Chapter 1

Theory and Method

In order to calculate T_c from first-principles, Lüders and his co-workers constructed the density functional theory for superconductors (SCDFT) [1]. By using SCDFT, it is able to calculate T_c from *ab-initio* electronic wave functions and electron-phonon matrix elements and so on. First, we will review their theory including electron-phonon interaction and Coulomb interaction. After that, we will review how to include the effect of spin fluctuations into the SCDFT.

1.1 Density functionals and Kohn-Sham system for superconductors

In order to treat the electron-phonon and Coulomb interactions in superconductors like the Hohenberg-Kohn way, we consider the many-body electron-nuclear Hamiltonian

$$\hat{H} = \hat{T}^{\mathrm{e}} + \hat{T}^{\mathrm{n}} + \hat{U}^{\mathrm{en}} + \hat{U}^{\mathrm{ee}} + \hat{V}^{\mathrm{e}}_{\mathrm{ext}} + \hat{V}^{\mathrm{n}}_{\mathrm{ext}} + \hat{\Delta}_{\mathrm{ext}} - \mu\hat{N}, \tag{1.1}$$

where $\hat{T}^{\mathrm{e}}$ represents the electronic kinetic energy, $\hat{T}^{\mathrm{n}}$ the nuclear kinetic energy, $\hat{U}^{\mathrm{en}}$ the electron-nuclear interaction, $\hat{U}^{\mathrm{ee}}$ the electron-electron interaction. The electronic external potential $\hat{V}^{\mathrm{e}}_{\mathrm{ext}}$ is defined as

$$\hat{V}^{\mathrm{e}}_{\mathrm{ext}} = \sum_{\sigma} \int d^3r \hat{\Psi}^{\dagger}_{\sigma}(\boldsymbol{r}) v^{\mathrm{e}}_{\mathrm{ext}}(\boldsymbol{r}) \hat{\Psi}_{\sigma}(\boldsymbol{r}), \tag{1.2}$$

where $\hat{\Psi}^{\dagger}_{\sigma}(\boldsymbol{r})$ is the electron creation operator. $\hat{V}^{\mathrm{n}}_{\mathrm{ext}}$ is a N-body operator with respect to the nuclear coordinates

$$\hat{V}^{\mathrm{n}}_{\mathrm{ext}} = \sum_{\sigma} \int d^3\underline{\boldsymbol{R}} v^{\mathrm{n}}_{\mathrm{ext}}(\underline{\boldsymbol{R}}) \hat{\Gamma}(\underline{\boldsymbol{R}}), \tag{1.3}$$

where $\underline{\boldsymbol{R}}$ represents a set of the coordinates of N-body nuclei and

$$\hat{\Gamma}(\underline{\boldsymbol{R}}) = \hat{\Phi}^{\dagger}(\boldsymbol{R}_1) \cdots \hat{\Phi}^{\dagger}(\boldsymbol{R}_N) \hat{\Phi}(\boldsymbol{R}_N) \cdots \hat{\Phi}(\boldsymbol{R}_1) \tag{1.4}$$

is the N-body nuclear density matrix operator in which nuclear creation and annihilation operators $\hat{\Phi}^{\dagger}$ and $\hat{\Phi}$ are used. The term

$$\hat{\Delta}_{\mathrm{ext}} = -\int d^3r \int d^3r' \left[\Delta^{*}_{\mathrm{ext}}(\boldsymbol{r}, \boldsymbol{r}') \hat{\Psi}_{\uparrow}(\boldsymbol{r}) \hat{\Psi}_{\downarrow}(\boldsymbol{r}') + \mathrm{H.c.} \right]. \tag{1.5}$$

indicates the external pairing field. This term must be included in order to break the gauge invariance of the Hamiltonian. We will take the limit $\Delta_{\mathrm{ext}} \to 0$ at the end of the derivation. In this thesis, it is assumed that we treat singlet superconductors. However, we can extend the formulation for triplet superconductors straightforwardly. Finally, μ means the chemical potential and $\hat{N}$ is the number operator of electrons.

The formulation of this theory is based on three densities: (i) The usual electronic density

$$n(\boldsymbol{r}) = \sum_{\sigma} \left\langle \hat{\Psi}^{\dagger}_{\sigma}(\boldsymbol{r})\, \hat{\Psi}_{\sigma}(\boldsymbol{r}) \right\rangle. \tag{1.6}$$

The bracket indicates the thermal average

$$\begin{aligned} \left\langle \hat{A} \right\rangle &= \mathrm{Tr}\hat{\rho}_0 \hat{A}, \\ \hat{\rho}_0 &= \frac{e^{-\beta \hat{H}}}{\mathrm{Tr} e^{-\beta \hat{H}}}, \end{aligned} \tag{1.7}$$

where $\hat{\rho}_0$ is the grand canonical density operator and β is the inverse temperature.

(ii) The anomalous density

$$\chi(\boldsymbol{r}, \boldsymbol{r'}) = \left\langle \hat{\Psi}^{\dagger}_{\uparrow}(\boldsymbol{r}) \hat{\Psi}_{\downarrow}(\boldsymbol{r'}) \right\rangle \tag{1.8}$$

is the order parameter for the singlet superconductors. This quantity becomes zero above the T_{c} and finite below it.

(iii) The diagonal part of nuclear N-body density matrix

$$\Gamma(\underline{\boldsymbol{R}}) = \left\langle \hat{\Gamma}(\underline{\boldsymbol{R}}) \right\rangle \tag{1.9}$$

is introduced to describe the nuclear degrees of freedom.

Extending the Hohenberg-Kohn theorem in usual DFT for present multicomponent theory straightforwardly, the existence of one-to-one mapping between the set of the densities $\{n(\boldsymbol{r}), \chi(\boldsymbol{r}, \boldsymbol{r'}), \Gamma(\underline{\boldsymbol{R}})\}$ and a set of the corresponding potentials $\left\{ v^{\mathrm{e}}_{\mathrm{ext}}(\boldsymbol{r}), \Delta_{\mathrm{ext}}(\boldsymbol{r}, \boldsymbol{r'}), v^{\mathrm{n}}_{\mathrm{ext}}(\underline{\boldsymbol{R}}) \right\}$ is guaranteed. Consequently, all observable quantities are functionals of these densities. This fact guarantees that the grand canonical potential

$$\begin{aligned} \Omega[n, \chi, \Gamma] = F[n, \chi, \Gamma] &+ \int d^3 r n(\boldsymbol{r}) [v^{\mathrm{e}}_{\mathrm{ext}}(\boldsymbol{r}) - \mu] \\ &- \int d^3 r \int d^3 r' \left[\chi(\boldsymbol{r}, \boldsymbol{r'}) \Delta^{*}_{\mathrm{ext}}(\boldsymbol{r}, \boldsymbol{r'}) + \mathrm{H.c.} \right] \\ &+ \int d^3 \underline{R} \Gamma(\underline{\boldsymbol{R}}) v^{\mathrm{n}}_{\mathrm{ext}}(\underline{\boldsymbol{R}}) \end{aligned} \tag{1.10}$$

is minimized by the ground state densities. The notation $A[f]$ means that A is a functional of f. The functional F is defined as

$$\begin{aligned} F[n, \chi, \Gamma] = T^{\mathrm{e}}[n, \chi, \Gamma] + T^{\mathrm{n}}[n, \chi, \Gamma] + U^{\mathrm{en}}[n, \chi, \Gamma] \\ + U^{\mathrm{ee}}[n, \chi, \Gamma] - \frac{1}{\beta} S[n, \chi, \Gamma], \end{aligned} \tag{1.11}$$

where S represents the entropy of the system

$$S[n, \chi, \Gamma] = -\mathrm{Tr}\left\{ \hat{\rho}_0[n, \chi, \Gamma] \ln \hat{\rho}_0[n, \chi, \Gamma] \right\}. \tag{1.12}$$

In this formulation, the Kohn-Sham system consists of noninteracting electrons and *interacting* nuclei. By including the interacting nuclei, we can treat lattice dynamics. The thermodynamic potential of the Kohn-Sham system is described as

$$\begin{aligned}\Omega_0[n,\chi,\Gamma] = F_0[n,\chi,\Gamma] + \int d^3r n(\boldsymbol{r}) \left[v_0^{\mathrm{e}}(\boldsymbol{r}) - \mu_0\right] \\ \int d^3r \int d^3r' \left[\chi(\boldsymbol{r},\boldsymbol{r'})\Delta_0^*(\boldsymbol{r},\boldsymbol{r'}) + \mathrm{H.c.}\right] \\ + \int d^3\underline{R}\Gamma(\underline{\boldsymbol{R}})v_0^{\mathrm{n}}(\underline{\boldsymbol{R}}),\end{aligned} \tag{1.13}$$

where $v_0^{\mathrm{n}}(\boldsymbol{r}), \Delta_0(\boldsymbol{r},\boldsymbol{r'})$, and $\Gamma(\underline{\boldsymbol{R}})$ are the Kohn-Sham potentials and F_0 is the counterpart of (1.11) for the Kohn-Sham system, defined as

$$\begin{aligned}F_0[n,\chi,\Gamma] = T_0^{\mathrm{e}}[n,\chi,\Gamma] + T_0^{\mathrm{n}}[n,\chi,\Gamma] \\ - \frac{1}{\beta}S_0[n,\chi,\Gamma].\end{aligned} \tag{1.14}$$

Here $T_0^{\mathrm{e}}[n,\chi,\Gamma], T_0^{\mathrm{n}}[n,\chi,\Gamma]$, and $S_0[n,\chi,\Gamma]$ represents the electronic and nuclear kinetic energy and the entropy of the Kohn-Sham system, respectively.

The exchange-correlation free energy is defined as

$$\begin{aligned}F_{\mathrm{xc}}[n,\chi,\Gamma] = F[n,\chi,\Gamma] - F_0[n,\chi,\Gamma] - U^{\mathrm{nn}}[\Gamma] \\ - E_{\mathrm{H}}^{\mathrm{ee}}[n,\chi,\Gamma] - E_{\mathrm{H}}^{\mathrm{en}}[n,\chi,\Gamma],\end{aligned} \tag{1.15}$$

where the Hartree terms are defined as

$$U^{\mathrm{nn}}[\Gamma] = \sum_{\alpha\neq\beta}\int d^3\underline{\boldsymbol{R}}\Gamma(\underline{\boldsymbol{R}})\frac{Z^2}{\left|\boldsymbol{R}_\alpha - \boldsymbol{R}_\beta\right|}, \tag{1.16}$$

$$E_{\mathrm{H}}^{\mathrm{ee}}[n,\chi,\Gamma] = \frac{1}{2}\int d^3r \int d^3r' \frac{n(\boldsymbol{r})n(\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|} + \int d^3r \int d^3r' \frac{|\chi(\boldsymbol{r},\boldsymbol{r'})|^2}{|\boldsymbol{r}-\boldsymbol{r'}|}, \tag{1.17}$$

$$E_{\mathrm{H}}^{\mathrm{en}}[n,\chi,\Gamma] = -Z\sum_\alpha \int d^3r \int d^3\underline{\boldsymbol{R}} \frac{n(\boldsymbol{r})\Gamma(\underline{\boldsymbol{R}})}{|\boldsymbol{r}-\boldsymbol{R}_\alpha|}. \tag{1.18}$$

Then we obtain the Kohn-Sham potentials

$$\begin{aligned}v_0^{\mathrm{e}}[n,\chi,\Gamma](\boldsymbol{r}) = -Z\sum_\alpha \int d^3\underline{\boldsymbol{R}} \frac{\Gamma(\underline{\boldsymbol{R}})}{|\boldsymbol{r}-\boldsymbol{R}_\alpha|} + \int d^3r' \frac{n(\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|} \\ + v_{\mathrm{xc}}^{\mathrm{e}}[n,\chi,\Gamma](\boldsymbol{r}),\end{aligned} \tag{1.19}$$

$$\Delta_0[n,\chi,\Gamma](\boldsymbol{r},\boldsymbol{r'}) = -\frac{\chi(\boldsymbol{r},\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|} + \Delta_{\mathrm{xc}}[n,\chi,\Gamma](\boldsymbol{r},\boldsymbol{r'}), \tag{1.20}$$

$$\begin{aligned}v_0^{\mathrm{n}}[n,\chi,\Gamma](\underline{\boldsymbol{R}}) = \sum_{\alpha\neq\beta}\frac{Z^2}{|\boldsymbol{R}_\alpha - \boldsymbol{R}_\beta|} - Z\sum_\alpha \int d^3r \frac{n(\boldsymbol{r})}{|\boldsymbol{r}-\boldsymbol{R}_\alpha|} \\ + v_{\mathrm{xc}}^{\mathrm{n}}[n,\chi,\Gamma](\underline{\boldsymbol{R}}),\end{aligned} \tag{1.21}$$

where exchange-correlation potentials are defined as

$$v_{\mathrm{xc}}^{\mathrm{e}}[n,\chi,\Gamma](\boldsymbol{r}) = \frac{\delta F_{\mathrm{xc}}[n,\chi,\Gamma]}{\delta n(\boldsymbol{r})}, \tag{1.22}$$

$$\Delta_{\mathrm{xc}}[n,\chi,\Gamma](\boldsymbol{r},\boldsymbol{r}') = -\frac{\delta F_{\mathrm{xc}}[n,\chi,\Gamma]}{\delta\chi(\boldsymbol{r},\boldsymbol{r}')}, \tag{1.23}$$

$$v^{\mathrm{e}}_{\mathrm{xc}}[n,\chi,\Gamma](\underline{\boldsymbol{R}}) = \frac{\delta F_{\mathrm{xc}}[n,\chi,\Gamma]}{\delta\Gamma(\underline{\boldsymbol{R}})}. \tag{1.24}$$

These definitions are analogous to the definition in the standard DFT.

1.2 The Kohn-Sham equations

We introduced the Kohn-Sham states in the previous section. Now the problem of minimizing the grand canonical potential (1.13) can be solved by solving a set of three differential equations self-consistently. Two of them describe the electronic degrees of freedom and the third desctibes the nuclear degrees of freedom.

The two coupled equations are as follows:

$$\left[-\frac{\nabla^2}{2} + v^{\mathrm{e}}_0(\boldsymbol{r}) - \mu\right] u_n(\boldsymbol{r}) + \int d^3r' \Delta_0(\boldsymbol{r},\boldsymbol{r}') v_n(r') = \widetilde{E}_n u_n(\boldsymbol{r}), \tag{1.25}$$

$$-\left[-\frac{\nabla^2}{2} + v^{\mathrm{e}}_0(\boldsymbol{r}) - \mu\right] v_n(\boldsymbol{r}) + \int d^3r' \Delta^*_0(\boldsymbol{r},\boldsymbol{r}') u_n(r') = \widetilde{E}_n v_n(\boldsymbol{r}), \tag{1.26}$$

where $u_n(\boldsymbol{r})$ and $v_n(\boldsymbol{r})$ are particle and hole wavefunctions respectively. These equations are equivalent to the Bogoliubov-de Gennes equations [2]. The equation for the nucleus

$$\left[-\sum_\alpha \frac{\nabla^2_\alpha}{2M} + v^{\mathrm{n}}_0(\underline{\boldsymbol{R}})\right] \Phi_n(\underline{\boldsymbol{R}}) = \mathcal{E}_n \Phi_n(\underline{\boldsymbol{R}}) \tag{1.27}$$

where $\Phi_n(\underline{\boldsymbol{R}})$ is many-body nuclear wavefunction has the same structure as the usual nuclear Born-Oppenheimer equation.

In priciple, when we solve the equations (1.25)-(1.27) iteratively, we can obtain the ground state densities $\{n,\chi,\Gamma\}$. However, it requires extraordinary high accuracy to resolve the superconducting energy gap because the magnitude of it is about $10^{-3} \sim 10^{-4}$ times typical electronic energy. In order to avoid this difficulty, so-called "decoupling approximation" is beneficial.

In the decoupling approximation, we approximate the particle and hole one-particle wavefunctions as follows

$$u_n(\boldsymbol{r}) \approx u_n \varphi_n(\boldsymbol{r}), v_n(\boldsymbol{r}) \approx v_n \varphi_n(\boldsymbol{r}), \tag{1.28}$$

where φ_n are calculated through the equation

$$\left[-\frac{\nabla^2}{2} + v^{\mathrm{n}}_0[n,\chi,\Gamma](\boldsymbol{r}) - \mu\right] \varphi_n(\boldsymbol{r}) = \epsilon_n \varphi_n(\boldsymbol{r}). \tag{1.29}$$

Then the eigenenergies in (1.25) (1.26) is calculated as

$$\widetilde{E}_n = \mathrm{sgn}(\xi_n)\sqrt{\xi_n^2 + |\Delta_n|^2} = \mathrm{sgn}(\xi_n) E_n \tag{1.30}$$

where $\xi_n = \epsilon_n - \mu$, and the matrix elements Δ_n are defined as

$$\Delta_n = \int d^3r \int d^3r' \varphi_n^*(\boldsymbol{r}) \Delta_0(\boldsymbol{r}, \boldsymbol{r'}) \varphi_n(\boldsymbol{r}). \tag{1.31}$$

In the decoupling approximation, the electronic densities and the anomalous densities can be obtained easily as follows

$$n(\boldsymbol{r}) = \sum_n \left[1 - \frac{\xi_n}{E_n} \tanh\left(\frac{\beta}{2} E_n \right) \right] |\varphi_n(\boldsymbol{r})|^2, \tag{1.32}$$

$$\chi(\boldsymbol{r}, \boldsymbol{r'}) = \sum_n \frac{\Delta_n}{2E_n} \tanh\left(\frac{\beta}{2} E_n \right) \varphi_n(\boldsymbol{r}) \varphi_n^*(\boldsymbol{r'}). \tag{1.33}$$

Next, we consider the nucear equation. Now we are interested in superconductors at relatively low tempereutre, so it is reasonable to introduce the harmonic approximation. Then the equation (1.27) reads

$$\hat{H}_0^{\mathrm{ph}} = \sum_{\lambda, \boldsymbol{q}} \Omega_{\lambda, \boldsymbol{q}} \left[\hat{b}_{\lambda, \boldsymbol{q}}^\dagger \hat{b}_{\lambda, \boldsymbol{q}} + \frac{1}{2} \right], \tag{1.34}$$

where $\Omega_{\lambda, \boldsymbol{q}}$ represents the phonon eigenfrequencies and $\hat{b}_{\lambda, \boldsymbol{q}}^\dagger$ and $\hat{b}_{\lambda, \boldsymbol{q}}$ are the creation and annihilation operator of the phonon from the branch λ and wavevector $\boldsymbol{q}$. Then the nuclear density matrix is as follows

$$\Gamma(\underline{\boldsymbol{R}}) = \sum_{\lambda, \boldsymbol{q}} n_\beta(\Omega_{\lambda, \boldsymbol{q}}) |h_{\lambda, \boldsymbol{q}}(\boldsymbol{Q})|^2, \tag{1.35}$$

where $n_\beta(\Omega)$ means the Bose occupation numbers and $h_{\lambda, \boldsymbol{q}}(\boldsymbol{Q})$ are harmonic oscillator wavefunctions with respect to the collective coordinates $\boldsymbol{Q}$.

Now we describe how to treat the density dependence of potentials in order to preceed calculations more simply. (i) For $v_0^{\mathrm{e}}[n, \chi, \Gamma]$, we neglect the dependense on χ and Γ because the typical electronic energies are three orders of magnitudes bigger than superconducting gap and phonons and consequently they do not modify electronic structures so much. (ii) For $v_0^{\mathrm{n}}[n, \chi, \Gamma]$, we neglect the dependence on n and χ because we use the Born-Oppenheimer approximation. This approximation is reasonable because it is known that the calculations executed within the Born-Oppenheimer approximation well reproduce the experimental phonon dispersions [3].

1.3 Gap equation

Now we derive the gap equation for the potential Δ_n. By inserting (1.32) and (1.33) in (1.20) and insert (1.20) into the right-hand side of (1.31), we get the gap equation

$$\Delta_n = \Delta_{\mathrm{Hxc}, n}[n, \chi, \Gamma], \tag{1.36}$$

where $\Delta_{\mathrm{Hxc}, n}$ means the sum of the Hartree and excanhge-correlation terms.

Around the transition temperature, the anomalous density χ becomes vanishingly small and the gap

equation (1.36) can be linearized as below

$$\Delta_i = -\frac{1}{2}\sum_j \mathcal{F}_{\mathrm{Hxc},i,j}[n,\chi,\Gamma]\frac{\tanh[(\beta/2)\xi_j]}{\xi_j}\Delta_j, \tag{1.37}$$

where $\mathcal{F}_{\mathrm{Hxc},i,j}$ are the Hartree exchange-correlation energy kernels which defined as

$$\mathcal{F}_{\mathrm{Hxc},i,j} = -\frac{\delta\Delta_{\mathrm{Hxc},i}}{\delta\chi_j}\bigg|_{\chi=0} = \frac{\delta^2(E_{\mathrm{H}}^{\mathrm{ee}}+F_{\mathrm{xc}})}{\delta\chi_i^*\delta\chi_j}\bigg|_{\chi=0}, \tag{1.38}$$

where we defined the matrix element of anomalous density χ_i as

$$\chi_i = \int d^3r \int d^3r' \varphi_i^*(\boldsymbol{r})\chi(\boldsymbol{r},\boldsymbol{r'})\varphi_i(\boldsymbol{r'}). \tag{1.39}$$

In practice, we solve the linearized gap equation (1.37) with changing the temperature. When we get the vanishingly-small Δ_i solution at some temperature, we regard that temperature as the superconducting transition temperature T_{c}.

1.4 Kernels of Gap Equation from functional derivatives

Through the previous sections, we derived the gap equation (1.37) from a density functional theory for superconductors. In principle, it is able to calculate the T_{c} by solving the gap equation for any superconductors. However, in order to calculate the kernels $\mathcal{F}_{\mathrm{Hxc},ij}$, we have to make approximations for Δ_{xc} in (1.20) which is defined in (1.23). In the following, we briefly review the Kohn-Sham perturbation theory, as described by Görling and Levy [4], and how to deribe the concrete expressions for $\mathcal{F}_{\mathrm{Hxc},ij}$.

We consider the electron-nuclear system which Hamiltonian is defined as (1.1). In order to apply the perturbation theory, we split the Hamiltonian into the unperturbed Hamiltonian $\hat{H}_0$ and the reminder which is treated as perturbation. In the unperturbed Hamiltonian, it is appropriate to consider that nuclei are fixed at their equiliblium position $\underline{\boldsymbol{R}}_0$, which are defined by nuclear Kohn-Sham Hamiltonian (1.27). When applied the harmonic approximation, it can be rewritten as the phonon Hamiltonian (1.34). Then we construct the Kohn-Sham Hamiltonian within the Born-Oppenheimer approximation as follows

$$\hat{H}_{\mathrm{BO}}^{\mathrm{e}} = \hat{T}^{\mathrm{e}} + \hat{V}_{\mathrm{latt},\underline{\boldsymbol{R}}_0}^{\mathrm{e}} + \hat{V}_{\mathrm{Hxc}}^{\mathrm{e}} + \hat{\Delta}_{\mathrm{Hxc}}, \tag{1.40}$$

where $\hat{V}_{\mathrm{latt},\underline{\boldsymbol{R}}_0}^{\mathrm{e}}$ is the potential from the nuclei fixed at their equilibrium position $\underline{\boldsymbol{R}}_0$ and

$$\hat{V}_{\mathrm{Hxc}}^{\mathrm{e}} = \sum_\sigma \int d^3r \hat{\Psi}_\sigma^\dagger(\boldsymbol{r})\hat{\Psi}_\sigma(\boldsymbol{r})\left[\int d^3r' \frac{n(\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|} + v_{\mathrm{xc}}^{\mathrm{e}}(\boldsymbol{r})\right] \tag{1.41}$$

$$\hat{\Delta}_{\mathrm{Hxc}} = -\int d^3r \int d^3r' \left\{\hat{\Psi}_\uparrow(\boldsymbol{r})\hat{\Psi}_\downarrow(\boldsymbol{r'})\left[\frac{\chi^*(\boldsymbol{r},\boldsymbol{r'})}{|\boldsymbol{r}-\boldsymbol{r'}|} + \Delta_{\mathrm{xc}}^*(\boldsymbol{r},\boldsymbol{r'})\right] + \mathrm{H.c.}\right\} \tag{1.42}$$

means the normal and anomalous Hartree term and exchange-correlation term.

When we define the unperturbed Hamiltonian as $\hat{H}_0 = \hat{H}_0^{\mathrm{ph}} + \hat{H}_{\mathrm{BO}}^{\mathrm{e}}$, the interaction Hamiltonian becomes

$$\hat{H}_1 = \hat{U}^{\mathrm{ee}} + \hat{U}_{\mathrm{BO}}^{\mathrm{el-ph}} - \hat{V}_{\mathrm{Hxc}}^{\mathrm{n}} - \hat{V}_{\mathrm{Hxc}}^{\mathrm{e}} - \hat{\Delta}_{\mathrm{Hxc}}. \tag{1.43}$$

The electron-phonon coupling operator within the Born-Oppenheimer approximation $\hat{U}_{\mathrm{BO}}^{\mathrm{el-ph}}$ is

$$\hat{U}_{\mathrm{BO}}^{\mathrm{el-ph}} = \sum_{\sigma} \sum_{\lambda,\boldsymbol{q}} \int d^3 r V_{\lambda,\boldsymbol{q}}^{\mathrm{BO}}(\boldsymbol{r}) \hat{\Psi}_{\sigma}^{\dagger}(\boldsymbol{r}) \hat{\Psi}_{\sigma}(\boldsymbol{r}) \hat{\Phi}_{\lambda,\boldsymbol{q}}, \tag{1.44}$$

where $V_{\lambda,\boldsymbol{q}}^{\mathrm{BO}}(\boldsymbol{r})$ is the gradient of the electronic Kohn-Sham potential with respect to the nuclear collective coordinates $\boldsymbol{Q}$ and $\hat{\Phi}_{\lambda,\boldsymbol{q}} = \hat{b}_{\lambda,-\boldsymbol{q}}^{\dagger} + \hat{b}_{\lambda,\boldsymbol{q}}$ is the phononic field operator. Using $V_{\lambda,\boldsymbol{q}}^{\mathrm{BO}}(\boldsymbol{r})$, the electron-phonon coupling constant is deined as

$$g_{\lambda\boldsymbol{q}}^{n\boldsymbol{k},n'\boldsymbol{k}+\boldsymbol{q}} = \int d^3 r \varphi_{n\boldsymbol{k}}^{*}(\boldsymbol{r}) V_{\lambda,\boldsymbol{q}}^{\mathrm{BO}}(\boldsymbol{r}) \varphi_{n'\boldsymbol{k}+\boldsymbol{q}}(\boldsymbol{r}). \tag{1.45}$$

We defined the Hamiltonian $\hat{H}_0$ and $\hat{H}_1$ above and now we can apply the perturbation approach in order to obtain the explicit expression for kernels in gap equation defined as (1.38). Considering the definition of F_{xc} in (1.15), F_{xc} can be obtained by applying the perturbative approach to the difference of thermodynamic potentials $\Delta\Omega = \Omega - \Omega_0$ (see (1.10) and (1.13)) and its functional derivatives with respect to the anomalous density become the kernels of the gap equation.

In the following, we introduce the explicit expressions for F_{xc} derived by Lüders *et al.*. They expanded $\Delta\Omega$ in the series of topologically distinct connected diagrams and brought the lowest-order diagrams to derive F_{xc}.

At first, we define and calculate the Kohn-Sham propagators which appear in considering diagrams. The usual Green's function is defined as

$$G_{\sigma\sigma'}^{\mathrm{s}}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') = -\langle \hat{\mathcal{T}} \hat{\psi}_{\sigma}(\boldsymbol{r}\tau) \hat{\psi}_{\sigma'}^{\dagger}(\boldsymbol{r}'\tau') \rangle_{\mathrm{s}}, \tag{1.46}$$

where $\hat{\mathcal{T}}$ is the time-ordering operator and $\langle \cdots \rangle_{\mathrm{s}}$ means the average with respect to the Kohn-Sham density operator $\hat{\rho}_{\mathrm{s}}$. The representation of this Green's function is Fig.1.1a. In addition to the usual Green's function, following average which is nonvanishing in superconductors should be considered:

$$F_{\sigma\sigma'}^{\mathrm{s}}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') = -\langle \hat{\mathcal{T}} \hat{\psi}_{\sigma}(\boldsymbol{r}\tau) \hat{\psi}_{\sigma'}(\boldsymbol{r}'\tau') \rangle_{\mathrm{s}}, \tag{1.47}$$

$$F_{\sigma\sigma'}^{\mathrm{s}\dagger}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') = -\langle \hat{\mathcal{T}} \hat{\psi}_{\sigma}^{\dagger}(\boldsymbol{r}\tau) \hat{\psi}_{\sigma'}^{\dagger}(\boldsymbol{r}'\tau') \rangle_{\mathrm{s}}. \tag{1.48}$$

These functions are represented in the Feynman diagrams as Fig.1.1b (for F^{s}) and Fig.1.1c (for $F^{\mathrm{s}\dagger}$). Finally, the phonon propagator represented as a wavy line is defined as

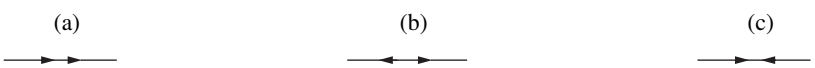

Figure1.1: Diagram corresponding to (a) G^{s}, (b) F^{s} and (c) $F^{\mathrm{s}\dagger}$

$$D^{\mathrm{s}}_{\lambda,\boldsymbol{q}}(\tau,\tau') = \langle \hat{\mathcal{T}}\hat{\Phi}_{\lambda,\boldsymbol{q}}(\tau)\hat{\Phi}^{\dagger}_{\lambda,\boldsymbol{q}}(\tau')\rangle_{\mathrm{s}}. \tag{1.49}$$

In practice, it is convenient to consider in the imaginary frequency space instead of the imaginary time space. The Fourier transform from the imaginary time space to the imaginary frequency space of the normal Green's function (1.46) is defined as

$$G^{\mathrm{s}}_{\sigma\sigma'}(\boldsymbol{r}\tau,\boldsymbol{r}'\tau') = \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n(\tau-\tau')} G^{\mathrm{s}}_{\sigma\sigma'}(\boldsymbol{r},\boldsymbol{r}',\omega_n), \tag{1.50}$$

where $\omega_n = (2n+1)/\beta$ are the odd Matsubara frequencies. The transform for the anomalous propagators are defined similarly. With these definitions and after some calculations, the frequency-dependent propagators read

$$G^{\mathrm{s}}_{\sigma\sigma'}(\boldsymbol{r},\boldsymbol{r}',\omega_n) = \delta_{\sigma\sigma'}\sum_i \left[\frac{u_i(\boldsymbol{r})u_i^*(\boldsymbol{r}')}{i\omega_n - E_i} - \frac{v_i(\boldsymbol{r})v_i^*(\boldsymbol{r}')}{i\omega_n + E_i}\right], \tag{1.51}$$

$$F^{\mathrm{s}}_{\sigma\sigma'}(\boldsymbol{r},\boldsymbol{r}',\omega_n) = \delta_{\sigma,-\sigma'}\mathrm{sgn}(\sigma')\sum_i \left[\frac{v_i^*(\boldsymbol{r})u_i(\boldsymbol{r}')}{i\omega_n + E_i} - \frac{u_i(\boldsymbol{r})v_i^*(\boldsymbol{r}')}{i\omega_n - E_i}\right], \tag{1.52}$$

$$F^{\mathrm{s}*}_{\sigma\sigma'}(\boldsymbol{r},\boldsymbol{r}',\omega_n) = \delta_{\sigma,-\sigma'}\mathrm{sgn}(\sigma)\sum_i \left[\frac{u_i^*(\boldsymbol{r})v_i(\boldsymbol{r}')}{i\omega_n + E_i} - \frac{v_i(\boldsymbol{r})u_i^*(\boldsymbol{r}')}{i\omega_n - E_i}\right], \tag{1.53}$$

in terms of the Kohn-Sham eigenfunctions and the Kohn-Sham eigenenergies (see from (1.28) to (1.30)). On the other hand, the Fourier transform of phonon propagator is defined as

$$D^{\mathrm{s}}_{\lambda,\boldsymbol{q}}(\nu_n) = -\frac{2\Omega_{\lambda,\boldsymbol{q}}}{\nu_n^2 + \Omega^2_{\lambda,\boldsymbol{q}}}, \tag{1.54}$$

where $\nu_n = 2n\pi/\beta$ are the even Matsubara frequencies. Now we are ready to derive the explicit expressions for lowest-order contributions to F_{xc}. As mentioned before, now we consider the contributions from the Coulomb interaction and the electron-phonon interaction but do not consider the effect of spin fluctuations.

Figure1.2: Lowest-order phononic contributions to F_{xc}.

Phononic kernels

Lowest-order contributions from electron-phonon interaction can be written as

$$F_{\rm xc}^{(1)} = \frac{1}{2}\sum_{\lambda,\boldsymbol{q}}\sum_{ij}|g_{\lambda,\boldsymbol{q}}^{ij}|^2\frac{\Delta_i\Delta_j^*}{E_iE_j}\left[I(E_i,E_j,\Omega_{\lambda,\boldsymbol{q}}) - I(E_i,-E_j,\Omega_{\lambda,\boldsymbol{q}})\right], \tag{1.55}$$

$$F_{\rm xc}^{(2)} = -\frac{1}{2}\sum_{\lambda,\boldsymbol{q}}\sum_{ij}|g_{\lambda,\boldsymbol{q}}^{ij}|^2\left[\left(1+\frac{\xi_i}{E_i}\frac{\xi_j}{E_j}\right)I(E_i,E_j,\Omega_{\lambda,\boldsymbol{q}}) + \left(1-\frac{\xi_i}{E_i}\frac{\xi_j}{E_j}\right)I(E_i,-E_j,\Omega_{\lambda,\boldsymbol{q}})\right], \tag{1.56}$$

where the explicit form of function I is

$$I(E_i,E_j,\Omega) = f_\beta(E_i)f_\beta(E_j)n_\beta(\Omega)\left[\frac{e^{\beta E_i}-e^{\beta(E_j+\Omega)}}{E_i-E_j-\Omega} - \frac{e^{\beta E_j}-e^{\beta(E_i+\Omega)}}{E_i-E_j+\Omega}\right]. \tag{1.57}$$

The diagrammatic expression for $F_{\rm xc}^{(1)}$ and $F_{\rm xc}^{(2)}$ is depicted in Figs.1.2a and 1.2b, respectively.

Now we can compute the phononic contributions to the exchange-correlation kernels $\mathcal{F}_{{\rm Hxc},ij}$ (see (1.38)). The exchange-correlation kernel arising from $F_{\rm xc}^{(1)}$ is nondiagonal and its form is

$$\mathcal{F}_{{\rm Hxc},ij}^{(1)} \equiv \mathcal{K}_{ij}^{\rm ph} = \frac{2}{\tanh[(\beta/2)\xi_i]\tanh[(\beta/2)\xi_j]}\sum_{\lambda,\boldsymbol{q}}|g_{\lambda,\boldsymbol{q}}^{ij}|^2\left[I(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}}) - I(\xi_i,-\xi_j,\Omega_{\lambda,\boldsymbol{q}})\right]. \tag{1.58}$$

On the other hand, the exchange-correlation kernel arising from $F_{\rm xc}^{(2)}$ is diagonal. Now we define the diagonal part of exchange-correlation kernel $\mathcal{Z}_i^{\rm ph,full}$ as

$$\mathcal{F}_{{\rm Hxc},ij}^{(2)} = \delta_{ij}\frac{E_i}{\tanh[(\beta/2)\xi_i]}\mathcal{Z}_i^{\rm ph,PT}, \tag{1.59}$$

and its explicit form derived by perturbation theory (PT) directly reads

$$\begin{aligned}\mathcal{Z}_i^{\rm ph,PT} = &-\frac{2}{\sum_j\frac{\beta/2}{\cosh^2[(\beta/2)\xi_j]}}\left[\frac{1}{\xi_i} - \frac{\beta/2}{\sinh[(\beta/2)\xi_i]\cosh[(\beta/2)\xi_i]}\right]\sum_{jl}\sum_{\lambda,\boldsymbol{q}}|g_{\lambda,\boldsymbol{q}}^{jl}|^2 I'(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}})\\ &+\frac{1}{\tanh[(\beta/2)\xi_i]}\sum_j\sum_{\lambda,\boldsymbol{q}}|g_{\lambda,\boldsymbol{q}}^{ij}|^2\left\{\frac{1}{\xi_j}[I(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}}) - I(\xi_i,-\xi_j,\Omega_{\lambda,\boldsymbol{q}})] - 2I'(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}})\right\},\end{aligned} \tag{1.60}$$

where the function I' is defined as

$$I'(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}}) = \frac{\partial}{\partial\xi_i}I(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}}). \tag{1.61}$$

However, it is found that the direct use of $\mathcal{Z}_i^{\rm ph,PT}$ leads numerical instabilities [1], then an alternative expression is developed. The numerically-stable expression for diagonal kernel is

$$\mathcal{Z}_i^{\rm ph} = \frac{1}{\tanh[(\beta/2)\xi_i]}\sum_j\sum_{\lambda,\boldsymbol{q}}|g_{\lambda,\boldsymbol{q}}^{ij}|^2\left[J(\xi_i,\xi_j,\Omega_{\lambda,\boldsymbol{q}}) + J(\xi_i,-\xi_j,\Omega_{\lambda,\boldsymbol{q}})\right], \tag{1.62}$$

where the function J is defined as

$$J(\xi,\xi,\Omega) = \tilde{J}(\xi,\xi,\Omega) + \tilde{J}(\xi,\xi,-\Omega), \tag{1.63}$$

$$\tilde{J}(\xi,\xi',\Omega) = -\frac{f_\beta(\xi)+n_\beta(\Omega)}{\xi-\xi'-\Omega}\left[\frac{f_\beta(\xi')+f_\beta(\xi-\Omega)}{\xi-\xi'-\Omega} - \beta f_\beta(\xi-\Omega)f_\beta(-\xi'+\Omega)\right]. \tag{1.64}$$

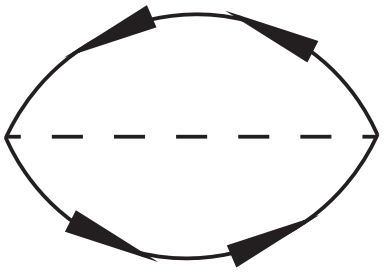

Figure1.3: Lowest-order electronic contributions to the F_{xc}. A dashed line means the screened Coulomb interaction.

Electron-electron kernels

We now develop the exchange-correlation kernels arising from the Coulomb interaction. From the definition of $\mathcal{F}_{\mathrm{Hxc},ij}$ (1.38), it can be seen that there are two terms that contribute to the kernels. The first is the anomalous Hartree energy (1.17), and the second is the exchange-correlation free energy $F_{\mathrm{xc}}^{(3)}$ (Fig.1.3). For convenience, an approximation is applied to *both* of the anomalous Hartree energy and F_{xc} as follows [1]:

$$F_{\mathrm{xc}}^{(3)} + E_{\mathrm{H}}^{\mathrm{ee},\chi} = \int d^3r \int d^3r' \left|\chi(\boldsymbol{r}-\boldsymbol{r}')\right|^2 v^{\mathrm{screen}}(\boldsymbol{r}-\boldsymbol{r}'), \tag{1.65}$$

where $v^{\mathrm{screen}}(\boldsymbol{r}-\boldsymbol{r}')$ means a static screened Coulomb interaction. Within this approximation, the exchange-correlation kernel from electron-electron interaction can be written as

$$\begin{aligned} \mathcal{K}_{ij}^{\mathrm{el}} &\equiv \frac{\delta^2\left(F_{\mathrm{xc}}^{(3)} + E_{\mathrm{H}}^{\mathrm{ee},\chi}\right)}{\delta\chi_i^*\delta\chi_j} \\ &= v_{ij}^{\mathrm{scr}}, \end{aligned} \tag{1.66}$$

where

$$v_{ij}^{\mathrm{scr}} = \int d^3r \int d^3r' \varphi_i^*(\boldsymbol{r})\varphi_i(\boldsymbol{r}')v^{\mathrm{scr}}(\boldsymbol{r},\boldsymbol{r}')\varphi_j(\boldsymbol{r})\varphi_j^*(\boldsymbol{r}'). \tag{1.67}$$

There are some way how to approximate the screened Coulomb interaction $v^{\mathrm{scr}}(\boldsymbol{r},\boldsymbol{r}')$. Lüders *et al.* applied the Thomas-Fermi interaction to the Coulomb interaction [1]. There are also some studies which applies the random phase approximation to v^{scr} [5]. In our calculation, we applied the adiabatic local density approximation(ALDA) [6] and so we now summarize the expression for the screened Coulomb interaction in ALDA. Furthermore, it should be taken account of the dynamical structure of the Coulomb interaction which is represented by the frequency-dependent polarization function Π. The polarization function Π is obtained by the following equation

$$\Pi(\boldsymbol{r},\boldsymbol{r}',\omega) = \Pi_0(\boldsymbol{r},\boldsymbol{r}',\omega) + \iint d^3r_1 d^3r_2 \Pi_0(\boldsymbol{r},\boldsymbol{r}_1,\omega)\left(\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} + \frac{\delta^2 E_{\mathrm{xc}}}{\delta\rho(\boldsymbol{r}_1)\delta\rho(\boldsymbol{r}_2)}\right)\Pi(\boldsymbol{r}_2,\boldsymbol{r}',\omega), \tag{1.68}$$

where Π_0 indicates the independent-particle polarization function

$$\Pi_0(\boldsymbol{r},\boldsymbol{r}',\omega) = \sum_{ij} \frac{\theta(-\xi_i) - \theta(\xi_j)}{\xi_j - \xi_i + i\omega} \varphi_i^*(\boldsymbol{r})\varphi_j^*(\boldsymbol{r}')\varphi_i(\boldsymbol{r}')\varphi_j(\boldsymbol{r}), \tag{1.69}$$

where $\theta(\xi)$ is the step function. We used adiabatic local density apploximation(ALDA) [7] to calculate the polarization function Π. Now the screened Coulomb interaction within the ALDA is written as

$$v^{\mathrm{scr}}(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} + \iint d^3r_1 d^3r_2 \left(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_1|} + \frac{\delta^2 E_{\mathrm{xc}}}{\delta\rho(\boldsymbol{r})\delta\rho(\boldsymbol{r}_1)} \right) \Pi(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega) \frac{1}{|\boldsymbol{r}_2-\boldsymbol{r}'|} \tag{1.70}$$

If we take into account of the frequency-dependent screened Coulomb interaction, the formulation for $\mathcal{K}_{ij}^{\mathrm{el}}$ should be modified as follows [8]:

$$\mathcal{K}_{n\boldsymbol{k},n'\boldsymbol{k}'}^{\mathrm{el,dyn}} = \lim_{\{\Delta_{n\boldsymbol{k}}\}\to 0} \frac{1}{\tanh[(\beta/2)E_{n\boldsymbol{k}}]} \frac{1}{\tanh[(\beta/2)E_{n'\boldsymbol{k}'}]} \frac{1}{\beta^2} \sum_{\tilde{\omega}_1\tilde{\omega}_2} F_{n\boldsymbol{k}}(\mathrm{i}\tilde{\omega}_1) F_{n'\boldsymbol{k}'}(\mathrm{i}\tilde{\omega}_2) W_{n\boldsymbol{k}n'\boldsymbol{k}'}[\mathrm{i}(\tilde{\omega}_1 - \tilde{\omega}_2)], \tag{1.71}$$

where $F_{n\boldsymbol{k}}(\mathrm{i}\tilde{\omega}) = \frac{1}{\mathrm{i}\tilde{\omega}+\mathrm{E_{nk}}} - \frac{1}{\mathrm{i}\tilde{\omega}-\mathrm{E_{nk}}}$ and $\tilde{\omega}$ means the bosonic Matsubara frequency and we defined $W_{n\boldsymbol{k}n'\boldsymbol{k}'}(\mathrm{i}\omega)$ as below

$$W_{n\boldsymbol{k}n'\boldsymbol{k}'}(\mathrm{i}\omega) = \int d^3r \int d^3r' \varphi_{n\boldsymbol{k}}(\boldsymbol{r})\varphi_{n-\boldsymbol{k}}(\boldsymbol{r}')v^{\mathrm{scr}}(\boldsymbol{r},\boldsymbol{r}',\omega)\varphi_{n'\boldsymbol{k}'}(\boldsymbol{r})\varphi_{n'-\boldsymbol{k}'}(\boldsymbol{r}'). \tag{1.72}$$

We describe how to calcurate the summation with respect to the even Matsubara frequency in (1.71) in Appendix. Using the kernels derived above, the resulting SCDFT gap equation is written as

$$\Delta_{n\boldsymbol{k}} = -\mathcal{Z}_{n\boldsymbol{k}}\Delta_{n\boldsymbol{k}} - \frac{1}{2}\sum_{n'\boldsymbol{k}'} \mathcal{K}_{n\boldsymbol{k}n\boldsymbol{k}'} \frac{\tanh[(\beta/2)E_{n'\boldsymbol{k}'}]}{E_{n'\boldsymbol{k}'}} \Delta_{n'\boldsymbol{k}'}, \tag{1.73}$$

where $\mathcal{Z}$ contains the phonon contribution (1.62) and $\mathcal{K}$ contains the phonon term (1.58) and Coulombic term (1.71).

1.5 Spin fluctuations kernel from Sham-Shlüter connection

In the previous section, we derived the phononic and electron-electron Coulomb kernel from functional derivatives. Now we review the derivation of the expression for kernels arising from spin fluctuations by Essenberger and coworkers [9]. In the following, we will construct the SCDFT gap equation from the Sham-Shlüter connection including the effect of spin fluctuations and derive the expression for the kernel from the spin fluctuations.

1.5.1 Spin fluctuations contribution to the self-energy

In order to surpass the GW approximation, at first the T-matrix [10, 11] is considered. The T-matrix is defined through the Bethe-Salpeter equation [12] as

$$T(1,2,3,4) = w(1,3)\delta_{13}\delta_{24} + w(1,2)G(1,5)G(2,6)T(5,6,3,4), \tag{1.74}$$

Figure1.4: Self-energy diagram of spin fluctuations described with particle-hole propagator Λ. A double-line indicates the full Green's function.

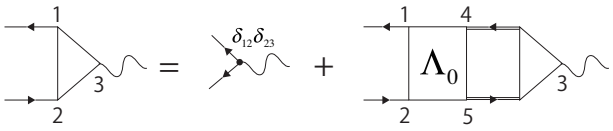

Figure1.5: Diagrammatic representation of one of the Hedin's equations.

where w indicates the screened Coulomb interaction. The coordinate 1 indicates that $1 = \{\boldsymbol{r}_1, \tau_1, \sigma_1\}$, where $\boldsymbol{r}_1$, τ_1, σ_1 is the real space coordinate, the Matsubara imaginary time and the spin index, respectively. Using this T-matrix, the contribution of spin fluctuations to the self-energy can be written as $\bar{\Sigma}^T = \bar{G}T$. Is is known that the response function within the T-matrix approximation reasonably describes the magnetic response function [11, 13]. However, due to the reason we discuss later, we do not directly use this T-matrix.

Alternatively, we start from particle-hole propagator Λ in order to take account of spin fluctuations in self-energy (Fig. 1.4). Particle-hole propagator Λ contains all irreducible diagrams with respect to Coulomb interaction and has two incoming and outgoing points. The T-matrix is fully contained in theΛ. In the following, we assume that we consider about the case of collinear magnetic systems and then the Green's function becomes diagonal with respect to spin indices. We consider one of the Hedin's equation [14] which is depicted in Fig.1.5

$$\Gamma(1,2,3) = \delta(1,2)\delta(1,3) + \int d(4,5,6,7)\Lambda_0(1,2,4,5)G(4,6)G(7,5)\Gamma(6,7,3), \tag{1.75}$$

where

$$\Lambda_0(1,2,3,4) = \frac{\delta\Sigma^{\mathrm{V}}(1,2)}{\delta G(3,4)}. \tag{1.76}$$

The coordinates 1 and 4 are connected to the lines which go outside, and the coordinates 2 and 3 are connected to the lines which come inside. Λ_0 is called an irreducible particle-hole propagator [15]. The self-energy used to calculate Λ_0 is written as Σ^{V}. We will apply an approximation for Σ^{V} later. The Λ_0 contains all connected and irreducible diagrams with respect to the Coulomb interaction and the particle-hole propagator. If we obtain the Λ_0, we can get the Λ by using the Bethe-Salpeter equation(BSE) [12] for Λ. However, before considering the BSE for Λ, we have to note that there can be two possible contributions

to Λ_0.

The functional derivative of the self-energy with respect to G correspond to the removal of one Green's function in self-energy. Hence, the two possible contributions to Λ_0 come from the type of the Green's function which is removed. If the removed Green's function was a factor of a loop, we call the resulting contribution to Λ_0 as direct contribution Λ^{d}. Otherwise, we call these contributions as crossed ones and define as Λ^{c}. Then we can write these contributions as follows:

$$\Lambda_0^{\mathrm{c}}(1,2,3,4) \equiv \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\Lambda_0^{\mathrm{c}}(1,2,3,4), \tag{1.77}$$

$$\Lambda_0^{\mathrm{d}}(1,2,3,4) \equiv \delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4}\Lambda_0^{\mathrm{d}}(1,2,3,4). \tag{1.78}$$

It should be noted that crossed and direct contributions have different signs because one loop is removed in case of direct ones:

$$\Lambda_0^{\mathrm{c}}(1,2,3,4) = \frac{\delta\Sigma^{\mathrm{V}}(1,2)}{\delta G(3,4)}, \tag{1.79}$$

$$\Lambda_0^{\mathrm{d}}(1,2,3,4) = -\frac{\delta\Sigma^{\mathrm{V}}(1,2)}{\delta G(3,4)}. \tag{1.80}$$

From Eqs. (1.76), (1.79) and (1.80), the total irreducible particle-hole propagator can be written as follows:

$$\Lambda_0(1,2,3,4) = \frac{\delta\Sigma^{\mathrm{V}}(1,2)}{\delta G(3,4)} = \Lambda_0^{\mathrm{c}} - \Lambda_0^{\mathrm{d}} \equiv \Lambda_0^{\mathrm{c-d}}. \tag{1.81}$$

Furthermore, we have to consider how higher order irreducible particle-hole propagators are constructed.

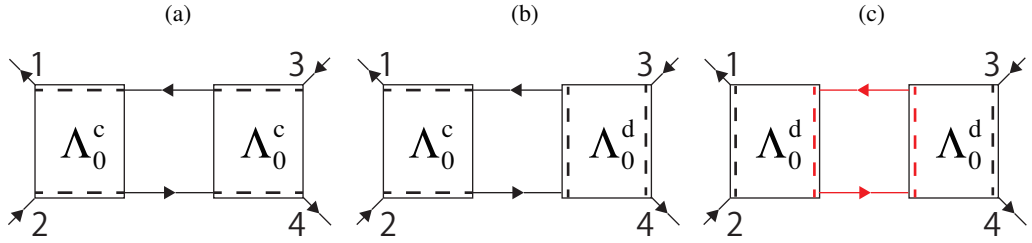

Figure1.6: Diagrammatic representation how higher order propagator is constructed. Bold dashed lines indicate that connected two points have the same spins.

There can be three patterns how crossed and direct contributions are linked: (a) If two crossed contributions are connected, the resulting contribution is also crossed one(Fig.1.6a). (b) If crossed and direct contributions are linked, the resulting contribution becomes direct one(Fig.1.6b). (c) If two direct contributions are linked, the resulting contribution is also direct one(Fig.1.6c). In this case, we have to pay attention to the sign of this contribution because one additional loop appears.

With these considerations, the BSE for Λ becomes as follows:

$$\Lambda = \sum_{n=0}^{\infty}\Lambda_{(n)}^{\mathrm{c}} + \sum_{n=0}^{\infty}\Lambda_{(n)}^{\mathrm{d}}, \tag{1.82}$$

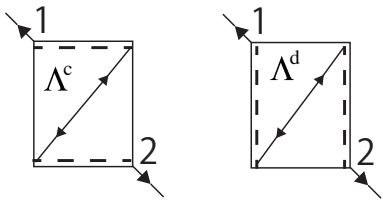

Figure1.7: Crossed and direct contribution to self-energy with anomalous Green's function F.

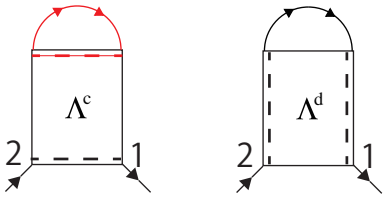

Figure1.8: Crossed and direct contribution to self-energy with normal Green's function G.

$$\Lambda^{c}_{(n+1)} = \Lambda^{c}_{0} GG\Lambda^{c}_{(n)}, \tag{1.83}$$

$$\Lambda^{d}_{(n+1)} = \Lambda^{d}_{0} GG\Lambda^{c}_{(n)} + \Lambda^{c}_{0} GG\Lambda^{d}_{(n)} - \Lambda^{d}_{0} GG\Lambda^{d}_{(n)}, \tag{1.84}$$

where (n) means the order of the irreducible particle-hole propagator and $\Lambda^{c,d}_{(0)}$ is equal to $\Lambda^{c,d}_{0}$ defined in Eqs.(1.77) and (1.78). From Eqs.(1.83) and (1.84), we obtain the BSE for Λ^{c-d} as

$$\Lambda^{c-d} = \Lambda_0 + \Lambda_0 GG\Lambda^{c-d}, \tag{1.85}$$

where Λ_0 is defined in Eq.(1.81).

So far, we considered only the normal Green's function because we neglected the effects of spin fluctuations on superconductors. We are interested in the theory in superconductors, so we have to construct the self-energy comes from spin fluctuations(Fig.1.4) with normal and anomalous Green's functions(Fig.1.1). In anomalous terms in which F and $F^{\dagger}$ appear, no loop is created when we construct the self-energy(Fig.1.7). Therefore, crossed and direct contribution to the self-energy have the same sign and the resulting expression reads

$$\bar{\Sigma}^{SF}_{F} \equiv \iint d34\tau^{z} \begin{pmatrix} 0 & F(3,4)\Lambda^{c+d}(1,3,4,2) \\ F^{\dagger}(3,4)\Lambda^{c+d}(3,1,2,4) & 0 \end{pmatrix}. \tag{1.86}$$

In this expression, the order of coordinates in Λ correspond to the definition of Λ as stated before. On the other hand, in normal contributions, the sign of crossed term and direct one is different because one extra loop appears in the crossed term(Fig.1.8). With this normal contributions, the equation of the self-energy from spin fluctuations can be written as follows:

$$\bar{\Sigma}^{SF} \equiv \iint d34\tau^{z} \begin{pmatrix} -G(3,4)\Lambda^{c-d}(1,3,2,4) & F(3,4)\Lambda^{c+d}(1,3,4,2) \\ F^{\dagger}(3,4)\Lambda^{c+d}(3,1,2,4) & -G^{\dagger}(3,4)\Lambda^{c-d}(3,1,4,2) \end{pmatrix}. \tag{1.87}$$

We obtained the equation for the self-energy from spin fluctuations with Λ^{c+d} and Λ^{c-d}. We can simplify

the expression because it is already assumed that we are now interested in singlet cuperconductor and magnetic collinear system. From this assumption, we already know that the normal Green's function conserves the spin while the anomalous one flips the spin(see from Eq. (1.46) to Eq.(1.48)). According to these spin properties of Green's functions, it can be seen that the 11 and 22 element of Eq.(1.87) depend only on $\Lambda^{\mathrm{c-d}}_{\sigma_1\sigma\sigma_2\sigma}$ while the 12 and 21 element depend only on $\Lambda^{\mathrm{c+d}}_{\sigma_1\sigma-\sigma\sigma_2}$.

Furthermore, considering the spin properties of Λ^{c} and Λ^{d} (see Eq.(1.77) and (1.78)), following relations can be straightforwardly derived:

$$\Lambda^{\mathrm{c+d}}_{\sigma\sigma-\sigma-\sigma} = \Lambda^{\mathrm{d}}_{\sigma\sigma-\sigma-\sigma} = -\Lambda^{\mathrm{c-d}}_{\sigma\sigma-\sigma-\sigma}, \tag{1.88}$$

$$\Lambda^{\mathrm{c+d}}_{\sigma-\sigma\sigma-\sigma} = \Lambda^{\mathrm{c}}_{\sigma-\sigma\sigma-\sigma} = \Lambda^{\mathrm{c-d}}_{\sigma-\sigma\sigma-\sigma}. \tag{1.89}$$

By using these relations, we can rewrite the expression of the self-energy as follows:

$$\bar{\Sigma}^{\mathrm{SF}}_{11} = -\delta_{\sigma_1\sigma_2} G_{\sigma_1} \sum_{\sigma} \Lambda^{\mathrm{c-d}}_{\sigma_1\sigma\sigma_1\sigma}, \tag{1.90}$$

$$\bar{\Sigma}^{\mathrm{SF}}_{22} = \delta_{\sigma_1\sigma_2} G^{\dagger}_{\sigma_1} \sum_{\sigma} \Lambda^{\mathrm{c-d}}_{\sigma\sigma_1\sigma\sigma_1}, \tag{1.91}$$

$$\bar{\Sigma}^{\mathrm{SF}}_{12} = \delta_{\sigma_1-\sigma_2} F_{\sigma_1} \sum_{\sigma} (1 - 2\delta_{\sigma\sigma_1}) \Lambda^{\mathrm{c-d}}_{\sigma_1\sigma-\sigma-\sigma_1}, \tag{1.92}$$

$$\bar{\Sigma}^{\mathrm{SF}}_{21} = -\delta_{\sigma_1-\sigma_2} F^{\dagger}_{\sigma_1} \sum_{\sigma} (1 - 2\delta_{\sigma\sigma_1}) \Lambda^{\mathrm{c-d}}_{\sigma\sigma_1-\sigma_1-\sigma}. \tag{1.93}$$

This is a more convenient result than Eq.(1.87) because we have to solve the BSE for only $\Lambda^{\mathrm{c-d}}$ and we do not have to compute both Λ^{c} and Λ^{d} separately. In the above expression, we omitted the integral and we will use this notation below unless the expression leads any ambiguity.

In the previous explanation, we derived the approximated expression of the self-energy from spin fluctuations. However, there is one problem in the previous expression. If we want to calculate the self-energy along with the expression from (1.90) to (1.93), we need to calculate the four-point function $\Lambda^{\mathrm{c-d}}$ and the resulting integration omitted in the previous expressions becomes too complex to execute. In order to avoid this difficulty, we apply a crude approximation to the self-energy Σ^V which is used to calculate Λ_0 (see Eq.(1.76)) and obtain the Λ as a two-point function. The approximation is that we use the Kohn-Sham potential as the Σ^V [14]:

$$\Sigma^V(1,2) \approx \delta_{\tau_1\tau_2}\delta_{\boldsymbol{r}_1\boldsymbol{r}_2} v^{\mathrm{xc}}_{\sigma_1\sigma_2}(\boldsymbol{r}_1\tau_1), \tag{1.94}$$

where v^{xc} means the Kohn-Sham potential. Within this approximation, the functional derivative of Σ^V can

be calculated using the following result:

$$\begin{aligned}\frac{\delta v^{\mathrm{xc}}_{\sigma_1\sigma_2}(\boldsymbol{x}_1)}{\delta G(3,4)} &= \sum_{\sigma_5\sigma_6}\int d\boldsymbol{x}_5 \frac{\delta v^{\mathrm{xc}}_{\sigma_1\sigma_2}(\boldsymbol{x}_1)}{\delta \rho_{\sigma_5\sigma_6}(\boldsymbol{x}_5)}\frac{\delta \rho_{\sigma_5\sigma_6}(\boldsymbol{x}_5)}{\delta G(3,4)} \\ &= \iint d5d6 f^{\mathrm{xc}}_{\sigma_1\sigma_2\sigma_5\sigma_6}(\boldsymbol{x}_1\boldsymbol{x}_5)\frac{\delta G(5,6)}{\delta G(3,4)}\delta_{\boldsymbol{x}_5\boldsymbol{x}_6} \\ &= f^{\mathrm{xc}}_{\sigma_1\sigma_2\sigma_5\sigma_6}(\boldsymbol{x}_1,\boldsymbol{x}_3)\delta_{\boldsymbol{x}_3\boldsymbol{x}_4},\end{aligned} \tag{1.95}$$

where $\boldsymbol{x}_1 = (\boldsymbol{r}_1\tau_1)$ and f^{xc} is defined as

$$f^{\mathrm{xc}}_{\sigma_1\sigma_2\sigma_5\sigma_6}(\boldsymbol{x}_1\boldsymbol{x}_5) \equiv \frac{\delta v^{\mathrm{xc}}_{\sigma_1\sigma_2}(\boldsymbol{x}_1)}{\delta \rho_{\sigma_5\sigma_6}(\boldsymbol{x}_5)}. \tag{1.96}$$

If we approximate the full Green's function in (1.85) by the Kohn-Sham one, the BSE for $\Lambda^{\mathrm{c-d}}$ can be written as

$$\Lambda^{\mathrm{c-d}}_{\sigma_1\sigma_1\sigma_2\sigma_2} = 4f^{\mathrm{xc}}_{\sigma_1\sigma_1\sigma_2\sigma_2} + 16\sum_{\sigma_6\sigma_7} f^{\mathrm{xc}}_{\sigma_1\sigma_1\sigma_6\sigma_6}P_{\sigma_6\sigma_6\sigma_7\sigma_7}f^{\mathrm{xc}}_{\sigma_7\sigma_7\sigma_2\sigma_2}, \tag{1.97}$$

$$\Lambda^{\mathrm{c-d}}_{\sigma-\sigma\sigma-\sigma} = 4f^{\mathrm{xc}}_{\sigma-\sigma\sigma-\sigma} + 16f^{\mathrm{xc}}_{\sigma-\sigma\sigma-\sigma}P_{\sigma-\sigma\sigma-\sigma}f^{\mathrm{xc}}_{\sigma-\sigma\sigma-\sigma}, \tag{1.98}$$

where P indicates the proper part of the response function. The full response function can be obtained by solving the following Dyson equation:

$$\chi_{\sigma_1\sigma_2\sigma_3\sigma_4} = P_{\sigma_1\sigma_2\sigma_3\sigma_4} + \delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4}\sum_{\sigma\sigma'} P_{\sigma_1\sigma_2\sigma\sigma}v\chi_{\sigma'\sigma'\sigma_3\sigma_4}, \tag{1.99}$$

where v indicates the bare Coulomb interaction. The full response function in the spin basis describes how the spin-resolved charge density is modified due to the external field:

$$\chi_{\sigma_1\sigma_2\sigma_3\sigma_4}(\boldsymbol{x}_1,\boldsymbol{x}_2) \equiv \frac{\delta\rho_{\sigma_1\sigma_2}(\boldsymbol{x}_1)}{\delta\varphi^{\mathrm{ext}}_{\sigma_3\sigma_4}(\boldsymbol{x}_2)}. \tag{1.100}$$

In equations from (1.90) to (1.93), $\Lambda^{\mathrm{c-d}}$ is still the four-point function with respect to spin and difficult to handle. To simplify these equations, we transform these four-point quantities into the quantities which have two labels of the Pauli matrices; i.e.,

$$\chi_{ij}(\boldsymbol{x}_1,\boldsymbol{x}_2) \equiv \frac{\delta\rho_i(\boldsymbol{x}_1)}{\delta\varphi^{\mathrm{ext}}_j(\boldsymbol{x}_2)}. \tag{1.101}$$

In this form, χ determines the change of the electronic charge ρ or magnetic moment $\boldsymbol{m}$ due to the external physical fields. The basis transformation between these two representations is defined as

$$\begin{aligned}A_{\alpha\beta\delta\gamma} &= \frac{1}{4}\sum_{ij}\sigma^i_{\alpha\beta}A_{ij}\sigma^j_{\gamma\delta}, \\ A_{ij} &= \sum_{\alpha\beta\gamma\delta}\sigma^i_{\beta\alpha}A_{\alpha\beta\gamma\delta}\sigma^i_{\delta\gamma},\end{aligned} \tag{1.102}$$

where σ^i is the Pauli matrices

$$\sigma^0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \sigma^x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \sigma^y = \begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}, \sigma^z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{1.103}$$

It should be noted that the full response function is sparse for the magnetic collinear system

$$\chi_{ij} = \begin{pmatrix} \chi_{xx} & \chi_{xy} & 0 & 0 \\ \chi_{yx} & \chi_{yy} & 0 & 0 \\ 0 & 0 & \chi_{zz} & \chi_{z0} \\ 0 & 0 & \chi_{0z} & \chi_{00} \end{pmatrix}, \tag{1.104}$$

and the full response function is equal to the proper one, i.e., $\chi_{ij} = P_{ij}$ if $i,j \in \{x,y\}$. Using these representations, we can rewrite the effective interaction $\Lambda^{\mathrm{c-d}}$ in more transparent form as follows

$$\Lambda^{\mathrm{c-d}}_{\sigma_1\sigma_1\sigma_2\sigma_2} = \sum_{ij\in\{0,z\}} f^{\mathrm{T}}_{i\sigma_1} P_{ij} (1 - \delta_{i0}\delta_{j0}) f_{j\sigma_2}, \tag{1.105}$$

$$\Lambda^{\mathrm{c-d}}_{\sigma-\sigma\sigma-\sigma} = 2 f^{\mathrm{F}}_{\sigma} \chi^{\mathrm{F}}_{\sigma} f^{\mathrm{F}}_{\sigma}, \tag{1.106}$$

where the two-point funtions are defined as ($z_\uparrow = 1, z_\downarrow = -1$)

$$\begin{aligned} f^{\mathrm{T}}_{z\sigma} &\equiv z_\sigma f^{\mathrm{xc}}_{zz} + f^{\mathrm{xc}}_{0z} \quad f_{z\sigma} \equiv z_\sigma f^{\mathrm{xc}}_{zz} + f^{\mathrm{xc}}_{z0}, \\ f^{\mathrm{T}}_{0\sigma} &\equiv f^{\mathrm{xc}}_{00} + z_\sigma f^{\mathrm{xc}}_{z0} \quad f_{0\sigma} \equiv f^{\mathrm{xc}}_{00} + z_\sigma f^{\mathrm{xc}}_{0z}, \\ f^{\mathrm{F}}_{\sigma} &\equiv f^{\mathrm{xc}}_{xx} + z_\sigma \mathrm{i} f^{\mathrm{xc}}_{xy} \quad \chi^{\mathrm{F}}_{\sigma} \equiv \chi_{xx} + z_\sigma \mathrm{i}\chi_{\mathrm{xy}}. \end{aligned} \tag{1.107}$$

In (1.105), we subtracted $f^{\mathrm{xc}}_{\sigma_1\sigma_1\sigma_2\sigma_2} + f^{\mathrm{T}}_{0\sigma_1} P_{00} f_{0\sigma_2}$ in order to avoid the double counting. In fact, this contribution is already included in the self-energy from the screened Coulomb interaction. In addition, we neglected $f^{\mathrm{xc}}_{\sigma-\sigma\sigma-\sigma}$ in (1.106) in order to avoid the physically unreasonable result. We will discuss this problem later.

So far we derived the two-point expression of the effective interaction $\Lambda^{\mathrm{c-d}}$. In addition, we make further two assumptions: The response functions and xc kernel f^{xc} are diagonal with respect to the Pauli index and the effect of the external magnetic field is degenerated in three directions. Within these assumptions, the effective interaction (1.105) and (1.106) can be written in simple form as follows:

$$\begin{aligned} &\Lambda^{\mathrm{c-d}}_{\sigma_1\sigma_1\sigma_2\sigma_2}(\boldsymbol{x}_1,\boldsymbol{x}_2) = z_{\sigma_1} z_{\sigma_2} \Lambda^{\mathrm{SF}}(\boldsymbol{x}_1,\boldsymbol{x}_2), \\ &\Lambda^{\mathrm{c-d}}_{\sigma-\sigma\sigma-\sigma}(\boldsymbol{x}_1,\boldsymbol{x}_2) = 2\Lambda^{\mathrm{SF}}(\boldsymbol{x}_1,\boldsymbol{x}_2), \\ &\Lambda^{\mathrm{SF}}(\boldsymbol{x}_1,\boldsymbol{x}_2) \equiv \iint d\boldsymbol{x} d\boldsymbol{x}' f^{\mathrm{xc}}_{zz}(\boldsymbol{x}_1,\boldsymbol{x}) \chi_{zz}(\boldsymbol{x},\boldsymbol{x}') f^{\mathrm{xc}}_{zz}(\boldsymbol{x}',\boldsymbol{x}_2), \end{aligned} \tag{1.108}$$

where χ_{zz} is the spin susceptibility which is obtained from the following equations (m indicates the spin density)

$$\chi_{zz}(\boldsymbol{x},\boldsymbol{x}') = \chi^{\mathrm{KS}}(\boldsymbol{x},\boldsymbol{x}') + \iint d\boldsymbol{x}_1 d\boldsymbol{x}_2 \chi^{\mathrm{KS}}(\boldsymbol{x},\boldsymbol{x}_1) f^{\mathrm{xc}}_{zz}(\boldsymbol{x}_1,\boldsymbol{x}_2) \chi_{zz}(\boldsymbol{x}_2,\boldsymbol{x}'), \tag{1.109}$$

$$f^{\mathrm{xc}}_{zz}(\boldsymbol{x},\boldsymbol{x}') = \frac{\delta^2 E_{\mathrm{xc}}}{\delta m(\boldsymbol{x}) \delta m(\boldsymbol{x}')}. \tag{1.110}$$

Inserting (1.108) into (1.90) to (1.93), we obtain the final form of the self-energy from spin fluctuations

$$\bar{\Sigma}^{\mathrm{SF}}_{ab}(\boldsymbol{x}_1,\boldsymbol{x}_2) = 3(-1)^{a+b+1} \Lambda^{\mathrm{SF}}(\boldsymbol{x}_1,\boldsymbol{x}_2) \bar{G}_{ab}(\boldsymbol{x}_1,\boldsymbol{x}_2), \tag{1.111}$$

where a,b indicate the Nambu index. The expression (1.111) has the GW form and then Λ^{SF} can be

interpreted as the effective interaction originated from the spin fluctuation. The present form of the effective interaction reduces to the formalism by Vignale and Singwi [16] in the limit of a homogeneous electron gas and the similar form can be derived from the paramagnon-pole model [17]. The xc kernel defined in (1.110) can be calculated using the Time-Dependent DFT(TDDFT) [18] within the ALDA.

1.5.2 Kernel originated from spin fluctuations

So far we have derived the spin fluctuations contribution to the self-energy in collinear superconductors. Then we can consider the effect of spin fluctuations in the framework of SCDFT using the Sham-Schlüter connection [19, 20]. The noninteracting Kohn-Sham system is mapped to the interacting system by the following self-energy

$$\bar{\Sigma}^{\mathrm{SS}} = \bar{\Sigma}^{\mathrm{GW}} + \bar{\Sigma}^{\mathrm{SF}} + \bar{\Sigma}^{\mathrm{ph}} - \begin{pmatrix} v_{\mathrm{xc}} & \Delta^{\mathrm{xc}} \\ \Delta^{\mathrm{xc}*} & -v_{\mathrm{xc}} \end{pmatrix}. \tag{1.112}$$

The Sham-Schlüter connection is the requirement that the ground state densities of the Kohn-Sham system and that of the interacting system should be same. Because the normal density and the anomalous density is defined as

$$\rho(\boldsymbol{r}_1) = \lim_{\boldsymbol{r}_1 \to \boldsymbol{r}_2} \frac{2}{\beta} \sum_{\omega_n} G(\boldsymbol{r}_1, \boldsymbol{r}_2, \omega_n), \tag{1.113}$$

$$\chi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{\beta} \sum_{\omega_n} F(\boldsymbol{r}_1, \boldsymbol{r}_2, -\omega_n), \tag{1.114}$$

then the Sham-Schlüter connection is written as follows:

$$0 = \delta_{ab} \lim_{\boldsymbol{r}_1 \to \boldsymbol{r}_2} \frac{2}{\beta} \sum_{\omega_n} e^{\mathrm{i}\omega_{\mathrm{n}} 0^+} [\bar{G}^{\mathrm{KS}} \bar{\Sigma}^{\mathrm{SS}} \bar{G}]_{ab}, \tag{1.115}$$

$$0 = (1 - \delta_{ab}) \frac{1}{\beta} \sum_{\omega_n} e^{\mathrm{i}\omega_{\mathrm{n}} 0^+} [\bar{G}^{\mathrm{KS}} \bar{\Sigma}^{\mathrm{SS}} \bar{G}]_{ab}, \tag{1.116}$$

In order to handle these equations, we approximate the full Green's function with the Kohn-Sham Green's function. Furthermore, we neglect all higher order term with respect to the xc potential Δ^{xc}. The Matsubara summation in (1.115) and (1.116) can be executed by means of the residue theorem:

$$\frac{1}{\beta} \sum_{n}^{\infty} A(\mathrm{i}\omega_{\mathrm{n}}) = \sum_{\mathrm{m}}^{\mathrm{Poles} \in \gamma} \mathrm{res}[\mathrm{f}_\beta(\mathrm{z}) \mathrm{A}(\mathrm{z}), \mathrm{z}_{\mathrm{m}}], \tag{1.117}$$

where $A(z)$ is an analytic function. After the Matsubara summation and some of algebra, we obtain the gap equation which is similar to the conventional one (1.73):

$$\Delta_k^{\mathrm{xc}} = -\mathcal{Z}_k \Delta_k^{\mathrm{xc}} - \frac{1}{2} \sum_{k'} \mathcal{K}_{kk'} \frac{\tanh[(\beta/2) E_{k'}]}{E_{k'}} \Delta_{k'}^{\mathrm{xc}}, \tag{1.118}$$

$$\mathcal{Z}_k = \mathcal{Z}_k^{\mathrm{ph}} - \mathcal{Z}_k^{\mathrm{SF}} \tag{1.119}$$

$$\mathcal{Z}^{\rm SF} = -\frac{1}{\beta^2}\frac{2}{\tanh[(\beta/2)\xi_k]}\sum_{n,m}\sum_{k'}\frac{1}{{\rm i}\omega_n + E_k}\frac{1}{{\rm i}\omega_m + E_{k'}}\left(\frac{1}{{\rm i}\omega_n + E_k} - \frac{1}{{\rm i}\omega_n - E_{k'}}\right)\Lambda^{\rm SF}_{kk'}(\omega_n - \omega_m)$$
$$+ \frac{2}{\beta^2}\left(\frac{1}{\xi_k} - \frac{(\beta/2)}{\sinh[(\beta/2)\xi_k]\cosh[(\beta/2)\xi_k]}\right)\sum_{nm}\sum_{k'k''}\frac{1}{({\rm i}\omega_n + E_{k'})^2}\frac{1}{{\rm i}\omega_m + E_{k''}}\frac{1}{\sum_{k'}\frac{\beta/2}{\cosh^2[(\beta/2)\xi_{k'}]}}\Lambda^{\rm SF}_{k'k''}(\omega_n - \omega_m), \tag{1.120}$$

$$\mathcal{K}_{kk'} = \mathcal{K}^{\rm ph}_{kk'} + \mathcal{K}^{\rm el}_{kk'} + \mathcal{K}^{\rm SF}_{kk'} \tag{1.121}$$

$$\mathcal{K}^{\rm SF}_{kk'} = \lim_{\{\Delta_k\}\to 0}\frac{1}{\tanh[(\beta/2)E_k]}\frac{1}{\tanh[(\beta/2)E_{k'}]}\frac{1}{\beta^2}\sum_{\omega_n\omega_m} F_k({\rm i}\omega_n)F_{k'}({\rm i}\omega_m)\Lambda^{\rm SF}_{kk'}(\omega_n - \omega_m), \tag{1.122}$$

$$F_k({\rm i}\omega_n) = \frac{1}{{\rm i}\omega_n + E_k} - \frac{1}{{\rm i}\omega_n - E_k}. \tag{1.123}$$

In the above equations, $k = \{n, \boldsymbol{k}\}$ and the kernels labeled ph and el are same as ones derived in the preivious section. Note that the contribution from spin fluctuations to $\mathcal{Z}$ has the different sign from phonon contribution, while in $\mathcal{K}$ they have same signs. This sign difference comes from the number of loops contained in diagrams discussed above (see (1.86)). The detail of derivation of these equations are described in Appendix.

1.6 Equation

1.6.1 Equation

1.7 Figure

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