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Resonating Mean-Field Theoretical Approach to Two-Gap Superconductivity with High- T_c

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Plan of the talk

- Introduction; **Motivation**
- Resonating HB eigenvalue equation;
- Application to two-gap superconductivity;
- SU(2) resonating HB approximation;
- Res-HB eigenvalue equation for two-gap state;
- Temperature-dependent Res-HB equation;
- Behaviour of the gap near T_c ;
- Summary.

Motivation:

A topical two-gap superconductivity has been recently discovered near 39 K in MgB₂.

1) Before the discovery of *high-T_c* superconductors, much effort had been devoted to raise critical temperatures T_c of the usual BCS superconductors in the weak coupling regime and Eliashberg's in the strong coupling.

2) $T_c = 39$ K in MgB₂ is close to or even above upper theoretical values predicted by the BCS theory.

- **Resonating (Res-) mean-field (MF) theories:**

- Resonating Hartree-Fock (Res-HF) theory ;
- Resonating Hartree-Bogoliubov (Res-HB) theory;
- Res-MF RPA;

- **Temperature dependent Res-MF theories:**

$$g_r^\dagger W_{rr}[\mathcal{F}_r]g_r = g_r^\dagger \frac{1}{1 + \exp\{\beta(\mathcal{F}_r + \{H[W_{rr}] - E\}|c_r|^2 \cdot 1_{2N})\}} g_r = \widetilde{W}_r = \begin{bmatrix} \tilde{w}_r & 0 \\ 0 & 1 - \tilde{w}_r \end{bmatrix},$$
$$\tilde{w}_{ri} = \frac{1}{1 + \exp\{\beta\tilde{\epsilon}_{ri}\}}, \quad 1 - \tilde{w}_{ri} = \frac{1}{1 + \exp\{-\beta\tilde{\epsilon}_{ri}\}}. \quad (r = 1, 2)$$

3) Then, it may be expected to open a new area in the vigorous pursuit by the radical sprit of the Res-MF theories.

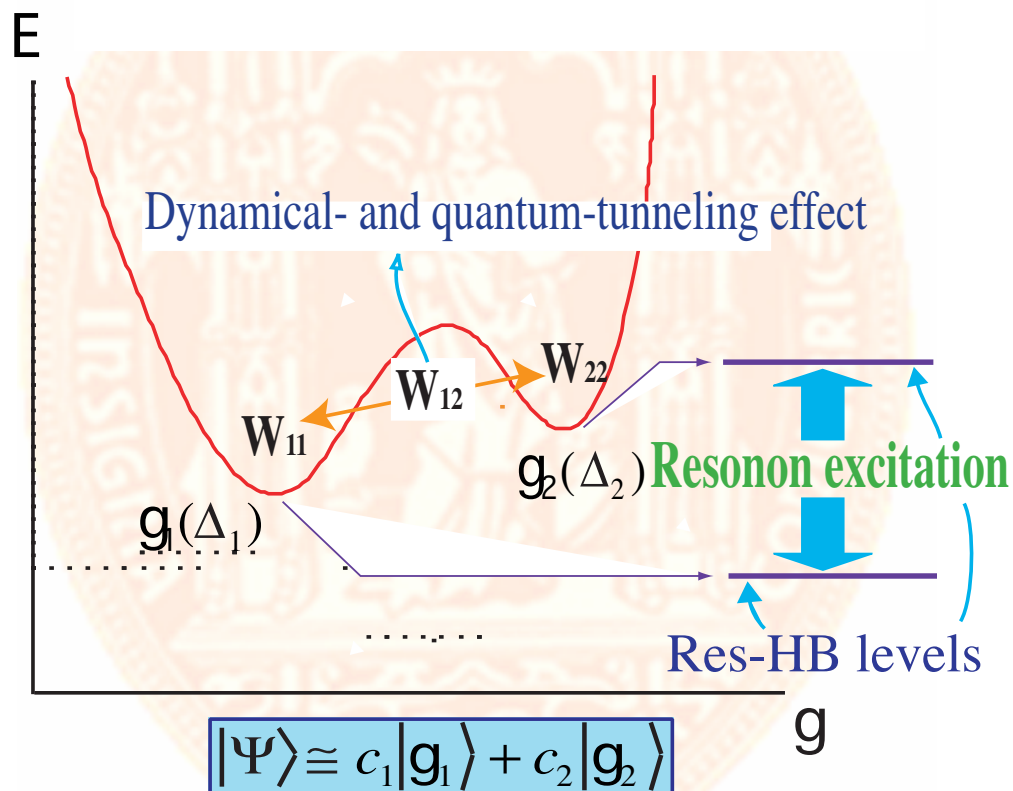
- H. Fukutome, PTP 80 (1988); PTP 81 (1989), S. Nishiyama and H. Fukutome, PTP 85 (1991); PTP 86 (1991).

Resonating HB eigenvalue equation:

- HB energy functional surface:

Res-HB levels and Resonon excitations

Two-Gap Superconductivity



Possible structure of the HB energy functional surface, the case where quantal resonance is present.

- Res-HB approximation:**

Approximate low energy eigenstate $|\Psi^{\text{Res}}\rangle$ by **discrete superposition** of HB WFs $|g_r\rangle, |g_s\rangle \dots$;
 ($|g_r\rangle$'s: Non-orthogonal and different correlation states)

$$|\Psi^{\text{Res}}\rangle = \sum_{s=1}^n |g_s\rangle c_s. \quad (1)$$

$N \times N$ matrix z and $2N \times 2N$ **HB interstate density matrix** W_{rs} between $|g_r\rangle$ and $|g_s\rangle$;

$$z_{rs} = u_r^\dagger u_s, \quad W_{rs} = u_s z_{rs}^{-1} u_r^\dagger, \quad W_{rs}^2 = W_{rs}, \quad (2)$$

Matrix form;

$$W_{rs} = \begin{bmatrix} R_{rs} & K_{rs} \\ -K_{sr}^* & 1_N - R_{sr}^* \end{bmatrix}. \quad (3)$$

- Normalization of mixing coefficients;**

$$\langle \Psi^{\text{Res}} | \Psi^{\text{Res}} \rangle = \sum_{r,s=1}^n \langle g_r | g_s \rangle c_r^* c_s = \sum_{r,s=1}^n [\det z_{rs}]^{\frac{1}{2}} c_r^* c_s = 1. \quad (4)$$

- Expectation value of the Hamiltonian;**

$$\langle \Psi^{\text{Res}} | H | \Psi^{\text{Res}} \rangle = \sum_{r,s=1}^n \langle g_r | H | g_s \rangle c_r^* c_s = \sum_{r,s=1}^n H[W_{rs}] \cdot [\det z_{rs}]^{\frac{1}{2}} c_r^* c_s. \quad (5)$$

- **Res-HB CI Eq. and Res-HB eigenvalue Eq.:**

- **Res-HB configuration interaction (CI) equation;**

$$\boxed{\sum_{s=1}^n \{H[W_{rs}] - E\} \cdot [\det z_{rs}]^{\frac{1}{2}} c_s = 0.} \quad (6)$$

- **Res-HB equation;**

$$\left. \begin{aligned} & \sum_{s=1}^n \mathcal{K}_{rs} c_r^* c_s = 0, \\ & \mathcal{K}_{rs} \equiv \{(1_{2N} - W_{rs}) \mathcal{F}[W_{rs}] + H[W_{rs}] - E\} \cdot W_{rs} \cdot [\det z_{rs}]^{\frac{1}{2}}, \end{aligned} \right\} \quad (7)$$

- **Fock-Bogoliubov (FB) operator;**

$$\mathcal{F}[W_{rs}] = \begin{bmatrix} F_{rs} & D_{rs} \\ -D_{sr}^* & -F_{sr}^* \end{bmatrix}, \quad (8)$$

- **$N \times N$ matrices F_{rs} and D_{rs} ;**

$$\left. \begin{aligned} F_{rs;\alpha\beta} & \equiv \frac{\delta H[W_{rs}]}{\delta R_{rs;\beta\alpha}} = h_{\alpha\beta} + [\alpha\beta|\gamma\delta] R_{rs;\delta\gamma}, \\ D_{rs;\alpha\beta} & \equiv \frac{\delta H[W_{rs}]}{\delta K_{sr;\alpha\beta}^*} = -\frac{1}{2} [\alpha\gamma|\beta\delta] K_{rs;\delta\gamma}. \end{aligned} \right\} \quad (9)$$

- **Res-HB coupled eigenvalue equations;**

$$\left. \begin{aligned} & [\mathcal{F}_r u_r]_i = \epsilon_{ri} u_{ri}, \quad \epsilon_{ri} \equiv \tilde{\epsilon}_{ri} - \{H[W_{rr}] - E\} |c_r|^2, \\ & \mathcal{F}_r \equiv \mathcal{F}[W_{rr}] |c_r|^2 + \sum_{s(s \neq r)=1}^n (\mathcal{K}_{rs} c_r^* c_s + \mathcal{K}_{rs}^\dagger c_r c_s^*). \end{aligned} \right\} \quad (10)$$

Hermitian $2N \times 2N$ matrices \mathcal{F}_r : Res-HB operator

Application to two-gap superconductivity:

- **A naive BCS Hamiltonian;**

$$H = \sum_{p, \sigma} \varepsilon_p c_{p\sigma}^\dagger c_{p\sigma} + \sum_{p, p'} V_{p, p'} c_{p\uparrow}^\dagger c_{-p\downarrow}^\dagger c_{-p'\downarrow} c_{p'\uparrow}. \quad (11)$$

- **Bogoliubov-Valatin transformation;**

$$\left[d_{p\downarrow(\downarrow)}, d_{-p\uparrow(\downarrow)}^\dagger \right] = \left[c_{p\downarrow(\downarrow)}, c_{-p\uparrow(\downarrow)}^\dagger \right] \begin{bmatrix} u_p & -v_{p\uparrow(\downarrow)}^* \\ -v_{p\downarrow(\downarrow)} & u_p^* \end{bmatrix}. \quad (12)$$

- **Parametrizations for u_p and v_p ; $|u_p|^2 + |v_p|^2 = 1$**

$$\left. \begin{aligned} u_p &= \cos \frac{\theta_p}{2} e^{-i\frac{\psi+\varphi}{2}}, & \cos \frac{\theta_p}{2} &\equiv \sqrt{\frac{1}{2} \left(1 + \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \Delta^2}} \right)}, \\ v_p &= \sin \frac{\theta_p}{2} e^{i\frac{\psi-\varphi}{2}}, & \sin \frac{\theta_p}{2} &\equiv \sqrt{\frac{1}{2} \left(1 - \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \Delta^2}} \right)}. \end{aligned} \right\} \quad (13)$$

- **Bogoliubov transformation g_p ;**

$$\left. \begin{aligned} g_p &= \begin{bmatrix} g_p^\uparrow & 0 \\ 0 & g_p^\downarrow \end{bmatrix}, & g_p^\dagger g_p &= I_{2N}, \\ g_p^{\uparrow(\downarrow)} &= \begin{bmatrix} \cos \frac{\theta_p}{2} e^{-i\frac{\psi+\varphi}{2}} I_2 & \{-(+)\} \sin \frac{\theta_p}{2} e^{-i\frac{\psi-\varphi}{2}} I_2 \\ \{+(-)\} \sin \frac{\theta_p}{2} e^{i\frac{\psi-\varphi}{2}} I_2 & \cos \frac{\theta_p}{2} e^{i\frac{\psi+\varphi}{2}} I_2 \end{bmatrix}. \end{aligned} \right\} \quad (14)$$

SU(2) resonating HB approximation:

SU(2) Res-HB WF; $|\Psi\rangle = c_1 |g_1\rangle + c_2 |g_2\rangle$

To regularize equations, $\sum_p \Rightarrow N(0) \int_{-\hbar\omega_D}^{\hbar\omega_D} d\varepsilon;$

$N(0)d\varepsilon$: Number of electronic states of one spin in the normal metal within $d\varepsilon$ near the Fermi surface;

$V_{p, p'} \Rightarrow$ Constant ($-V$) for all the p and p' ;

Two HB WFs with $\psi_2 = \pi, \psi_1 = 0; \varphi_2 = -\psi_2, \varphi_1 = -\psi_1$ but with equal gaps $\Delta_2 = \Delta_1 = \Delta$

Formula: $\ln \left(\frac{1}{x} + \sqrt{1 + \frac{1}{x^2}} \right) = \operatorname{arcsinh} \left(\frac{1}{x} \right), \left(x = \frac{\Delta}{\hbar\omega_D} \right),$

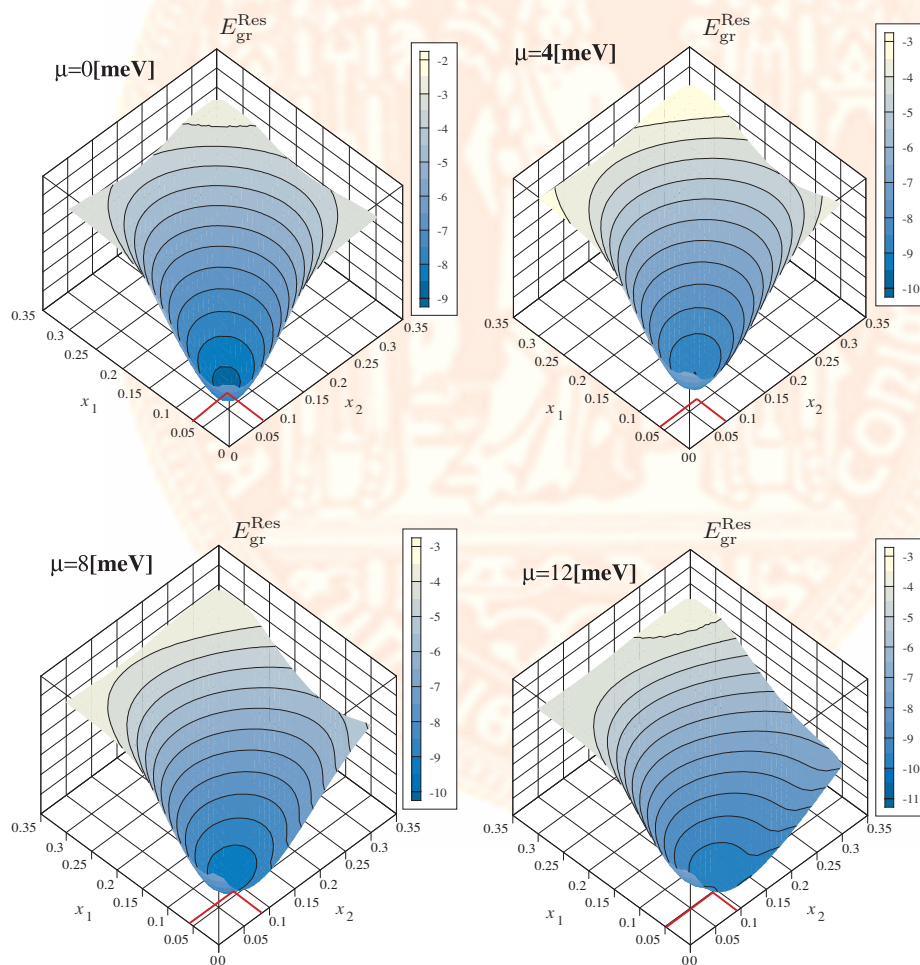
$$H[W_{11}(\Delta)] = H[W_{22}(\Delta)] = H[W(\Delta)] = -2\hbar\omega_D N(0)\hbar\omega_D \times \left[\sqrt{1+x^2} - x^2 \cdot \operatorname{arcsinh} \left(\frac{1}{x} \right) + N(0)V \left\{ x \cdot \operatorname{arcsinh} \left(\frac{1}{x} \right) \right\}^2 \right], \quad (15)$$

$$H[W_{12}(\Delta, \Delta)] = -2\hbar\omega_D N(0)\hbar\omega_D \left[\sqrt{1+x^2} + x^2 \cdot \operatorname{arcsinh} \left(\frac{1}{x} \right) \right], \quad (16)$$

$$[\det z_{12}(\Delta, \Delta)]^{\frac{1}{2}} = \exp \left[-2N(0)\hbar\omega_D \left\{ \ln(1+x^2) + 2x \cdot \arctan \left(\frac{1}{x} \right) \right\} \right]. \quad (17)$$

Solution of the coupled two-gap equations;

	Input				Output		
	$N(0)\hbar\omega_D$	$N(0)V$	$\hbar\omega_D$ [meV]	μ [meV]	Δ_1 [meV]	Δ_2 [meV]	$E_{\text{resonon}}^{\text{Res}}$ [meV]
Res-HB	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 ~ 3	6.5 ~ 7.5	



Res-HB eigenvalue equation for two-gap state:

Res-FB operators;

$$\mathcal{F}_1 = [\mathcal{F}[W_{11}] - (H[W_{11}] - E_{\text{gr}}^{\text{Res}})] \times \left\{ W_{12} + W_{12}^\dagger + \frac{(1_{2N} - W_{12})\mathcal{F}[W_{12}]W_{12}}{H[W_{12}] - E_{\text{gr}}^{\text{Res}}} + \frac{W_{12}^\dagger \mathcal{F}^\dagger[W_{12}](1_{2N} - W_{12}^\dagger)}{H^*[W_{12}] - E_{\text{gr}}^{\text{Res}}} \right\} |c_1|^2, \quad (18)$$

$$\mathcal{F}_2 = [\mathcal{F}[W_{22}] - (H[W_{22}] - E_{\text{gr}}^{\text{Res}})] \times \left\{ W_{12} + W_{12}^\dagger + \frac{W_{12}\mathcal{F}[W_{12}](1_{2N} - W_{12})}{H[W_{12}] - E_{\text{gr}}^{\text{Res}}} + \frac{(1_{2N} - W_{12}^\dagger)\mathcal{F}^\dagger[W_{12}]W_{12}^\dagger}{H^*[W_{12}] - E_{\text{gr}}^{\text{Res}}} \right\} |c_2|^2. \quad (19)$$

Equal gaps: $\Delta_2 = \Delta_1 = \Delta \Rightarrow \theta_{2p} = \theta_{1p} = \theta_p.$

Res-FB operators $\mathcal{F}_{1p}^\uparrow$ and $\mathcal{F}_{2p}^\uparrow$ for the spin-up state;

$$\mathcal{F}_{1p}^\uparrow = \begin{bmatrix} \mathcal{F}_{+\varepsilon p}^\uparrow \cdot I_2 & \mathcal{F}_{\Delta p}^\uparrow \cdot I_2 \\ \mathcal{F}_{\Delta p}^\uparrow \cdot I_2 & -\mathcal{F}_{-\varepsilon p}^\uparrow \cdot I_2 \end{bmatrix}. \quad \mathcal{F}_{2p}^\uparrow \text{ essentially has the same form.} \quad (20)$$

$$\left. \begin{aligned} \mathcal{F}_{+\varepsilon p}^\uparrow &\equiv \frac{1}{2} \left\{ \varepsilon_p + 2(H[W] - E_{\text{gr}}^{\text{Res}}) \frac{\sin^2 \frac{\theta_p}{2}}{\cos \theta_p} \mp \frac{\Delta^2}{\varepsilon_p} \cdot [\det z_{12}]^{\frac{1}{2}} \right\} \cdot \frac{1}{1 \pm [\det z_{12}]^{\frac{1}{2}}}, \\ \mathcal{F}_{-\varepsilon p}^\uparrow &\equiv \frac{1}{2} \left\{ \varepsilon_p + 2(H[W] - E_{\text{gr}}^{\text{Res}}) \frac{\cos^2 \frac{\theta_p}{2}}{\cos \theta_p} \mp \frac{\Delta^2}{\varepsilon_p} \cdot [\det z_{12}]^{\frac{1}{2}} \right\} \cdot \frac{1}{1 \pm [\det z_{12}]^{\frac{1}{2}}}, \\ \mathcal{F}_{\Delta p}^\uparrow = \mathcal{F}_\Delta^\uparrow &\equiv -\frac{1}{2} \Delta \left\{ N(0)V \cdot \operatorname{arcsinh} \left(\frac{1}{x} \right) \pm [\det z_{12}]^{\frac{1}{2}} \right\} \cdot \frac{1}{1 \pm [\det z_{12}]^{\frac{1}{2}}}. \end{aligned} \right\} \quad (21)$$

upper sign \rightarrow Case I, lower sign \rightarrow Case II.

Diagonalization of \mathcal{F}_{1p}^\dagger by a unitary matrix \mathcal{F}_{1p}^\dagger ;

$$\hat{g}_{1p}^\dagger = \begin{bmatrix} \cos \frac{\hat{\theta}_{1p}}{2} \cdot I_2 & -\sin \frac{\hat{\theta}_{1p}}{2} e^{-i\hat{\psi}_1} \cdot I_2 \\ \sin \frac{\hat{\theta}_{1p}}{2} e^{i\hat{\psi}_1} \cdot I_2 & \cos \frac{\hat{\theta}_{1p}}{2} \cdot I_2 \end{bmatrix}. \quad (22)$$

Diagonalization condition;

$$\tan \hat{\theta}_{1p} = -\frac{\mathcal{F}_\Delta^\dagger}{\frac{1}{2} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger)}, \quad \text{and} \quad (23)$$

$$\left. \begin{aligned} & \mathcal{F}_{+\varepsilon p}^\dagger \cos^2 \frac{\hat{\theta}_{1p}}{2} - \mathcal{F}_{-\varepsilon p}^\dagger \sin^2 \frac{\hat{\theta}_{1p}}{2} - \mathcal{F}_\Delta^\dagger \sin \hat{\theta}_{1p} \\ &= \frac{\mathcal{F}_{+\varepsilon p}^\dagger - \mathcal{F}_{-\varepsilon p}^\dagger}{2} + \frac{\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger}{2} \sqrt{1 + \tan^2 \hat{\theta}_{1p}}, \\ & \mathcal{F}_{+\varepsilon p}^\dagger \sin^2 \frac{\hat{\theta}_{1p}}{2} - \mathcal{F}_{-\varepsilon p}^\dagger \cos^2 \frac{\hat{\theta}_{1p}}{2} + \mathcal{F}_\Delta^\dagger \sin \hat{\theta}_{1p} \\ &= \frac{\mathcal{F}_{+\varepsilon p}^\dagger - \mathcal{F}_{-\varepsilon p}^\dagger}{2} - \frac{\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger}{2} \sqrt{1 + \tan^2 \hat{\theta}_{1p}}. \end{aligned} \right\} \quad (24)$$

To get the usual type of the HB orbital energies, we should add a **term**

$$(H[W] - E_{\text{gr}}^{\text{Res}}) |c_1|^2 \cdot I_2 = \frac{1}{2} \frac{H[W] - E_{\text{gr}}^{\text{Res}}}{1 \pm [\det z_{12}]^{\frac{1}{2}}} \cdot I_2 = -\frac{1}{2} (\mathcal{F}_{+\varepsilon p}^\dagger - \mathcal{F}_{-\varepsilon p}^\dagger) \cdot I_2. \quad (25)$$

Eigenvalues $\tilde{\epsilon}_{+p}^\dagger$ and $\tilde{\epsilon}_{-p}^\dagger$, **orbital energies** in the Res-HB states:

$$\left. \begin{aligned} \tilde{\epsilon}_{+p}^\dagger &= \sqrt{\left\{ \frac{1}{2} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger) \right\}^2 + \mathcal{F}_\Delta^{\dagger 2}}, \\ \tilde{\epsilon}_{-p}^\dagger &= -\sqrt{\left\{ \frac{1}{2} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger) \right\}^2 + \mathcal{F}_\Delta^{\dagger 2}}. \end{aligned} \right\} \quad (26)$$

Temperature-dependent Res-HB equation:

Tilde Res-HB density operator \widetilde{W}_{1p} for equal gaps case;

$$\widetilde{W}_{1p} = \begin{bmatrix} \widetilde{W}_{1p}^{\uparrow} \cdot I_2 & 0 \\ 0 & \widetilde{W}_{1p}^{\downarrow} \cdot I_2 \end{bmatrix}, \quad \widetilde{W}_{1p}^{\uparrow(\downarrow)} = \begin{bmatrix} \widetilde{w}_{1p}^{\uparrow(\downarrow)} \cdot I_2 & 0 \\ 0 & (1 - \widetilde{w}_{1p}^{\uparrow(\downarrow)}) \cdot I_2 \end{bmatrix}, \quad (27)$$

where

$$\widetilde{w}_{1p}^{\uparrow(\downarrow)} = \frac{1}{1 + \exp\{\beta\epsilon_{1p}^{\uparrow(\downarrow)}\}}. \quad (28)$$

Final form of the Res-HB density matrix W_{1p} ;

$$\begin{aligned} W_{1p}^{\uparrow(\downarrow)} &= \widehat{g}_{1p}^{\uparrow(\downarrow)} \widetilde{W}_{1p}^{\uparrow(\downarrow)} \widehat{g}_{1p}^{\uparrow(\downarrow)\dagger} = \widehat{g}_{1p}^{\uparrow(\downarrow)} \begin{bmatrix} \widetilde{w}_{1p}^{\uparrow(\downarrow)} \cdot I_2 & 0 \\ 0 & (1 - \widetilde{w}_{1p}^{\uparrow(\downarrow)}) \cdot I_2 \end{bmatrix} \widehat{g}_{1p}^{\uparrow(\downarrow)\dagger} \\ &= \begin{bmatrix} \frac{1}{2} \left\{ 1 - \cos \widehat{\theta}_{1p} \left(1 - 2\widetilde{w}_{1p}^{\uparrow(\downarrow)} \right) \right\} I_2 & \{-(+)\} \frac{1}{2} \sin \widehat{\theta}_{1p} e^{-i\widehat{\psi}_1} \left(1 - 2\widetilde{w}_{1p}^{\uparrow(\downarrow)} \right) I_2 \\ \{-(+)\} \frac{1}{2} \sin \widehat{\theta}_{1p} e^{i\widehat{\psi}_1} \left(1 - 2\widetilde{w}_{1p}^{\uparrow(\downarrow)} \right) I_2 & \frac{1}{2} \left\{ 1 + \cos \widehat{\theta}_{1p} \left(1 - 2\widetilde{w}_{1p}^{\uparrow(\downarrow)} \right) \right\} I_2 \end{bmatrix}. \end{aligned} \quad (29)$$

W_{2p} essentially has the same form as the above.

At finite temperature, we require correspondence relations

$$\boxed{\cos \theta_p \Rightarrow \cos \hat{\theta}_{1p}} \quad \text{and} \quad \boxed{\sin \theta_p \Rightarrow \sin \hat{\theta}_{1p}} ;$$

$$\left. \begin{aligned} \cos \theta_p &= \frac{\varepsilon_p}{\sqrt{\varepsilon_p^2 + \Delta_T^2}} = \frac{\frac{1}{2} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger)}{\tilde{\varepsilon}_{1p}^\dagger} (1 - 2\tilde{w}_{1p}^\dagger), \\ \sin \theta_p &= \frac{\Delta_T}{\sqrt{\varepsilon_p^2 + \Delta_T^2}} = -\frac{\mathcal{F}_{\Delta_T}^\dagger}{\tilde{\varepsilon}_{1p}^\dagger} (1 - 2\tilde{w}_{1p}^\dagger), \end{aligned} \right\} \quad (30)$$

SCF \Rightarrow

$$\frac{\Delta_T}{\varepsilon_p} = \frac{\mathcal{F}_{\Delta_T}^\dagger (1 - 2\tilde{w}_{1p}^\dagger)}{\frac{1}{2} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger) (1 - 2\tilde{w}_{1p}^\dagger)}, \quad (31)$$

dividing numerator and denominator by $(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}$, which is rewritten as

$$1 = \frac{\frac{\varepsilon_p^2}{(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}} \left(-\frac{2\mathcal{F}_{\Delta_T}^\dagger}{\Delta_T} \right) (1 - 2\tilde{w}_{1p}^\dagger)}{\frac{\varepsilon_p}{(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger) (1 - 2\tilde{w}_{1p}^\dagger)}. \quad (32)$$

New temperature-dependent gap equation;

$$\sum_p \left\{ \frac{\varepsilon_p}{(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}} (\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger) - \frac{\varepsilon_p^2}{(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}} \left(-\frac{2\mathcal{F}_{\Delta_T}^\dagger}{\Delta_T} \right) \right\} (1 - 2\tilde{w}_{1p}^\dagger) = 0, \quad (33)$$

\Rightarrow

$$\left\{ 1 - N(0)V \cdot \operatorname{arcsinh} \left(\frac{1}{x_T} \right) \mp [\det z_{12T}]^{\frac{1}{2}} \right\} \sum_p A_p + \tilde{E}_{\text{gr}}^{\text{Res}(\pm)} \hbar\omega_D \sum_p B_p \mp \Delta_T^2 \cdot [\det z_{12T}]^{\frac{1}{2}} \sum_p C_p = 0, \quad \left(x_T \equiv \frac{\Delta_T}{\hbar\omega_D} \right), \quad (34)$$

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

Summations of A_p , B_p and C_p are defined as

$$\left[\sum_p A_p, \sum_p B_p, \sum_p C_p \right] \equiv \sum_p \left[\frac{\varepsilon_p^2}{(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}}, \frac{1}{\varepsilon_p^2 + \Delta_T^2}, \frac{1}{(\varepsilon_p^2 + \Delta_T^2)^{\frac{3}{2}}} \right] (1 - 2\tilde{w}_{1p}^\uparrow). \quad (35)$$

\Rightarrow **Thermal gap equations;**

$$\frac{1}{N(0)V} = \operatorname{arcsinh} \left(\frac{1}{x_T} \right) \left[1 \pm 2N(0)\hbar\omega_D \frac{\operatorname{arcsinh} \left(\frac{1}{x_T} \right)}{\sum_p A_p} \frac{x_T \Delta_T \sum_p B_p}{1 \pm [\det z_{12T}]^{\frac{1}{2}}} [\det z_{12T}]^{\frac{1}{2}} \right] \\ \times \left[1 + \left\{ \mp 1 \mp \frac{\Delta_T^2 \sum_p C_p}{\sum_p A_p} \pm 4N(0)\hbar\omega_D \frac{\operatorname{arcsinh} \left(\frac{1}{x_T} \right)}{\sum_p A_p} \frac{x_T \Delta_T \sum_p B_p}{1 \pm [\det z_{12T}]^{\frac{1}{2}}} \right\} [\det z_{12T}]^{\frac{1}{2}} \right]^{-1}, \quad (36)$$

which reduce to the previous Res-HB gap equations as $T \rightarrow 0$.

$\sum_p A_p$, $\sum_p B_p$ and $\sum_p C_p$ near $T = 0$ can be computed to be

$$\left. \begin{aligned} \frac{\sum_p A_p}{2N(0)} &= \operatorname{arcsinh} \left(\frac{1}{x_T} \right) - \frac{1}{\sqrt{1+x_T^2}} + A(T), \quad A(T) = -T^{\frac{1}{2}} + \dots, \\ \frac{\Delta_T \sum_p B_p}{2N(0)} &= \arctan \left(\frac{1}{x_T} \right) + B(T), \quad B(T) = -T^{\frac{1}{2}} + \frac{1}{2}T^{\frac{3}{2}} - \dots, \\ \frac{\Delta_T^2 \sum_p C_p}{2N(0)} &= \frac{1}{\sqrt{1+x_T^2}} + C(T), \quad C(T) = -T^{\frac{1}{2}} + T^{\frac{3}{2}} - \dots, \end{aligned} \right\} \quad (37)$$

and

$$T^{\frac{n}{2}} \equiv \sqrt{2\pi} \left\{ \tilde{\Delta}_T^{I(\text{II})} \right\}^{-\frac{n}{2}} \left\{ \frac{k_B T}{\hbar\omega_D} \right\}^{\frac{n}{2}} \exp \left(-\frac{\hbar\omega_D}{k_B T} \tilde{\Delta}_T^{I(\text{II})} \right), \quad (n = 1, 3, \dots). \quad (38)$$

In the limit $T \rightarrow T_c^I$ for the Case I, the gap should be extremely small, which brings us $[\det z_{12T}]^{\frac{1}{2}} \rightarrow 1$, $\mathcal{F}_{\Delta T}^\dagger \rightarrow 0$ and $\frac{1}{2}(\mathcal{F}_{+\varepsilon p}^\dagger + \mathcal{F}_{-\varepsilon p}^\dagger) \rightarrow \frac{1}{4}\varepsilon_p$. Approximate QP energy $\rightarrow \tilde{\varepsilon}_p^\dagger \simeq \frac{1}{4}\varepsilon_p$.

Gap equation for the Case I at the limit $T \rightarrow T_c^I$ reduces to

$$1 = \frac{V}{2} \sum_p \frac{4}{\varepsilon_p} \tanh\left(\frac{\varepsilon_p}{8k_B T_c^I}\right) = 4N(0)V \int_0^{\hbar\omega_D} d\varepsilon \frac{1}{\varepsilon} \tanh\left(\frac{\varepsilon}{8k_B T_c^I}\right), \quad (39)$$

integrating by parts, which is approximated as follows:

$$\begin{aligned} \frac{1}{4N(0)V} &= \frac{\tanh y}{\frac{1}{\ln y}} \Bigg|_0^{y_{T_c^I}^I} - \int_0^{y_{T_c^I}^I} dy \ln y \operatorname{sech}^2 y \simeq \ln y_{T_c^I}^I - \int_0^\infty dy \ln y \operatorname{sech}^2 y \\ &= \ln y_{T_c^I}^I + \ln\left(\frac{4e^\gamma}{\pi}\right) = \ln\left(\frac{e^\gamma \hbar\omega_D}{2\pi k_B T_c^I}\right). \end{aligned} \quad (40)$$

The number γ is the Euler's constant ($\gamma \simeq 0.5772$) and $e^\gamma \simeq 1.781$. Finally a small rearrangement yields

$$\boxed{k_B T_c^I = 0.283 \hbar\omega_D e^{-1/4N(0)V}, \quad (T_c^I = 0.283 \theta_D e^{-1/4N(0)V}),} \quad (41)$$

which should be compared with the usual HB formula for T_c

$$k_B T_c = 1.13 \hbar\omega_D e^{-1/N(0)V}, \quad (T_c = 1.130 \theta_D e^{-1/N(0)V}). \quad (42)$$

θ_D : **Debye temperature**. The present formula gives, for example, $T_c^I = 72.87$ K for $N(0)V = 0.25$ and $\theta_D = 700$ K.

The HB formula: $T_c = 14.49$ K for the same values of $N(0)V$ and θ_D .

Behaviour of the gap near T_c :

$\sqrt{T_c^I - T}$ dependence of Δ_T^I and T_c^{II-T} dependence of Δ_T^{II} :

Using the QP energy near T_c , namely, $\tilde{\epsilon} = \frac{1}{4} \sqrt{\varepsilon^2 + \left\{ \Delta_T N(0) V \cdot \operatorname{arcsinh} \left(\frac{\hbar\omega_D}{\Delta_T} \right) \right\}^2}$,

the gap equation is approximately calculated as

$$\frac{1}{N(0)V} = \ln \left(\frac{\hbar\omega_D}{k_B \tilde{T}} \right) - \frac{7}{8\pi^2} \zeta(3) \left(\frac{\pi}{2e^\gamma} \right)^2 \left(\frac{\hbar\omega_D}{k_B \tilde{T}} \right)^2 \left\{ N(0)V x_T \cdot \operatorname{arcsinh} \left(\frac{1}{x_T} \right) \right\}^2$$

$$\ln \left(\frac{\hbar\omega_D}{k_B \tilde{T}_c^I} \right) + \frac{\tilde{T}_c^I - \tilde{T}}{\tilde{T}_c^I} - \frac{7}{8\pi^2} \zeta(3) \left(\frac{\pi}{2e^\gamma} \right)^2 \left(1 - \frac{\tilde{T}_c^I - \tilde{T}}{\tilde{T}_c^I} \right)^{-2} \left(\frac{\hbar\omega_D}{k_B \tilde{T}_c^I} \right)^2 \left\{ N(0)V x_T \cdot \operatorname{arcsinh} \left(\frac{1}{x_T} \right) \right\}^2, \quad (43)$$

where $\frac{\hbar\omega_D}{k_B \tilde{T}} \equiv \frac{e^\gamma}{2\pi} \cdot \frac{\hbar\omega_D}{k_B T}$. Using $\operatorname{arcsinh} \left(\frac{1}{x_T} \right) \simeq \ln \left(\frac{2}{x_T} \right) \simeq -\frac{x_T - 2}{2} + \dots \left(\frac{2}{x_T} > \frac{1}{2} \right)$,

(40) and (43), we get Δ_T^I near T_c^I as

$$\Delta_T^I \simeq 8\pi \sqrt{\frac{2}{7\zeta(3)} \frac{k_B T_c^I}{N(0)V} \left(1 - \frac{T_c^I - T}{T_c^I} \right) \sqrt{\frac{T_c^I - T}{T_c^I}}}. \quad (44)$$

The QP energy $\tilde{\epsilon}_p^\uparrow$ is obtained as

$$\tilde{\epsilon}_p^\uparrow = \frac{\sqrt{\varepsilon_p^2 + \Delta_T^2}}{\varepsilon_p} \frac{1}{2} \left\{ \varepsilon_p + \frac{\sqrt{\varepsilon_p^2 + \Delta_T^2}}{\varepsilon_p} \hbar\omega_D \tilde{E}_{\text{gr}}^{\text{Res}(-)} + \frac{\Delta_T^2}{\varepsilon_p} \cdot [\det z_{12T}]^{\frac{1}{2}} \right\} \cdot \frac{1}{1 - [\det z_{12T}]^{\frac{1}{2}}}. \quad (45)$$

At $T \simeq T_c^{II}$, Δ_T^{II} almost disappears. Then, we have an approximate relation $\frac{\tilde{\epsilon}}{k_B T} =$

$\left(1 - [\det z_{12T}]^{\frac{1}{2}} \right)^{-1} \frac{\sqrt{\varepsilon^2 + \Delta_T^2}}{2k_B T}$. If $\varepsilon \gg \Delta_T$, equation (35) becomes to be

$$\left. \begin{aligned} \frac{\sum_p A_p}{2N(0)} &= \int_0^{\hbar\omega_D} d\varepsilon \frac{\varepsilon^2}{(\varepsilon^2 + \Delta_T^2)^{\frac{3}{2}}} \tanh \left(\frac{\tilde{\epsilon}}{2k_B T} \right) = \ln \left(\frac{4e^\gamma}{\pi} y_T^{II} \right) - \frac{21}{2\pi^2} \zeta(3) (y_T^{II} x_T)^2, \\ \frac{\Delta_T \sum_p B_p}{2N(0)} &= 0, \quad \frac{\Delta_T^2 \sum_p C_p}{2N(0)} = \int_0^{\hbar\omega_D} d\varepsilon \frac{1}{(\varepsilon^2 + \Delta_T^2)^{\frac{3}{2}}} \tanh \left(\frac{\tilde{\epsilon}}{2k_B T} \right) = \frac{7}{\pi^2} \zeta(3) (y_T^{II} x_T)^2. \end{aligned} \right\} \quad (46)$$

At T_c^{II} , y_T^{II} is approximated as

$$\frac{\text{II}}{T_c} = \frac{1}{4} \frac{1}{\left(1 - [\det z_{12T_c^{\text{II}}}]^{\frac{1}{2}}\right)} \frac{\hbar\omega_D}{k_B T_c^{\text{II}}} \simeq \frac{1}{16\pi N(0)\hbar\omega_D} \frac{\hbar\omega_D}{k_B T_c^{\text{II}}} \frac{2}{x_c} \equiv \frac{1}{2} \left(\frac{\pi}{2e^\gamma}\right) \left(\frac{\hbar\omega_D}{k_B \tilde{T}_c^{\text{II}}}\right) \frac{2}{x_c}, \quad (47)$$

using $1 - [\det z_{12T_c^{\text{II}}}]^{\frac{1}{2}} \simeq 2\pi N(0)\hbar\omega_D x_c$ ($0 < x_c \ll 1$). x_c means its value at T_c^{II} .

Expanding leading terms in (46) in terms of \tilde{T} near \tilde{T}_c^{II} , we have

$$\begin{aligned} \text{arcsinh}^2\left(\frac{1}{x_T}\right) - \left\{ \frac{2}{N(0)V} - \ln\left(\frac{\hbar\omega_D}{k_B \tilde{T}_c^{\text{II}}}\right) + \frac{\tilde{T}_c^{\text{II}} - \tilde{T}}{\tilde{T}_c^{\text{II}}} + \alpha \left(1 + 2\frac{\tilde{T}_c^{\text{II}} - \tilde{T}}{\tilde{T}_c^{\text{II}}}\right) \right\} \text{arcsinh}\left(\frac{1}{x_T}\right) \\ - \frac{2}{N(0)V} \left\{ \ln\left(\frac{\hbar\omega_D}{k_B \tilde{T}_c^{\text{II}}}\right) + \frac{\tilde{T}_c^{\text{II}} - \tilde{T}}{\tilde{T}_c^{\text{II}}} - \frac{2}{3}\alpha \left(1 + 2\frac{\tilde{T}_c^{\text{II}} - \tilde{T}}{\tilde{T}_c^{\text{II}}}\right) \right\} = 0, \end{aligned} \quad (48)$$

$$\alpha \equiv \frac{21}{2\pi^2} \zeta(3) \left(\frac{\pi}{2e^\gamma}\right)^2 \left(\frac{\hbar\omega_D}{k_B \tilde{T}_c^{\text{II}}}\right)^2. \quad (49)$$

Then we have

$$- \left\{ \text{arcsinh}\left(\frac{1}{x_T}\right) - \text{arcsinh}\left(\frac{1}{x_c}\right) \right\} \left\{ \frac{2}{3} \frac{1}{N(0)V} - \alpha \right\} \simeq 2\alpha^2 \cdot \frac{\tilde{T}_c^{\text{II}} - \tilde{T}}{\tilde{T}_c^{\text{II}}}. \quad (50)$$

Using $\text{arcsinh}\left(\frac{1}{x}\right) \simeq \text{arcsinh}\left(\frac{1}{a}\right) - \frac{1}{a\sqrt{a^2+1}} \cdot (x-a)$ ($a \ll 1$), finally Δ_T^{II} near T_c^{II} can be obtained approximately as

$$\Delta_T^{\text{II}} \simeq \frac{21}{16\pi^2} \frac{1}{\{2\pi N(0)\hbar\omega_D\}^2} \left(\frac{\hbar\omega_D}{k_B T_c^{\text{II}}}\right)^2 \cdot \frac{T_c^{\text{II}} - T}{T_c^{\text{II}}} \cdot \Delta_{T_c}, \quad (51)$$

which is **linearly dependent** on $T_c^{\text{II}} - T$. It is very interesting to find such a dependence, comparing with the usual dependence $\sqrt{T_c^{\text{II}} - T}$ of Δ_T^{II} .

Summary:

- At $T = 0$ two-gap superconductivity in MgB_2 is well described by the Res-HB approximation;
- Provide a finite temperature Res-HB approximation;
- Use a Res-HB subspace spanned by Res-ground and -excited states;
- The temperature dependence of gap near $T = 0$ and T_c becomes more complicated than the temperature dependence of the usual HB and Abrikosov descriptions;
- Equating the numerator to the denominator, we sum up over p , namely, integrate over ε both sides of the equation, to achieve good optimization. Then we may obtain coupled thermal Res-HB gap equations and reach our ultimate goal of computing temperature-dependent two-gaps;
- Partition function in an $SO(2N)$ CS rep $|g\rangle$;

$$\text{Tr}(e^{-\beta H}) = 2^{N-1} \int \langle g | e^{-\beta H} | g \rangle dg \quad (\beta = \frac{1}{k_B T});$$

Thermal path-integral with Matsubara frequency is also useful to calculate the partition function.

Summation $\sum_p A_p$, $\sum_p B_p$ and $\sum_p C_p$ are converted to

$$\frac{\sum_p A_p}{2N(0)V} = \int_0^{\frac{1}{x}} d\xi \frac{\xi^2}{(\xi^2+1)^{\frac{3}{2}}} - 2 \int_0^{\frac{1}{x}} d\xi \frac{\xi^2}{(\xi^2+1)^{\frac{3}{2}}} \frac{1}{1+e^{d^{(II)}} \sqrt{\xi^2+1}}, \quad d^{(II)} \equiv \frac{\hbar\omega_D}{k_B T} \tilde{\Delta}_T^{(II)}, \quad (52)$$

$d^{(II)} \gg 1$ for large $\hbar\omega_D$. Introducing $y = \sqrt{\xi^2+1}$, (52) is integrated as

$$\begin{aligned} \frac{\sum_p A_p}{2N(0)V} \simeq & \operatorname{arcsinh}\left(\frac{1}{x}\right) - \frac{1}{\sqrt{1+x^2}} - 2 \int_1^\infty dy \frac{1}{\sqrt{y^2-1}} e^{-d^{(II)}y} \\ & - 2 \int_1^\infty dy \frac{1}{y^2} \frac{1}{\sqrt{y^2-1}} e^{-d^{(II)}y}, \end{aligned} \quad (53)$$

$$\frac{\Delta_T \sum_p B_p}{2N(0)V} \simeq \arctan\left(\frac{1}{x}\right) - 2 \int_1^\infty dy \frac{1}{y} \frac{1}{\sqrt{y^2-1}} e^{-d^{(II)}y}, \quad (54)$$

$$\frac{\Delta_T^2 \sum_p C_p}{2N(0)V} \simeq \frac{1}{\sqrt{1+x^2}} - 2 \int_1^\infty dy \frac{1}{y^2} \frac{1}{\sqrt{y^2-1}} e^{-d^{(II)}y}. \quad (55)$$

The Bessel function of order ν is represented as

$$K_\nu(z) = \frac{\sqrt{\pi} \left(\frac{z}{2}\right)^\nu}{\Gamma\left(\nu + \frac{1}{2}\right)} \int_1^\infty dy (y^2 - 1)^{\nu-\frac{1}{2}} e^{-zy}, \quad K_0(z) = \sqrt{\frac{\pi}{2z}} e^{-z}, \quad \left(\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}\right). \quad (56)$$

Using (56), integral calculations of (53) ~ (55) are made in the following ways:

$$\begin{aligned} \int_1^\infty dy \frac{1}{y} \frac{1}{\sqrt{y^2-1}} e^{-dy} &= \int_1^\infty dy \frac{1}{\sqrt{y^2-1}} \int_d^\infty dz e^{-zy} = \int_d^\infty dz K_0(z) \\ &= \sqrt{\frac{\pi}{2}} \left(d^{-\frac{1}{2}} - \frac{1}{2} d^{-\frac{3}{2}} + \frac{3}{4} d^{-\frac{5}{2}} - \dots \right) e^{-d}, \end{aligned} \quad (57)$$

$$\begin{aligned} \int_1^\infty dy \frac{1}{y^2} \frac{1}{\sqrt{y^2-1}} e^{-dy} &= \int_1^\infty dy \frac{1}{y} \frac{1}{\sqrt{y^2-1}} \int_d^\infty dw e^{-wy} = \int_d^\infty dw \int_w^\infty dz K_0(z) \\ &= \sqrt{\frac{\pi}{2}} \left(d^{-\frac{1}{2}} - d^{-\frac{3}{2}} + \frac{9}{4} d^{-\frac{5}{2}} - \dots \right) e^{-d}. \end{aligned} \quad (58)$$

The QP energy $\tilde{\varepsilon}$ is expressed as $\tilde{\varepsilon} = \left(1 - [\det z_{12T}]^{\frac{1}{2}}\right)^{-1} \frac{\sqrt{\varepsilon^2 + \Delta_T^2}}{2}$. Let us introduce y by $\varepsilon = 4\left(1 - [\det z_{12T}]^{\frac{1}{2}}\right) k_B T y$ and $y_T^{\text{H}} = \left(1 - [\det z_{12T}]^{\frac{1}{2}}\right)^{-1} \cdot \frac{\hbar\omega_D}{4k_B T}$. If $\varepsilon \gg \Delta_T$, $\sum_p B_p = 0$ and $\sum_p A_p$ and $\sum_p C_p$ in (35) are recast to integrals up to Δ_T^2 :

$$\begin{aligned} \frac{\sum_p A_p}{2N(0)} &\simeq \int_0^{\hbar\omega_D} d\varepsilon \frac{1}{\sqrt{\varepsilon^2 + \Delta_T^2}} \tanh\left(\frac{\tilde{\varepsilon}}{2k_B T}\right) - \int_0^{\hbar\omega_D} d\varepsilon \frac{\Delta_T^2}{\varepsilon^2 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh\left(\frac{\tilde{\varepsilon}}{2k_B T}\right) \\ &= \int_0^{y_T^{\text{H}}} dy \left\{ 1 - \frac{(y_T^{\text{H}} x_T)^2}{y^2} \right\} \frac{1}{\sqrt{y^2 + (y_T^{\text{H}} x_T)^2}} \tanh\left[\sqrt{y^2 + (y_T^{\text{H}} x_T)^2}\right], \end{aligned} \quad (59)$$

$$\begin{aligned} \frac{\Delta_T^2 \sum_p C_p}{2N(0)} &\simeq \int_0^{\hbar\omega_D} d\varepsilon \frac{1}{\varepsilon^2 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh\left(\frac{\tilde{\varepsilon}}{2k_B T}\right) - \int_0^{\hbar\omega_D} d\varepsilon \frac{\Delta_T^2}{\varepsilon^4 \sqrt{\varepsilon^2 + \Delta_T^2}} \tanh\left(\frac{\tilde{\varepsilon}}{2k_B T}\right) \\ &= (y_T^{\text{H}} x_T)^2 \int_0^{y_T^{\text{H}}} dy \left\{ 1 - \frac{(y_T^{\text{H}} x_T)^2}{y^2} \right\} \frac{1}{y^2} \frac{1}{\sqrt{y^2 + (y_T^{\text{H}} x_T)^2}} \tanh\left[\sqrt{y^2 + (y_T^{\text{H}} x_T)^2}\right]. \end{aligned} \quad (60)$$

Expanding around $(y_T^{\text{H}} x_T)$, (59) and (60) are boldly approximated as

$$\frac{\sum_p A_p}{2N(0)} \simeq \int_0^{y_T^{\text{H}}} dy \frac{1}{y} \tanh y - \frac{3}{2} (y_T^{\text{H}} x_T)^2 \int_0^{y_T^{\text{H}}} dy \left\{ \frac{1}{y^3} \tanh y - \frac{1}{y^2} \text{sech}^2 y \right\}, \quad (61)$$

$$\frac{\Delta_T^2 \sum_p C_p}{2N(0)} \simeq (y_T^{\text{H}} x_T)^2 \int_0^{y_T^{\text{H}}} dy \left\{ \frac{1}{y^3} \tanh y - \frac{1}{y^2} \text{sech}^2 y \right\}. \quad (62)$$

We further use the famous mathematical formulas

$$\left. \begin{aligned} \frac{1}{y} \tanh y &= 8 \sum_{m=1}^{\infty} \frac{1}{(2m-1)^2 \pi^2 + 4y^2}, \\ \frac{1}{y^3} \tanh y - \frac{1}{y^2} \text{sech}^2 y &= 64 \sum_{m=1}^{\infty} \frac{1}{\{(2m-1)^2 \pi^2 + 4y^2\}^2}. \end{aligned} \right\} \quad (63)$$

Putting $y = \frac{\pi}{2} (2m-1) \tan \theta$, integration of the second in (63) is made for $\hbar\omega_D \gg 1$ as

$$64 \int_0^{y_T^{\text{H}} \rightarrow \infty} dy \sum_{m=1}^{\infty} \frac{1}{\{(2m-1)^2 \pi^2 + 4y^2\}^2} = \frac{7}{\pi^2} \zeta(3), \quad (64)$$

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