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Resonating Mean-Field Theoretical Approach to Two-Gap Superconductivity*

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Dedicated to the Memory of Hideo Fukutome

Abstract

We have developed the resonating mean-field theories (Res-MFTs) both for normal and superconducting fermion systems with large quantum fluctuations. We have successfully applied them to descriptions of exact solvable Lipkin model in nuclei, deformed-shape coexistence in superconducting nuclei and low-energy light-mesons mass spectra in hadrons. To show their effectiveness, we also apply the Res-MFT to a superconducting metal to describe one of current and hot topics, the two-gap superconductivity. A state with large quantum fluctuations is approximated by superposition of two MF wave functions (WFs) composed of non-orthogonal Hartree-Bogoliubov (HB) WFs with different correlation structures. We make a direct optimization of the Res-HB ground-state energy with respect to the energy gaps at $T=0$. Adopting a suitable chemical potential, the two-gap superconductivity in MgB_2 is well described by the Res-HB approximation. The Res-HB ground state generated with HB WFs is expected to explain almost the value of the ground-state correlation energy in all the correlation regimes.

Keywords: Res-MF theory, BCS model, Two-gap superconductivity

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1 Introduction

A topical two-gap superconductivity with critical temperature $T_c = 39$K has been recently discovered in MgB_2 [2]. It is a stimulating challenge for the radical sprit of the Resonating Mean-Field Theories (Res-MFTs) [3, 4] to develop a theoretical framework appropriate to explore the problem of the so-called two- or multi-gap superconductivity. In particular fermion systems with large quantum fluctuations present serious difficulties in many-body problems. To approach such problems, Fukutome has developed the resonating Hartree-Fock theory (Res-HFT) [3] 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 [4] (referred to as I). The essential points of the Res-MFTs consist of the discrete superposition of MF wave functions (WFs), the introduction of interstate density matrix between MF WFs and the introduction of Res-MF interstate Fock operator between MF WFs. Both the mixing coefficients and the MF WFs are determined variationally. The essential idea of the Res-MFT is illustrated as follows:

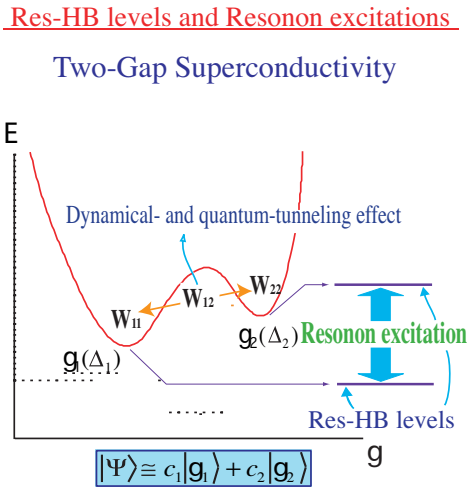

Figure 1: Illustration of essential idea of the Res-MFT

In a system with small quantum fluctuations, the ground state is well approximated by a usual MF WF, namely the HF Slater determinantal (S-det) or the HB WF. The quantum fluctuations are given by small-amplitude harmonic oscillations of orbitals around a MF minimum in an energy functional surface. Such fluctuations and collective excitations due to them are well described by the random phase approximation (RPA). If the energy functional surface has a large anharmonicity in its low energy portion, nonlinear couplings between RPA excitation modes become important. The ground state,

however, may remain describable by a perturbative correction of the MF WF. If the anharmonicity is so large that the surface has multiple low-energy minima, then the situation becomes essentially different. It turns out that it is not possible to approximate the ground state by a single MF WF. It becomes a superposition of multiple MF WFs, namely, it is resonating between different correlation structures. If the ground state has such a resonating character, any perturbative approach starting from a reference MF WF is no longer valid. Such a resonance may also be present in superconducting metals as well as in transitional nuclei and in hadrons.

In a series of papers, we have succeeded in applying the Res-MFTs to description of the following systems: exact solvable Lipkin model [5] (referred to as II), deformed-shape coexistence in superconducting nuclei [6] and low-energy phenomena in light mesons [7] (referred to as III). A direct optimization of the Res-MF energy functional is achieved by variation of the Res-MF ground-state energies with respect to the Res-MF variational parameters. These are exactly the self-consistency conditions in the Res-MF approximation (Res-MFA). Notice that the similarity between these conditions and the so-called *gap equation* in the BCS theory [8, 9] is a manifestation of the analogy of the Res-MFTs with the BCS theory.

Before the discovery of *high-*T_c superconductor, much effort had been devoted to raising the critical temperature T_c of usual BCS superconductor in the weak coupling regime [8, 9, 10] and to obtaining Eliashberg's critical temperature in the strong coupling [11, 12, 13]. The T_c for MgB_2 is 39K, which is close to or even above the upper theoretical value predicted by the BCS theory [14]. This implies that MgB_2 is possibly regarded as an unusual superconductor. Even if superconductivity in MgB_2 is phonon-mediated, a model beyond simple BCS model or Eliashberg model is required. The T_c for MgB_2 has been estimated phenomenologically as 22K by Kortus et al. [15]. The existence of two energy gaps in MgB_2 has been predicted theoretically by Liu et al. [16] employing a BCS-like weak-coupling multi-gap model with the use of the effective σ and π two-band model. They have got $\Delta_\sigma = 7.4$ [meV] and $\Delta_\pi = 2.4$ [meV] at $T = 0$, their temperature dependencies and $T_c = 40$K. On the other hand, employing the Eliashberg's strong-coupling theory [11], Choi et al. [17] have got $\Delta_\sigma = 6.8$ [meV] and $\Delta_\pi = 1.8$ [meV] at $T = 0$ and $T_c = 39.4$K.

In spite of the above theoretical great successes by the two-band model and the Eliashberg's strong-coupling theory, also the present Res-HBT itself is considered to be contributory to such theoretical approaches. This is because the Res-HBT is equivalent to the coupled Res-HB eigenvalue equations, which has already been proved in I. This fact means that the orbital concept or the band picture is still surviving in the Res-HB approximation, though orbitals or bands of different structures are resonating. Then the Res-HBT may be related to a microscopic theory for the two-band model. In the Res-HBT we have

started with a general Hamiltonian based on first principle without assuming some models such as the two-band model. From the Res-Fock-Bogoliubov (FB) one-body operators, we have derived two FB operators and an interstate FB operator in matrix forms each of which, in a certain sense, may imply microscopic descriptions of two-band Hamiltonians and an interaction between the two bands, respectively. The Res-HB ground state generated with HB WFs that are the coherent state representations (CS reps) [18], is expected to almost explain the value of the ground-state correlation energy in all the correlation regimes including an intermediate coupling regime due to the superposition of the HB WFs. It is worthwhile to apply the Res-HBT to the problem of the so-called two-gap superconductivity in MgB_2. Koshelev and Golubov have investigated the vortex state in the σ and π two-band superconductor and provided qualitative interptretation of scanning tunneling microscopy experiments on the vortex structure [19] solving the coupled Usadel equations and the self-consistency conditions for the order parameters [20]. The structure of the coupled Res-HB eigenvalue equations resembles that of the above coupled quasiclassic Usadel equations for an anisotoropic two-band superconductor. It is very interesting to study a methodological relationship between the coupled Res-HB eigenvalue equations and the coupled Usadel equations.

Being inspired by the preceding phenomenologies and the previous series of papers I, II and III, we will here develop a Res-HBT. A variation, direct optimization or orbital optimization, is made to find the diagonalization condition for the Res-FB operators along a way different from those in the BCS theory [21, 22, 23], so-called the two-band model and the Eliashberg's theory. We aim at deriving a formula to determine behaviour of gaps at $T = 0$. In the extremely special case of single-gap, we find a new formula for the gap different from the usual HB formula.

This paper is organized as follows: In Sec. 2, starting from a naive BCS Hamiltonian, we give expressions for Res-HB interstate density matrices after introducing new parametrization for coefficients of the Bogoliubov-Valatin transformations (BVTs) [9, 24]. In Sec. 3, we consider two HB WFs with *different energy gaps*. After calculating Hamiltonian matrix elements and the overlap integral, we carry out the $SU(2)$ Res-HBA. Instead of solving the Res-HB equation self-consistently, we make a direct optimization of the Res-HB energy, variation of the Res-HB ground-state energy. In Sec. 4, to make the essentials of the Res-HBT clearer, we treat the Res-HB equation with *equal energy gaps* and obtain a relation of interaction-strength to gap. Finally in Section 5, we give a summary and a discussion on the validity of the Res-MF approach. We also give further perspectives of the thermal Res-MFA. In Appendices, we calculate the overlap integral to perform a tractable direct-optimization and discuss on the relation between coupled Res-HB eigenvalue equations and coupled Usadel equations.

2 BCS Hamiltonian and interstate density matrix

We consider a naive BCS Hamiltonian [8] which describes a system of many fermions interacting via a two-body interaction

$$H = \sum_{\boldsymbol{p},\,\sigma} \varepsilon_{\boldsymbol{p}} c^{\dagger}_{\boldsymbol{p}\sigma} c_{\boldsymbol{p}\sigma} + \sum_{\boldsymbol{p},\,\boldsymbol{p}\prime} V_{\boldsymbol{p},\,\boldsymbol{p}\prime} c^{\dagger}_{\boldsymbol{p}\uparrow} c^{\dagger}_{-\boldsymbol{p}\downarrow} c_{-\boldsymbol{p}\prime\downarrow} c_{\boldsymbol{p}\prime\uparrow}, \tag{1}$$

where $c^{\dagger}_{\boldsymbol{p}\sigma}$ and $c_{\boldsymbol{p}\sigma}$ are electron creation and annihilation operators. Indices $\boldsymbol{p}$ and σ stand for the momentum and the spin index. We assume that the chemical potential μ is absorbed into the single-electron energy $\varepsilon_{\boldsymbol{p}}$.

According to the BVT [9, 24], quasi-particle (QP) operators $d_{\boldsymbol{p}\sigma}$ ($d^{\dagger}_{\boldsymbol{p}\sigma}$) and $d_{-\boldsymbol{p}\sigma}$ ($d^{\dagger}_{-\boldsymbol{p}\sigma}$) are introduced by canonical transformations

$$\left.\begin{aligned} \left[d_{\boldsymbol{p}\downarrow},\ d^{\dagger}_{-\boldsymbol{p}\uparrow}\right] &= \left[c_{\boldsymbol{p}\downarrow},\ c^{\dagger}_{-\boldsymbol{p}\uparrow}\right] \begin{bmatrix} u_p & -v^{*}_{p\uparrow} \\ -v_{p\downarrow} & u^{*}_p \end{bmatrix}, \\ \left[d_{\boldsymbol{p}\uparrow},\ d^{\dagger}_{-\boldsymbol{p}\downarrow}\right] &= \left[c_{\boldsymbol{p}\uparrow},\ c^{\dagger}_{-\boldsymbol{p}\downarrow}\right] \begin{bmatrix} u_p & -v^{*}_{p\downarrow} \\ -v_{p\uparrow} & u^{*}_p \end{bmatrix}, \end{aligned}\right\} \tag{2}$$

where the transformation coefficients satisfy the relations $v^{\uparrow}_p = -v^{\downarrow}_p = v_p$ and $|u_p|^2 + |v_p|^2 = 1$ for $p = |\boldsymbol{p}|$. We have similar transformations to the above for the QP operators if we replace the momentum $\boldsymbol{p}$ by $-\boldsymbol{p}$.

Introducing the well-known parametrization for u_p and v_p (BCS ansatz [8])

$$\left.\begin{aligned} u_p &= \cos\frac{\theta_p}{2} e^{-i\frac{\psi+\varphi}{2}}, \quad \cos\frac{\theta_p}{2} \equiv \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \Delta^2}}\right)}, \\ v_p &= \sin\frac{\theta_p}{2} e^{i\frac{\psi-\varphi}{2}}, \quad \sin\frac{\theta_p}{2} \equiv \sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \Delta^2}}\right)}, \end{aligned}\right\} \tag{3}$$

then the above canonical transformation is represented in a lump as

$$\begin{aligned} &\left[d_{\boldsymbol{p}\downarrow},\ d_{-\boldsymbol{p}\downarrow},\ d^{\dagger}_{-\boldsymbol{p}\uparrow},\ d^{\dagger}_{\boldsymbol{p}\uparrow},\ d_{\boldsymbol{p}\uparrow},\ d_{-\boldsymbol{p}\uparrow},\ d^{\dagger}_{-\boldsymbol{p}\downarrow},\ d^{\dagger}_{\boldsymbol{p}\downarrow}\right] \\ &= U(g_p)\left[c_{\boldsymbol{p}\downarrow},\ c_{-\boldsymbol{p}\downarrow},\ c^{\dagger}_{-\boldsymbol{p}\uparrow},\ c^{\dagger}_{\boldsymbol{p}\uparrow},\ c_{\boldsymbol{p}\uparrow},\ c_{-\boldsymbol{p}\uparrow},\ c^{\dagger}_{-\boldsymbol{p}\downarrow},\ c^{\dagger}_{\boldsymbol{p}\downarrow}\right] U^{\dagger}(g_p) \\ &= \left[c_{\boldsymbol{p}\downarrow},\ c_{-\boldsymbol{p}\downarrow},\ c^{\dagger}_{-\boldsymbol{p}\uparrow},\ c^{\dagger}_{\boldsymbol{p}\uparrow},\ c_{\boldsymbol{p}\uparrow},\ c_{-\boldsymbol{p}\uparrow},\ c^{\dagger}_{-\boldsymbol{p}\downarrow},\ c^{\dagger}_{\boldsymbol{p}\downarrow}\right] g_p, \\ &U(g_p)U(g'_p) = U(g_p g'_p),\ U({g_p}^{-1}) = U^{-1}(g_p) = U^{\dagger}(g_p),\ U(1) = 1. \end{aligned} \tag{4}$$

$U(g_p)$ is a unitary operator to induce the Thouless transformation [25, 26] and g_p is given in the form of the direct sum as

$$g_p = \begin{bmatrix} g^{\uparrow}_p & 0 \\ 0 & g^{\downarrow}_p \end{bmatrix},\ g^{\uparrow(\downarrow)}_p = \begin{bmatrix} \cos\frac{\theta_p}{2} e^{-i\frac{\psi+\varphi}{2}} \cdot I_2 & \{-(+)\} \times \sin\frac{\theta_p}{2} e^{-i\frac{\psi-\varphi}{2}} \cdot I_2 \\ \{+(-)\} \times \sin\frac{\theta_p}{2} e^{i\frac{\psi-\varphi}{2}} \cdot I_2 & \cos\frac{\theta_p}{2} e^{i\frac{\psi+\varphi}{2}} \cdot I_2 \end{bmatrix}, \tag{5}$$

where I_2 is the 2-dimensional unit matrix. In the case of spin down ($\downarrow$) we take the parenthetical sign. The 8×8 matrix g_p satisfies $g_p g_p^\dagger = g_p^\dagger g_p = I_8$ and $\det g_p = 1$ where $\det g_p$ is the determinant of matrix g_p. The matrix g_p is essentially the direct sum of $SU(2)$ matrices. Then, the physical situation is very similar to the one in the $SU(2M)$ Thouless transformation for the Lipkin model with M particles [5]. In the $SU(2)$ Res-HBA, the order parameter Δ (energy gap) is treated as a variational parameter. An energy-cutoff parameter $\hbar\omega_D$ (Debye energy) is introduced in order to regularize the $SU(2)$ Res-HBA.

Along quite the same method as the one developed in II, acting with $U(g_p)$ on a vacuum $|0\rangle$ ($c_{\boldsymbol{p}\sigma}|0\rangle = 0$), any HB WF $|g_p\rangle$ is constructed as $|g_p\rangle = U(g_p)|0\rangle$ in which the HB WF is the CS-rep of a superconducting fermion system [18]. We denote two HB states of possible local energy minima with variable gaps Δ_1 and Δ_2 as $|g_{1p}\rangle$ and $|g_{2p}\rangle$, distinguished by writing explicitly subscripts 1 and 2, which correspond to orbital or band indices whose characteristics result from eigenvalues obtained by solving the coupled Res-HB eigenvalue equations.

To construct an approximate $SU(2)$ Res-HB WF $|\Psi\rangle$, it is useful to introduce an isometric matrix in the following way:

$$u^{\uparrow}_{1(2)p} = \begin{bmatrix} \sin\frac{\theta_{1(2)p}}{2} e^{i\frac{1}{2}(\psi_{1(2)}-\varphi_{1(2)})}\cdot I_2 \\ \cos\frac{\theta_{1(2)p}}{2} e^{-i\frac{1}{2}(\psi_{1(2)}+\varphi_{1(2)})}\cdot I_2 \end{bmatrix}, u^{\downarrow}_{1(2)p} = \begin{bmatrix} -\sin\frac{\theta_{1(2)p}}{2} e^{i\frac{1}{2}(\psi_{1(2)}-\varphi_{1(2)})}\cdot I_2 \\ \cos\frac{\theta_{1(2)p}}{2} e^{-i\frac{1}{2}(\psi_{1(2)}+\varphi_{1(2)})}\cdot I_2 \end{bmatrix}, \quad (6)$$

which satisfy $u^{\uparrow\dagger}_{1(2)p} u^{\uparrow}_{1(2)p} = I_2$ and $u^{\downarrow\dagger}_{1(2)p} u^{\downarrow}_{1(2)p} = I_2$, respectively.

We introduce $z^{\uparrow}_{12p} = u^{\uparrow\dagger}_{1p} u^{\uparrow}_{2p}$ and $z^{\downarrow}_{12p} = u^{\downarrow\dagger}_{1p} u^{\downarrow}_{2p}$. So that $z^{\uparrow(\downarrow)}_{12p}$ is a 2×2 matrix and $z^{\uparrow(\downarrow)}_{21p} = z^{\uparrow(\downarrow)\dagger}_{12p}$. Then, we also have the form of the direct sum for z_{12p}

$$z_{12p} = \begin{bmatrix} z^{\uparrow}_{12p} & 0 \\ 0 & z^{\downarrow}_{12p} \end{bmatrix}, \quad z^{\uparrow}_{12p} = z^{\downarrow}_{12p} = \mathring{z}_{12p}\, e^{-i\frac{\varphi}{2}}\cdot I_2, \quad (7)$$

where

$$\left.\begin{aligned} &\mathring{z}_{12p} = \cos\tfrac{\theta_p}{2}\cos\tfrac{\psi}{2} - i\cos\tfrac{\Theta_p}{2}\sin\tfrac{\psi}{2},\ \ \mathring{z}_{21p} = \mathring{z}^*_{12p}, \\ &\theta_p \equiv \theta_{2p} - \theta_{1p},\ \ \Theta_p \equiv \theta_{2p} + \theta_{1p},\ \ \psi \equiv \psi_2 - \psi_1,\ \ \Psi \equiv \psi_2 + \psi_1,\ \ \varphi \equiv \varphi_2 - \varphi_1. \end{aligned}\right\} \quad (8)$$

The overlap integral $\langle g_{1p}|g_{2p}\rangle$ is calculated as

$$\left.\begin{aligned} \langle g_{1p}|g_{2p}\rangle &= [\det z_{12p}]^{\frac{1}{2}} = [\det z^{\uparrow}_{12p}]^{\frac{1}{2}}[\det z^{\downarrow}_{12p}]^{\frac{1}{2}}, \\ \det z^{\uparrow}_{12p} &= \det z^{\downarrow}_{12p} = \mathring{z}^2_{12p} e^{-i\varphi}. \end{aligned}\right\} \quad (9)$$

The 4×4 HB interstate density matrix $W^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p})$ ($\equiv W^{\uparrow}_{12p}$) is represented as

$$W^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p}) = u^{\uparrow}_{2p} z^{\uparrow -1}_{12p} u^{\uparrow\dagger}_{1p} = \begin{bmatrix} R^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p})\cdot I_2 & K^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p})\cdot I_2 \\ -K^{\uparrow *}(g^{\uparrow}_{2p}, g^{\uparrow}_{1p})\cdot I_2 & \{1 - R^{\uparrow *}(g^{\uparrow}_{2p}, g^{\uparrow}_{1p})\}\cdot I_2 \end{bmatrix}, \quad (10)$$

where

$$\left.\begin{aligned} R^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p}) &= \sin\tfrac{\theta_{2p}}{2}\mathring{z}^{-1}_{12p}\sin\tfrac{\theta_{1p}}{2}e^{i\frac{\psi}{2}}, \\ K^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p}) &= \sin\tfrac{\theta_{2p}}{2}\mathring{z}^{-1}_{12p}\cos\tfrac{\theta_{1p}}{2}e^{i\frac{\Psi}{2}}, \\ -K^{\uparrow *}(g^{\uparrow}_{2p}, g^{\uparrow}_{1p}) &= \cos\tfrac{\theta_{2p}}{2}\mathring{z}^{-1}_{12p}\sin\tfrac{\theta_{1p}}{2}e^{-i\frac{\Psi}{2}}, \\ 1-R^{\uparrow *}(g^{\uparrow}_{2p}, g^{\uparrow}_{1p}) &= \cos\tfrac{\theta_{2p}}{2}\mathring{z}^{-1}_{12p}\cos\tfrac{\theta_{1p}}{2}e^{-i\frac{\psi}{2}}, \end{aligned}\right\} \tag{11}$$

which satisfies the idempotency condition $W^{\uparrow 2}_{12p} = W^{\uparrow}_{12p}$ but is not hermitian. By putting $\theta_{2p} = \theta_{1p}$ and $\psi_2 = \psi_1$, so that $\theta_p = 0$ and $\psi = 0$, from (10) and (11) the usual HB density matrix $W^{\uparrow}_{11(22)p} (= u^{\uparrow}_{1(2)p} u^{\uparrow\dagger}_{1(2)p})$ is obtained as

$$W^{\uparrow}_{11(22)p} = \begin{bmatrix} \sin^2\frac{\theta_{1(2)p}}{2}\cdot I_2 & \frac{1}{2}\sin\theta_{1(2)p}e^{i\psi_{1(2)}}\cdot I_2 \\ \frac{1}{2}\sin\theta_{1(2)p}e^{-i\psi_{1(2)}}\cdot I_2 & \cos^2\frac{\theta_{1(2)p}}{2}\cdot I_2 \end{bmatrix}, \tag{12}$$

which satisfies the idempotency condition $W^{\uparrow 2}_{11(22)p} = W^{\uparrow}_{11(22)p}$ but is hermitian this time. Hereafter we denote $W^{\uparrow}_{11(22)p}$ simply as $W^{\uparrow}_{1(2)p}$.

Concerning the $SU(2)$ Res-HB parameters, we consider the two variables θ_{1p} and θ_{2p} as the essential parameters to be determined by the variation. For the remainder, we assume the values of the phases; $\psi_2 = \pi$, $\psi_1 = 0$ and the phase conventions: $\varphi_2 = -\psi_2$, $\varphi_1 = -\psi_1$ because this assumption brings the very excellent result for the ground-state energy of the Lipkin-model Hamiltonian as was done in II. Strongly suggested by the above fact, here we also adopt such an assumption. Then, from (8), we obtain more simplified expressions for the above quantities in the following forms:

$$\mathring{z}_{12p} = -i\cos\left(\frac{\theta_{1p}+\theta_{2p}}{2}\right), \tag{13}$$

$$W^{\uparrow}_{12p} = \begin{bmatrix} -\sin\frac{\theta_{2p}}{2}\dfrac{1}{\cos\left(\frac{\theta_{1p}+\theta_{2p}}{2}\right)}\sin\frac{\theta_{1p}}{2}\cdot I_2 & -\sin\frac{\theta_{2p}}{2}\dfrac{1}{\cos\left(\frac{\theta_{1p}+\theta_{2p}}{2}\right)}\cos\frac{\theta_{1p}}{2}\cdot I_2 \\ \cos\frac{\theta_{2p}}{2}\dfrac{1}{\cos\left(\frac{\theta_{1p}+\theta_{2p}}{2}\right)}\sin\frac{\theta_{1p}}{2}\cdot I_2 & \cos\frac{\theta_{2p}}{2}\dfrac{1}{\cos\left(\frac{\theta_{1p}+\theta_{2p}}{2}\right)}\cos\frac{\theta_{1p}}{2}\cdot I_2 \end{bmatrix}, \tag{14}$$

and

$$W^{\uparrow}_{1(2)p} = \begin{bmatrix} \sin^2\frac{\theta_{1(2)p}}{2}\cdot I_2 & \{+(-)\}\times\frac{1}{2}\sin\theta_{1(2)p}\cdot I_2 \\ \{+(-)\}\times\frac{1}{2}\sin\theta_{1(2)p}\cdot I_2 & \cos^2\frac{\theta_{1(2)p}}{2}\cdot I_2 \end{bmatrix}. \tag{15}$$

In the case of subscript (2) we take a parenthetical sign. The spin-down $\downarrow$ case is made quite parallel to the spin-up $\uparrow$ case except the opposite sign of non-diagonal blocks of the matrix. In (14) it is self-evident that if we take

$\theta_{2p} = -\theta_{1p}$ the HB interstate density matrix $W^{\uparrow}_{12p}$ becomes identical to the usual HB density matrix $W^{\uparrow}_{1p}$ $(= W^{\uparrow}_{2p})$. Then, as a matter of the course, all the HB interstate density matrix W_p in the whole space of both spin-up and -down are represented in the form of a direct sum as

$$W_p = \begin{bmatrix} W^{\uparrow}_p & 0 \\ 0 & W^{\downarrow}_p \end{bmatrix}. \tag{16}$$

The HB interstate density matrix, particularly W_{12p} plays a crucial role in taking quantum- and dynamical-tunneling effects into account. It really produces matrix elements of the one and two-body operators in the BCS Hamiltonian between HB WFs with different correlation structures.

3 SU(2) resonating HB approximation

Following II and III, an $SU(2)$ Res-HB WF is approximated as a superposition of two HB WFs, $|\Psi\rangle = c_1 |g_1\rangle + c_2 |g_2\rangle$. The Hamiltonian matrix element $\langle g_1|H|g_2\rangle = H[W_{12}] \cdot [\det z_{12}]^{\frac{1}{2}}$ $(H[W_{21}] = H^*[W_{12}])$ and overlap integral $[\det z_{12}]^{\frac{1}{2}}$ $(= [\det z^*_{12}]^{\frac{1}{2}})$ are expressed as

$$\begin{aligned} H[W_{12}] = & \sum_p \mathrm{Tr}\Big[\varepsilon_p \Big\{R^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p}) + R^{\downarrow}(g^{\downarrow}_{1p}, g^{\downarrow}_{2p})\Big\} \cdot I_2\Big] \\ & - \frac{1}{4} \sum_{p,\ p'} V_{p,\ p'} \mathrm{Tr}\Big\{K^{\uparrow *}(g^{\uparrow}_{2p}, g^{\uparrow}_{1p}) \cdot I_2\Big\} \mathrm{Tr}\Big\{K^{\uparrow}(g^{\uparrow}_{1p}, g^{\uparrow}_{2p}) \cdot I_2\Big\} \\ & - \frac{1}{4} \sum_{p,\ p'} V_{p,\ p'} \mathrm{Tr}\Big\{K^{\downarrow *}(g^{\downarrow}_{2p}, g^{\downarrow}_{1p}) \cdot I_2\Big\} \mathrm{Tr}\Big\{K^{\downarrow}(g^{\downarrow}_{1p}, g^{\downarrow}_{2p}) \cdot I_2\Big\} \\ = & 4 \sum_p \varepsilon_p \sin \frac{\theta_{2p}}{2} \mathring{z}^{-1}_{12p} \sin \frac{\theta_{1p}}{2} e^{i\frac{\pi}{2}} \\ & + 2 \sum_{p,\ p'} V_{p,\ p'} \cos \frac{\theta_{2p}}{2} \mathring{z}^{-1}_{12p} \sin \frac{\theta_{1p}}{2} \cdot \sin \frac{\theta_{2p'}}{2} \mathring{z}^{-1}_{12p'} \cos \frac{\theta_{1p'}}{2}, \end{aligned} \tag{17}$$

$$[\det z_{12}]^{\frac{1}{2}} = \Pi_p [\det z_{12p}]^{\frac{1}{2}} = \exp\left\{\sum_p \ln \cos^2\left(\frac{\theta_{1p} + \theta_{2p}}{2}\right)\right\}, \tag{18}$$

and from (13), the $\mathring{z}_{12p}$ is rewritten as

$$\mathring{z}_{12p} = -i\left(\cos\frac{\theta_{2p}}{2}\cos\frac{\theta_{1p}}{2} - \sin\frac{\theta_{2p}}{2}\sin\frac{\theta_{1p}}{2}\right). \tag{19}$$

The usual HB energy $\langle g_{1(2)}|H|g_{1(2)}\rangle = H[W_{11(22)}]$ is obtained as

$$H[W_{11(22)}] = 4\sum_p \varepsilon_p \sin^2\frac{\theta_{1(2)p}}{2} + \frac{1}{2}\sum_{p,\ p'} V_{p,\ p'} \sin\theta_{1(2)p} \sin\theta_{1(2)p'}. \tag{20}$$

Using the definitions (3) for $\cos\frac{\theta_{1(2)p}}{2}$ and $\sin\frac{\theta_{1(2)p}}{2}$, the Hamiltonian matrix elements and the overlap integral are tranformed to

$$
\begin{aligned}
H[W_{12}(\Delta_1,\Delta_2)] &= 2\sum_p \varepsilon_p - 2\frac{\Delta_1}{\Delta_1+\Delta_2}\sum_p \sqrt{\varepsilon_p^2+\Delta_2^2} - 2\frac{\Delta_2}{\Delta_1+\Delta_2}\sum_p \sqrt{\varepsilon_p^2+\Delta_1^2} \\
&\quad -\frac{1}{2}\frac{1}{(\Delta_1+\Delta_2)^2}\sum_{p,\ p'} V_{p,\ p'} \\
&\quad \times\left\{\varepsilon_p - \frac{\Delta_1\Delta_2}{\varepsilon_p} - \left(\sqrt{\varepsilon_p^2+\Delta_1^2}-\sqrt{\varepsilon_p^2+\Delta_2^2}\right) - \frac{\sqrt{\varepsilon_p^2+\Delta_1^2}\sqrt{\varepsilon_p^2+\Delta_2^2}}{\varepsilon_p}\right\} \\
&\quad \times\left\{\varepsilon_{p'} - \frac{\Delta_1\Delta_2}{\varepsilon_{p'}} + \left(\sqrt{\varepsilon_{p'}^2+\Delta_1^2}-\sqrt{\varepsilon_{p'}^2+\Delta_2^2}\right) - \frac{\sqrt{\varepsilon_{p'}^2+\Delta_1^2}\sqrt{\varepsilon_{p'}^2+\Delta_2^2}}{\varepsilon_{p'}}\right\},
\end{aligned}
\tag{21}
$$

$$
[\det z_{12}(\Delta_1,\Delta_2)]^{\frac{1}{2}} = \exp\left[\sum_p \ln\left\{\frac{1}{2}\left(1+\frac{\varepsilon_p^2-\Delta_1\Delta_2}{\sqrt{\varepsilon_p^2+\Delta_1^2}\sqrt{\varepsilon_p^2+\Delta_2^2}}\right)\right\}\right], \tag{22}
$$

$$
\begin{aligned}
H[W_{11(22)}(\Delta_{1(2)})] &= 2\sum_p \varepsilon_p\left(1-\frac{\varepsilon_p}{\sqrt{\varepsilon_p^2+\Delta_{1(2)}^2}}\right) \\
&\quad +\frac{1}{2}\sum_{p,\ p'} V_{p,\ p'}\frac{\Delta_{1(2)}}{\sqrt{\varepsilon_p^2+\Delta_{1(2)}^2}}\cdot\frac{\Delta_{1(2)}}{\sqrt{\varepsilon_{p'}^2+\Delta_{1(2)}^2}}.
\end{aligned}
\tag{23}
$$

To regularize (21) $\sim$ (23), the summation $\sum_p$ is converted to an integration $N(0)\int_{-\hbar\omega_D}^{\hbar\omega_D} d\varepsilon$. $N(0)d\varepsilon$ is the number of electronic states of one spin in the normal metal within energy interval $d\varepsilon$ near the Fermi surface.

Assuming the $V_{p,\ p'}$ to be a constant $-V(V>0)$ for all the p and p' and introducing new dimensionless variables $x_{1(2)} = \dfrac{\Delta_{1(2)}}{\hbar\omega_D}$. To show a direct effect of the chemical potential μ on the energy and overlap, we here approximate the integration $\int_{-\hbar\omega_D}^{\hbar\omega_D} d\varepsilon$ as $\int_{-\hbar\omega_D}^{\hbar\omega_D} d\epsilon$ which is converted to $\int_{-\hbar\omega_D-\mu}^{\hbar\omega_D-\mu} d\xi$ if we introduce a shifted variable $\xi(=\epsilon-\mu=\varepsilon)$ where ϵ denotes the original single-electron energy. First for chemical potential $\mu=0$, we calculate (21) as

$$
\begin{aligned}
H[W_{12}(\Delta_1,\Delta_2)] &= -\frac{2\hbar\omega_D N(0)\hbar\omega_D}{x_1+x_2} \\
&\quad \times\Bigg[x_2\left\{\sqrt{1+x_1^2}+x_1^2\cdot\operatorname{arcsinh}\left(\frac{1}{x_1}\right)\right\}+x_1\left\{\sqrt{1+x_2^2}+x_2^2\cdot\operatorname{arcsinh}\left(\frac{1}{x_2}\right)\right\} \\
&\quad +\frac{N(0)V}{4(x_1+x_2)}\left[\left\{\sqrt{1+x_1^2}+x_1^2\cdot\operatorname{arcsinh}\left(\frac{1}{x_1}\right)\right\}-\left\{\sqrt{1+x_2^2}+x_2^2\cdot\operatorname{arcsinh}\left(\frac{1}{x_2}\right)\right\}\right]^2\Bigg],
\end{aligned}
\tag{24}
$$

in which we have discarded a divergent integration of the type $\int_{-\hbar\omega_D}^{\hbar\omega_D} d\epsilon\dfrac{1}{\epsilon}$. Using the overap integral (A.1) in Appendix A, equation (22) is also computed as

$$\left.\begin{aligned}
&[\det z_{12}(\Delta_1,\Delta_2)]^{\frac{1}{2}} \equiv \exp[2N(0)\hbar\omega_D z(x_1,x_2)],\\
&z(x_1,x_2) = 1-\ln 2-\left\{x_1\cdot\arctan\left(\frac{1}{x_1}\right)+x_2\cdot\arctan\left(\frac{1}{x_2}\right)\right\}-\sqrt{\frac{1+x_1^2}{1+x_2^2}}\\
&+\ln\left\{1+\frac{1-x_1x_2}{\sqrt{1+x_1^2}\sqrt{1+x_2^2}}\right\}\\
&+x_1E\left\{\arctan\left(\frac{1}{x_2}\right),\sqrt{1-\frac{x_2^2}{x_1^2}}\right\}-x_2F\left\{\arctan\left(\frac{1}{x_2}\right),\sqrt{1-\frac{x_2^2}{x_1^2}}\right\}.\ (x_1\geq x_2)
\end{aligned}\right\} \quad (25)$$

Then, equation (23) is easily converted to

$$\begin{aligned}
&H[W_{11(22)}(\Delta_{1(2)})] = -2\hbar\omega_D N(0)\hbar\omega_D\\
&\times\left[\sqrt{1+x_{1(2)}^2}-x_{1(2)}^2\cdot\operatorname{arcsinh}\left(\frac{1}{x_{1(2)}}\right)+N(0)Vx_{1(2)}^2\cdot\operatorname{arcsinh}^2\left(\frac{1}{x_{1(2)}}\right)\right].
\end{aligned} \quad (26)$$

The Res-HB configuration interaction (CI) equation $\sum_{s=1}^{2}\{H[W_{rs}]-E\}\cdot[\det z_{rs}]^{\frac{1}{2}}c_s=0$ $(r=1,2)$ determines the mixing coefficients c_1 and c_2 under the normalization condition $\langle\Psi|\Psi\rangle=1$. Due to the simplicity of the Res-HB CI equation, putting $S_{12}=[\det z_{12}]^{\frac{1}{2}}$, we easily obtain the Res-HB energy E

$$\left.\begin{aligned}
&E=\begin{bmatrix}E_{\rm gr}^{\rm Res}\\ \\ E_{\rm ex}^{\rm Res}\end{bmatrix}=\frac{1}{2(1-|S_{12}|^2)}\left\{H[W_{11}]+H[W_{22}]-2H[W_{12}]\cdot|S_{12}|^2\mp E_{\rm dis}^{\frac{1}{2}}\right\},\\
&E_{\rm dis}\equiv(H[W_{11}]-H[W_{22}])^2+4\{H[W_{11}]-H[W_{12}]\}\{H[W_{22}]-H[W_{12}]\}\cdot|S_{12}|^2.
\end{aligned}\right\} \quad (27)$$

Following II and III, the direct optimization of E is easily achieved by a variation of the Res-HB ground-state energy $E_{\rm gr}^{\rm Res}$ with respect to the variational parameters x_1 and x_2, $\dfrac{\partial}{\partial x_1}E_{\rm gr}^{\rm Res}(x_1,x_2)=0$ and $\dfrac{\partial}{\partial x_2}E_{\rm gr}^{\rm Res}(x_1,x_2)=0$. There are actually four parameters $\hbar\omega_D$ (Debye energy), V (interaction-strength), $N(0)$ (density of electronic states) and μ (chemical potential) in the present regularization of the integration over the single-electron energy and the adopted naive BCS Hamiltonian. Instead of making an orbital optimization, we search for the energy minimum in the two directions of the quadratic steepest descent Δx_1 and Δx_2.

4 Res-HB equation with equal gaps

For simplicity, we here consider two HB WFs with different correlation structures $\psi_2=\pi, \psi_1=0$ and $\varphi_2=-\psi_2, \varphi_1=-\psi_1$ but with *equal gaps* $\Delta_1=\Delta_2=\Delta$. Then,

for $\mu=0$ by using the formula $\ln\left(\frac{1}{x}+\sqrt{1+\frac{1}{x^2}}\right)=\mathrm{arcsinh}\left(\frac{1}{x}\right)$, $\left(x=\frac{\Delta}{\hbar\omega_D}\right)$, Eqs. (26), (24) and (25) are rewritten in compact forms as

$$\begin{aligned} H[W_{11}(\Delta)]=H[W_{22}(\Delta)]=H[W(\Delta)]=-2\hbar\omega_D N(0)\hbar\omega_D \\ \times\left[\sqrt{1+x^2}-x^2\cdot\mathrm{arcsinh}\left(\frac{1}{x}\right)+N(0)V\left\{x\cdot\mathrm{arcsinh}\left(\frac{1}{x}\right)\right\}^2\right], \end{aligned} \tag{28}$$

$$H[W_{12}(\Delta,\Delta)]=-2\hbar\omega_D N(0)\hbar\omega_D\left[\sqrt{1+x^2}+x^2\cdot\mathrm{arcsinh}\left(\frac{1}{x}\right)\right], \tag{29}$$

$$[\det z_{12}(\Delta,\ \Delta)]^{\frac{1}{2}}=\exp\left[-2N(0)\hbar\omega_D\left\{\ln(1+x^2)+2x\cdot\arctan\left(\frac{1}{x}\right)\right\}\right]. \tag{30}$$

Due to the relation $H[W_{11}]=H[W_{22}]=H[W]$, we get the Res-HB energy E

$$E=\frac{1}{1-([\det z_{12}]^{\frac{1}{2}})^2}\cdot\left\{H[W]-H[W_{12}]\cdot\det z_{12}\mp|H[W]-H[W_{12}]|\cdot[\det z_{12}]^{\frac{1}{2}}\right\}, \tag{31}$$

where E is classified into two cases, according to the solutions for the Res-HB CI equation:

$$\left.\begin{aligned} \text{Case I} \quad &: \quad H[W]-H[W_{12}]>0, \\ E^{\mathrm{Res}}_{\mathrm{gr(ex)}} \ &= \ \frac{1}{1+(-)[\det z_{12}]^{\frac{1}{2}}}\cdot\left(H[W]+(-)H[W_{12}]\cdot[\det z_{12}]^{\frac{1}{2}}\right), \end{aligned}\right\} \tag{32}$$

$$\left.\begin{aligned} \text{Case II} \quad &: \quad H[W]-H[W_{12}]<0, \\ E^{\mathrm{Res}}_{\mathrm{gr(ex)}} \ &= \ \frac{1}{1-(+)[\det z_{12}]^{\frac{1}{2}}}\cdot\left(H[W]-(+)H[W_{12}]\cdot[\det z_{12}]^{\frac{1}{2}}\right). \end{aligned}\right\} \tag{33}$$

We also make a direct optimization of E. This is easily achieved by a variation of the Res-HB ground-state energy $E^{\mathrm{Res}}_{\mathrm{gr}}$ with respect to the variational parameter x, $\frac{d}{dx}E^{\mathrm{Res}}_{\mathrm{gr}}=0$, which leads to

$$\left.\begin{aligned} &\frac{d}{dx}H[W]\cdot(1+[\det z_{12}]^{\frac{1}{2}})+\frac{d}{dx}H[W_{12}]\cdot[\det z_{12}]^{\frac{1}{2}}\cdot(1+[\det z_{12}]^{\frac{1}{2}}) \\ &\qquad -(H[W]-H[W_{12}])\cdot\frac{d}{dx}[\det z_{12}]^{\frac{1}{2}}=0, \quad \text{(for Case I)} \\ &\frac{d}{dx}H[W]\cdot(1-[\det z_{12}]^{\frac{1}{2}})-\frac{d}{dx}H[W_{12}]\cdot[\det z_{12}]^{\frac{1}{2}}\cdot(1-[\det z_{12}]^{\frac{1}{2}}) \\ &\qquad +(H[W]-H[W_{12}])\cdot\frac{d}{dx}[\det z_{12}]^{\frac{1}{2}}=0. \quad \text{(for Case II)} \end{aligned}\right\} \tag{34}$$

These are self-consistency conditions for Case I and Case II, respectively in the Res-HBA and just gap equations in the BCS theory [8, 9] and Res-HBT [4].

Substitution of differential formulas for Hamiltonian matrix elements and overlap integral

$$\left.\begin{aligned}\frac{d}{dx}H[W]&=-4\hbar\omega_D N(0)\hbar\omega_D x\left\{\frac{1}{\sqrt{1+x^2}}-\operatorname{arcsinh}\left(\frac{1}{x}\right)\right\}\\&\qquad\times\left\{1-N(0)V\cdot\operatorname{arcsinh}\left(\frac{1}{x}\right)\right\},\\\frac{d}{dx}H[W_{12}]&=-4\hbar\omega_D N(0)\hbar\omega_D x\cdot\operatorname{arcsinh}\left(\frac{1}{x}\right),\\\frac{d}{dx}[\det z_{12}]^{\frac{1}{2}}&=-4N(0)\hbar\omega_D\cdot\arctan\left(\frac{1}{x}\right)\cdot[\det z_{12}]^{\frac{1}{2}},\end{aligned}\right\}\tag{35}$$

into (34) leads the following formulas connecting V with x for both Cases:

$$\begin{aligned}\frac{1}{N(0)V}=\operatorname{arcsinh}\left(\frac{1}{x}\right)&\left[1\pm2N(0)\hbar\omega_D\frac{\operatorname{arcsinh}\left(\frac{1}{x}\right)}{\operatorname{arcsinh}\left(\frac{1}{x}\right)-\frac{1}{\sqrt{1+x^2}}}\ \frac{x\cdot\arctan\left(\frac{1}{x}\right)}{1\pm[\det z_{12}]^{\frac{1}{2}}}\cdot[\det z_{12}]^{\frac{1}{2}}\right]\\&\times\left[1\mp\frac{\operatorname{arcsinh}\left(\frac{1}{x}\right)}{\operatorname{arcsinh}\left(\frac{1}{x}\right)-\frac{1}{\sqrt{1+x^2}}}\left\{1-4N(0)\hbar\omega_D\frac{x\cdot\arctan\left(\frac{1}{x}\right)}{1\pm[\det z_{12}]^{\frac{1}{2}}}\right\}\cdot[\det z_{12}]^{\frac{1}{2}}\right]^{-1},\end{aligned}$$

(upper sign for Case I and lower sign for Case II) (36)

Equation (36) just coincides with the well-known BCS gap equation [8] if $\det z_{12}=0$. It turns out that occurrence of the above relations of $N(0)V$ to x is attributed to the consequence of taking quantum- and dynamical-tunnelling effects into account.

First we solve the Res-HB equation for the *equal-gap* case. For $\mu=0$, we investigate a sign difference of $H[W]-H[W_{12}]$ as a function of dimensionless $\frac{1}{N(0)V}$. The sign is positive at $N(0)V=0.1\sim1.0$ if x is larger than 0.28. At an extreamely small value of x it becomes negative as $N(0)V$ becomes larger than about 0.2. If $N(0)V=0.4\sim1.0$ the difference has a negative and large value when $x=0.005\sim0.1$. Then for Case I if $N(0)\hbar\omega_D$ is smaller than 0.4 we have no good solution within $N(0)V=0.3\sim1.0$. For Case II we have an interesting solution within $N(0)V=0.4\sim0.6$ when $N(0)\hbar\omega_D$ is smaller than 0.05. Solving (36) numerically for various values of the two parameters $N(0)V$ and $N(0)\hbar\omega_D$, the behaviour of $\frac{1}{N(0)V}$ against x for Case II is illustrated at $x=0.01\sim0.1$ for each $N(0)\hbar\omega_D$. They show a gradual decrease as x becomes large for a certain value of $N(0)\hbar\omega_D$. On the other hand, as $N(0)\hbar\omega_D$ becomes smaller than 0.1, exotic behaviour of sudden increase and decrease in $\frac{1}{N(0)V}$ occurs at a point x lying inside $x\simeq0.3$. We find suitable parameters $N(0)V=1.00$ (strong coupling regime) and $N(0)\hbar\omega_D=0.02$ and arrive at a solution associated with the gap $\Delta=4.24$ [meV] for $\hbar\omega_D=60.00$ [meV]. For $\mu\neq0$, numerical calulations

are carried out parallel to the $\mu=0$ case. The μ dependence of Res-HB ground-state energy for Case II is shown in Fig. 2. In Fig. 3, R.H.S. of (36) for Case II is plotted as a function of x for $N(0)\hbar\omega_D = 0.02$, $N(0)V = 1.0$, $\hbar\omega_D = 60$ [meV] and $\mu=0$ [meV]. It gives a solution $x=0.071$ ($\Delta=4.24$ [meV]), mixing coefficients $c_{1,\mathrm{gr}} = -c_{2,\mathrm{gr}} = 7.609$ and an overlap integral $\det z_{12} = 0.991$ which produce the Res-HB ground-state energy $E_{\mathrm{gr}}^{\mathrm{Res}} = -8.680$ [meV] considerably smaller than the ground-state energy in the usual BCS theory $E_{\mathrm{gr}}^{\mathrm{BCS}} = -2.500$ [meV]. The numerical result justifies the advantage of the present Res-MF theory compared with that given by the usual BCS theory. The μ dependence of the gap is given in Table 1. Both the mixing coefficients and overlap integral gradually increase as the chemical potential grows upward though the gap gradually decreases. Then, it is concluded that the gap for Case II can not present a value such as $\Delta=8.45$ [meV], larger than the BCS value.

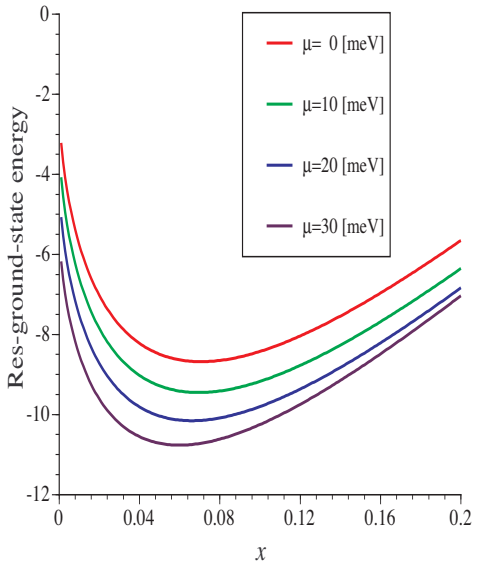

Figure 2: The μ dependence of the Res-ground-state energy with *equal gaps* for $N(0)\hbar\omega_D = 0.02$, $N(0)V = 1.00$ and $\hbar\omega_D = 60$ [meV].

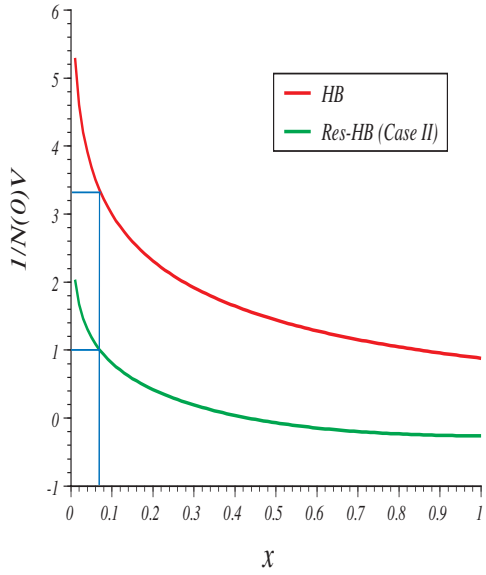

Figure 3: Solutions of the gap equation, Case II and of the BCS gap equation for $N(0)\hbar\omega_D = 0.02$, $N(0)V = 1.00$ and $\hbar\omega_D = 60$ [meV].

μ [meV]	0	10	20	30	40
Δ [meV]	4.24	4.17	3.96	3.58	3.02

Table 1: Relation between the chemical potential and energy gap in the case of *equal-gaps* at $N(0)\hbar\omega_D = 0.02$, $N(0)V = 1.00$ and $\hbar\omega_D = 60$ [meV].

To solve the Res-HB equations for gaps Δ_1 and Δ_2, we optimize by quadratic steepest-descent method until the convergence is achived. The μ dependence

of $H[W]$, $H[W_{12}]$ and $\det z_{12}$ causes an essentially different behaviour of the ground-state energy from that in the BCS approximation. In particular $H[W_{12}]$ and $\det z_{12}$ are asymmetry with respect to Δ_1 and Δ_2 which are brought through the integration $\int_{-\hbar\omega_D-\mu}^{\hbar\omega_D-\mu} d\xi_p = \int_{-\hbar\omega_D-\mu}^{-\hbar\omega_D+\mu} d\xi_p + \int_{-\hbar\omega_D+\mu}^{\hbar\omega_D-\mu} d\xi_p$ ($\xi_p = \epsilon_p - \mu = \varepsilon_p$). Calculations for case II are carried out at the region $N(0)V = 0.10 \sim 1.00$ and $N(0)\hbar\omega_D = 0.01 \sim 1.00$. As illustrated in Fig. 3, with the increase of μ the solution is shifted to asymmetrical directions, i.e., difference between Δ_1 and Δ_2 becomes larger, due to the above asymmetry. For $\mu = 12$ [meV], we arrive at the optimized-numerical values for $N(0)V = 1.00$ (strong coupling regime), $N(0)\hbar\omega_D = 0.02$ and $\hbar\omega_D = 60.00$ [meV] giving $\Delta_1 = 2.84$ [meV] and $\Delta_2 = 5.60$ [meV] and $c_{1,\mathrm{gr}} = 7.862$ and $c_{2,\mathrm{gr}} = -7.810$ and $\det z_{12} = 0.992$. If the value of the chemical potential becomes larger than 12 [meV], Δ_1 vanishes. These

	Input[meV]				Output[meV]		
	$N(0)\hbar\omega_D$	$N(0)V$	$\hbar\omega_D$	μ	Δ_1	Δ_2	$E^{\mathrm{Res}}_{\mathrm{resonon}}$
Res-MF	0.02	1.00	60	0	4.24	4.24	6.21
				4	3.94	4.53	6.21
				8	3.53	4.93	6.23
				12	2.84	5.60	6.31
Exp.	0.014		75.9		$2 \sim 3$	$6.5 \sim 7.5$	

Table 2: Energy gaps and *resonon* excitation energy against at μ

values reach good agreements with the theoretical [15, 16, 17] values of gaps and a density of states ($N(0) = 0.36$ states eV^{-1}/spin) [15] in MgB_2.

Generally it is very difficult to calculate the Res-HB excited-state energy self-consistently by the direct-orbital-optimization algorithm. We, however, easily calculate the approximate Res-HB excited-state energy $E^{\mathrm{Res}}_{\mathrm{ex}}$ given by the second solution of the Res-HB CI equation called a *resonon*, which it is evaluated by using the value of Res-HB variational parameter already determined in the Res-HB ground state. Each of energy difference $E^{\mathrm{Res}}_{\mathrm{ex}} - E^{\mathrm{Res}}_{\mathrm{gr}}$ for Case II and Case I corresponds to the excitation energy $E^{\mathrm{Res}}_{\mathrm{exc}}$ for the Res-excited state above the Res-ground state. This predicts an existence of *resonon* excitation of gaps and $E^{\mathrm{Res}}_{\mathrm{exc,\ II}} \simeq 6.20$ [meV] and $E^{\mathrm{Res}}_{\mathrm{exc,\ I}} \simeq 2.33$ [meV], respectively, for $\mu = 0$.

The physical motivation of the Res-MFT approach, like the above-mentioned two gaps observed in MgB_2, lies in an explicit realization of the radical spirit of the Res-MFT since this approach suffers any no problems of two different Fermi-surface sheets and their individual structures. This model, behaving as a two-band system, has been regarded as a good approximation adopted in the previous phenomenological theories. In this paper, however, we have pointed out another possibility of the approach, different from such phenomenologies, to the two gaps in MgB_2. Up to the present stage, instead of making an orbital

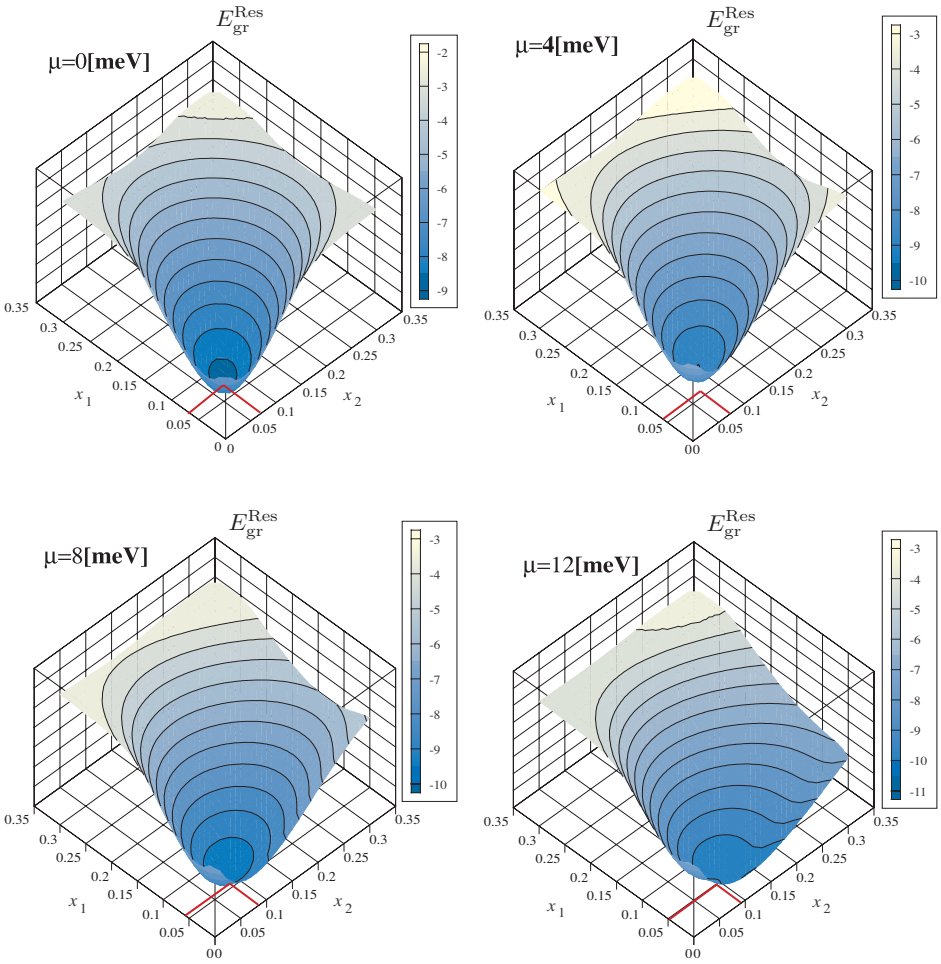

Figure 4: Chemical-potential dependence of the Res-ground-state energy for $N(0)\hbar\omega_D = 0.02$, $N(0)V = 1.00$, $\hbar\omega_D = 60$ [meV] and $\mu = 0, 4, 8, 12$ [meV]. Going from left to right, starting with the upper left figure, finishing with the bottom right. The optimized solution for E_{gr}^{Res} is given by the intersection of the red solid-line from the x_1-axis and the one from the x_2-axis.

optimization, we have searched for the minimum of the Res-HB ground-state energy in two directions of the quadratic steepest descent of the two gaps.

5 Summary and further perspectives

To show the superiority of the Res-HBT for superconducting fermion systems with large quantum fluctuations over the usual BCS and Eliashberg theories, we have applied it to the naive BCS Hamiltonian with singlet-pairing. A state with large quantum fluctuations is approximated by the superposition of two non-orthogonal CS reps, HB WFs with different correlation structures. At $T=0$, we have optimized directly the Res-HB energy by variation of the Res-HB ground-state energy with respect to the *energy-gaps*. The Res-HB ground and excited states generated with the two HB WFs explain most of the two-gap state in MgB_2. It predicts existence of *resonon* excitation which may be observed experimentally. It is also possible to start from the Res-FB operators $\mathcal{F}_{rp}$ $(r=1,2)$. Transforming by a unitary matrix $\widehat{g}_{rp}$, $\mathcal{F}_{rp}$ is easily diagonalized. Then we may obtain coupled Res-HB gap equations and reach our ultimate goal of computing two-gaps basing on the orbital-optimization. The validity of the Res-MFA is strongly dependent on the justice of such diagonalization conditions and optimization processes for the Res-FB operators in all the correlation regimes.

We will develop the present theory to include thermal effects and derive thermal *gap equations* within the same framework of Res-HBA. The temperature dependence of gap near $T=0$ and T_c becomes more complicated than that of the usual HBT and Abrikosov's [22, 23]. For *equal-gaps* of Case I, a small rearrangement after troublesome calculations yields a formula as

$$T_c^{\mathrm{I}} = 0.283\theta_D e^{-\frac{1}{4N(0)V}}, \tag{37}$$

which should be compared with the Eliashberg's formula [27] and the usual HB's one for T_c

$$T_c = 1.130\theta_D e^{-\frac{1}{N(0)V}}, \tag{38}$$

where θ_D denotes the Debye temperature. The formula (37) gives a *high* critical temperature, e.g., $T_c^{\mathrm{I}}=72.87$K for $N(0)V=0.25$ and $\theta_D=700$K. This T_c^{I} is nearly five times higher than the T_c obtained by the usual HBT formula (38), giving $T_c=14.49$K for the same values of $N(0)V$ and θ_D. The solution for Case II, however, has an anomolous behaviour for too small x_c. The derivation of such remarks is straightforward but the expression is longthy. So, their detailed descriptions will be given in a forthcoming paper. Finally, to approach such a problem we must provide a rigorous thermal Res-HBA. We have an expression for the partition function in an $SO(2N)$(N:Number of single-particle states) CS rep $|g\rangle$ [18], $\mathrm{Tr}\left(e^{-\beta H}\right)=2^{N-1}\int\langle g|e^{-\beta H}|g\rangle dg\left(\beta=\frac{1}{k_BT}\right)$ ($\int dg$ is the group integration on group $SO(2N)$). Following Fukutome [3], introducing the projection

operator P to the Res-HB subspace, partition function in the Res-HB subspace is computed as $\mathrm{Tr}\left(Pe^{-\beta H}\right)$. A group action on a quadratic HB Hamiltonian and an HB statistical density matrix at finite temperature can be defined exactly. The thermal variation of the Res-HB free energy is made along the same line as the usual thermal BCS and HB theories, which will be given elsewhere in a separate paper.

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Appendix

A Calculation of the overlap integral

Using (18) and (3), the overlap integral $[\det z_{12}]^{\frac{1}{2}}$ is transformed to

$$\begin{aligned}
[\det z_{12}]^{\frac{1}{2}} &= \exp\left\{\sum_p \ln\left(1+\frac{\varepsilon_p^2-\Delta_1\Delta_2}{\sqrt{\varepsilon_p^2+\Delta_1^2}\sqrt{\varepsilon_p^2+\Delta_2^2}}\right)-\ln 2\sum_p\right\} \\
&= \exp\left\{2N(0)\int_0^{\hbar\omega_D} d\epsilon \ln\left(\frac{\sqrt{\epsilon^2+\Delta_1^2}\sqrt{\epsilon^2+\Delta_2^2}+\epsilon^2-\Delta_1\Delta_2}{\sqrt{\epsilon^2+\Delta_1^2}\sqrt{\epsilon^2+\Delta_2^2}}\right)-\ln 2\cdot 2N(0)\hbar\omega_D\right\} \\
&= \exp\left\{2N(0)\hbar\omega_D\sqrt{x_1x_2}\int_0^{\frac{1}{\sqrt{x_1x_2}}} dy \ln\left(\sqrt{y^2+\frac{x_1}{x_2}}\sqrt{y^2+\frac{x_2}{x_1}}+y^2-1\right)\right. \\
&\quad \left. -N(0)\hbar\omega_D\sqrt{x_1x_2}\int_0^{\frac{1}{\sqrt{x_1x_2}}} dy\left[\ln\left(y^2+\frac{x_1}{x_2}\right)+\ln\left(y^2+\frac{x_2}{x_1}\right)\right]-\ln 2\cdot 2N(0)\hbar\omega_D\right\},
\end{aligned} \tag{A.1}$$

where we have introduced a new variable $y=\dfrac{\epsilon}{\sqrt{\Delta_1\Delta_2}}$. The first term in the last line of the above equation and second one are calculated by using the Elliptic functions E and F. We omit the explicit expression for the overlap integral here since it is very lengthy.

B Relation between coupled Res-HB eigenvalue equations and coupled Usadel equations

The coupled Res-HB **eigenvalue** equations $\mathcal{F}_{1(2)}u_{1(2)i} = \epsilon_{1(2)i}u_{1(2)i}$ in I are given through the **Res-FB operators** which are represented explicitly in the following forms:

$$\mathcal{F}_1 = \Big[\mathcal{F}[W_{11}] - (H[W_{11}] - E_{\rm gr}^{\rm Res}) \times \left\{ W_{12} + W_{12}^\dagger + \frac{(1_{2N} - W_{12})\mathcal{F}[W_{12}]W_{12}}{H[W_{12}] - E_{\rm gr}^{\rm Res}} + \frac{W_{12}^\dagger \mathcal{F}^\dagger[W_{12}](1_{2N} - W_{12}^\dagger)}{H^*[W_{12}] - E_{\rm gr}^{\rm Res}} \right\} \Big] |c_1|^2, \tag{B.1}$$

$$\mathcal{F}_2 = \Big[\mathcal{F}[W_{22}] - (H[W_{22}] - E_{\rm gr}^{\rm Res}) \times \left\{ W_{12} + W_{12}^\dagger + \frac{W_{12}\mathcal{F}[W_{12}](1_{2N} - W_{12})}{H[W_{12}] - E_{\rm gr}^{\rm Res}} + \frac{(1_{2N} - W_{12}^\dagger)\mathcal{F}^\dagger[W_{12}]W_{12}^\dagger}{H^*[W_{12}] - E_{\rm gr}^{\rm Res}} \right\} \Big] |c_2|^2. \tag{B.2}$$

Mixing coefficients $|c_1|^2$ and $|c_2|^2$ are obtained by solving the Res-HB CI equation. The interstate density matrix and interstate FB operator make important roles to take quantum- and dynamical-tunnelling effects into account. The self-consistency condition, i.e., the gap equation determines gaps together with the realization of the Res-HB ground-state energy.

Following [19], the coupled Usadel equations [20] for components (F_1, F_2), (F_1^*, F_2^*) and (G_1, G_2) of a matrix-valued Green's function read as follows:

$$\omega F_1 - \frac{\mathcal{D}_1}{2}\left[G_1\left(\nabla - \frac{2\pi i}{\Phi_0}\mathbf{A}\right)^2 F_1 - F_1\nabla^2 G_1\right] = \Delta_1 G_1, \tag{B.3}$$

$$\omega F_2 - \frac{\mathcal{D}_2}{2}\left[G_2\left(\nabla - \frac{2\pi i}{\Phi_0}\mathbf{A}\right)^2 F_2 - F_2\nabla^2 G_2\right] = \Delta_2 G_2, \tag{B.4}$$

where Φ_0 (flux quantum), $\mathcal{D}_{1(2)}$ (Diffusion constants), $\omega = (2n+1)\pi T$ (Matsubara frequency) and pair potentials and normalization conditions are given by

$$\left.\begin{aligned} \Delta_1 &= 2\pi T \textstyle\sum_n \left(\Lambda_{11}F_1 + \Lambda_{12}F_2\right), \ G_1^2 + F_1^* F_1 = 1, \\ \Delta_2 &= 2\pi T \textstyle\sum_n \left(\Lambda_{21}F_1 + \Lambda_{22}F_2\right), \ G_2^2 + F_2^* F_2 = 1. \end{aligned}\right\} \tag{B.5}$$

The Λ is the matrix of effective coupling constants. The index 1 corresponds to σ band and index 2 to π band in MgB_2. The Green's functions in different bands are coupled only indirectly, via the self-consistent equation in (B.5). Then the way of couplings is simpler than that of the Res-HBT. It should be noticed that the coupled Usadel equations are **not eigenvalue** equations contrary to the coupled Res-HB **eigenvalue** equations.

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