

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

$$\chi_{ij} = \begin{pmatrix} \chi_{xx} & \chi_{xy} & 0 & 0 \\ \chi_{yx} & \chi_{yy} & 0 & 0 \\ 0 & 0 & \chi_{zz} & \chi_{z0} \\ 0 & 0 & \chi_{0z} & \chi_{00} \end{pmatrix}, \quad (1)$$

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 $\Lambda^{\text{c-d}}$ in more transparent form as follows

$$\Lambda_{\sigma_1\sigma_1\sigma_2\sigma_2}^{\text{c-d}} = \sum_{ij \in \{0, z\}} f_{i\sigma_1}^T P_{ij} (1 - \delta_{i0}\delta_{j0}) f_{j\sigma_2}, \quad (2)$$

$$\Lambda_{\sigma-\sigma\sigma-\sigma}^{\text{c-d}} = 2f_{\sigma}^F \chi_{\sigma}^F f_{\sigma}^F, \quad (3)$$

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

$$\begin{aligned} f_{z\sigma}^T &\equiv z_{\sigma} f_{zz}^{\text{xc}} + f_{0z}^{\text{xc}} & f_{z\sigma} &\equiv z_{\sigma} f_{zz}^{\text{xc}} + f_{z0}^{\text{xc}}, \\ f_{0\sigma}^T &\equiv f_{00}^{\text{xc}} + z_{\sigma} f_{z0}^{\text{xc}} & f_{0\sigma} &\equiv f_{00}^{\text{xc}} + z_{\sigma} f_{0z}^{\text{xc}}, \\ f_{\sigma}^F &\equiv f_{xx}^{\text{xc}} + z_{\sigma} i f_{xy}^{\text{xc}} & \chi_{\sigma}^F &\equiv \chi_{xx} + z_{\sigma} i \chi_{xy}. \end{aligned} \quad (4)$$

In (2), we subtracted $f_{\sigma_1\sigma_1\sigma_2\sigma_2}^{\text{xc}} + f_{0\sigma_1}^T P_{00} f_{0\sigma_2}$ 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 $f_{\sigma-\sigma\sigma-\sigma}^{\text{xc}}$ in (3) 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 $\Lambda^{\text{c-d}}$. 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 (2) and (3) can be written in simple form as follows:

$$\begin{aligned} \Lambda_{\sigma_1\sigma_1\sigma_2\sigma_2}^{\text{c-d}}(\mathbf{x}_1, \mathbf{x}_2) &= z_{\sigma_1} z_{\sigma_2} \Lambda^{\text{SF}}(\mathbf{x}_1, \mathbf{x}_2), \\ \Lambda_{\sigma-\sigma\sigma-\sigma}^{\text{c-d}}(\mathbf{x}_1, \mathbf{x}_2) &= 2\Lambda^{\text{SF}}(\mathbf{x}_1, \mathbf{x}_2), \\ \Lambda^{\text{SF}}(\mathbf{x}_1, \mathbf{x}_2) &\equiv \iint d\mathbf{x} d\mathbf{x}' f_{zz}^{\text{xc}}(\mathbf{x}_1, \mathbf{x}) \chi_{zz}(\mathbf{x}, \mathbf{x}') f_{zz}^{\text{xc}}(\mathbf{x}', \mathbf{x}_2), \end{aligned} \quad (5)$$

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

$$\chi_{zz}(\mathbf{x}, \mathbf{x}') = \chi^{\text{KS}}(\mathbf{x}, \mathbf{x}') + \iint d\mathbf{x}_1 d\mathbf{x}_2 \chi^{\text{KS}}(\mathbf{x}, \mathbf{x}_1) f_{zz}^{\text{xc}}(\mathbf{x}_1, \mathbf{x}_2) \chi_{zz}(\mathbf{x}_2, \mathbf{x}'), \quad (6)$$

$$f_{zz}^{\text{xc}}(\mathbf{x}, \mathbf{x}') = \frac{\delta^2 E_{\text{xc}}}{\delta m(\mathbf{x}) \delta m(\mathbf{x}')}. \quad (7)$$

Inserting (5) into (??) to (??), we obtain the final form of the self-energy from spin fluctuations

$$\bar{\Sigma}_{ab}^{\text{SF}}(\mathbf{x}_1, \mathbf{x}_2) = 3(-1)^{a+b+1} \Lambda^{\text{SF}}(\mathbf{x}_1, \mathbf{x}_2) \bar{G}_{ab}(\mathbf{x}_1, \mathbf{x}_2), \quad (8)$$

where a, b indicate the Nambu index. The expression (8) 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 [?] in the limit of a homogeneous electron gas and the similar form can be derived from the paramagnon-pole model [?]. The xc kernel defined in (7) can be calculated using the Time-Dependent DFT(TDDFT) [?] within the ALDA.

0.0.1 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 [?, ?]. The noninteracting Kohn-Sham system is mapped to the interacting system by the following self-energy

$$\bar{\Sigma}^{\text{SS}} = \bar{\Sigma}^{\text{GW}} + \bar{\Sigma}^{\text{SF}} + \bar{\Sigma}^{\text{ph}} - \begin{pmatrix} v_{\text{xc}} & \Delta^{\text{xc}} \\ \Delta^{\text{xc}*} & -v_{\text{xc}} \end{pmatrix}. \quad (9)$$

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

$$\rho(\mathbf{r}_1) = \lim_{\mathbf{r}_1 \rightarrow \mathbf{r}_2} \frac{2}{\beta} \sum_{\omega_n} G(\mathbf{r}_1, \mathbf{r}_2, \omega_n), \quad (10)$$

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\beta} \sum_{\omega_n} F(\mathbf{r}_1, \mathbf{r}_2, -\omega_n), \quad (11)$$

then the Sham-Schlüter connection is written as follows:

$$0 = \delta_{ab} \lim_{\mathbf{r}_1 \rightarrow \mathbf{r}_2} \frac{2}{\beta} \sum_{\omega_n} e^{i\omega_n 0^+} [\bar{G}^{\text{KS}} \bar{\Sigma}^{\text{SS}} \bar{G}]_{ab}, \quad (12)$$

$$0 = (1 - \delta_{ab}) \frac{1}{\beta} \sum_{\omega_n} e^{i\omega_n 0^+} [\bar{G}^{\text{KS}} \bar{\Sigma}^{\text{SS}} \bar{G}]_{ab}, \quad (13)$$

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 (12) and (13) can be executed by means of the residue theorem:

$$\frac{1}{\beta} \sum_n^{\infty} A(i\omega_n) = \sum_{\text{Poles} \in \gamma}^{\infty} \text{res}[f_{\beta}(z)A(z), z_m], \quad (14)$$

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 (??):

$$\Delta_k^{\text{xc}} = -\mathcal{Z}_k \Delta_k^{\text{xc}} - \frac{1}{2} \sum_{k'} \mathcal{K}_{kk'} \frac{\tanh[(\beta/2)E_{k'}]}{E_{k'}} \Delta_{k'}^{\text{xc}}, \quad (15)$$

$$\mathcal{Z}_k = \mathcal{Z}_k^{\text{ph}} + \mathcal{Z}_k^{\text{SF}} \quad (16)$$

$$\begin{aligned} \mathcal{Z}^{\text{SF}} = & -\frac{1}{\beta^2} \frac{2}{\tanh[(\beta/2)\xi_k]} \sum_{n,m} \sum_{k'} \frac{1}{i\omega_n + E_k} \frac{1}{i\omega_m + E_{k'}} \left(\frac{1}{i\omega_n + E_k} - \frac{1}{i\omega_n - E_{k'}} \right) \Lambda_{kk'}^{\text{SF}}(\omega_n - \omega_m) \\ & + \frac{2}{\beta^2} \left(\frac{1}{\xi_k} - \frac{(\beta/2)}{\sinh[(\beta/2)\xi_k] \cosh[(\beta/2)\xi_k]} \right) \sum_{nm} \sum_{k'k''} \frac{1}{(i\omega_n + E_{k'})^2} \frac{1}{i\omega_m + E_{k''}} \frac{1}{\sum_{k'} \frac{\beta/2}{\cosh^2[(\beta/2)\xi_k']}} \Lambda_{k'k''}^{\text{SF}}(\omega_n - \omega_m), \end{aligned} \quad (17)$$

$$\mathcal{K}_{kk'} = \mathcal{K}_{kk'}^{\text{ph}} + \mathcal{K}_{kk'}^{\text{el}} + \mathcal{K}_{kk'}^{\text{SF}} \quad (18)$$

$$\mathcal{K}_{kk'}^{\text{SF}} = \lim_{\{\Delta_k\} \rightarrow 0} \frac{1}{\tanh[(\beta/2)E_k]} \frac{1}{\tanh[(\beta/2)E_{k'}]} \frac{1}{\beta^2} \sum_{\omega_n \omega_m} F_k(i\omega_n) F_{k'}(i\omega_m) \Lambda_{kk'}^{\text{SF}}(\omega_n - \omega_m), \quad (19)$$

$$F_k(i\omega_n) = \frac{1}{i\omega_n + E_k} - \frac{1}{i\omega_n - E_k}. \quad (20)$$

In the above equations, $k = \{n, \mathbf{k}\}$ and the kernels labeled ph and el are same as derived in the previous section.