An attempt at a resonating mean-field theoretical description of thermal behavior of two-gap superconductivity

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Dedicated to the Memory of Hideo Fukutome
May 2, 2014

Abstract

The resonating mean-field theory (Res-MFT) has been applied and shown to effectively describe two-gap superconductivity (SC). Particularly at $T = 0$ using a suitable chemical potential, the two-gap SC in MgB$_2$ has been well described by the Res-Hartree-Bogoliubov theory (Res-HBT). The Res-HB ground state generated with HB wave functions almost exhausts the ground-state correlation energy in all the correlation regimes. In this paper we make an attempt at a Res-MF theoretical description of thermal behavior of the two-gap SC. In an equal energy-gap case we find a new formula leading to a higher $T_c$ than the $T_c$ of the usual HB formula.

Keywords: Res-MF theory; BCS model; Two-gap superconductivity
1 Introduction

A two-gap superconductivity (SC) of magnesium diboride MgB$_2$ with critical temperature $T_c = 39$K has been discovered nearly a decade ago [1]. Hitherto, intensive studies had been made to raise the $T_c$ of usual BCS superconductor in the weak coupling regime [2, 3, 4] and to obtain Eliashberg’s critical temperature in the strong coupling [5, 6, 7]. The $T_c = 39$K is close to or even above the upper theoretical value predicted by the BCS theory [8]. Through ab initio density functional computations it has been estimated as 22K by Kortus et al. [9]. The existence of two energy gaps in MgB$_2$ has been predicted theoretically by Liu et al. [10] employing the effective $\sigma$ and $\pi$ two-band model. They have obtained gaps at $T = 0$, $\Delta_\sigma = 7.4$ [meV] and $\Delta_\pi = 2.4$ [meV] and also their temperature dependencies and $T_c = 40$K. The two-band model was first proposed by Suhl et al. [11] and next introduced by Kondo [12].

In spite of theoretical great successes by the two-band model and the Eliashberg’s strong-coupling theory, the resonating mean-field theory (Res-MFT) [13, 14] may stand as a candidate for a possible theory and is considered to be useful for such a theoretical approach. Fermion systems with large quantum fluctuations show serious difficulties in many-body problems at finite temperature. To approach such problems, Fukutome has developed the Res-Hartree-Fock theory (Res-HFT) [13] and Fukutome and one of the present authors (S.N.) have extended it directly to the Res-Hartree-Bogoliubov theory (Res-HBT) to include pair correlations [14, 15], basing on the Lie algebra $U(N)$ and $SO(2N)$ of fermion pair operators (N: number of single-particle states), respectively. Steadily the Res-HBT has succeeded to describe effectively the two-gap SC [16] (referred to as I). If we get a Thermal Gap Equation in the Res-HBT, it is a strong manifestation of analogy of the Res-HBT with the usual BCS and HBT [2, 3, 17, 18]. The Res-HBT has a surprising fact that every HB eigenfunction in a Res-HB state has its own orbital-energy. Due to this fact, thus the Res-HBT, namely the Res-MFT, is considered to be a possible candidate for approaching to such subjects. This is because that the Res-HBT has the following characteristic feature: The Res-HBT is equivalent to the coupled Res-HB eigenvalue equations and the orbital concept is still surviving in the Res-HB approximation (Res-HBA) though the orbitals are resonating. This feature permits us to say that in some sense the band picture has a correspondence to the orbital concept in the Res-HBA though bands of different structures are resonating. The structure of the coupled Res-HB eigenvalue equations resembles considerably the structure of the coupled quasiclassic Usadel equations [19] derived by Gurevich for an anisotropic two-band superconductor [20]. The Res-HB ground state generated with HB wave functions (WFs) which are the coherent state representations (CS reps) [21], is expected to almost exhausts the ground-state correlation energy in all the correlation regimes. The generator coordinate method (GCM) is also a powerful tool for such the problem. The modern GCM is widely used in nuclear and molecular physics [22, 23].

To demonstrate the advantage of the Res-HBT for superconducting fermion systems with large quantum fluctuations over the usual BCS and Eliashberg theories, we already have applied it to a naive BCS Hamiltonian of singlet-pairing. 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, i.e., energy-gaps. The Res-MF ground and excited states generated with the two HB WFs explain most of the magnitudes of 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 the fermions [16].
To go beyond the above mentioned *ab initio* density functional computations and phenomenologies, we develop a thermal Res-HBT which enables us to describe exactly a superconducting fermion system with $N$ single-particle states. A thermal Res-Fock-Bogoliubov (Res-FB) operator plays a central and crucial role in the thermal Res-HBT \cite{13,14}. Using such an operator, a temperature dependent variation should be made necessarily along a way different from the usual thermal-BCS theory \cite{24,25,26}. Let us now prepare a Res-HB subspace spanned by Res-HB ground and excited states. We also introduce the projection operator $P$ to the Res-HB subspace. A partition function in a CS rep of the Lie algebra $SO(2N)$, $\langle g |$ \cite{21} is expressed as $\text{Tr}(e^{-\beta H})=2^{N-1}\int \langle g|e^{-\beta H}|g \rangle dg$ ($\beta = 1/k_BT$) where $\text{Tr}$ means trace and the integration is the group integration on the Lie group $SO(2N)$. Making use of the projection operator $P$, the partition function in the Res-HB subspace is given as $\text{Tr}(Pe^{-\beta H})$. This kind of trace formula is calculated within the Res-HB subspace by using the Laplace transform of $e^{-\beta H}$ and the projection operator method \cite{27,28,29,30} which leads us to an infinite matrix continued fraction (IMCF). For the moment such a trace formula is assumed to be calculated appropriately. A group action on an HB-Hamiltonian and -density matrix at finite temperature are exactly defined. The variation of the Res-HB free energy is made parallel to the usual thermal BCS theory \cite{2,3,24,25,26}, which leads to a thermal HB density matrix $W^\text{thermal}_{\text{Res}}$ expressed in terms of the thermal Res-FB operator $F^\text{thermal}_{\text{Res}}$ as $W^\text{thermal}_{\text{Res}}=[1_{2N}+\exp\{\beta F^\text{thermal}_{\text{Res}}\}]^{-1}$. Then the Res-HB coupled eigenvalue equation is extended to the thermal Res-HB coupled eigenvalue equation in a formal way whose eigenvalue is obtained by diagonalization of the thermal Res-FB operator. For the sake of simplicity here the whole Res-HB subspace is assumed to be superposition of two HB WFs. In this simplest case we apply the present tentative of the thermal Res-HBT to the naive BCS Hamiltonian of singlet-pairing and then derive formulas for determining $T_c$ and thermal behaviors of the gaps near $T=0$ and $T_c$. Particularly in the case of equal magnitude of two gaps but with different phases, we find new formulas for $T_c$ boosting up $T_c$ to higher values than the usual HB values and get new analytical expressions for gaps near $T=0$ and $T_c$. In the intermediate temperature region, we solve a thermal resonating gap equation numerically. Finally in the last Section, we give a summary and further perspectives. In Appendices we give a proof of trace formula and a derivation of the expression for thermal HB density matrix in terms of thermal Res-FB operator. We further provide the formulas to calculate the gap at zero and intermediate temperatures.
2 Thermal resonating HB eigenvalue equation

According to the principles of quantum statistical physics, the free energy \( F \) is given in terms of the statistical density matrix \( \hat{W} \) as follows:

\[
F = \text{Tr}(\hat{W} H) + \frac{1}{\beta} \text{Tr}(\hat{W} \ln \hat{W}), \quad \hat{W} = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})}. \tag{2.1}
\]

Consider the whole Res-HB subspace \( |\Psi_{\text{Res}}^{(k)}\rangle = \sum_{r=1}^{n} c_r^{(k)} |g_r\rangle \) \( (k = 1, \cdots, n) \), namely the superposition of HB WFs \( |g_r\rangle \), in which the Res-state with index \( k = 1 \) and the Res-states with indices \( k = 2, \cdots, n \) stand for the Res-ground state and the Res-excited states, respectively. Let us introduce a projection operator \( P \) to the Res-HB subspace, \( P|\Psi\rangle = |\Psi_{\text{Res}}\rangle \), as

\[
P = \sum_{r,s=1}^{n} |g_r\rangle \langle S^{-1}_{rs} |g_s\rangle = P^\dagger, \quad Q = 1 - P,
\]

\[
P^2 = P, \quad Q^2 = Q, \quad PQ = Q P = 0,
\]

where \( S = (S_{rs}) \left( = [\det z_{rs}]^\frac{1}{2} \right) \) is an \( n \times n \) matrix composed of the overlap integrals and \( S^\dagger = S \). Here we propose a quantum statistical Res-HB theory along the same way as the Peierls-Bogoliubov’s quantum statistical approach [31, 3, 4]. Using the projection operator \( P \), we can extend the HB free energy corresponding to the form of the free energy (2.1) naturally to the Res-HB free energy in the following form:

\[
F_{\text{Res}} = \text{Tr}(\hat{W}_{\text{Res}} H) + \frac{1}{\beta} \text{Tr}\left\{ \hat{W}_{\text{Res}} \ln \hat{W}_{\text{Res}} \right\}, \quad \hat{W}_{\text{Res}} = \frac{P e^{-\beta H} P}{\text{Tr}(P e^{-\beta H})}, \tag{2.3}
\]

which leads directly to

\[
F_{\text{Res}} = \langle H \rangle_{\text{Res}} + \frac{1}{\beta} \text{Tr}\left\{ P e^{-\beta H} P \ln(P e^{-\beta H}) \right\} - \frac{1}{\beta} \ln \text{Tr}(P e^{-\beta H}), \quad \langle H \rangle_{\text{Res}} = \frac{\text{Tr}(P e^{-\beta H} P)}{\text{Tr}(P e^{-\beta H})}. \tag{2.4}
\]

In the denominator of resonating statistical density matrix \( \hat{W}_{\text{Res}} \) (2.3) and in that of Res-HB free energy \( F_{\text{Res}}^{\text{thermal}} \) (2.4), there appears the partition function in the Res-HB subspace, which is computed as

\[
\text{Tr}(P e^{-\beta H}) = \sum_{r,s=1}^{n} \langle g_r | e^{-\beta H} | g_s \rangle (S^{-1})_{sr}, \tag{2.5}
\]

the detailed proof of which is given in Appendix A.

On the other hand, using the entropy \( S_{\text{thermal}}^{\text{Res}} \) in the Res-HB subspace and the relation \( F_{\text{Res}}^{\text{thermal}} = \langle H \rangle_{\text{Res}} - T S_{\text{Res}}^{\text{Res}} \), we have another form of the Res-HB free energy, i.e., a well-known formula expressed in terms of a thermal Res-HB density matrix \( \hat{W}_{\text{Res}}^{\text{thermal}} \) as

\[
F_{\text{Res}}^{\text{thermal}} = \langle H \rangle_{\text{Res}} + \frac{1}{2} \frac{1}{\beta} \text{Tr}\left\{ \hat{W}_{\text{Res}}^{\text{thermal}} \ln \hat{W}_{\text{Res}}^{\text{thermal}} + (12N - \hat{W}_{\text{Res}}^{\text{thermal}}) \ln(12N - \hat{W}_{\text{Res}}^{\text{thermal}}) \right\}, \quad \hat{W}_{\text{Res}}^{\text{thermal}} = \left[ \begin{array}{c|c}
\hat{R}_{\text{Res}}^{\text{thermal}} & \hat{K}_{\text{Res}}^{\text{thermal}} \\
\hline
-\hat{K}^{\text{thermal}*}_{\text{Res}} & 1 N - \hat{R}^{\text{thermal}*}_{\text{Res}}
\end{array} \right], \quad \hat{R}_{\text{Res}}^{\text{thermal}} = (R_{\text{Res};\alpha\beta}^{\text{thermal}}), \quad \hat{K}_{\text{Res}}^{\text{thermal}} = (K_{\text{Res};\alpha\beta}^{\text{thermal}}), \tag{2.6}
\]

where, using the resonating statistical density matrix \( \hat{W}_{\text{Res}} \), the quantities \( \hat{R}_{\text{Res};\alpha\beta}^{\text{thermal}} \) and \( \hat{K}_{\text{Res};\alpha\beta}^{\text{thermal}} \) are defined as

\[
\hat{R}_{\text{Res};\alpha\beta}^{\text{thermal}} \equiv \text{Tr}\left\{ \hat{W}_{\text{Res}} \left( \frac{E_{\alpha}^\beta + \frac{1}{2} \delta_{\beta\alpha}}{2} \right) \right\}, \quad \hat{K}_{\text{Res};\alpha\beta}^{\text{thermal}} \equiv \text{Tr}\left\{ \hat{W}_{\text{Res}} E_{\beta\alpha} \right\}. \tag{2.7}
\]
Applying the trace manipulation, the last equation of (2.7), developed in Appendix A, to the trace formulas (2.7), the second equation in (2.4) can be expressed as

$$\langle H \rangle_{\text{Res}} = h_{\beta_\alpha} \text{Tr} \left\{ \tilde{W}_{\text{Res}} \left( E^\beta_\alpha + \frac{1}{2} \delta_{\beta_\alpha} \right) \right\} + \frac{1}{4} [\alpha/\beta] [\gamma/\delta] \text{Tr} \left\{ \tilde{W}_{\text{Res}} E^{\gamma/\delta} E^{\beta/\alpha} \right\}, \quad (2.8)$$

where

$$\text{Tr} \left\{ \tilde{W}_{\text{Res}} \left( E^\beta_\alpha + \frac{1}{2} \delta_{\beta_\alpha} \right) \right\} = \sum_{k=1}^{n} \sum_{r,s=1}^{n} \frac{c^{(k)*}_r c^{(k)}_s}{\text{Tr}(Pe^{-\beta H})} \sum_{r',s'=1}^{n} \langle g_r | e^{-\beta H} | g_{r'} \rangle (S^{-1})_{r'r'} \times \langle g_{s'} | E^\beta_\alpha + \frac{1}{2} \delta_{\beta_\alpha} | g_s \rangle, \quad (2.9)$$

$$\text{Tr} \left\{ \tilde{W}_{\text{Res}} E^\beta_\alpha \right\} = \sum_{k=1}^{n} \sum_{r,s=1}^{n} \frac{c^{(k)*}_r c^{(k)}_s}{\text{Tr}(Pe^{-\beta H})} \sum_{r',s'=1}^{n} \langle g_r | e^{-\beta H} | g_{r'} \rangle (S^{-1})_{r'r'} \langle g_{s'} | E^\beta_\alpha | g_s \rangle.$$

The relation $$\sum_{k=1}^{n} c^{(k)*}_r c^{(k)}_s = (S^{-1})_{rs}$$ is satisfied if the thermal Res-HB CI equation, which is given later, could be solved and all the mixing coefficients could be determined completely. We have a simpler expression for $$\langle H \rangle_{\text{Res}}$$, redenoted as $$\langle H \rangle_{\text{Res}}^{\text{thermal}}$$, in the following form:

$$\langle H \rangle_{\text{Res}}^{\text{thermal}} = \sum_{k=1}^{n} \sum_{r,s=1}^{n} H \left[ W_{\text{Res};rs}^{\text{thermal}} \right] \cdot \left[ \text{det} \ z_{rs} \right]^{\frac{1}{2}} \frac{c^{(k)*}_r c^{(k)}_s}{\text{Tr}(Pe^{-\beta H})}, \quad (2.10)$$

$$W_{\text{Res};rs}^{\text{thermal}} \equiv \left[ \begin{array}{cc} R_{\text{Res};rs}^{\text{thermal}} & K_{\text{Res};rs}^{\text{thermal}} \\ -K_{\text{Res};sr}^{\text{thermal}} & 1 - R_{\text{Res};sr}^{\text{thermal}} \end{array} \right],$$

in which the explicit form of the Hamiltonian matrix element is given as

$$H \left[ W_{\text{Res};rs}^{\text{thermal}} \right] = h_{\alpha_\beta} R_{\text{Res};rs;\beta\alpha}^{\text{thermal}}$$

$$+ \frac{1}{2} [\alpha/\beta] [\gamma/\delta] \left\{ R_{\text{Res};rs;\beta\alpha}^{\text{thermal}} R_{\text{Res};sr;\alpha\gamma}^{\text{thermal}} - \frac{1}{2} K_{\text{Res};sr;\alpha\gamma}^{\text{thermal}} K_{\text{Res};rs;\beta\delta}^{\text{thermal}} \right\}, \quad (2.11)$$

where

$$R_{\text{Res};rs;\beta\alpha}^{\text{thermal}} \cdot \left[ \text{det} \ z_{rs} \right]^{\frac{1}{2}} = \sum_{r',s'=1}^{n} \langle g_r | e^{-\beta H} | g_{r'} \rangle (S^{-1})_{r'r'} \langle g_{s'} | E^\beta_\alpha + \frac{1}{2} \delta_{\beta_\alpha} | g_s \rangle,$$

$$K_{\text{Res};rs;\beta\alpha}^{\text{thermal}} \cdot \left[ \text{det} \ z_{rs} \right]^{\frac{1}{2}} = \sum_{r',s'=1}^{n} \langle g_r | e^{-\beta H} | g_{r'} \rangle (S^{-1})_{r'r'} \langle g_{s'} | E^\beta_\alpha | g_s \rangle. \quad (2.12)$$

To determine $$|g_r\rangle$$’s and $$c^{(k)}_r$$’s by the variational method, we adopt a thermal Lagrangian with Lagrange multiplier term $$E^{(k)}$$ to secure normalization condition $$\langle \Psi^{\text{Res}(k)}_r | \Psi^{\text{Res}(k)}_s \rangle = 1$$,

$$L_{\text{Res}}^{\text{thermalHB}} = \sum_{k=1}^{n} \sum_{r,s=1}^{n} \left( H \left[ W_{\text{Res};rs}^{\text{thermal}} \right] - E^{(k)} \right) \cdot \left[ \text{det} \ z_{rs}^{\text{thermal}} \right]^{\frac{1}{2}} c^{(k)*}_r c^{(k)}_s. \quad (2.13)$$

The variation of (2.13) is made in a quite parallel manner to the previous ones [13, 14]. From the variation of $$L_{\text{Res}}^{\text{thermalHB}}$$ with respect to $$c^{(k)*}_r$$ for ground state ($$k = 1$$) and any $$k$$th excited state, we get the thermal Res-HB CI equation to determine thermal mixing coefficients $$c^{(k)}_s$$

$$\sum_{s=1}^{n} \left( H \left[ W_{\text{Res};rs}^{\text{thermal}} \right] - E^{(k)} \right) \cdot \left[ \text{det} \ z_{rs}^{\text{thermal}} \right]^{\frac{1}{2}} c^{(k)}_s = 0. \quad (k = 1, \cdots, n) \quad (2.14)$$

We also make the variation of the Hamiltonian matrix element $$H[W_{\text{Res};rs}^{\text{thermal}}]$$ as
\[ \delta H_{\text{Res,FB}} = \frac{1}{2} \text{Tr} \left\{ \mathcal{F}[W_{\text{thermal}}_{\text{Res,FB}}] \delta W_{\text{thermal}}_{\text{Res,FB}} \right\}, \quad \mathcal{F}[W_{\text{thermal}}_{\text{Res,FB}}] = \begin{pmatrix} F_{\text{thermal,Res,FB}} & D_{\text{thermal,Res,FB}} \\ -D_{\text{thermal,Res,FB}} & -F_{\text{thermal,Res,FB}} \end{pmatrix}, \]

\[ F_{\text{thermal,Res,FB};\alpha\beta} = \frac{\delta H_{\text{thermal,Res,FB}}}{\delta R_{\text{Res,FB};\alpha\beta}} = h_{\alpha\beta} + [\alpha\beta|\gamma\delta]_{\text{thermal,Res,FB};\gamma\delta}, \]

\[ D_{\text{thermal,Res,FB};\alpha\beta} = -\frac{1}{2} [\alpha\gamma|\beta\delta]_{\text{thermal,Res,FB};\gamma\delta}. \]

The variation of the thermal HB interstate density matrix \( W_{\text{thermal}}_{\text{Res,FB}} \) and the overlap integral \( [\text{det} z_{\text{thermal}}]^{1/2} \) are also given by

\[ \delta W_{\text{thermal,Res,FB}} = D_{rs} (12N - W_{\text{thermal,Res,FB}}) + (12N - W_{\text{thermal,Res,FB}}) \tilde{D}_{rs}, \]

\[ D_{rs} \equiv u_{rs}^{\text{thermal},-1} \delta u_{rs}^{\text{thermal},+1}, \quad \tilde{D}_{rs} \equiv \delta u_{rs}^{\text{thermal},-1} u_{rs}^{\text{thermal},+1}, \]

\[ \delta [\text{det} z_{\text{thermal}}]^{1/2} = \frac{1}{2} \text{Tr} (D_{rs} + \tilde{D}_{rs}) \cdot [\text{det} z_{\text{thermal}}]^{1/2}. \]

Following I and the Res-HFT [13], writing \( L_{\text{thermal,Res,FB}} = \sum_{k=1}^{n} \sum_{s=1}^{n} K_{\text{thermal,Res,FB};s}^{(k)} c_{r}^{(k)s} c_{s}^{(k)} \) and \( L_{\text{Res,FB}} = \{ H[W_{\text{thermal,Res,FB}}] - E^{(k)} \} [\text{det} z_{\text{thermal}}]^{1/2} \), then from the variation of \( L_{\text{Res,FB}} \), namely (2.15) and (2.16), we obtain the thermal Res-HB equation to determine the MF WF \( u_{rs} \) as

\[ \sum_{k=1}^{n} \sum_{s=1}^{n} K_{\text{thermal,Res,FB};s}^{(k)} c_{r}^{(k)s} c_{s}^{(k)} = 0, \]

\[ K_{\text{thermal,Res,FB};s}^{(k)} \equiv \{ (12N - W_{\text{thermal,Res,FB}}) \mathcal{F}[W_{\text{thermal,Res,FB}}] + H[W_{\text{thermal,Res,FB}}] - E^{(k)} \} \cdot W_{\text{thermal,Res,FB}} \cdot [\text{det} z_{\text{thermal}}]^{1/2}, \]

from which we can derive the following thermal Res-HB coupled eigenvalue equations:

\[ \left\{ \mathcal{F}_{\text{thermal,Res,FB}} u_{rs} \right\} = \epsilon_{rs}^{\text{thermal}} u_{rs}, \quad \epsilon_{rs}^{\text{thermal}} \equiv \epsilon_{rs}^{\text{thermal}} - \sum_{k=1}^{n} \{ H[W_{\text{thermal,Res,FB}}] - E^{(k)} \} |c_{r}^{(k)}|^{2}, \]

\[ \mathcal{F}_{\text{thermal,Res,FB}} = \mathcal{F}[W_{\text{thermal,Res,FB}}] \sum_{k=1}^{n} |c_{r}^{(k)}|^{2} + \sum_{k=1}^{n} \sum_{s=1}^{n} \left\{ K_{\text{thermal,Res,FB};s}^{(k)} c_{r}^{(k)s} c_{s}^{(k)} + K_{\text{thermal,Res,FB};r}^{(k)} c_{r}^{(k)s} + K_{\text{thermal,Res,FB};s}^{(k)} c_{r}^{(k)s} \right\}. \]

We call the hermitian \( 2N \times 2N \) matrix \( \mathcal{F}_{\text{Res,FB}} \) the thermal Res-FB operator. Finally, we derive the expression for thermal HB density matrix in terms of thermal Res-FB operator. From the relations \( [\mathcal{F}_{\text{thermal,Res,FB}}, W_{\text{thermal,Res,FB}}] = 0 \) (3.2) and (3.5), we can reach the \( r \)th thermal HB density matrix \( W_{\text{thermal,Res,FB}} \), which is expressed in terms of the \( r \)th thermal Res-FB operator \( \mathcal{F}_{\text{Res,FB}}^{(r)} \), as

\[ W_{\text{thermal,Res,FB}} = \frac{1}{12N + \exp(\beta F_{\text{Res,FB}}^{(r)})}, \]

which is the generalizations of the usual thermal density matrix to the Res-MFT. In this section, a thermal Res-HB theory has been developed in a formal way.

For the moment the trace formula, \( \text{Tr}(P e^{-\beta H}) \) (2.5) is assumed to be computed suitably. For our sake of simplicity, in the next Section, the whole Res-HB subspace is assumed to be superposition of two HB WFs. In this simplest case, keeping an intimate connection with the usual BCS theory, we apply a tentative of the thermal Res-HBT to the naive BCS Hamiltonian of singlet-pairing and derive formulas for determining \( T_{c} \) and thermal behaviors of the gaps near \( T=0 \) and \( T_{c} \). We denote \( W_{\text{thermal,Res,FB}} \), \( \mathcal{F}_{\text{Res,FB}}^{(r)} \) and \( \mathcal{F}[W_{\text{thermal,Res,FB}}] \) simply as \( W_{rs}, \mathcal{F}_{rs} \) and \( \mathcal{F}[W_{rs}] \), respectively.
3 Thermal resonating gap equation

From [2.19] the thermal HB density matrix is given as $W_{rrp}[\mathcal{F}_{rp}] = [1 + \exp\{\beta F_{rp}\}]^{-1}$ ($r = 1, 2$) in momentum $p$. Using a Bogoliubov transformation $g_{1(2)p}$, $W_{11(22)p}[\mathcal{F}_{1(2)p}]$ are diagonalized as

$$
\tilde{W}_{rp} = g_{rp}^\dagger W_{rrp}[\mathcal{F}_{rp}] g_{rp} = \begin{bmatrix}
\hat{w}_{rp} & 0 \\
0 & 1 - \hat{w}_{rp}
\end{bmatrix}, \quad \hat{w}_{rp} = \frac{1}{1 + e^{\beta \epsilon_{rp}}}, \quad 1 - \hat{w}_{rp} = \frac{1}{1 + e^{-\beta \epsilon_{rp}}}. \tag{3.1}
$$

By making the Bogoliubov transformation $g_{rp}$, eigenvalues $\tilde{c}_{rp}$ are obtained by diagonalization of the thermal Res-FB operators $F_{rp}$ with additional terms $(H[W_{rrp}] - E)|c_{rp}|^2$ ($r = 1, 2$). The thermal HB interstate density matrix in the whole Res-HB subspace is given as the direct sum:

$$
W_p[\mathcal{F}_p] = g_p \tilde{W}_p g_p^\dagger = \bigoplus_{r=1}^{2} W_{rrp}[\mathcal{F}_{rp}], \quad W_{rr}[\mathcal{F}_r] = g_{rp} \tilde{W}_{rp} g_{rp}^\dagger. \tag{3.2}
$$

Suppose a tilde thermal Res-HB density operator $\tilde{W}_{1(2)p}$ for equal-gaps to be

$$
\tilde{W}_{1(2)p} = \begin{bmatrix}
\tilde{W}_{11(2)p}^\dagger & I_2 \\
0 & \tilde{W}_{11(2)p}^\dagger
\end{bmatrix}, \quad \tilde{W}_{11(2)p}^{\dagger (1)} = \begin{bmatrix}
\tilde{w}_{11(2)p}^{\dagger (1)} & 0 \\
0 & (1 - \tilde{w}_{11(2)p}^{\dagger (1)}) \cdot I_2
\end{bmatrix}. \tag{3.3}
$$

Here $I_2$ is the two-dimensional unit matrix. Performing the unitary transformation by $\tilde{g}_{(1(2)p)}^{\dagger}$, we obtain the following thermal Res-HB density matrix $\tilde{W}_{11(2)p}^{\dagger}$.

$$
W_{11(2)p}^{\dagger} = \tilde{g}_{(1(2)p)}^{\dagger} \tilde{W}_{11(2)p} \tilde{g}_{(1(2)p)}^{\dagger} = \tilde{g}_{11(2)p}^{\dagger} \begin{bmatrix}
\tilde{w}_{11(2)p}^{\dagger (1)} & 0 \\
0 & (1 - \tilde{w}_{11(2)p}^{\dagger (1)}) \cdot I_2
\end{bmatrix} \cdot \tilde{g}_{11(2)p}^{\dagger \dagger} \tag{3.4}
$$

In the equal-gaps case ($H[W_{11}] = H[W_{22}] = H[W]$), following I, the Res-HB ground (excited) energy $E_{\text{gr(ex)}}^{\text{Res}}$ is classified into two cases, according to the solutions for the Res-HB CI equation:

Case I: $H[W] - H[W_{12}] > 0$,

$$
E_{\text{gr(ex)}}^{\text{Res}} = \frac{1}{1 + (-)[\det z_{12}]^{\frac{1}{2}}} \cdot (H[W] + (-)H[W_{12}] \cdot [\det z_{12}]^{\frac{1}{2}}), \tag{3.5}
$$

Case II: $H[W] - H[W_{12}] < 0$,

$$
E_{\text{gr(ex)}}^{\text{Res}} = \frac{1}{1 - (+)[\det z_{12}]^{-\frac{1}{2}}} \cdot (H[W] - (+)H[W_{12}] \cdot [\det z_{12}]^{\frac{1}{2}}). \tag{3.6}
$$

From now we keep a close connection with the BCS theory, especially in relation to the gap. The Res-FB operator $F_{1(2)p}$ for spin-up state, accompanying quantities with upper or lower sign corresponding to Case I (3.5) and Case II (3.6), is expressed as

$$
F_{1(2)p} = \begin{bmatrix}
F_{+\epsilon_p}^\dagger \cdot I_2 & \{+(-)\} \times F_{\Delta p}^\dagger \cdot I_2 \\
\{+(-)\} \times F_{\Delta p}^\dagger \cdot I_2 & -F_{-\epsilon_p}^\dagger \cdot I_2
\end{bmatrix}. \tag{3.7}
$$

The quantities $F_{+\epsilon_p}^\dagger$ and $F_{-\epsilon_p}^\dagger$ for Case I(upper sign) and Case II(lower sign) are defined as

$$
F_{+\epsilon_p}^\dagger = \frac{1}{2} \left\{ \epsilon_p + 2 \tilde{E}_{\text{gr}}^{\text{Res}} \cdot \frac{\sin^2 \theta_p}{\cos^2 \theta_p} \cdot [\det z_{12}]^{-\frac{1}{2}} + \Delta^2 \cdot [\det z_{12}]^{\frac{1}{2}} \right\} \cdot \frac{1}{1 \pm [\det z_{12}]^{\frac{1}{2}}}, \tilde{E}_{\text{gr}}^{\text{Res}} = H[W] - E_{\text{gr(ex)}}^{\text{Res}}, \tag{3.8}
$$

7
\[ \mathcal{F}_\Delta^\pm = \mathcal{F}_\Delta^\pm \equiv - \frac{1}{2} \left\{ \frac{N(0)V \cdot \arcsinh \left( \frac{1}{x} \right) \pm [\det z_{12}]^{\frac{1}{2}}}{1 \pm [\det z_{12}]^{\frac{1}{2}}} \right\}, \]

where
\[ [\det z_{12}]^{\frac{1}{2}} = \exp \left\{ -2N(0)\hbar \omega_D \left\{ \ln(1 + x^2) + 2x \cdot \arctan \left( \frac{1}{x} \right) \right\} \right\}. \tag{3.9} \]

At finite temperature, the quantities \( \mathcal{F}_{\mp \epsilon_p}^\pm, \mathcal{F}_{\pm \epsilon_p}^\pm, \mathcal{F}_\Delta^\pm \) and \( \Delta \) become temperature-dependent. This is explicitly expressed by a subscript \( T \). Using the distributions \( (3.11) \) we require correspondence relations \( \cos \theta_p \Rightarrow \cos \tilde{\theta}_1 \) and \( \sin \theta_p \Rightarrow \sin \tilde{\theta}_1 \) given through

\[
\begin{align*}
\cos \theta_p &= - \frac{\epsilon_p}{\sqrt{\epsilon_p^2 + \Delta_T^2}} \left( \frac{2\mathcal{F}_\Delta^\pm}{\Delta_T} \right) (1 - 2\tilde{\omega}_1^\pm), \\
\sin \theta_p &= \frac{\Delta_T}{\sqrt{\epsilon_p^2 + \Delta_T^2}} = - \frac{\mathcal{F}_\Delta^\pm}{\epsilon_p} (1 - 2\tilde{\omega}_1^\pm),
\end{align*}
\tag{3.11}
\]

Notice the multiplication factor \( 1 - 2\tilde{\omega}_1^\pm \). The \( \epsilon_p \) is the quasi-particle (QP) energy: \( \epsilon_p = \sqrt{\mathcal{F}_{\mp \epsilon_p}^\pm + \mathcal{F}_{\pm \epsilon_p}^\pm} \) and \( \Delta_T \) are computed in Appendix A. Substituting \( \epsilon_p \) for \( \tilde{\epsilon}_1 \) in \( (3.11) \) we have

\[
1 = \frac{\epsilon_p^2}{(\epsilon_p^2 + \Delta_T^2)^{\frac{1}{2}}} \left( \mathcal{F}_\Delta^\pm \right) (1 - 2\tilde{\omega}_1^\pm), \quad \tilde{\omega}_1^\pm = \tilde{\omega}_1^\pm.
\tag{3.12}
\]

Now we demand a new condition for Thermal Gap Equation

\[
\sum_p \left\{ \frac{\epsilon_p}{(\epsilon_p^2 + \Delta_T^2)^{\frac{1}{2}}} \left( \mathcal{F}_\Delta^\pm + \mathcal{F}_\Delta^\mp \right) - \frac{\epsilon_p^2}{(\epsilon_p^2 + \Delta_T^2)^{\frac{1}{2}}} \left( - \frac{\mathcal{F}_\Delta^\pm}{\Delta_T} \right) \right\} (1 - 2\tilde{\omega}_1^\pm) = 0, \tag{3.13}
\]

which leads to

\[
\begin{align*}
1 - N(0)V \cdot \arcsinh \left( \frac{1}{x_T} \right) \mp [\det z_{12}]^{\frac{1}{2}} \sum_p A_p \\
+ \bar{E}_{\text{Resp}}(\pm) \hbar \omega_D \sum_p B_p \mp \Delta^{\frac{1}{2}} \cdot [\det z_{12}]^{\frac{1}{2}} \sum_p C_p = 0,
\end{align*}
\tag{3.14}
\]

which we have calculated using the solutions for the Res-HB CI equation obtained in I. We also give the following definitions for \( \sum_p A_p, \sum_p B_p \) and \( \sum_p C_p \):

\[
\left[ \sum_p A_p, \sum_p B_p, \sum_p C_p \right] \equiv \sum_p \left[ \frac{\epsilon_p^2}{(\epsilon_p^2 + \Delta_T^2)^{\frac{1}{2}}} \cdot \frac{1}{\epsilon_p^2 + \Delta_T^2}, \frac{1}{\epsilon_p^2 + \Delta_T^2} \right] (1 - 2\tilde{\omega}_1^\pm).
\tag{3.15}
\]

Rearranging \( (3.14) \), it is cast to a Thermal Gap Equation with similar form to the one in I:

\[
\frac{1}{N(0)V} = \arcsinh \left( \frac{1}{x_T} \right) \left[ 1 + 2N(0) \sum_p A_p \Delta_T \cdot [\det z_{12}]^{\frac{1}{2}} \right] \\
\times \left[ 1 + \left\{ \mp [\det z_{12}]^{\frac{1}{2}} \right\} \Delta_T \cdot [\det z_{12}]^{\frac{1}{2}} \right]^{-1}.
\tag{3.16}
\]

The summations \( \sum_p A_p, \sum_p B_p \) and \( \sum_p C_p \) near \( T = 0 \) are computed in Appendix A. Substituting \( (C.11), (C.12) \) and \( (C.11) \) into \( (3.16) \), then, near \( T = 0 \) we have the gaps for Case I \( (3.5) \) as
\[
\Delta_T = \Delta_0 \left[ 1 - \frac{\det z_{12}}{N(0)V} \left\{ \arcsinh \left( \frac{\hbar \omega_D}{\Delta_0} \right) - 1 + \frac{\det z_{12}}{N(0)V} \right\}^{-1} \right] T_\frac{1}{2}.
\] (3.17)

On the other hand, with the aid of \( \left[ \det z_{12} \right]^{1/2} \approx 1 - 2\pi N(0)\hbar \omega_D x_0 (0 < x_0 \ll 1) \) which is easily derived from Taylor expansion of (3.10), we obtain the gap for Case II \( \Delta^{II}_T \) as
\[
\Delta^{II}_T = \Delta_0 \left[ 1 + \frac{1}{\pi \sqrt{1 + (N(0)V)^2}} \left\{ 1 - \arcsinh \left( \frac{\hbar \omega_D}{\Delta_0} \right) \right\} \right] \cdot T_\frac{1}{2}.
\] (3.18)

where we have used the approximate relation
\[
\frac{1}{2} \left\{ \arcsinh \left( \frac{\hbar \omega_D}{\Delta_0} \right) - 1 \right\} \approx \arcsinh \left( \frac{\hbar \omega_D}{\Delta_0} \right) - 1.
\] (3.19)

In (3.17) and (3.18), as shown from Appendix A, the quantity \( T_2^{(II)} \) is defined by
\[
T_2^{(II)} \equiv 2\pi \left\{ \Delta^{II}_T \right\} \frac{\hbar \omega_D}{k_B T} \exp \left( -\frac{\hbar \omega_D}{k_B T} \right) \cdot (n = 1, 3, \cdots).
\] (3.20)

In the opposite limit \( T \to T_c^{I} \) (\( T_c \) for Case I) the gap becomes very small, \( \left[ \det z_{12} \right]^{1/2} \to 1 \), then \( \mathcal{F}_{\mathcal{S}_T} \to -\Delta N(0)V\arcsinh(\hbar \omega_D/\Delta)/4 \) and \( (\mathcal{F}_{\mathcal{S}_T} + \epsilon_p) \to 2\epsilon_p/4 \) if we use the relations (3.8) and (3.9). We have an approximate QP energy \( \tilde{\epsilon}_p^{I} \approx \left\{ \left[ \epsilon_p^2 \right] - \left\{ \Delta N(0)V\arcsinh(\hbar \omega_D/\Delta) \right\} \right\}^{1/2}/4 \) in which the appearance of numerical factor 1/4 should be become aware carefully. This is because two HB WFs have different correlation structures \( \psi_{\alpha} = \psi_{\alpha} \) and \( \psi_{\beta} = 0 \). In such a case, returning to the original form of the BCS gap equation but with the modified QP energy \( \tilde{\epsilon}_p^{I} \), the thermal gap equation is expressed as \( 1 = 4N(0)V \int_{0}^{\hbar \omega_D} d\epsilon \frac{1}{\epsilon} \tanh \left( \frac{\epsilon}{8k_BT} \right) \).

We should emphasize that this form results from the above numerical factor 1/4. Introduce a dimensionless variable \( y_{T}^{I} \equiv \epsilon / 8k_BT^{4} \), its upper-value \( y_{T}^{I} \equiv \hbar \omega_D / 8k_BT^{I} \), and the Debye temperature \( \theta_D \equiv \hbar \omega_D / k_B \). Integrating R.H.S. of (3.21) by parts, it is approximated as follows:
\[
\int_{0}^{\hbar \omega_D} d\epsilon \frac{1}{\epsilon} \tanh \left( \frac{\epsilon}{8k_BT} \right) = \ln \frac{\epsilon}{8k_BT} \bigg|_{\epsilon = 8k_BT} \left( \frac{8k_BT}{\epsilon} \right) \equiv \ln \left( \frac{\theta_D}{T} \right).
\] (3.22)

where we have used the formula given in textbook [33]. The number \( C \) is the Euler’s constant \( (C \approx 0.5772) \) and \( e^C \approx 1.781 \). Finally a small rearrangement yields
\[
T_c^{I} = 0.283 \theta_D e^{-\frac{1}{N(0)V} V}.
\] (3.23)

It should be compared with the Eliashberg’s formula [34] and the usual HB’s one for \( T_c \) [8]
\[
T_c = 1.130 \theta_D e^{-\frac{1}{N(0)V} V}.
\] (3.24)

The new formula (3.23) gives a high critical-temperature, e.g., \( T_c^{I} = 72.87K \) for \( N(0)V = 0.25 \) and \( \theta_D = 700K \). This \( T_c^{I} \) is in contrast to \( T_c \) obtained by the famous HB formula (3.24) given by Rickayzen and Cohen in [8], namely, \( T_c = 14.49K \) for the same values of \( N(0)V \) and \( \theta_D \).

From now on we discuss behaviour of the gap near \( T_c \). In the above the modified QP energy \( \tilde{\epsilon} \equiv \left\{ \left[ \epsilon_p^2 \right] - \left\{ \Delta N(0)V\arcsinh(\hbar \omega_D/\Delta) \right\} \right\}^{1/2}/4 \) plays a crucial role to boost the \( T_c \) (3.23) comparing with \( T_c = 14.49K \) by (3.24). Note the numerical factor 1/4 in \( \tilde{\epsilon} \). First consider \( \Delta_T^{I} \) near \( T_c^{I} \). Using this form of the modified QP energy, the gap equation is roughly rewritten as
\[
\left\{ \Delta N(0)V\cdot \arcsinh \left( \frac{\hbar \omega_D}{\Delta_T} \right)^2 \right\} \int_{0}^{\hbar \omega_D} d\epsilon \left\{ \frac{1}{6} \epsilon^3 \tanh \left( \frac{\epsilon}{8k_BT} \right) - \frac{1}{8k_BT} \tanh \left( \frac{\epsilon}{8k_BT} \right) \right\}.
\] (3.25)
\[
\begin{align*}
\frac{1}{4N(0)V} &= \ln \left( \frac{h\omega_p}{k_BT} \right) - \frac{7}{8\pi^2} \zeta(3) \left( \frac{2\pi}{\epsilon_C} \right)^2 \left( \frac{h\omega_p}{k_BT} \right)^2 \left\{ N(0)Vx_T \cdot \arcsinh \left( \frac{1}{x_T} \right) \right\}^2 \\
\cong & \ln \left( \frac{h\omega_p}{k_BT} \right) + \frac{T_1^c - T}{T_1^c} - \frac{7}{8\pi^2} \zeta(3) \left( \frac{2\pi}{\epsilon_C} \right)^2 \left( 1 - \frac{T_1^c - T}{T_1^c} \right)^2 \left( \frac{h\omega_p}{k_BT} \right)^2 \left\{ N(0)Vx_T \cdot \arcsinh \left( \frac{1}{x_T} \right) \right\}^2
d(3.26)
\end{align*}
\]

where \( h\omega_p/k_BT \equiv e^C/2\pi \cdot h\omega_p/k_BT \) and we have used the famous integral-formula (C.18). Using \( \arcsinh(1/x_T) \cong \ln(2/x_T) \) \( 0 < x_T < 1 \), \( (3.22) \) and \( (3.26) \), we get \( \Delta_T \) near \( T_1^c \) as
\[
\Delta_T \cong 2\pi \sqrt{\frac{2}{7\zeta(3)}} \frac{k_BT_1^c}{\sqrt{N(0)V}} \left( 1 - \frac{T_1^c - T}{T_1^c} \right) \sqrt{\frac{T_1^c - T}{T_1^c}}
d(3.27)
\]

Such a formula has been brought through the use of the modified QP energy \( \tilde{\epsilon} \) which owes to a resonant feature of the multi-band SC. This new formula shows a more complicated temperature-dependence of \( \Delta_T \) than the \( \sqrt{T_1^c - T} \) dependence of \( \Delta_T \) presented by equation (36.6) in textbook [25] and by equations (16.32) and (16.33) in textbook [26], respectively.

Next, for Case II, \( (F_{+\epsilon_p T}^\dagger + F_{-\epsilon_p T}^\dagger) \), \( \mathcal{F}_{\Delta T} \) and \( c_p^\dagger \) become infinite simultaneously in the limit \( \Delta_T \to 0 \) \( (x_T \to 0) \) due to the existence of \( 1 - |\det z_{12}|^{1/2} \) in the denominator. Then mathematical handling for such a problem is too difficult and therefore we can not easily get a formula for \( T_{II}^c \) in an analytical way as we did in Case I. Let us denote \( T_c \) for Case II as \( T_{II}^c \). At \( T \cong T_{II}^c \), \( \Delta_{II}^T \) almost vanishes and \( 1 - |\det z_{12}|^{1/2} \to 2\pi N(0)h\omega_D x_T \). Using the \( \mathcal{F}_{\Delta T}^1 \) expressed as \( (3.2) \), we reach to the following asymptotic forms: \( \mathcal{F}_{\Delta T}^1 \to - (4\pi N(0))^{-1} N(0) V \arcsinh (h\omega_D/\Delta_T) \) and \( (\mathcal{F}_{+\epsilon_p T}^\dagger + \mathcal{F}_{-\epsilon_p T}^\dagger)/2 \to (4\pi N(0))^{-1} \epsilon_p/\Delta_T \). The QP energy \( \tilde{\epsilon}_p = (\mathcal{F}_{+\epsilon_p T}^\dagger + \mathcal{F}_{-\epsilon_p T}^\dagger)^2/4 + \mathcal{F}_{\Delta T}^{1(2)} \) is approximately calculated as \( \tilde{\epsilon}_p \equiv (4\pi N(0))^{-1} \epsilon_p/\Delta_T \) \( 0 < \Delta_T \ll 1 \). Here we discard the contribution from \( \mathcal{F}_{\Delta T}^1 \) comparing with the contribution from \( (\mathcal{F}_{+\epsilon_p T}^\dagger + \mathcal{F}_{-\epsilon_p T}^\dagger)/2 \). Returning again to the original form of the BCS gap equation but with another modified QP energy \( \tilde{\epsilon}_p^{II} \), the thermal gap equation is obtained as \( 1 = V/2 \sum_p (1 - 2\tilde{w}_{p}^\dagger)/\epsilon_p^{II} \) which also leads to the integral form
\[
1 = N(0)V \int_{0}^{\omega_D} \frac{d\epsilon}{\epsilon} \frac{4\pi N(0)\Delta_{II}^T}{\epsilon} \tanh \left( \frac{\epsilon}{2k_BT_{II}^c \cdot 4\pi N(0)\Delta_{II}^T} \right)
d(3.28)
\]

We introduce the dimensionless variable \( y_{II}^c \equiv \epsilon/(2k_BT \cdot 4\pi N(0)\Delta_{II}^T) \) and its upper-value \( y_{II}^c \equiv h\omega_D/(2k_BT_{II}^c \cdot 4\pi N(0)\Delta_{II}^T) \). Integrating \( (3.28) \) by parts \( (\theta_D/k_BT_{II}^c \equiv e^C/2\pi \cdot h\omega_D/k_BT_{II}^c) \), we have
\[
\frac{1}{4N(0)V} \pi N(0)\Delta_{II}^T \cong \ln y_{II}^c + \ln \left( \frac{4e^C}{\pi} \right) = \ln \left( \frac{1}{\pi N(0)\Delta_{II}^T} \frac{\theta_D}{T_{II}^c} \right)
d(3.29)
\]

which reads
\[
\Delta_{II}^T = \frac{\theta_D}{\pi N(0)T_{II}^c} \exp \left\{ - \frac{1}{4N(0)V \pi N(0)\Delta_{II}^T} \right\} \approx \frac{\theta_D}{\pi N(0)\Delta_{II}^T} \left( 1 - \frac{1}{4N(0)V \pi N(0)\Delta_{II}^T} \right)
d(3.30)
\]

From \( (3.30) \) we obtain a quadratic equation for \( \Delta_{II}^T \) very near \( T_c \) and then we have a solution
\[
\Delta_{II}^T = \frac{1}{\pi N(0)\Delta_{II}^T} \frac{\theta_D}{T_{II}^c} - \frac{1}{4N(0)V \pi N(0)}
d(3.31)
\]

in which at \( T_{II}^c = T_c \), the \( \Delta_{II}^T \) vanishes. Finally we can determine the critical temperature \( T_{II}^c \) for Case II as
\[
T_{II}^c = \frac{2e^C}{\pi} \theta_D N(0)V = 1.334\theta_D N(0)V
(3.32)
\]
The simple formula (3.32) gives a high critical temperature, e.g., \( T^1_c = 198 \text{K} \) for \( N(0)V = 0.25 \) and \( \theta_D = 700 \text{K} \). Finally \( \Delta^\|_T \) near \( T^\|_c \) can be approximately obtained as

\[
\Delta^\|_T \approx -\frac{e^C}{2\pi} \frac{1}{\pi N(0)} \frac{\theta_D}{T^\|_c} \left( \frac{T - T^\|_c}{T^\|_c} \right),
\]

which is linearly dependent on \( T - T^\|_c \). It is very interesting that we could find such a dependence of \( \Delta^\|_T \), comparing with the usual dependence \( \sqrt{T - T^\|_c} \) of \( \Delta^\|_T \). The numerical results for \( N(0)V = 0.25 \) and \( \theta_D = 700 \text{K} \), obtained from (3.23), (3.24) and (3.32), are illustrated in Fig. 1 below:

![Critical Temperature](image)

Figure 1: Critical Temperature \( T_c \): 1. \( T^1_c = 72.87 \text{K} \); 2. \( T_c = 14.49 \text{K} \); 3. \( T^\|_c = 198 \text{K} \)

In the intermediate temperature region, substituting (C.16) and (C.17) into (3.16), we have

\[
\begin{equation}
\left[ \frac{e^C}{\pi} \frac{1}{1 + |\text{det } z_{12}|^2 T} \right]^2 x_T \left( \frac{N(0)V \text{arcsinh} \left( \frac{1}{x_T} \right)}{T^\|_c} \right)^2 - \frac{2\pi^2}{21\zeta(3)} \ln \left( \frac{e^C}{\pi} \frac{1}{1 + |\text{det } z_{12}|^2 T} \right) \left( \frac{T}{\theta_D} \right)^2 \right] \times \left\{ \frac{N(0)V \text{arcsinh} \left( \frac{1}{x_T} \right)}{T^\|_c} - \left( 1 - |\text{det } z_{12}|^2 \right) \right\} = \frac{2}{3} \left( \frac{e^C}{\pi} \frac{1}{1 + |\text{det } z_{12}|^2 T} \right)^2 x_T^2 |\text{det } z_{12}|^2 \frac{1}{T^\|_c}.
\end{equation}
\]

Using the relation and the approximations

\[
\text{arcsinh} \left( \frac{1}{x} \right) = \ln \left( \frac{1}{x} + \sqrt{1 + \frac{1}{x^2}} \right), \quad \frac{1}{x} + \sqrt{1 + \frac{1}{x^2}} \approx 1 + \frac{1}{2x^2},
\]

and \( e^x \approx 1 + x + \frac{1}{2} x^2 \), for \( |\text{det } z_{12}|^2 \approx 0.3 \) we have

\[
x_T + \frac{1}{2} = -\frac{\sqrt{0.782}}{0.436 N(0)V} \ln \left( \frac{0.436 \theta_D}{T} \right) \left( \frac{T}{\theta_D} \right) x_T + \frac{1}{2} \frac{0.782}{0.436 N(0)V^2} \ln \left( \frac{0.436 \theta_D}{T} \right) \left( \frac{T}{\theta_D} \right)^2,
\]

from which, finally we have a very simple solution for \( x_T \) \((N(0)V = 0.25\) and \( \theta_D = 700 \text{K} \)) as

\[
x_T = -\frac{1}{2} \left\{ 1 - \frac{\sqrt{0.782}}{0.436 \times 0.25} \sqrt{\ln(0.436) - \ln \left( \frac{T}{700} \right) \left( \frac{T}{700} \right)} \right\}.
\]
Case II: Using \(1-[\det z_{12}]^{1/2}\approx 2\pi N(0)\hbar \omega_D x_T\), from (3.34) we have

\[
(0.283)^2 \{N(0)\}^2 \arcsinh^2 \left(\frac{2}{x_T}\right) - 0.782 \{\pi N(0)\hbar \omega_D\}^2 \left[\ln \left(\frac{0.283}{2\pi N(0)\hbar \omega_D}\right) - \ln \left(\frac{T}{\theta_D}\right) + \arcsinh \left(\frac{2}{x_T}\right) \left(\frac{T}{\theta_D}\right)^2\right] \\
\times \left\{N(0)\arcsinh \left(\frac{2}{x_T}\right) - (1-[\det z_{12}]^{1/2})\right\} = -\frac{2}{3} (0.283)^2 [\det z_{12}]^{1/2}.
\]

Expanding (3.39) with respect to \(\arcsinh(2/x_T)\) and neglecting a constant term which is very small for \([\det z_{12}]^{1/2}\approx 0.3\) and for \((N(0)V=0.25, N(0)\hbar \omega_D=0.01 and \theta_D=700K)\), (3.39) becomes to be a quadratic equation for \(\arcsinh(2/x_T)\). Finally we have the following solution for \(x_T\):

\[
x_T = 2/\sinh \left[\frac{1}{2} - \frac{0.3}{0.25} + \frac{0.782(\pi \times 0.01)^2}{(0.283)^2(0.25)^2} \left(\frac{T}{700}\right)^2\right] \]

\[
+ \frac{1}{4} \left[\frac{1-0.3}{0.25} - \frac{0.782(\pi \times 0.01)^2}{(0.283)^2(0.25)^2} \left(\frac{T}{700}\right)^2 + \frac{0.782(\pi \times 0.01)^2}{(0.283)^2(0.25)^3} \left[\frac{0.25}{\ln \left(\frac{0.283}{2\pi \times 0.01}\right) - \ln \left(\frac{T}{700}\right)}\right] \left(\frac{T}{700}\right)^2\right].
\]

We draw below the numerical results of the solutions for Case I and Case II.

Figure 2: Temperature dependence of the gap, Case I for \([\det z_{12}]^{1/2} = 0.3, N(0)V=0.25 and \theta_D=700K\).

Figure 3: Temperature dependence of the gap, Case II for \([\det z_{12}]^{1/2} = 0.3, N(0)V=0.25, N(0)\hbar \omega_D=0.01 and \theta_D=700K\).

The formula for Case I gives a high \(T_c^I\), e.g., \(T_c^I = 72.87K\) for parameters \(N(0)V=0.25\) and \(\theta_D=700K\). This is in contrast with \(T_c\) of the usual HB formula giving \(T_c=14.49K\) for the same values, \(N(0)V=0.25\) and \(\theta_D=700\). The formula for Case II gives also a very high \(T_c^{II}\), e.g., \(T_c^{II}=198K\) for the same values of the parameters. They are illustrated together in Fig.1. The temperature dependence of gap near \(T=0\) and \(T_c\) becomes more complicated than that of the HB and Abrikosov’s descriptions [25, 26]. At intermediate temperature, as shown in Figs. 2 and 3, we have got the solutions of \(\Delta_T\) for Cases I and II. We assume \([\det z_{12}]^{1/2}\approx 0.3\) (Cases I and II) and \(N(0)\hbar \omega_D=0.01\) (Case II) to acquire real solutions. Anyway we could obtain really the solutions \(x_T=0.030\) (Case I) and 0.243 (Case II) for \(T=80K\). The former has a negative gap below 72K. To our great interest, that value is almost equal to the \(T_c\) given by (3.23). It, however, recovers a positive and small gap. Further it increases as temperature rises up to around 190K but shows vividly a decreasing tendency beyond around 200K. In this sense the former is considerably good solution. On the contrary, the latter solution naturally decreases to 0.198 as temperature rises up to around 2000K but never vanishes. This means the latter solution has no tendency approaching the \(T_c\) given by (3.32). Much improvement of the above results should be possible if the original equation (3.34) can be solved more accurately.
4 Summary and further perspectives

In this paper, keeping an intimate connection with the usual BCS theory, we have made
an attempt at a Res-MF theoretical description of the thermal behavior of the two-gap SC.
To show the predominance of the Res-HBT for superconducting fermion systems with large
quantum fluctuations over the usual BCS and Eliashberg’s theories, we have applied the Res-
HBT to the naive BCS Hamiltonian of singlet-pairing. We have obtained gap equations within
the framework of Res-HBA. From the Res-FB operators $\mathcal{F}_1$ and $\mathcal{F}_2$ with equal-gaps, we have
found the diagonalization condition for them, which is essentially the same form as that of the
BCS theory. It leads to the self-consistent Res-HB gap equation, from which we could derive
the present gap. Here we have concentrated on the derivation of the Thermal Gap Equation
with the use of the thermal Res-HBA. From the thermal Res-FB operators $\mathcal{F}_{1T}$ and $\mathcal{F}_{2T}$ with
equal-gaps we also have found the diagonalization condition, which is just the same form of the
condition at $T=0$. This reads the self-consistent Res-HB Thermal Gap Equation and makes
possible derivation of the new formulas to determine the $T_c$ and the gaps near $T=0$ and $T_c$.

For unequal two-gaps, it is also possible to realize the above diagonalization condition
for Res-FB operators $\mathcal{F}_{rp}$ ($r=1, 2$). Transforming by a unitary matrix $\hat{g}_{rp}$, $\mathcal{F}_{rp}$ is easily
diagonalized. Noticing the same correspondence as the correspondence in (3.11), $\cos \theta_{rp} \rightarrow \cos \hat{\theta}_{rp}$ and $\sin \theta_{rp} \rightarrow \sin \hat{\theta}_{rp}$, we assume each diagonalization condition (3.12) holds even in this
case. Then we obtain coupled equations through a function of $\Delta_{1T}$ and $\Delta_{2T}$ expressed as

\[
1 = \frac{\epsilon_p^2 + (\Delta_{2T}^2)^{3/2}}{(\epsilon_p^2 + \Delta_{2T}^2)^{3/2}} \left( -\frac{2\mathcal{F}_{1T} \Delta_{2T}}{\Delta_{2T}} \right) \left( 1 - 2\tilde{w}_{rp}^+ \right), \quad \tilde{w}_{rp}^+ = \frac{1}{1 + e^{\beta \epsilon_p}}, \quad \Delta_{1T} \Delta_{2T} = 0, \quad (4.1)
\]

which reduces to equation in R.H.S. of (3.11) if $\Delta_{1T} = \Delta_{2T}$. The quantities $\mathcal{F}_{r,\Delta T}$ and $\mathcal{F}_{r,\pm \epsilon p}$
are given by the equations similar to (5.9) in I but with more complicated forms of $\Delta_{1T}$ and
$\Delta_{2T}$. For the time being, as was done in the previous section we here also use the function
$(\epsilon_p^2 + \Delta_{2T}^2)^{3/2}$ by which we divide numerator and denominator, respectively, in (4.1). After
equating the numerator to the denominator and using the relation $1 - 2\tilde{w}_{rp}^+ = \tanh(\epsilon_{rp}/2k_B T)$,
we sum up over $p$, namely integrate both sides of the equation over $\epsilon$, to achieve the optimized
conditions. Thus we obtain Res-HB coupled Thermal Gap Equations and reach our temporary
goal of computing thermal two-gaps. Along such a strategy and method, at the moment, we
will make a numerical analysis to demonstrate the thermal behavior of two-gaps.

To describe a superconducting fermion system and to approach such fundamental problems,
it is absolutely necessary to provide a rigorous thermal Res-HBA and MF approximation. As
mentioned in Introduction, we have the partition function as $\text{Tr}(e^{-\beta H})=\int \langle g | e^{-\beta H} | g \rangle dg$ and
the projection operator $P$ onto the Res-HB subspace. Then, the partition function in the Res-
HB subspace is computed as $\text{Tr}(P e^{-\beta H})$. This can be calculated within the Res-HB subspace,
e.g., by using the Laplace transform of $e^{-\beta H}$ and the projection method. The result leads
to an infinite matrix continued fraction IMCF, a concrete computation for which, however,
is very difficult. As a realistic problem, it is better to seek for another possible and more
practical way of computing approximately the partition function and the Res-HB free energy
within the framework of the Res-MFT. For this aim, it may be useful to introduce a quadratic
Res-HB Hamiltonian consisting of the Res-FB operators which satisfy the Res-HB eigenvalue
equations $[\mathcal{F}_r u_{ri}] = \epsilon_{ri} u_{ri}$. This will be given elsewhere in a separate paper in a near future.
Appendix

A Proof of the equation (2.5)

The formula for the partition function in the Res-HB subspace, (2.5), is proved as follows: Consider the whole Res-HB subspace

$$|\Psi^{\text{Res}(k)}\rangle = \sum_{t=1}^{n} c_{t}^{(k)} |g_{t}\rangle, \quad (k = 1, \ldots, n)$$

(A.1)

in which the Res-state with index $k=1$ and the Res-states with indices $k=2, \ldots, n$ stand for the Res-ground one and the Res-excited ones, respectively. For each $k$ and $k'$ state, we regard the mixing coefficients $c_{t}^{(k)}$ and their products $c_{t}^{(k)} c_{t'}^{(k')}$ as components of a column vector $\{c_{t}^{(k)}\}$ and matrix elements of a matrix $\{c_{t}^{(k)} e^{(k')}\}$, respectively. Then, we require the following ortho-normalization condition:

$$\langle \Psi^{\text{Res}(k)} | \Psi^{\text{Res}(k')} \rangle = \sum_{t,t'=1}^{n} c_{t}^{(k)} c_{t'}^{(k')} S_{tt'} = \text{Tr}\left(\{c_{t}^{(k)} e^{(k')}\} S^{T}\right) = 0, \quad (k \neq k'),$$

$$\frac{1}{n} \sum_{k=1}^{n} |\Psi^{\text{Res}(k)}\rangle \langle \Psi^{\text{Res}(k)}| = \frac{1}{n} \text{Tr}\left(\sum_{k=1}^{n} \{c_{t}^{(k)} e^{(k')}\} S^{T}\right) = 1, \quad \langle \Psi^{\text{Res}(k)} | \Psi^{\text{Res}(k')} \rangle = 1, \quad \forall k.$$  

(A.2)

On the Res-WF $|\Psi^{\text{Res}}\rangle$ we also demand the completeness condition

$$\frac{1}{n} \sum_{k=1}^{n} |\Psi^{\text{Res}(k)}\rangle \langle \Psi^{\text{Res}(k)}| = \frac{1}{n} \sum_{t,t'=1}^{n} |g_{t}\rangle \sum_{k=1}^{n} c_{t}^{(k)} c_{t'}^{(k')} \langle g_{t'}| = 1. \quad \text{(A.3)}$$

From (A.2) and (A.3), we have an important relation

$$\left\{ \sum_{k=1}^{n} e^{(k)} c^{(k)} \right\}_{tt'} = (S^{-1})_{tt'} \quad \text{(A.4)}$$

Using the definition of the projection operator $P$ (2.2) and considering the meaning of the trace manipulation in the present thermal Res-HBT, the partition function in the Res-HB subspace $\text{Tr}(P e^{-\beta H})$ is computed as

$$\text{Tr}(P e^{-\beta H}) = \text{Tr}\left(\sum_{r,s=1}^{n} |g_{r}\rangle (S^{-1})_{rs} \langle g_{s}| e^{-\beta H}\right)$$

$$= \sum_{k=1}^{n} \sum_{t,t'=1}^{n} c_{t}^{(k)} \langle g_{t}| \sum_{r,s=1}^{n} |g_{r}\rangle (S^{-1})_{rs} \langle g_{s}| e^{-\beta H} |g_{t'}\rangle c_{t'}^{(k)}$$

$$= \sum_{k=1}^{n} \sum_{t,t=1}^{n} c_{t}^{(k)} c_{t'}^{(k')} S_{tt'}(S^{-1})_{tt'} \langle g_{t}| e^{-\beta H} |g_{t'}\rangle = \sum_{t,t'=1}^{n} c_{t}^{(k)} c_{t'}^{(k')} |g_{t}| e^{-\beta H} |g_{t'}\rangle.$$  

(A.5)

Substituting (A.4) into (A.5), thus, we obtain (2.5) exactly. This is our desired result for the partition function. This kind of trace formula is calculated within the Ress-HB subspace by using the Laplace transform of $e^{-\beta H}$ and the projection operator method [27, 28, 29, 30] which leads us to an infinite matrix continued fraction (IMCF). In (A.5) if we put the unit operator instead of $e^{-\beta H}$ we get $\text{Tr}(P) = \sum_{t,t'=1}^{n} c_{t}^{(k)} c_{t'}^{(k')} |g_{t}| e^{-\beta H} |g_{t'}\rangle = \sum_{t,t'=1}^{n} S_{tt'}(S^{-1})_{tt'}(S)_{tt'} = n$. This means that the entropy $S^{\text{thermalHB}}_{\text{Res}}$ (See $F^{\text{thermalHB}}_{\text{Res}}$ in (3.1)) is at most $\ln n$. One expects that for sufficiently low temperatures the main effect of temperature consists in inducing jumps from one resonating state to another. This effect may be described by the projection operator $P$. In the case of $n=2$, $S^{\text{thermalHB}}_{\text{Res}} < \ln 2$. This fact means, of course that the extrapolations to higher temperatures may not be entirely reliable. Nevertheless, we assume that by extrapolating the temperature behavior of the gaps we may guess the critical temperatures.

As suggested in the last Section, the partition function is also capable of computation if we introduce a quadratic Res-HB Hamiltonian consisting of the Res-FB operators which satisfy the Res-HB eigenvalue equations $[F_{r} u_{r}]_{i} = \epsilon_{r} u_{r}$. This may give another possible partition function within the framework of the Res-MFT.
We here introduce the following Res-HB free energy $F_{\text{Res}}^{\text{thermalHB}}$ quite similar to (2.6). We adopt the thermal Lagrangian $L_{\text{Res}}^{\text{thermalHB}}$ (2.13) without Lagrange multiplier term $F^{(k)}$ instead of the $\langle H \rangle_{\text{Res}}$ but use the entropy $S_{\text{Res}}^{\text{thermalHB}}$, namely, multiplication of $(-1/T)$ by $F_{\text{Res}}^{\text{thermalHB}}(2)$ given right below, which is expressed in terms of the thermal HB density matrix $W_{\text{Res}:rs}^{\text{thermal}}$:

$$
F_{\text{Res}}^{\text{thermalHB}} = F_{\text{Res}}^{\text{thermalHB}(1)} + F_{\text{Res}}^{\text{thermalHB}(2)},
$$

(B.1)

$$
F_{\text{Res}}^{\text{thermalHB}(1)} = \frac{1}{2} \sum_{s=1}^{n} \sum_{r,s=1}^{n} W_{\text{Res}:rs}^{\text{thermal}} \ln W_{\text{Res}:rs}^{\text{thermal}} + \left( 1_{2N} - W_{\text{Res}:rs}^{\text{thermal}} \right) \ln \left( 1_{2N} - W_{\text{Res}:rs}^{\text{thermal}} \right),
$$

(B.2)

Multiplying the second equation of (2.18) by $W_{\text{Res}:rr}^{\text{thermal}}$ from the right and using the explicit form of $K_{\text{Res}:rr}^{\text{thermal}}(k)$ obtained from (2.17) and the idempotency relation $W_{\text{Res}:rr}^{\text{thermal}2} = W_{\text{Res}:rr}^{\text{thermal}}$, we can prove the equivalence relation and the commutability relation

$$\sum_{k=1}^{n} \sum_{s=1}^{n} K_{\text{Res}:rs}^{\text{thermal}(k)} c_{r}^{(k)} c_{s}^{* (k)} \equiv F_{\text{Res}:rr}^{\text{thermal}} W_{\text{Res}:rr}^{\text{thermal}} - W_{\text{Res}:rr}^{\text{thermal}} F_{\text{Res}:rr}^{\text{thermal}} W_{\text{Res}:rr}^{\text{thermal}},$$

which is identical to the thermal Res-HB equation (2.17). Further using the formulas (2.16) and (B.2), the direct variation of the Res-HB free energy is made parallel to the variations carried out in [13, 14] as follows:

$$
\delta F_{\text{Res}}^{\text{thermalHB}(1)} = \sum_{r=1}^{n} \frac{1}{2} \text{Tr} \left\{ \sum_{k=1}^{n} \sum_{s=1}^{n} K_{\text{Res}:rs}^{\text{thermal}(k)} c_{r}^{(k)} c_{s}^{* (k)} u_{r} \delta u_{r} \right\} + \sum_{r=1}^{n} \frac{1}{2} \text{Tr} \left\{ \delta u_{r} u_{r}^{\dagger} \sum_{k=1}^{n} \sum_{s=1}^{n} K_{\text{Res}:rs}^{\text{thermal}(k)} c_{r}^{(k)} c_{s}^{* (k)} \right\}
$$

(B.3)

$$
\delta F_{\text{Res}}^{\text{thermalHB}(2)} = \frac{1}{2} \beta \sum_{r=1}^{n} \text{Tr} \left\{ \left[ F_{\text{Res}:rr}^{\text{thermal}} W_{\text{Res}:rr}^{\text{thermal}} - W_{\text{Res}:rr}^{\text{thermal}} F_{\text{Res}:rr}^{\text{thermal}} W_{\text{Res}:rr}^{\text{thermal}} \right] \delta W_{\text{Res}:rr}^{\text{thermal}} \right\},
$$

(B.4)

second line of (B.4) has no contribution since $(1_{2N} - W_{\text{Res}:rr}^{\text{thermal}}) W_{\text{Res}:rs}^{\text{thermal}} = 0$. Then, the variational equation $\delta F_{\text{Res}}^{\text{thermalHB}} = \delta F_{\text{Res}}^{\text{thermalHB}(1)} + \delta F_{\text{Res}}^{\text{thermalHB}(2)} = 0$ leads to

$$
\ln \left\{ W_{\text{Res}:rr}^{\text{thermal}} \left( 1_{2N} - W_{\text{Res}:rr}^{\text{thermal}} \right)^{-1} \right\} = -\beta F_{\text{Res}:rr}^{\text{thermal}},
$$

(B.5)

in which we have used the variational relations $\delta W_{\text{Res}:rr}^{\text{thermal}} = u_{r} \delta u_{r}^{\dagger} + \delta u_{r} u_{r}^{\dagger}$ and $\delta u_{r}^{\dagger} u_{r} + u_{r}^{\dagger} \delta u_{r} = 0$.

From (B.5) we get $W_{\text{Res}:rr}^{\text{thermal}} \left( 1_{2N} - W_{\text{Res}:rr}^{\text{thermal}} \right)^{-1} = \exp \{ -\beta F_{\text{Res}:rr}^{\text{thermal}} \}$. Multiplication of the matrix $(1_{2N} - W_{\text{Res}:rr}^{\text{thermal}})$ from the right casts into

$$
W_{\text{Res}:rr}^{\text{thermal}} = \exp \{ -\beta F_{\text{Res}:rr}^{\text{thermal}} \} \left( 1_{2N} - W_{\text{Res}:rr}^{\text{thermal}} \right).
$$

(B.6)

From (B.6) we can reach to the final goal of the desired equation (2.19).
C Calculations of $\sum_p A_p$, $\sum_p B_p$ and $\sum_p C_p$ at zero and intermediate temperature

First, equation (3.16) is shown to reduce to the Res-HB gap equation (4.10) in I as $T \to 0$. Using a variable $\varepsilon = x \Delta_T$ instead of $\varepsilon$, summations $\sum_p A_p$, $\sum_p B_p$ and $\sum_p C_p$ near $T = 0$ are computed as follows:

\[
\begin{align*}
\frac{\sum_p A_p}{2N(0)} &= \arcsinh \left( \frac{1}{x_T} \right) - \frac{1}{\sqrt{1 + x_T^2}} + A(T), \quad A(T) = -T^{I(I)}_T + \cdots, \\
\frac{\Delta T \sum_p B_p}{2N(0)} &= \arctan \left( \frac{1}{x_T} \right) + B(T), \quad B(T) = -T^{I(I)}_T + \frac{1}{2} T^{I(I)}_T - \cdots, \\
\frac{\Delta^2 T \sum_p C_p}{2N(0)} &= \frac{1}{\sqrt{1 + x_T^2}} + C(T), \quad C(T) = -T^{I(I)}_T + T^{I(I)}_T - \cdots,
\end{align*}
\]

(C.1)

detailed calculation of which is given below. With the use of the relations (3.9) and $\Delta T / \varepsilon_p = -2 \mathcal{J}_T \mathcal{J}_T / (\mathcal{J}_T + \mathcal{J}_T)$ which lead to $\tilde{\varepsilon} = \sqrt{\varepsilon^2 + \hbar \omega_D \Delta T^{I(I)}_T}$, $\sum_p A_p$ in (3.15) is converted to

\[
\frac{\sum_p A_p}{2N(0)} \approx \int_0^1 d\xi - \xi^2 \left( \frac{1}{(\xi + 1)^2} \right) - 2 \int_0^1 d\xi \frac{\xi^2}{(\xi + 1)^2} \frac{1}{1 + e^{d^{I(I)}_{T}} \sqrt{\xi^2 + 1}}, \quad d^{I(I)}_{T} \equiv \hbar \omega_D \tilde{\Delta}^{I(I)}_T,
\]

(C.2)

where $d^{I(I)}_{T} \gg 1$ for large $\hbar \omega_D$ and for Case I and Case II, $\tilde{\Delta}^{I(I)}_T$ is defined as

\[
\tilde{\Delta}^{I(I)}_T \equiv \frac{1}{2} x_T \left\{ N(0) V \cdot \arcsinh \left( \frac{1}{x_T} \right) + (-)[\det z_{12}]^2 \right\} \frac{1}{1 + (-)[\det z_{12}]^2}.
\]

Introducing a new variable $y = \sqrt{\xi^2 + 1}$, (C.2) is integrated partly and approximated to be

\[
\frac{\sum_p A_p}{2N(0)} \approx \arcsinh \left( \frac{1}{x_T} \right) - \frac{1}{\sqrt{1 + x_T^2}} - \frac{1}{2} \int_1^\infty dy \frac{1}{\sqrt{y^2 - 1}} e^{-d^{I(I)}_{T} y} + 2 \int_1^\infty dy \frac{1}{y^2} \frac{1}{\sqrt{y^2 - 1}} e^{-d^{I(I)}_{T} y}.
\]

(C.4)

Similarly, we get approximate formulas for $\sum_p B_p$ and $\sum_p C_p$ as

\[
\frac{\Delta T \sum_p B_p}{2N(0)} \approx \arctan \left( \frac{1}{x_T} \right) - 2 \int_1^\infty dy \frac{1}{y \sqrt{y^2 - 1}} e^{-d^{I(I)}_{T} y},
\]

(C.5)
\[
\frac{\Delta^2 T \sum_p C_p}{2N(0)} \approx \frac{1}{\sqrt{1 + x_T^2}} - 2 \int_1^\infty dy \frac{1}{y^2 \sqrt{y^2 - 1}} e^{-d^{I(I)}_{T} y}.
\]

(C.6)

To carry out integral calculations in (C.4) ~ (C.6), it is convenient to use an integral representation of Bessel function [35]. The Bessel function of order $\nu$ is represented as

\[
K_{\nu}(z) = \frac{\sqrt{\pi} (\frac{z}{2})^\nu}{\Gamma (\nu + \frac{1}{2})} \int_0^\infty dy (y^2 - 1)^{\nu - \frac{1}{2}} e^{-zy}.
\]

(C.7)

Then, the integral form of the Bessel function of order 0 and its exact result are given by

\[
K_0(z) = \frac{\sqrt{\pi}}{\Gamma (\frac{1}{2})} \int_1^\infty dy \frac{1}{\sqrt{y^2 - 1}} e^{-zy} = \sqrt{\frac{\pi}{2z}} e^{-z}, \quad (\Gamma (\frac{1}{2}) = \sqrt{\pi}).
\]

(C.8)

Using (C.8), integral calculations of (C.4) ~ (C.6) are made in the following ways:

\[
\int_1^\infty dy \frac{1}{y \sqrt{y^2 - 1}} e^{-d y} = \int_1^\infty dy \frac{1}{\sqrt{y^2 - 1}} \int_1^\infty dz e^{-z y} = \int_1^d dz K_0(z)
\]

\[
= \sqrt{\frac{\pi}{2}} \left( d^{-\frac{1}{2}} - \frac{1}{2} d^{-\frac{3}{2}} + \frac{3}{4} d^{-\frac{5}{2}} - \cdots \right) e^{-d},
\]

(C.9)
\[ \int_1^\infty dy \frac{1}{y^2 \sqrt{y^2 - 1}} e^{-dy} = \int_1^\infty dy \frac{1}{y \sqrt{y^2 - 1}} \int_0^\infty dw e^{-wy} = \int_d^\infty dw \int_0^\infty dz K_0(z) \]

\[ = \sqrt{\frac{\pi}{2}} \left( d^{-\frac{1}{2}} - d^{-\frac{3}{2}} + \frac{9}{4} d^{-\frac{5}{2}} - \cdots \right) e^{-d}. \]

As a result, we obtain the approximation for \( A(T), B(T) \) and \( C(T) \) near \( T = 0 \) as

\[ A(T) \simeq 0, \quad B(T) = C(T) \simeq -T^4, \quad (11) \]

Further in the above near \( T = 0 \) we make the following approximations:

\[ \arctan \left( \frac{1}{x_T} \right) \simeq \frac{\pi}{2} - x_T, \quad \frac{1}{\sqrt{1+x_T^2}} \simeq 1 - x_0 x_T, \quad (0 < x_0 \ll 1) \]

\[ \arcsinh \left( \frac{1}{x_T} \right) \simeq \arcsinh \left( \frac{1}{x_0} \right) - \frac{1}{x_0} (x_T - x_0), \quad [\det z_{12}]^\frac{1}{T} \simeq [\det z_{12}]^\frac{1}{T=0}. \]

Next, let us introduce a new variable \( y \) by \( \varepsilon = 4(1 + [\det z_{12}]^{1/2}) k_B T y \) and quantities \( y_T \) and \( y_T^{(\pm)} = \sqrt{\varepsilon^2 + \Delta_T^2 / 2} \{ 4(1 + [\det z_{12}]^{1/2}) \}^{-1} \varepsilon \omega_D / k_B T \) where \( \Delta_T \equiv \Delta_T N(0) V \arcsinh (\hbar \omega_D / \Delta_T) \). In intermediate temperature region the modified QP energy \( \tilde{\varepsilon} \) is approximated as \( \tilde{\varepsilon}^{(\pm)} = \sqrt{\varepsilon^2 + \Delta_T^2 / 2} \{ 2(1 + [\det z_{12}]^{1/2}) \}^{-1} \). If \( \varepsilon \gg \Delta_T \), \( \sum_p A_p, \sum_p B_p \) and \( \sum_p C_p \) in (3.15) are recast to the following integrals up to \( \Delta_T \):

\[ \frac{\sum_p A_p}{2N(0)} \simeq \int_0^{\hbar \omega_D} d\varepsilon \frac{1}{\sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) - \int_0^{\hbar \omega_D} d\varepsilon \frac{\Delta_T^2}{\varepsilon^2 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) \]

\[ \simeq \int_0^{y_T^{(\pm)}} dy \left\{ 1 - \left( \frac{y_T^{(\pm)} \tilde{x}_T}{y^2} \right)^2 \right\} \frac{1}{\sqrt{y^2 + \left( \frac{y_T^{(\pm)} \tilde{x}_T}{y^2} \right)^2}} \tanh \left[ \sqrt{y^2 + \left( \frac{y_T^{(\pm)} \tilde{x}_T}{y^2} \right)^2} \right]. \]

\[ \frac{\Delta_T^2 \sum_p B_p}{N(0)} \simeq \int_{-\hbar \omega_D}^{\hbar \omega_D} d\varepsilon \frac{\Delta_T}{\sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) - \frac{1}{2} \int_{-\hbar \omega_D}^{\hbar \omega_D} d\varepsilon \frac{\Delta_T^3}{\varepsilon^3 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) = 0, \]

\[ \frac{\Delta_T^2 \sum_p C_p}{2N(0)} \simeq \int_0^{\hbar \omega_D} d\varepsilon \frac{\Delta_T^2}{\varepsilon^2 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) - \int_0^{\hbar \omega_D} d\varepsilon \frac{\Delta_T^4}{\varepsilon^4 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) \]

\[ = \left( y_T^{(\pm)} \tilde{x}_T \right)^2 \int_0^{y_T^{(\pm)}} dy \left\{ 1 - \left( \frac{y_T^{(\pm)} \tilde{x}_T}{y^2} \right)^2 \right\} \frac{1}{y^2 \sqrt{y^2 + \left( \frac{y_T^{(\pm)} \tilde{x}_T}{y^2} \right)^2}} \tanh \left[ \sqrt{y^2 + \left( \frac{y_T^{(\pm)} \tilde{x}_T}{y^2} \right)^2} \right]. \]

Further equations (C.13) and (C.15) are approximately computed, respectively, as

\[ \frac{\sum_p A_p}{2N(0)} = \int_0^{\hbar \omega_D} d\varepsilon \frac{\varepsilon^2}{\varepsilon^2 + \Delta_T^2} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) \simeq \ln \left( \frac{4e^C}{\pi y_T^{(\pm)}} \right) - \frac{21}{2\pi^2} \zeta(3) \left( y_T^{(\pm)} \tilde{x}_T \right)^2, \]

\[ \frac{\Delta_T^2 \sum_p C_p}{2N(0)} \simeq \int_0^{\hbar \omega_D} d\varepsilon \frac{1}{\varepsilon^2 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh \left( \frac{\tilde{\varepsilon}^{(\pm)}}{2k_B T} \right) \simeq \frac{7}{\pi^2} \zeta(3) \left( y_T^{(\pm)} \tilde{x}_T \right)^2. \]
Taking only a leading term, finally terms $A_p$ and $C_p$ in (C.16) are approximated to be

$$
\frac{\sum_p A_p}{2N(0)} \simeq \ln \left( \frac{e^C}{\pi} \frac{1}{1 \pm \det z_{12}} \right) - \alpha_T^{(\pm)}, \quad \frac{\tilde{\Delta}_T^2 \sum_p C_p}{2N(0)} \simeq \frac{2}{3} \alpha_T^{(\pm)},
$$

(C.17)

$$
\alpha_T^{(\pm)} \equiv \frac{21\zeta(3)}{2\pi^2} \left( \frac{e^C}{\pi} \frac{1}{1 \pm \det z_{12}} \right)^2 \left( \frac{\tilde{\Delta}_T}{k_BT} \right)^2.
$$

To derive (C.16) we give an integral formula

$$
\int_0^\infty dy \left\{ \frac{1}{y^3} \tanh y - \frac{1}{y^2} \sech^2 y \right\} = \frac{7}{\pi^2} \zeta(3),
$$

(C.18)

which can be derived by using the famous mathematical formulas [33]

$$
\frac{1}{y} \tanh y = 8 \sum_{m=1}^{\infty} \frac{1}{(2m-1)^2 \pi^2 + 4y^2}, \quad \frac{1}{y^3} \tanh y - \frac{1}{y^2} \sech^2 y = 64 \sum_{m=1}^{\infty} \frac{1}{(2m-1)^2 \pi^2 + 4y^2}.
$$

(C.19)

Adopting a new integral variable $y = (2m-1)\pi/2 \cdot \tan \theta$, an integral of the second formula in (C.19) is easily carried out for $\hbar \omega_D \gg 1$ as

$$
64 \int_0^{\pi/2} d\theta \sum_{m=1}^{\infty} \frac{1}{((2m-1)^2 \pi^2 + 4y^2)^2} = 32 \sum_{m=1}^{\infty} \frac{1}{(2m-1)^3 \pi^3} \int_0^{\pi/2} \frac{\hat{\tilde{x}}}{1 + \tan^2 \theta} = \frac{7}{2\pi^2} \zeta(3),
$$

(C.20)

where we have used $\sum_{m=1}^{\infty} (2m-1)^{-3} = (7/8) \cdot \zeta(3)$, and $\zeta(3) = \pi^3/25.79436$ [33].

To get a finite value of $\sum_p A_p$, expanding (C.13) around $y_T^{(\pm)} \tilde{x}_T$, (C.13) is boldly approximated as

$$
\frac{\sum_p A_p}{2N(0)} \simeq \int_0^{y_T^{(\pm)}} dy \frac{1}{y^3} \tanh y - \frac{3}{2} \left( y_T^{(\pm)} \tilde{x}_T \right)^2 \int_0^{y_T^{(\pm)}} dy \left\{ \frac{1}{y^3} \tanh y - \frac{1}{y^2} \sech^2 y \right\}.
$$

(C.21)

In a similar way we also get a roughly approximated integral form for (C.15) as

$$
\frac{\tilde{\Delta}_T^2 \sum_p C_p}{2N(0)} \simeq \left( y_T^{(\pm)} \tilde{x}_T \right)^2 \int_0^{y_T^{(\pm)}} dy \left\{ \frac{1}{y^3} \tanh y - \frac{1}{y^2} \sech^2 y \right\}.
$$

(C.22)

Integrations of (C.21) and (C.22) are easily made by using the integration formula (C.18) if we take the upper-value $y_T^{(\pm)}$ to be infinite.

**Acknowledgements**

S. N. would like to express his sincere thanks to Professor Manuel Fiolhais for kind and warm hospitality extended to him at the Centro de Física Computacional, Universidade de Coimbra, Portugal. This work was supported by FCT (Portugal) under the project CERN/FP/83505/2008.
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