximation, a new aspect of the top is described in our recent work [50]. Using the expression for $H$ (5.17), the $< H >_{Z:Res}$ defined by second of (5.8) is computed as

$$< H >_{Z:Res} = \frac{\text{Tr}(P e^{-g_t H_{gt}} |S>_{Res})}{\text{Tr}(P e^{-g_t H_{gt}} |S>_{Res})} \sum_{s=1}^{n} \sum_{r=1}^{n} \sum_{i=1}^{N} \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) F_{\alpha i}^{g_t} + \frac{1}{4} \left( b_{\beta_i} b_{\alpha i}^{\beta_j} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) D_{\beta_i}^{g_t} + \frac{1}{2} \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j*} \right) D_{\alpha i}^{g_t}$$

$$+ \frac{1}{2} \left( b_{\beta_i} b_{\alpha i}^{\beta_j} - b_{\beta_i} b_{\alpha i}^{\beta_j} \right) D_{\beta_i}^{g_t} + \frac{1}{4} \left( a_{\alpha i}^{\beta_j*} - b_{\beta_i} b_{\alpha i}^{\beta_j*} \right) D_{\alpha i}^{g_t}$$

$$+ \frac{1}{16} \left[ \alpha \beta \right] \delta \left[ \left( a_{\alpha i}^{\gamma_j*} - a_{\alpha i}^{\gamma_j} \right) \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) + \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) \left( b_{\delta_i} b_{\beta_i} - b_{\delta_i} b_{\beta_i} \right) \right] \left( E_{\alpha i}^{g_t*} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$+ \frac{1}{16} \left[ \alpha \beta \right] \delta \left[ \left( a_{\alpha i}^{\gamma_j*} - a_{\alpha i}^{\gamma_j} \right) \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) + \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) \left( b_{\delta_i} b_{\beta_i} - b_{\delta_i} b_{\beta_i} \right) \right] \left( E_{\alpha i}^{g_t*} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$+ \frac{1}{8} \left[ \alpha \beta \right] \delta \left[ \left( a_{\alpha i}^{\gamma_j*} - a_{\alpha i}^{\gamma_j} \right) \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) + \left( b_{\beta_j} b_{\alpha i}^{\gamma_j*} - b_{\beta_j} b_{\alpha i}^{\gamma_j} \right) \left( b_{\delta_i} b_{\beta_i} - b_{\delta_i} b_{\beta_i} \right) \right] \left( E_{\alpha i}^{g_t*} + \frac{1}{2} \delta_{\alpha i} \right)$$

$$= \frac{1}{2} \delta_{\alpha \beta} < H >_{gt} + \frac{1}{4} \left[ \alpha \beta \right] \delta < H >_{gt} + \frac{1}{8} \left[ \alpha \beta \right] \delta < H >_{gt}. \tag{5.18}$$
where we have used the definitions \(2.23\) and the following ensemble averages of the new fermion \(SO(2N)\) Lie operators in the \(g_t\) quasi-particle frame:

\[
\begin{align*}
\text{Tr}\left\{ P e^{-\beta H|Z|_{\text{Res}}} P \left( E^{g_{\text{rit}} g_{\text{rj}} + \frac{1}{2} \delta_{ij}} \right) \right\} &= \delta_{ij} \text{Tr}\left\{ P e^{-\beta H|Z|_{\text{Res}}} P n_{g_{ij}} \right\}, \\
\text{Tr}\left\{ P e^{-\beta H|Z|_{\text{Res}}} P E^{g_{\text{rit}} g_{\text{rj}}} \right\} &= 0, \quad \text{Tr}\left\{ P e^{-\beta H|Z|_{\text{Res}}} P E^{g_{\text{rit}} g_{\text{rj}}} \right\} = 0, \\
\text{Tr}\left\{ P e^{-\beta H|Z|_{\text{Res}}} P E^{g_{\text{rit}} g_{\text{rj}}} \right\} &= \left( \delta_{ij} \delta_{ij} - \delta_{ij} \delta_{ij} \right) \text{Tr}\left\{ P e^{-\beta H|Z|_{\text{Res}}} P n_{g_{ij}} g_{ij} \right\}.
\end{align*}
\]

(5.20)

The trace manipulation \(\text{tr}\) is made as was done previously and the eigenvalue of \(n_{g_{ij}}\) is taken to be either 0 or 1. Using this, further computation of (5.19) can be made approximately as

\[
\langle H \rangle_{Z, \text{Res}} \approx \sum_{t=1}^{n} \langle H \rangle_{g_t} + \sum_{i=1}^{n} \frac{1}{4} [\alpha | \beta | \gamma | \delta]
\]

\[
\times \left[ 2 \left( b_{\alpha i} b_{\beta i} - a_{\alpha i} a_{\beta i} \right) \right] \text{tr}\left\{ \left( \sum_{r=1}^{s} S_{rr'} (S^{-1})_{r' s} S_{s' s} (S^{-1})_{s r} \right) \right\}
\]

(5.21)

where we have used \(5.18\) and the equation in the last line of (5.10). Taking only the term with \(t = s\) in the denominator, equation (5.21) is converted into

\[
\langle H \rangle_{Z, \text{Res}} \approx \sum_{t=1}^{n} \langle H \rangle_{g_t} + \sum_{t=1}^{n} \frac{1}{4} [\alpha | \beta | \gamma | \delta]
\]

\[
\times \left[ 2 \left( b_{\alpha i} b_{\beta i} - a_{\alpha i} a_{\beta i} \right) \right] \text{tr}\left\{ \left( \sum_{r=1}^{s} S_{rr'} (S^{-1})_{r' s} S_{s' s} (S^{-1})_{s r} \right) \right\}
\]

(5.22)
Using the usual HB orbital energy $\tilde{c}_{ri}$, (2.24), (1.9) and (1.10) but with the modification $\tilde{w}_{ri} \rightarrow w_{ri} - \frac{w_{ri}}{f_r}$, equation (5.22) is rewritten into a more compact form

$$\langle H \rangle_{z;\text{Res}} \simeq \sum_{r=1}^{n} <H>_{g_r}$$

$$+ \sum_{r=1}^{n} \frac{1}{2} \left[ R_{\text{thermal}}^{\alpha,\delta} \alpha \beta - \delta_{\alpha\beta} - K_{\text{thermal}}^{\alpha,\delta} \right] F_{\alpha,\beta}^{g_r} - K_{\text{thermal}}^{\alpha,\delta} D_{\alpha,\beta}^{g_r}$$

$$+ \sum_{r=1}^{n} \left\{ \frac{1}{2} F_{\alpha,\beta}^{g_r} + \sum_{i_1=1}^{N} \tilde{c}_{ri} b_{\alpha i}^{*} b_{\alpha i} \right\}$$

$$+ \sum_{r=1}^{n} \frac{1}{4} [\alpha | \beta | \gamma \delta]$$

$$\times 2 \left[ \left( - R_{\text{Res;R};\alpha,\beta} b_{\alpha i}^{*} + b_{\alpha i}^{*} \right) - R_{\text{Res;R};\alpha,\beta} \right] + \left( - K_{\text{Res;R};\alpha,\beta} \right) - a_{\gamma,\alpha}^{*} b_{\alpha i}^{*} - b_{\alpha i}^{*} a_{\delta,\beta}^{*}$$

$$= \sum_{r=1}^{n} <H>_{g_r} + \frac{1}{2} \sum_{r=1}^{n} \sum_{i_1=1}^{N} <E_{r;\gamma}>_{g_r} + \sum_{i_1=1}^{N} \tilde{c}_{ri}$$

$$+ \sum_{r=1}^{n} \frac{1}{4} [\alpha | \beta | \gamma \delta]$$

$$\times 2 \left[ R_{\text{Res;R};\alpha,\beta} - R_{\text{Res;R};\alpha,\beta} - K_{\text{Res;R};\alpha,\beta} - 2 R_{\text{Res;R};\alpha,\beta} \right] + \left( - K_{\text{Res;R};\alpha,\beta} \right) - a_{\gamma,\alpha}^{*} b_{\alpha i}^{*} - b_{\alpha i}^{*} a_{\delta,\beta}^{*}$$

$$+ <E_{\delta,\beta}>_{g_r} - <E_{\alpha,\gamma}>_{g_r} K_{\text{Res;R};\delta,\gamma} - 2 <E_{\delta,\beta}>_{g_r} <E_{\alpha,\gamma}>_{g_r}$$

Owing to the relations (2.23), i.e., $F_{\alpha,\beta}^{g_r} = h_{\alpha,\beta}^{\gamma} <E_{\delta,\beta}>_{g_r}$, and $D_{\alpha,\gamma}^{g_r} = \frac{1}{2} [\alpha | \beta | \gamma | \delta] <E_{\delta,\beta}>_{g_r}$, the final expression for equation (5.23) leads to the following simple form:

$$\langle H \rangle_{z;\text{Res}} = \sum_{r=1}^{n} <H>_{g_r} + \sum_{r=1}^{n} \frac{1}{2} [\alpha | \beta | \delta]$$

$$+ \sum_{r=1}^{n} \sum_{i_1=1}^{N} \tilde{c}_{ri}$$

$$+ \sum_{r=1}^{n} \frac{1}{2} [\alpha | \beta | \gamma | \delta]$$

$$\times 2 \left[ R_{\text{Res;R};\alpha,\beta} - R_{\text{Res;R};\alpha,\beta} - K_{\text{Res;R};\alpha,\beta} - 2 R_{\text{Res;R};\alpha,\beta} \right] + \left( - K_{\text{Res;R};\alpha,\beta} \right) - a_{\gamma,\alpha}^{*} b_{\alpha i}^{*} - b_{\alpha i}^{*} a_{\delta,\beta}^{*}$$

The first three terms in the last line of the above equation (5.24) are temperature independent while the last term is temperature dependent and is defined as

$$<H>_{g_r}^{\text{thermal}} = h_{\alpha,\beta}^{\gamma} R_{\text{Res;R};\alpha,\beta} + \frac{1}{2} [\alpha | \beta | \gamma | \delta]$$

$$\times 2 \left[ R_{\text{Res;R};\alpha,\beta} - R_{\text{Res;R};\alpha,\beta} - K_{\text{Res;R};\alpha,\beta} - 2 R_{\text{Res;R};\alpha,\beta} \right] + \left( - K_{\text{Res;R};\alpha,\beta} \right) - a_{\gamma,\alpha}^{*} b_{\alpha i}^{*} - b_{\alpha i}^{*} a_{\delta,\beta}^{*}$$

which is a thermal expectation value of the Hamiltonian (48-49) in the $g_r$ quasi-particle frame but the numerical factor in the curl brackets is modified from $-\frac{1}{2}$ to $-\frac{3}{2}$. Such a modification can take place since the HB WFs with different structures are resonating.
Let us remind the variable \( w_{ri} (\equiv [1 + e^{\beta \epsilon_{ri}}]^{-1}) \). Then the variation of the Res-HB free energy \( F[Z]_{\text{Res}} \) with respect to the variable \( \frac{w_{ri}}{f_r} \) is calculated as

\[
\delta F[Z]_{\text{Res}} = \delta \langle H \rangle_{Z; \text{Res}} - \delta \left\{ \langle H[Z]_{\text{Res}} \rangle_{Z; \text{Res}} + \frac{1}{\beta} \ln \text{Tr} \left( P e^{-\beta H[Z]}_{\text{Res}} \right) \right\}. \tag{5.26}
\]

First we give the variational formula for the variable \( \frac{w_{ri}}{f_r} \) as follows:

\[
\delta \left( \frac{w_{ri}}{f_r} \right) = \frac{\delta w_{ri}}{f_r} f_r - \frac{w_{ri}}{f_r} \frac{\delta f_r}{f_r} \]

\[
= - \frac{w_{ri}}{f_r} (1 - w_{ri}) \delta (\beta \epsilon_{ri}) - \frac{w_{ri}}{f_r} \frac{1}{f_r} S_{rr} \frac{1}{1 - w_{ri}} \frac{1}{1 - w_{ri}} \delta w_{ri} (S^{-1})_{rr} \]

\[
= - \frac{w_{ri}}{f_r} (1 - w_{ri}) \delta (\beta \epsilon_{ri}) + \frac{w_{ri}}{f_r} \frac{1}{f_r} S_{rr} \frac{w_{ri}}{1 - w_{ri}} \delta (\beta \epsilon_{ri}) (S^{-1})_{rr} \]

\[
= - \frac{w_{ri}}{f_r} \left\{ 1 - w_{ri} \frac{1}{f_r} S_{rr} \frac{w_{ri}}{1 - w_{ri}} (S^{-1})_{rr} \right\} \delta (\beta \epsilon_{ri}) \equiv \Delta w_{ri} \delta (\beta \epsilon_{ri}). \tag{5.27}
\]

Using (5.27), the variational formula for the \( R^{\text{thermal}}_{\text{Res}} \) and \( K^{\text{thermal}}_{\text{Res}} \) matrices are given as

\[
\delta R^{\text{thermal}}_{\text{Res}; \alpha \beta} = a^{\alpha *}_{\beta i} \delta \left( \frac{w_{ri}}{f_r} \right) a^{\beta}_{i \alpha} - b_{\alpha i} \delta \left( \frac{w_{ri}}{f_r} \right) b^{*}_{\beta i}, \tag{5.28}
\]

\[
\delta K^{\text{thermal}}_{\text{Res}; \alpha \beta} = a^{\alpha *}_{\beta i} \delta \left( \frac{w_{ri}}{f_r} \right) b^{*}_{\beta i} - b_{\alpha i} \delta \left( \frac{w_{ri}}{f_r} \right) a^{\beta *}_{i \alpha} \]

The second part of the variation in (5.26) is computed as

\[
- \delta \left\{ \langle H[Z]_{\text{Res}} \rangle_{Z; \text{Res}} + \frac{1}{\beta} \ln \text{Tr} \left( P e^{-\beta H[Z]}_{\text{Res}} \right) \right\}
\]

\[
= \frac{1}{\beta} \sum_{n=1}^{N} \sum_{i=1}^{N} \delta \left[ \frac{w_{ri}}{f_r} \frac{\ln w_{ri}}{f_r} + \frac{w_{ri}}{f_r} \frac{\ln (1 - w_{ri})}{f_r} \right] \]

\[
= - \frac{1}{\beta} \sum_{n=1}^{N} \sum_{i=1}^{N} \ln \left[ \frac{f_r - w_{ri}}{w_{ri}} \right] \Delta w_{ri} \delta (\beta \epsilon_{ri}). \tag{5.29}
\]

The variational formula for the thermal expectation value \( \langle H \rangle_{g_r}^{\text{thermal}} \) is calculated as

\[
\delta \langle H \rangle_{g_r}^{\text{thermal}} = \frac{1}{2} \left\{ F^{\text{thermal}}_{\text{Res}; \alpha \beta} \delta R^{\text{thermal}}_{\text{Res}; \alpha \beta} + F^{\text{thermal} *}_{\text{Res}; \alpha \beta} \delta R^{\text{thermal} *}_{\text{Res}; \alpha \beta} \right\}
\]

\[
- 3 D^{\text{thermal}}_{\text{Res}; \alpha \beta} \delta K^{\text{thermal} *}_{\text{Res}; \alpha \beta} - 3 D^{\text{thermal} *}_{\text{Res}; \alpha \beta} \delta K^{\text{thermal}}_{\text{Res}; \alpha \beta} \tag{5.30}
\]

\[
= \frac{1}{2} \sum_{n=1}^{N} \left[ F^{\text{thermal}}_{\text{Res}; \alpha \beta} \left\{ a^{\alpha *}_{\beta i} \delta \left( \frac{w_{ri}}{f_r} \right) a_{i \alpha} - b_{\alpha i} \delta \left( \frac{w_{ri}}{f_r} \right) b^{*}_{\beta i} \right\} \right] + F^{\text{thermal} *}_{\text{Res}; \alpha \beta} \left\{ a^{\alpha *}_{\beta i} \delta \left( \frac{w_{ri}}{f_r} \right) a_{i \alpha} - b_{\alpha i} \delta \left( \frac{w_{ri}}{f_r} \right) b^{*}_{\beta i} \right\}
\]

\[
- 3 D^{\text{thermal}}_{\text{Res}; \alpha \beta} \left\{ a^{\alpha *}_{\beta i} \delta \left( \frac{w_{ri}}{f_r} \right) b^{*}_{\beta i} - b_{\alpha i} \delta \left( \frac{w_{ri}}{f_r} \right) a^{\beta *}_{i \alpha} \right\} - 3 D^{\text{thermal} *}_{\text{Res}; \alpha \beta} \left\{ a^{\alpha *}_{\beta i} \delta \left( \frac{w_{ri}}{f_r} \right) b^{*}_{\beta i} - b_{\alpha i} \delta \left( \frac{w_{ri}}{f_r} \right) a^{\beta *}_{i \alpha} \right\},
\]

where we have used the relations (4.10) and (5.28).
Finally, by adding (5.30) to (5.29), the variation of the $F[Z]_{\text{Res}}$ is made as follows:

$$
\delta F[Z]_{\text{Res}} = \frac{1}{2} \sum_{r=1}^{n} \sum_{i=r}^{N} \left[ F_{\text{thermal}}^{\text{Res}\,rr\beta} \left\{ a_{ri}^{\alpha} \Delta w_{ri} \alpha_{i} - b_{ri} \Delta w_{ri} \beta_{i} \right\} + F_{\text{thermal}}^{\text{Res}\,rr\beta} \left\{ a_{ri}^{\alpha} \Delta w_{ri} \beta_{i} - b_{ri}^{*} \Delta w_{ri} \alpha_{i} \right\} - 3D_{\text{Res}\,rr\beta}^{\text{thermal}} \left\{ a_{ri}^{\alpha} \Delta w_{ri} \beta_{i} - b_{ri}^{*} \Delta w_{ri} \alpha_{i} \right\} \right]
\times \left[ 3D_{\text{Res}\,rr\beta}^{\text{thermal}} - F_{\text{Res}\,rr\beta}^{\text{thermal}} \right] \Delta w_{ri} \left[ a_{ri}^{\alpha} \right] - \frac{2}{\beta} \ln \left[ \frac{f_{r} - w_{ri}}{w_{ri}} \right] \Delta w_{ri} \left[ a_{ri}^{\alpha} \right] \delta (\beta \varepsilon_{ri}).
$$

Then the variation equation of the Res-HB free energy $F[Z]_{\text{Res}}$ is given by

$$
\delta F[Z]_{\text{Res}} = 0, \quad (5.32)
$$

from which, for $r=1, \ldots, n$, we have

$$
\left[ F_{\text{Res}\,rr}^{\text{thermal}} - \frac{1}{\beta} \ln \left[ \frac{f_{r} - w_{ri}}{w_{ri}} \right] I_N \right] \Delta w_{ri} \left[ a_{ri}^{\alpha} \right] = \left[ 3D_{\text{Res}\,rr}^{\text{thermal}} - F_{\text{Res}\,rr}^{\text{thermal}} \right] \left[ a_{ri}^{\alpha} \right] \delta (\beta \varepsilon_{ri}). \quad (5.33)
$$

The $E_{ri}^{\text{thermal}}$ is a new quasi-particle energy different from the one arisen in $w_{ri} \equiv \frac{1}{1 + e^{\beta \varepsilon_{ri}}}$. We write (5.33) as $H_{\text{thermal}}^{\text{Res}\,rr} = E_{\text{thermal}}^{\text{Res}\,rr} \left( r=1, \ldots, n, \right)$. In it there exist factors $f_{r}$ defined in (5.10) which contains $S_{rs}$ directly and $\Delta w_{ri}$ defined in (5.27) which has a diagonal element of inverse matrix of overlap integral $(S^{-1})_{rr} = \sum_{k=1}^{n} c_{r}^{(k)} c_{r}^{(k)^{*}}$; See II. This means that the equation $H_{\text{thermal}}^{\text{Res}\,rr} = E_{\text{thermal}}^{\text{Res}\,rr} \left( r=1, \ldots, n, \right)$ forces us to couple the HB WF $|g_r\rangle$ with the other $|g_s\rangle$ and $\ldots$, though no direct couplings among the mixing coefficients manifestly exist. Thus we can reach our ultimate goal, i.e., the thermal Res-HB coupled eigenvalue equation within the present approximation of partition function and free energy. This thermal Res-HB coupled eigenvalue equation, however, has the very different form from that of the previous thermal Res-HB coupled one proposed in II [22], for $r=1, \ldots, n$, which is described as

$$
F_{\text{Res}\,rr}^{\text{thermal}} \equiv \sum_{k=1}^{n} c_{r}^{(k)} c_{r}^{(k)^{*}} \left( r=1, \ldots, n, \right), \quad (r, s = 1, \ldots, n).
$$

The quantity $K_{\text{Res}\,rr}^{\text{thermal}(k)}$ is defined by (4.3). This is the reason why we have started from the quadratic Res-HB Hamiltonian (5.3) and why we also have used the solved set of the Res-HB eigenvalue equations $F_{\text{Res}\,rr}^{\text{thermal}} \equiv \sum_{k=1}^{n} c_{r}^{(k)} c_{r}^{(k)^{*}}$, for $r=1, \ldots, n) \left( r=1, \ldots, n \right) \left( r=1, \ldots, n \right)$.
6 Summary and further perspectives

In this paper we have given a rigorous thermal Res-HBT and Res-MF approximation, to describe a superconducting fermion system. We have used a Res-HB subspace spanned by Res-HB ground and excited states. Using the projection operator $P$ to the Res-HB subspace, the partition function in the Res-HB subspace is given as $\text{Tr}(Pe^{-\beta H}) = \sum_{r,s=1}^{n} \langle g_r | e^{-\beta H} | g_s \rangle (S^{-1})_{sr}$. In principle this trace formula can be computed within the Res-HB subspace by using the Laplace transform of $e^{-\beta H}$ and the projection method \[26, 27, 28, 38\], however, whose computation by the IMCF is cumbersome. A group action on a HB-Hamiltonian and -density matrix at finite temperature are defined. The variation of the Res-HB free energy is made parallel to the usual thermal BCS theory \[6, 7, 23, 24\]. It leads to the thermal Res-HB CI equation and the thermal Res-HB equation which is equivalent with the thermal Res-HB coupled eigenvalue equations $\mathcal{F}_{\text{Res}} = \epsilon_{\text{thermal}} u_r$ for the thermal Res-FB operator $\mathcal{F}_{\text{Res}}$. The variation of the Res-MF free energy brings us the thermal Res-HF approximation.

Recently, to demonstrate the predominance of the Res-HB MF theory for superconducting fermion systems with large quantum fluctuations, in II we have applied it to a naive BCS Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation Hamiltonian for singlet pairing \[19\].

Recently, to demonstrate the predominance of the Res-HB MF theory for superconducting fermion systems with large quantum fluctuations, in II we have applied it to a naive BCS Hamiltonian for singlet pairing \[19\]. A state with large quantum fluctuations is approximated by superposition of two HB WFs which are non-orthogonal CS reps with different correlation structures. We have optimized directly the Res-MF energy functionals by variations of the Res-MF ground-state energy with respect to the Res-MF parameters, the so-called energy-gaps. The Res-MF ground and excited states generated with the two HB WFs explain most of the two energy-gaps in MgB$_2$. Both the large energy-gap and the small one have a significant physical meaning because electron systems, composed of condensed electron pairs, have now strong correlations among fermions. We also have treated the special case of equal energy-gaps and obtained interesting analytic solutions \[22\].

A time-reversed single-particle state $\bar{\alpha}$ is obtained from $\alpha$ and a phase factor is used $s_\alpha$ in the time reversal of physical quantities. For the naive singlet-pairing interaction $|\alpha\beta| = -gs_\alpha \delta_{\alpha\beta} s_\gamma \delta_{\gamma\delta}$, (g : force strength), the thermal pairing potential $D^{\text{thermal}}_{\text{Res}_{rr};\alpha\beta}$ is expressed as

$$D^{\text{thermal}}_{\text{Res}_{rr};\alpha\beta} = -s_\alpha \delta_{\alpha\beta} \Delta^{\text{thermal}}_{\text{Res}_{rr}}, \quad \Delta^{\text{thermal}}_{\text{Res}_{rr}} = \frac{g}{2} s_\delta \mathcal{F}^{\text{thermal}}_{\text{Res}_{rr};\alpha\beta}, \quad (r = 1, \ldots, n) \quad (6.1)$$

Combining \[6.1\] with $\mathcal{H}_{\text{Res}_{rr}} u_{r\alpha} = E_r u_{r\alpha}$, (r = 1, ..., n), i.e., \[5.33\], we reach our ultimate goal of the coupled thermal Res-HB multi-gap equations. It may be expected to open a new research area in the vigorous pursuit by the radical spirit of the Res-HBT to develop a theoretical framework appropriate for exploring the problem of high-$T_c$ superconductors.

Finally, it should be emphasized that we may also provide a thermal Res-HF approximation. We already have an expression for partition function in a U(N) CS rep $|u\rangle$ \[25\], Tr$(e^{-\beta H}) = N \int_0^1 \langle u | e^{\beta H} | u \rangle du$, $N C_u = N! / (N - n)!$ (n: Number of occupied orbitals) where the integration is the group integration on the group U(N). Following Fukutome \[17\], using the projection operator $P$ to the Res-HF subspace, the partition function in the Res-HF subspace can also be computed. The variation of the Res-HF free energy is made in the same way as the present thermal Res-HBT and it may be applied to a 1-D half-filled Hubbard model \[20\] and a simple LMG nuclear-model \[32\]. These works will appear elsewhere.
Appendix

A Calculation of the first few matrices $S_{rs}^{(l)}$ and $\mathbb{L}_{ur}^{(l)}$

In (3.3) by inserting the explicit expression for the projection operators $P^{(1)}$ into $Q^{(1)}$,

$$Q^{(1)} \equiv 1 - \sum_{u,v=1}^{n} |g_{u}^{(1)})(S^{(1)-1})_{uv}g_{v}^{(1)}| = 1 - \sum_{u,v=1}^{n} QH|g_{u})(S^{(1)-1})_{uv}g_{v}|HQ,$$

and denoting $\langle g_{r}|H^{m}|g_{s} \rangle$ as $(H^{m})_{rs}$, first few matrices $S_{rs}^{(l)}$ and $\mathbb{L}_{ur}^{(l)}$ can be calculated as

$$S_{rs}^{(1)} = \langle g_{r}|H^{(1)}|g_{s}^{(1)} \rangle = \langle g_{r}|HQHQ|g_{s} \rangle = (H^{2})_{rs} - (HS^{-1}H)_{rs},$$

$$\left( (H^{2})_{rs} = \frac{1}{n} \sum_{t,t'=1}^{n} (H)_{rt} \sum_{k=1}^{n} c_{t}^{(k)} c_{t'}^{(k)*} (H^{2})_{ts} = \frac{1}{n} (HS^{-1}H)_{rs}, \right)$$

$$S_{rs}^{(2)} = \langle g_{r}|H^{(1)}Q^{(1)}H^{(1)}|g_{s}^{(1)} \rangle = \langle g_{r}|HQHQQ \langle 1 \rangle HQH|g_{s} \rangle$$

$$= \langle g_{r}|HQHQHQ|g_{s} \rangle - (\mathbb{L}^{(1)}S^{(1)-1}L^{(1)})_{rs},$$

where

$$\langle g_{r}|HQHQHQ|g_{s} \rangle = (H^{4})_{rs} - (HS^{-1}H^{3} + H^{3}S^{-1}H + H^{2}S^{-1}H^{2})_{rs}$$

$$+ (HS^{-1}HS^{-1}H^{2} + H^{2}S^{-1}HS^{-1}H + HS^{-1}H^{2}S^{-1}H)_{rs} - (HS^{-1}HS^{-1}HS^{-1}H)_{rs},$$

$$\mathbb{L}_{rs}^{(2)} = -\langle g_{r}^{(2)}|H^{(2)}|g_{s}^{(2)} \rangle = -\langle g_{r}|HQHQQ \langle 1 \rangle HQQ \langle 1 \rangle HQH|g_{s} \rangle$$

$$= -\langle g_{r}|HQHQHQ|g_{s} \rangle - \left\{ (S^{(2)} + \mathbb{L}^{(1)}S^{(1)-1}L^{(1)}) S^{(1)-1}L^{(1)} + (S^{(2)} + \mathbb{L}^{(1)}S^{(1)-1}L^{(1)}) \right\}_{rs}$$

$$- \left( (L^{(1)}S^{(1)-1}L^{(1)}S^{(1)-1}L^{(1)}) \right)_{rs},$$

where

$$\langle g_{r}|HQHQHQ|g_{s} \rangle = (H^{5})_{rs} - (HS^{-1}H^{4} + H^{2}S^{-1}H^{3} + H^{3}S^{-1}H^{2} + H^{4}S^{-1}H)_{rs}$$

$$+ (HS^{-1}HS^{-1}H^{3} + HS^{-1}H^{2}S^{-1}H + H^{2}S^{-1}HS^{-1}H)_{rs}$$

$$+ (HS^{-1}H^{2}S^{-1}H^{2} + H^{2}S^{-1}HS^{-1}H^{2} + H^{2}S^{-1}H^{2}S^{-1}H)_{rs}$$

$$- (HS^{-1}HS^{-1}HS^{-1}H^{2} + HS^{-1}HS^{-1}H^{2}S^{-1}H + HS^{-1}H^{2}S^{-1}HS^{-1}H + H^{2}S^{-1}HS^{-1}HS^{-1}H)_{rs}$$

$$+ (HS^{-1}HS^{-1}HS^{-1}S^{-1}H)_{rs}.$$
B Proof of relations (4.1) and (4.2)

The two Res-HB equations (2.24) and (2.21) are equivalent. The two thermal Res-HB ones derived in II, whose respective forms are the same as those of two Res-HB equations, also turn out to be equivalent. Here, following I, we prove this equivalence. From now let us denote \( W_{\text{thermal}}^{\text{Res:rs}} \), \( W_{\text{thermal}}^{\text{Res:r}} \), \( K^{(k)_{\text{thermal}}} \) and \( F[W_{\text{thermal}}^{\text{Res:rs}}] \) simply as \( W_{rs} \), \( F_r \), \( K^{(k)}_{rs} \) and \( F[W_{rs}] \).

First, due to idempotent-like product properties \( W_{rs}W_{rr} = W_{rs} \) and \( W_{sr}W_{rr} = W_{rr} \), we have important relations \( K^{(k)}_{rs}W_{rr} = K^{(k)}_{rr} \) and \( K^{(k)}_{rs}W_{rr} = \{H[W_{sr}] - E(k)\} W_{rr} \cdot [\det z_{sr}]^{\frac{1}{2}} \). Next multiplication of the second equation in (2.24) by \( W_{rr} \) from the right yields

\[
F_rW_{rr} = F[W_{rr}]W_{rr} \sum_{k=1}^{n} |c_r^{(k)}|^2 \\
+ \sum_{k=1}^{n} \sum_{s=1}^{n} \left[ K^{(k)}_{rs} c_r^{(k)*} c_s + \{H[W_{sr}] - E(k)\} W_{rr} \cdot [\det z_{sr}]^{\frac{1}{2}} c_r^{(k)*} c_s \right] \\
= F[W_{rr}]W_{rr} \sum_{k=1}^{n} |c_r^{(k)}|^2 - \sum_{k=1}^{n} K^{(k)}_{rr} |c_r^{(k)}|^2 - \sum_{k=1}^{n} \{H[W_{rr}] - E(k)\} W_{rr} |c_r^{(k)}|^2 \\
+ \sum_{k=1}^{n} \sum_{s=1}^{n} \left[ K^{(k)}_{rs} c_r^{(k)*} c_s + \{H[W_{sr}] - E(k)\} \cdot [\det z_{sr}]^{\frac{1}{2}} c_r^{(k)*} c_s \right].
\]

Using (2.20), the second term in the last line of R. H. S. of (B.1) is vanished. Substituting to \( K^{(k)}_{rs} \), whose explicit form is obtained from (2.21), thus, \( F_rW_{rr} \) is cast into

\[
F_rW_{rr} = F[W_{rr}]W_{rr} \sum_{k=1}^{n} |c_r^{(k)}|^2 \\
- \sum_{k=1}^{n} \left[ (12n - W_{rr}) F[W_{rr}] + 2 \{H[W_{rr}] - E(k)\} \right] \cdot W_{rr} |c_r^{(k)}|^2 + \sum_{k=1}^{n} \sum_{s=1}^{n} K^{(k)}_{rs} c_r^{(k)*} c_s \quad (B.2)
\]

\[
= W_{rr} F[W_{rr}] W_{rr} \sum_{k=1}^{n} |c_r^{(k)}|^2 - \sum_{k=1}^{n} 2 \{H[W_{rr}] - E(k)\} W_{rr} |c_r^{(k)}|^2 + \sum_{k=1}^{n} \sum_{s=1}^{n} K^{(k)}_{rs} c_r^{(k)*} c_s.
\]

Further taking the hermitian conjugate of both sides of (B.2), we have

\[
F_rW_{rr} = W_{rr} F_r. 
\]

This means the two hermitian matrices \( F_r \) and \( W_{rr} \) have common eigenvectors to diagonalize them so that it leads to (2.24). Therefore, (2.24) and (B.3) are equivalent. Due to the idempotency relation \( W_{rr}^2 = W_{rr} \), (B.3) is equivalent to

\[
F_rW_{rr} - W_{rr} F_r W_{rr} = 0. 
\]

Thus the relations (4.1) and (4.2) are proved. Further multiplying (B.2) by \( W_{rr} \) from the left and using the explicit form of \( K^{(k)}_{rs} \), we obtain

\[
W_{rr} F_r W_{rr} = W_{rr}^2 F[W_{rr}] W_{rr} \sum_{k=1}^{n} |c_r^{(k)}|^2 - \sum_{k=1}^{n} 2 \{H[W_{rr}] - E(k)\} W_{rr}^2 |c_r^{(k)}|^2 \\
+ \sum_{k=1}^{n} \sum_{s=1}^{n} W_{rr} \left[ (12n - W_{rs}) F[W_{rs}] + H[W_{rs}] - E(k) \right] \cdot W_{rs} \cdot [\det z_{rs}]^{\frac{1}{2}} c_r^{(k)*} c_s \quad (B.5)
\]

\[
= W_{rr} F[W_{rr}] W_{rr} \sum_{k=1}^{n} |c_r^{(k)}|^2 - \sum_{k=1}^{n} 2 \{H[W_{rr}] - E(k)\} W_{rr} |c_r^{(k)}|^2.
\]

Subtracting (B.5) from (B.2), it is easy to derive an equivalence relation

\[
\sum_{k=1}^{n} \sum_{s=1}^{n} K^{(k)}_{rs} c_r^{(k)*} c_s = F_r W_{rr} - W_{rr} F_r W_{rr}. 
\]

Thus, the equivalence of two types of the thermal Res-HB equations in II is proved. The equivalent relation (B.6) also makes a crucial role in the variation of Res-HB free energy.
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