

Superconducting Pairing Correlations and Form of Anomalous Green's Functions

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(2024)

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1 Nambu-Gor'kov Green's functions

Here we derive the Nambu-Gorkov Green's functions and self-consistency equation for the gap equation.

1.1 Anomalous Green's Function

Consider the reduced BdG Hamiltonian kernel in $\Psi = (\mathbf{c}, \mathbf{c}^\dagger)^T$ Nambu space. Here, c_μ is the annihilation operator, in which label μ runs over any internal degrees of freedom (spin, orbital, valley, etc.). The BdG Hamiltonian kernel may be expressed as

$$\mathcal{H}_{\text{BdG}} = \begin{pmatrix} \mathcal{H}_{\text{kin}} & \Delta \\ \Delta^\dagger & -\mathcal{H}_{\text{kin}}^T \end{pmatrix} \quad (1.1)$$

Here, $\mathcal{H}_{\text{kin},a(b)}$ represents the corresponding band Hamiltonians. Note, that we have disregarded the overall factor of $1/2$ in this convention.

Consider Nambu Matsubara Green's functions,

$$\mathcal{G}_{\text{BdG}}(\tau) = -\left\langle \mathcal{T}_\tau \Psi(\tau) \Psi^\dagger(0) \right\rangle = \begin{pmatrix} -\langle \mathcal{T}_\tau c_\mu(\tau) c_\nu^\dagger(0) \rangle & -\langle \mathcal{T}_\tau c_\mu(\tau) c_\nu(0) \rangle \\ -\langle \mathcal{T}_\tau c_\mu^\dagger(\tau) c_\nu^\dagger(0) \rangle & -\langle \mathcal{T}_\tau c_\mu^\dagger(\tau) c_\nu(0) \rangle \end{pmatrix} = \begin{pmatrix} \mathcal{G}_p(\tau) & \mathcal{F}(\tau) \\ \mathcal{F}^\dagger(\tau) & \mathcal{G}_h(\tau) \end{pmatrix}, \quad (1.2)$$

with \mathcal{T}_τ being the imaginary time-ordering operator. \mathcal{G}_p and \mathcal{G}_p are the particle-like and hole-like Matsubara Green's functions, and $\mathcal{F}_{\mu,\nu}(\tau) = -\langle \mathcal{T}_\tau c_\mu(\tau) c_\nu(0) \rangle$ is the anomalous Green's function. The hole-like Matsubara Green's function is related by

$$\begin{aligned}\mathcal{G}_h(\tau) &= -\langle \mathcal{T}_\tau c_\mu^\dagger(\tau) c_\nu(0) \rangle \\ &= +\langle \mathcal{T}_\tau c_\nu(0) c_\mu^\dagger(\tau) \rangle \\ &= +\langle \mathcal{T}_\tau c_\nu(-\tau) c_\mu^\dagger(0) \rangle \\ &= -\mathcal{G}_p^T(-\tau)\end{aligned}\quad (1.3)$$

Hence, we express the Nambu-Gorkov Green's function as

$$\boxed{\mathcal{G}_{\text{BdG}}(\tau) = \begin{pmatrix} \mathcal{G}_p(\tau) & \mathcal{F}(\tau) \\ \mathcal{F}^\dagger(\tau) & -\mathcal{G}_p^T(-\tau) \end{pmatrix}.}\quad (1.4)$$

Time evolution is defined as $\Psi(\tau) \equiv e^{H\tau} \Psi e^{-H\tau}$ in the imaginary-time representation.

We solve in imaginary frequency space using equations of motion. As we are working with the mean-field BdG Hamiltonian which can be regarded as a non-interacting Hamiltonian, the Nambu-Gor'kov Green's function is given by

$$\mathcal{G}^{-1}(\tau) = -\partial_\tau - \mathcal{H}_{\text{BdG}},\quad (1.5)$$

where $i\partial_t = i\partial_{-i\tau} = -\partial_\tau$. Rewriting in terms of imaginary frequency, the inverse Green's function is given by

$$\boxed{\mathcal{G}_{\text{BdG}}^{-1}(i\omega) = i\omega - \mathcal{H}_{\text{BdG}}}\quad (1.6)$$

in which we have used $\mathcal{G}(\tau) = \frac{1}{\beta} \sum_{i\omega} e^{-i\omega_n \tau} \mathcal{G}(i\omega)$. Similarly, we define the Green's functions for the band Hamiltonians to satisfy

$$(i\omega \mathbb{1} - \mathcal{H}_{\text{kin}}) \mathcal{G}_{\text{kin},p}(i\omega) = (i\omega \mathbb{1} - \mathcal{H}_{\text{kin}}) \mathcal{G}_{\text{kin}}(i\omega) = \mathbb{1},\quad (1.7a)$$

$$(i\omega \mathbb{1} - [-\mathcal{H}_{\text{kin}}^T]) (\mathcal{G}_{\text{kin},h}^T(i\omega)) = (i\omega \mathbb{1} + \mathcal{H}_{\text{kin}}^T) (-\mathcal{G}_{\text{kin}}^T(-i\omega)) = \mathbb{1},\quad (1.7b)$$

with $\mathcal{G}_{\text{kin},p}$ denoting the band Green's function for the “particle-like” part, and $\mathcal{G}_{\text{kin},h}$ for the “hole-like part”. In the second line, we have used $(\mathbb{1} - M)^T = (\mathbb{1} - M^T)$ for matrices M and also reexpressed the “hole-like” band Green's function in terms of the “particle-like” band Green's function, $\mathcal{G}_{\text{kin}} \equiv \mathcal{G}_{\text{kin},p}$ (dropping the subscript p).

To find the matrix elements of the Nambu-Gorkov Green's equation, we must find the inverse of $i\omega \mathbb{1} - \mathcal{H}_{\text{BdG}}$. As reviewed in Appendix A, the inverse of the block matrix

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

is given by

$$M^{-1} = \begin{pmatrix} [A - BD^{-1}C]^{-1} & -A^{-1}B[D - CA^{-1}B]^{-1} \\ -[D - CA^{-1}B]^{-1}CA^{-1} & [D - CA^{-1}B]^{-1} \end{pmatrix}.\quad (1.8)$$

Here,

$$M = i\omega - \mathcal{H}_{\text{BdG}} = \begin{pmatrix} i\omega - \mathcal{H}_{\text{kin}} & -\Delta \\ -\Delta^\dagger & i\omega + \mathcal{H}_{\text{kin}}^T \end{pmatrix}\quad (1.9)$$

Correspondingly, the elements of the Nambu Green's function are given by

$$\boxed{\begin{aligned}[\mathcal{G}_{\text{BdG}}(i\omega)]_{1,1} &= \mathcal{G}_p(i\omega) = \left[\mathcal{G}_{\text{kin},p}^{-1}(i\omega) - \Delta \mathcal{G}_{\text{kin},h}(i\omega) \Delta^\dagger \right]^{-1} \\ &= (1 - \mathcal{G}_{\text{kin},p}(i\omega) \Delta \mathcal{G}_{\text{kin},h}(i\omega) \Delta^\dagger)^{-1} \mathcal{G}_{\text{kin},p} \\ &= (1 + \mathcal{G}_{\text{kin}}(i\omega) \Delta \mathcal{G}_{\text{kin}}^T(-i\omega) \Delta^\dagger)^{-1} \mathcal{G}_{\text{kin}}(i\omega)\end{aligned}}\quad (1.10)$$

$$\begin{aligned}
[\mathcal{G}_{\text{BdG}}(i\omega)]_{1,2} &= \mathcal{F}(i\omega) = -\mathcal{G}_{\text{kin},p}(i\omega)(-\Delta) \left[\mathcal{G}_{\text{kin},h}^{-1}(i\omega) - \Delta^\dagger \mathcal{G}_{\text{kin},p}(i\omega) \Delta \right]^{-1} \\
&= \mathcal{G}_{\text{kin},p}(i\omega) \Delta \left[1 - \mathcal{G}_{\text{kin},h}(i\omega) \Delta^\dagger \mathcal{G}_{\text{kin},p}(i\omega) \Delta \right]^{-1} \mathcal{G}_{\text{kin},h}(i\omega) \\
&= -\mathcal{G}_{\text{kin}}(i\omega) \Delta \left[1 + \mathcal{G}_{\text{kin}}^T(-i\omega) \Delta^\dagger \mathcal{G}_{\text{kin}}(i\omega) \Delta \right]^{-1} \mathcal{G}_{\text{kin}}^T(-i\omega) \\
&= -\mathcal{G}_{\text{kin}}(i\omega) \Delta [\mathcal{G}_{\text{BdG}}(i\omega)]_{2,2}
\end{aligned} \tag{1.11}$$

Above, $\mathcal{G}_{\text{kin},p}(i\omega) = (i\omega - \mathcal{H}_{\text{kin}})^{-1} \equiv \mathcal{G}_{\text{kin}}(i\omega) (= A^{-1})$ is the particle-like Green's function in the absence of superconductivity, and similarly for the hole-like $\mathcal{G}_{\text{kin},h}(i\omega) = (i\omega + \mathcal{H}_{\text{kin}}^T)^{-1} = -(-i\omega - \mathcal{H}_{\text{kin}}^T)^{-1} = -\mathcal{G}_{\text{kin}}^T(-i\omega)$.

We typically consider the case where Δ is small, in which the term in brackets is unity to leading order, *i.e.* $[\mathcal{G}_{\text{BdG}}(i\omega)]_{1,1} \approx \mathcal{G}_{\text{kin}}(i\omega)$. This approximation gives rise to the commonly used linearized gap equation. The assumption is justified near T_c , where the magnitude of Δ is small. Higher order corrections would correspond to higher-order terms in the Ginzburg-Landau theory [1].

1.2 Self-consistent gap equation

The interacting Bardeen-Cooper-Schreiffer (BCS) Hamiltonian is given by

$$H_{\text{BCS}} = \sum_{\sigma, \sigma'} c_\sigma^\dagger [\mathcal{H}_{\text{kin}}]_{\sigma, \sigma'} c_{\sigma'} + \frac{1}{2} \sum_{\sigma, \sigma'; \nu, \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} c_\sigma^\dagger c_\nu^\dagger c_{\nu'} c_{\sigma'}, \tag{1.12}$$

in which \mathcal{V} describes the attractive interaction which destabilizes the Fermi surface. Above, the summations over σ, σ' go over all internal degrees of freedom (*e.g.* momentum or position, orbital, valley, *etc.*). In the mean-field approximation ($AB \approx \langle A \rangle B + A \langle B \rangle - \langle A \rangle \langle B \rangle$), the Hamiltonian reduces to

$$\begin{aligned}
H_{\text{BCS}} &= \sum_{\sigma, \sigma'} c_\sigma^\dagger [\mathcal{H}_{\text{kin}}]_{\sigma, \sigma'} c_{\sigma'} \\
&+ \frac{1}{2} \sum_{\sigma, \sigma'; \nu, \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} \langle c_{\nu'} c_{\sigma'} \rangle c_\sigma^\dagger c_\nu^\dagger + \frac{1}{2} \sum_{\sigma, \sigma'; \nu, \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} \langle c_\sigma^\dagger c_\nu^\dagger \rangle c_{\nu'} c_{\sigma'} \\
&- \frac{1}{2} \sum_{\sigma, \sigma'; \nu, \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} \langle c_\sigma^\dagger c_\nu^\dagger \rangle \langle c_{\nu'} c_{\sigma'} \rangle
\end{aligned} \tag{1.13}$$

These averaged terms correspond to the anomalous Green's functions, *i.e.* $\langle c_\nu c_\sigma \rangle = -\langle c_\sigma c_\nu \rangle = [\mathcal{F}(\tau = 0^+)]_{\sigma, \nu}$, consistent with Eq. (1.1). The BCS pairing order parameter is defined by the self-consistent equation,

$$\begin{aligned}
[\Delta]_{\sigma, \nu} &= \sum_{\sigma', \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} \langle c_{\nu'} c_{\sigma'} \rangle = \frac{1}{2} \sum_{\sigma', \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} \left(-\langle c_{\sigma'} c_{\nu'} \rangle \right) \\
&= \sum_{\sigma', \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} [\mathcal{F}(\tau = 0^+)]_{\sigma', \nu'}.
\end{aligned} \tag{1.14}$$

Note, we have taken the $1/2$ factor outside the BdG Hamiltonian, which already doubles the BCS Hamiltonian. To evaluate, one takes the Fourier transform and performs the Matsubara frequency summation

$$[\Delta]_{\sigma, \nu} = \frac{1}{\beta} \sum_{i\omega_n} \sum_{\sigma', \nu'} [\mathcal{V}]_{\sigma, \nu; \sigma', \nu'} e^{-i\omega_n \tau} \Big|_{\tau=0^+} [\mathcal{F}(i\omega_n)]_{\sigma', \nu'} \tag{1.15}$$

Above, $i\omega_n = (2n + 1)\pi/\beta$, $n \in \mathbb{Z}$ is the fermion frequency.

For $T \approx T_c$, it is a good approximation to take Δ to be small. In other words,

$$\mathcal{F}(i\omega) \approx -\mathcal{G}_{\text{kin}}(i\omega) \Delta \mathcal{G}_{\text{kin}}^T(-i\omega), \tag{1.16}$$

which is equivalent to taking $[\mathcal{G}_{\text{BdG}}(i\omega)]_{2,2} \approx \mathcal{G}_{\text{kin}}^T(-i\omega)$. This corresponds to the *linearized gap equation* and can be used, for example, to compare BCS theory to Ginzburg-Landau theory [2, 3].

2 General form of anomalous Green's function for spin-degenerate band Hamiltonian

We now solve for the general form spin-1/2 system considering the mean-field Hamiltonian. In this simplified scenario, we assume that the band Hamiltonians are spin-degenerate. The Green's function of a spin degenerate band Hamiltonian takes the form

$$\mathcal{G}_{\text{kin}}(\mathbf{k}, i\omega) = (i\omega - \xi_{\mathbf{k}}\sigma_0)^{-1} = \frac{1}{i\omega - \xi_{\mathbf{k}}}\sigma_0, \quad (2.1)$$

with $\xi_{\mathbf{k}}$ being the band dispersion and σ_0 being the 2×2 identity matrix. We also assume the dispersion is invariant under parity, $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$. The pairing order parameter can be expressed as

$$\Delta(\mathbf{k}) = (d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma})(i\sigma_y), \quad (2.2)$$

with d_0 denoting the spin-singlet pairing and $\mathbf{d}(\mathbf{k})$ being the d -vector corresponding to spin-triplet pairing.

It follows that the anomalous Green's function simplifies as

$$\begin{aligned} \mathcal{F}(\mathbf{k}, i\omega_n) &= -\mathcal{G}_{\text{kin}}(\mathbf{k}, i\omega)\Delta \left[1 + \mathcal{G}_{\mathbf{k}, \text{kin}}^T(-\mathbf{k}, -i\omega)\Delta^\dagger \mathcal{G}_{\text{kin}}(\mathbf{k}, i\omega)\Delta \right]^{-1} \mathcal{G}_{\text{kin}}^T(-\mathbf{k}, -i\omega) \\ &= -[i\omega - \xi_{\mathbf{k}}]^{-1}\Delta \left[1 + [-i\omega - \xi_{\mathbf{k}}]^{-1}\Delta^\dagger [i\omega - \xi_{\mathbf{k}}]^{-1}\Delta \right]^{-1} [-i\omega - \xi_{\mathbf{k}}]^{-1} \\ &= -\frac{1}{\omega^2 + \xi_{\mathbf{k}}^2}\Delta \left[1 + \frac{\Delta^\dagger\Delta}{\omega^2 + \xi_{\mathbf{k}}^2} \right]^{-1} \\ &= -\frac{1}{\omega^2 + \xi_{\mathbf{k}}^2}\Delta \left[\frac{\omega^2 + \xi_{\mathbf{k}}^2 + \Delta^\dagger\Delta}{\omega^2 + \xi_{\mathbf{k}}^2} \right]^{-1} \\ &= -\Delta \left[\omega^2 + \xi_{\mathbf{k}}^2 + \Delta^\dagger\Delta \right]^{-1} \end{aligned} \quad (2.3)$$

In the case where $\Delta^\dagger\Delta \propto \sigma_0$, *i.e.* a singlet superconductor or a unitary triplet superconductor, the inverse is easily found. Here, we consider the more general case. Recall that the inverse of a general 2×2 matrix is given by

$$[u_0\sigma_0 + \mathbf{u} \cdot \boldsymbol{\sigma}]^{-1} = \frac{u_0\sigma_0 - \mathbf{u} \cdot \boldsymbol{\sigma}}{u_0^2 - \mathbf{u} \cdot \mathbf{u}}. \quad (2.4)$$

for $u_0, u_{i=1,2,3} \in \mathbb{C}$. Here, we have made use of the anticommutativity of the Pauli matrices, $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$. Defining $\alpha \equiv \omega^2 + \xi_{\mathbf{k}}^2$, it follows that (dropping the \mathbf{k} for notation and using implied summation over repeated indices)

$$\begin{aligned} \alpha^2 + \Delta^\dagger\Delta &= \alpha^2\sigma_0 + (-i\sigma_y)(d_0^*\sigma_0 + d_i^*\sigma_i)(d_0\sigma_0 + d_j\sigma_j)(i\sigma_y) \\ &= \alpha^2\sigma_0 + \sigma_y \left[|d_0|^2 + (d_i^*d_0 + d_0^*d_i)\sigma_i + d_i^*d_j \underbrace{\sigma_i\sigma_j}_{\delta_{ij} + i\epsilon_{ijk}\sigma_k} \right] \sigma_y \\ &= \alpha^2\sigma_0 + \sigma_y \left[|d_0|^2 + (d_i^*d_0 + d_0^*d_i)\sigma_i + |\mathbf{d}|^2 + i\epsilon_{ijk}d_i^*d_j\sigma_k \right] \sigma_y \\ &= \alpha^2\sigma_0 + \left[|d_0|^2 + |\mathbf{d}|^2 - (d_i^*d_0 + d_0^*d_i)\sigma_i^* - i\epsilon_{ijk}d_i^*d_j\sigma_k^* \right] \\ &\equiv \beta_0\sigma_0 - \boldsymbol{\beta} \cdot \boldsymbol{\sigma}^* \end{aligned} \quad (2.5)$$

Above, we have used $\sigma_j\sigma_y = -\sigma_y\sigma_j^*$ in the last equality. For shorthand, we have defined

$$\begin{aligned} \beta_0 &= \omega^2 + \xi_{\mathbf{k}}^2 + |d_0|^2 + |\mathbf{d}|^2 = \omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2}\text{Tr}(\Delta^\dagger\Delta) \\ \beta_k &= (d_k^*d_0 + d_0^*d_k) + i\epsilon_{ijk}d_i^*d_j. \end{aligned} \quad (2.6)$$

In calculating β_0 , we have used the fact that

$$\text{Tr}[\Delta^\dagger\Delta] = [\Delta]_{ij}[\Delta^\dagger]_{ji} = \Delta_{ij}\Delta_{ij}^*. \quad (2.7)$$

$$\begin{aligned}
\Rightarrow \text{Tr}(\Delta^\dagger \Delta) &= \text{Tr} \left[\begin{pmatrix} -d_x + id_y & d_0 + d_z \\ -d_0 + d_z & d_x + id_y \end{pmatrix} \begin{pmatrix} \# & \# \\ \# & \# \end{pmatrix}^\dagger \right] \\
&= | -d_x + id_y|^2 + |d_x + id_y|^2 + |d_0 + d_z|^2 + | -d_0 + d_z|^2 \\
&= 2|d_x|^2 + 2|d_y|^2 + 2|d_0|^2 + 2|d_z|^2 \\
&\quad \underbrace{-d_x(-id_y^*)}_{-a} \underbrace{-d_x^*(id_y)}_{-b} \underbrace{+d_x(-id_y^*)}_{+a} \underbrace{+d_x^*(id_y)}_{+b} \underbrace{+d_0(d_z^*)}_{+c} \underbrace{+d_0^*(d_z)}_{+d} \underbrace{-d_0(d_z^*)}_{-c} \underbrace{-d_0^*(d_z)}_{-d} \\
&= 2(|d_x|^2 + |d_y|^2 + |d_0|^2 + |d_z|^2)
\end{aligned} \tag{2.8}$$

The above result is generally true when you can express the pairing matrix as a superposition of the identity matrix and traceless anticommuting matrices (as is the case for the spin-1/2 representation). For example, consider the set of Hermitian matrices M_i . The conditions follow from:

$$\text{Tr}[(m_0^* + m_i^* M_i)(m_0 + m_j M_j)] = \text{Tr} \left[|m_0|^2 + \underbrace{m_i^* m_j (M_i M_j)}_{\text{should be } \propto \delta_{ij}} + \underbrace{(m_i^* m_0 + m_0 m_i)^* M_i}_{\text{should be traceless}} \right] \tag{2.9}$$

Note that the form of the inverse in Eq. (2.4) is still true for the complex conjugated Pauli matrices. It follows that

$$[\omega^2 + \xi_{\mathbf{k}}^2 + \Delta^\dagger \Delta]^{-1} = \frac{1}{\beta_0^2 - \boldsymbol{\beta} \cdot \boldsymbol{\beta}} [\beta_0 \sigma_0 + \boldsymbol{\beta} \cdot \boldsymbol{\sigma}^*]. \tag{2.10}$$

The second term in the denominator simplifies as

$$\begin{aligned}
\boldsymbol{\beta} \cdot \boldsymbol{\beta} &= \beta_k \beta_k \\
&= [(d_k^* d_0 + d_0^* d_k) + i \epsilon_{ijk} d_i^* d_j] [(d_k^* d_0 + d_0^* d_k) + i \epsilon_{lmk} d_l^* d_m] \\
&= (\mathbf{d}^* \cdot \mathbf{d}^*)(d_0^2) + 2|\mathbf{d}|^2 |d_0|^2 + (d_0^*)^2 (\mathbf{d} \cdot \mathbf{d}) - \underbrace{\epsilon_{ijk} \epsilon_{lmk}}_{\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}} d_i^* d_j d_l^* d_m + \underbrace{2i \epsilon_{ijk} d_i^* d_j (d_k^* d_0 + d_0^* d_k)}_{=0, \epsilon_{ijk} = -\epsilon_{ikj}} \\
&= (\mathbf{d}^* \cdot \mathbf{d}^*)(d_0^2) + 2|\mathbf{d}|^2 |d_0|^2 + (d_0^*)^2 (\mathbf{d} \cdot \mathbf{d}) - (|\mathbf{d} \cdot \mathbf{d}|^2 - |\mathbf{d}|^4)
\end{aligned} \tag{2.11}$$

The latter term can also be expressed as $(|\mathbf{d} \cdot \mathbf{d}|^2 - |\mathbf{d}|^4) = -|\mathbf{d} \times \mathbf{d}^*|^2$. In other words,

$$\begin{aligned}
(|\mathbf{d} \cdot \mathbf{d}|^2 - |\mathbf{d}|^4) &= d_i d_i d_j^* d_j^* - d_i d_i^* d_j d_j^* \\
&= d_i d_j^* (d_i d_j^* - d_i^* d_j)
\end{aligned} \tag{2.12}$$

and

$$\begin{aligned}
|\mathbf{d} \times \mathbf{d}^*|^2 &= d_i d_j^* d_l^* d_m \epsilon_{ijk} \epsilon_{lmk} \\
&= d_i d_j^* d_l^* d_m (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) \\
&= d_i d_j^* d_i^* d_j - d_i d_j^* d_j^* d_i \\
&= -(|\mathbf{d} \cdot \mathbf{d}|^2 - |\mathbf{d}|^4)
\end{aligned} \tag{2.13}$$

For the numerator, we are interested in inserting the inverse into Eq. (2.3). The terms of interest are

$$\begin{aligned}
\Delta[\omega^2 + \xi_{\mathbf{k}}^2 + \Delta^\dagger \Delta]^{-1} (\beta_0^2 - \boldsymbol{\beta} \cdot \boldsymbol{\beta}) &= (d_0 \sigma_0 + \mathbf{d} \cdot \boldsymbol{\sigma})(\beta_0 \sigma_0 + \boldsymbol{\beta} \cdot \boldsymbol{\sigma}^*) \\
&= (d_0 \sigma_0 + d_j \sigma_j)(\beta_0 \sigma_0 - \beta_k \sigma_k)(i \sigma_y) \\
&= [d_0 \beta_0 + (d_k \beta_0 - d_0 \beta_k) \sigma_k - d_j \beta_k \sigma_j \sigma_k](i \sigma_y) \\
&= \underbrace{[(d_0 \beta_0 - d_k \beta_k)]}_{\equiv f_0} + \underbrace{[(d_n \beta_0 - d_0 \beta_n) - i \epsilon_{jkn} d_j \beta_k]}_{\equiv f_n} \sigma_n (i \sigma_y), \tag{2.14}
\end{aligned}$$

in which we have defined “effective” singlet and triplet channels, f_0 and \mathbf{f} (note that the units are inverse energy). They simplify as

$$\begin{aligned}
f_0 &= d_0\beta_0 - d_k\beta_k \\
&= d_0 \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] - d_k \left[(d_k^* d_0 + d_0^* d_k) + i\epsilon_{ijk} d_i^* d_j \right] \\
&= d_0 \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] - \left[|\mathbf{d}|^2 d_0 + (\mathbf{d} \cdot \mathbf{d}) d_0^* + i \underbrace{(\mathbf{d}^* \times \mathbf{d}) \cdot \mathbf{d}}_{=0} \right] \\
&= d_0 \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] - \left[|\mathbf{d}|^2 d_0 + (\mathbf{d} \cdot \mathbf{d}) d_0^* \right]
\end{aligned} \tag{2.15}$$

and

$$\begin{aligned}
f_n &= d_n\beta_0 - d_0\beta_n - i\epsilon_{lkn} d_l \beta_k \\
&= d_n \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] - d_0 \left[(d_n^* d_0 + d_0^* d_n) + i\epsilon_{ijn} d_i^* d_j \right] - i\epsilon_{lkn} d_l \left[(d_k^* d_0 + d_0^* d_k) + i\epsilon_{ijk} d_i^* d_j \right] \\
&= d_n [\dots] - d_0 [\dots] - i\epsilon_{lkn} d_l d_k^* d_0 - \underbrace{i\epsilon_{lkn} d_l d_k d_0^*}_{=0} + \epsilon_{nlk} \epsilon_{ijk} d_l d_i^* d_j \\
&= d_n [\dots] - d_0 [\dots] - id_0 (\mathbf{d} \times \mathbf{d}^*)_n + d_l d_i^* d_j (\delta_{ni} \delta_{lj} - \delta_{li} \delta_{nj}) \\
&= d_n [\dots] - d_0 [\dots] + id_0 (\mathbf{d}^* \times \mathbf{d})_n + (\mathbf{d} \cdot \mathbf{d}) d_n^* - |\mathbf{d}|^2 d_n
\end{aligned} \tag{2.16}$$

$$\begin{aligned}
\implies \mathbf{f} &= + \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] \mathbf{d} - d_0^2 \mathbf{d}^* - |\mathbf{d}_0|^2 \mathbf{d} - id_0 (\mathbf{d}^* \times \mathbf{d}) + id_0 (\mathbf{d}^* \times \mathbf{d}) + (\mathbf{d} \cdot \mathbf{d}) \mathbf{d}^* - |\mathbf{d}|^2 \mathbf{d} \\
&= + \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] \mathbf{d} - d_0^2 \mathbf{d}^* - |\mathbf{d}_0|^2 \mathbf{d} + \underbrace{(\mathbf{d} \cdot \mathbf{d}) \mathbf{d}^* + |\mathbf{d}|^2 \mathbf{d}}_{\sim (\mathbf{a} \cdot \mathbf{b}) \mathbf{c} - (\mathbf{a} \cdot \mathbf{c}) \mathbf{b} = -\mathbf{a} \times (\mathbf{b} \times \mathbf{c})} \\
&= + \left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] \mathbf{d} - d_0^2 \mathbf{d}^* - |\mathbf{d}_0|^2 \mathbf{d} - \mathbf{d} \times (\mathbf{d} \times \mathbf{d}^*)
\end{aligned} \tag{2.17}$$

Hence, the anomalous Green’s function has the form

$$\begin{aligned}
\mathcal{F}(\mathbf{k}, i\omega) &= -\Delta[\omega^2 + \xi_{\mathbf{k}}^2 + \Delta^\dagger \Delta]^{-1} \\
&= \frac{-[f_0 + \mathbf{f} \cdot \boldsymbol{\sigma}](i\sigma_y)}{\left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right]^2 - \left[(\mathbf{d}^* \cdot \mathbf{d}^*)^2 (d_0^2) + 2|\mathbf{d}|^2 |d_0|^2 + (d_0^*)^2 (\mathbf{d} \cdot \mathbf{d}) - (|\mathbf{d} \cdot \mathbf{d}|^2 - |\mathbf{d}|^4) \right]} \\
&= \boxed{\frac{-[f_0 + \mathbf{f} \cdot \boldsymbol{\sigma}](i\sigma_y)}{\left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right]^2 - \left[(\mathbf{d}^* \cdot \mathbf{d}^*)^2 (d_0^2) + 2|\mathbf{d}|^2 |d_0|^2 + (d_0^*)^2 (\mathbf{d} \cdot \mathbf{d}) + |\mathbf{d} \times \mathbf{d}^*|^2 \right]}}
\end{aligned} \tag{2.18}$$

For the case of pure singlet pairing, this reduces to

$$\mathcal{F}_{\text{sing}}(\mathbf{k}, i\omega) = -\frac{d_0(i\sigma_y)}{\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta)} = -\frac{d_0(i\sigma_y)}{\omega^2 + E_{\mathbf{k}}^2}. \tag{2.19}$$

For just triplet pairing (unitary or non-unitary), the result simplifies to

$$\begin{aligned}
\mathcal{F}_{\text{trip}}(\mathbf{k}, i\omega) &= \frac{-\left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] \mathbf{d} + \mathbf{d} \times (\mathbf{d} \times \mathbf{d}^*)}{\left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right]^2 + \left(|\mathbf{d} \cdot \mathbf{d}|^2 + |\mathbf{d}|^4 \right)} \cdot \boldsymbol{\sigma}(i\sigma_y) \\
&= -\frac{\left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right] \mathbf{d} + (\mathbf{d} \times \mathbf{d}^*) \times \mathbf{d}}{\left[\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2} \text{Tr}(\Delta^\dagger \Delta) \right]^2 - |\mathbf{d} \times \mathbf{d}^*|^2} \cdot \boldsymbol{\sigma}(i\sigma_y)
\end{aligned} \tag{2.20}$$

in agreement with Ref. 1 up to a sign convention. To note, other references, *e.g.* Eq. (17.15) of Ref. 4, write the anomalous Green's function for non-unitary triplet superconductors as

$$\mathcal{F}_{\text{trip}}(\mathbf{k}, i\omega) = -\frac{(\omega^2 + \xi_{\mathbf{k}}^2 + |\mathbf{d}|^2)\mathbf{d} + (\mathbf{d} \times \mathbf{d}^*) \times \mathbf{d}}{(\omega^2 + E_{\mathbf{k},+}^2)(\omega^2 + E_{\mathbf{k},-}^2)} \cdot \boldsymbol{\sigma}(i\sigma_y), \quad (2.21)$$

with $E_{\mathbf{k},\pm} \equiv \sqrt{\xi_{\mathbf{k}}^2 + (|\mathbf{d}|^2 \pm |\mathbf{d} \times \mathbf{d}^*|)}$. It is quick to show that $(\omega^2 + E_{\mathbf{k},+}^2)(\omega^2 + E_{\mathbf{k},-}^2) = (\omega^2 + \xi_{\mathbf{k}}^2 + |\mathbf{d}|^2)^2 - |\mathbf{d} \times \mathbf{d}^*|^2 = (\omega^2 + \xi_{\mathbf{k}}^2 + \text{Tr}(\Delta^\dagger \Delta)/2)^2 - |\mathbf{d} \times \mathbf{d}^*|^2$, which agrees with the above results.

As a side note, consider the non-unitary pairing with conserved spin $s_z = \pm 1$. The d -vector in this case reads $\mathbf{d} = (-\Delta(\mathbf{k})/2)(\zeta, i, 0)^T$, with $\zeta = \pm$. Then,

$$\mathbf{d} \times \mathbf{d}^* = -\frac{i}{2} |\Delta(\mathbf{k})|^2 (0, 0, \zeta)^T$$

and also

$$\mathbf{d} \times (\mathbf{d} \times \mathbf{d}^*) = -\frac{1}{4} \Delta(\mathbf{k}) |\Delta(\mathbf{k})|^2 (\zeta, +i, 0)^T = \frac{1}{2} |\Delta|^2 \mathbf{d}.$$

It is additionally useful to note that

$$\text{Tr} \left[\begin{pmatrix} \Delta^* & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta & 0 \\ 0 & 0 \end{pmatrix} \right] = \text{Tr} \left[\begin{pmatrix} 0 & 0 \\ 0 & \Delta^* \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \Delta \end{pmatrix} \right] = |\Delta|^2. \quad (2.22)$$

It follows that

$$\begin{aligned} \mathcal{F}_{\text{trip}}^{(\uparrow\uparrow/\downarrow\downarrow)}(\mathbf{k}, i\omega) &= -\frac{(\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2}|\Delta|^2)\mathbf{d} - \frac{1}{2}|\Delta|^2\mathbf{d}}{(\omega^2 + \xi_{\mathbf{k}}^2 + \frac{1}{2}|\Delta|^2)^2 - (\frac{1}{2}|\Delta|^2\mathbf{d})} \cdot \boldsymbol{\sigma}(i\sigma_y) \\ &= -\frac{(\omega^2 + \xi_{\mathbf{k}}^2)\mathbf{d}}{(\omega^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2)(\omega^2 + \xi_{\mathbf{k}}^2)} \cdot \boldsymbol{\sigma}(i\sigma_y) \\ &= -\frac{\mathbf{d}}{(\omega^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2)} \cdot \boldsymbol{\sigma}(i\sigma_y) \end{aligned} \quad (2.23)$$

which is nearly the same as that of the unitary triplet pairing, save for the denominator (which has $\text{Tr}(\Delta^\dagger \Delta)$ as opposed to $\text{Tr}(\Delta^\dagger \Delta)/2$). This can be seen as essentially projecting to the $\uparrow\uparrow$ or $\downarrow\downarrow$ pairing (which reduces the space from two-dimensions to one-dimension). This is discussed more in the following section.

3 Projected Pairing

We now discuss the case in which the pairing is projected to the states at the Fermi level. This is particularly aimed towards describing the monopole superconducting pairing [5, 6].

3.1 Effective pairing channels

We derive the effective monopole pairing order in the weak coupling limit upon projecting to the helical band eigenstates and show the effective pairing channels inherited from the nontrivial spin texture of the Fermi surface. Consider the general Hamiltonian of a monopole superconductor,

$$\mathcal{H}_{\text{BdG}}(\mathbf{k}) = \begin{pmatrix} \mathcal{H}_{\text{kin},1}(\mathbf{k}) & \Delta_{\text{inter}}(\mathbf{k}) \\ \Delta_{\text{inter}}^\dagger(\mathbf{k}) & -\mathcal{H}_{\text{kin},2}^T(-\mathbf{k}) \end{pmatrix}, \quad (3.1)$$

with $\Delta_{\text{inter}}(\mathbf{k})$ describing the inter-Fermi surface pairing between Fermi surfaces FS₁ and FS₂. Here, we treat the inter-Fermi surface pairing potential perturbatively. Suppose that band Hamiltonians $\mathcal{H}_{\text{kin},1}$ and $\mathcal{H}_{\text{kin},2}$ are diagonalized by the unitary transformations $U_1(\mathbf{k})$ and $U_2(\mathbf{k})$ respectively. Without loss of generalization, we define projection to the band eigenstates at the Fermi level by the idempotent matrix $P_+ = \text{diag}(1, 0, 0, \dots)$.

Note: We have chosen to arrange the states according to the energy eigenvalue without loss of generalization. If instead, for example, projecting to some off-diagonal part (*e.g.* intra-Fermi surface pairing in this case, in which e.g. $\Delta^{(b)} \propto \sigma_+$,) then the projection operator would be different for the left and right side, *i.e.*

$$\Delta^{(b)} \equiv P_{1,+}\Delta P_{2,+}. \quad (3.2)$$

The following discussion is nonetheless unchanged.

The effective pairing order written in the band-diagonal representation is given by

$$\Delta_{\text{MSC}}^{(b)}(\mathbf{k}) = P_+ U_1^\dagger(\mathbf{k}) \Delta_{\text{inter}}(\mathbf{k}) U_2^*(-\mathbf{k}) P_+. \quad (3.3)$$

Upon transforming the projected effective pairing back to the original basis, the effective pairing order reads

$$\Delta_{\text{MSC}}(\mathbf{k}) = U_1(\mathbf{k}) \Delta_{\text{MSC}}^{(b)}(\mathbf{k}) U_2^T(-\mathbf{k}) \equiv \tilde{P}_1(\mathbf{k}) \Delta_{\text{inter}}(\mathbf{k}) \tilde{P}_2^T(-\mathbf{k}). \quad (3.4)$$

Here, $\tilde{P}_{i=1,2}(\mathbf{k}) \equiv U_i(\mathbf{k}) P_+ U_i^\dagger(\mathbf{k})$ describes the momentum-dependent projection operator. For example, consider a spin- $\frac{1}{2}$ basis and suppose that band eigenstates at the Fermi surface FS_{i=1,2} are given by $|\chi_{i,+}(\mathbf{k})\rangle = (u_i(\mathbf{k}), v_i(\mathbf{k}))^\text{T}$. It follows that the projection operator is

$$\tilde{P}_{i=1,2}(\mathbf{k}) = \begin{pmatrix} |u_i(\mathbf{k})|^2 & u_i(\mathbf{k})v_i^*(\mathbf{k}) \\ u_i^*(\mathbf{k})v_i(\mathbf{k}) & |v_i(\mathbf{k})|^2 \end{pmatrix}. \quad (3.5)$$

When the Fermi surface has nontrivial spin textures, for example when both $u_i(\mathbf{k})$ and $v_i(\mathbf{k})$ have momentum dependence, this can lead to superconducting pairing in new spin channels which differ from that of the original inter-Fermi surface pairing.

As an example, we show the effective spin-triplet pairing channels in the $\Delta_{\text{MSC}}^{(q_p=-1, l_z=0)}$ monopole superconducting order. To recap, we consider a system with Fermi surfaces FS₁ and FS₂, surrounding Weyl nodes $+\mathbf{K}_0$ and $-\mathbf{K}_0$ respectively, which are related by parity, $\mathcal{H}_{\text{kin},1}(\mathbf{k}) = \sigma_z \mathcal{H}_{\text{kin},2}(-\mathbf{k}) \sigma_z$. The respective unitary transformations which diagonalize the band Hamiltonians are given by

$$U_1(\mathbf{k}) = \sqrt{2\pi} \begin{pmatrix} \mathcal{Y}_{+\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) & \mathcal{Y}_{-\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \\ -\mathcal{Y}_{+\frac{1}{2}; \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) & -\mathcal{Y}_{-\frac{1}{2}; \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \end{pmatrix} \quad (3.6a)$$

$$U_2(-\mathbf{k}) = \sqrt{2\pi} \begin{pmatrix} \mathcal{Y}_{+\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) & \mathcal{Y}_{-\frac{1}{2}; \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \\ \mathcal{Y}_{+\frac{1}{2}; \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) & \mathcal{Y}_{-\frac{1}{2}; \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \end{pmatrix} \quad (3.6b)$$

in which $\Omega_{\tilde{\mathbf{k}}}$ is the spherical coordinate, with $\tilde{\mathbf{k}} = \mathbf{k} - \mathbf{K}_0$. When inter-Fermi surface s -wave pairing is introduced, $\Delta_{\text{inter}}(\mathbf{k}) = \Delta_0 i\sigma_y$, it follows that the effective pairing order (in the spin-1/2 basis) becomes

$$\begin{aligned} & \Delta_{\text{MSC}}(\mathbf{k}) \\ &= 8\pi^2 \Delta_0 \begin{pmatrix} -|\mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}})|^2 \mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \mathcal{Y}_{-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) & |\mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}})|^2 \\ -|\mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}})|^2 & -|\mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}})|^2 \mathcal{Y}_{+\frac{1}{2}, \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \mathcal{Y}_{-\frac{1}{2}, \frac{1}{2}, +\frac{1}{2}}(\Omega_{\tilde{\mathbf{k}}}) \end{pmatrix} \\ &= \Delta_0 \begin{pmatrix} -\cos^2 \frac{\theta_{\tilde{\mathbf{k}}}}{2} \sin \theta_{\tilde{\mathbf{k}}} e^{-i\varphi_{\tilde{\mathbf{k}}}} & \frac{1}{2} \sin^2 \theta_{\tilde{\mathbf{k}}} \\ -\frac{1}{2} \sin^2 \theta_{\tilde{\mathbf{k}}} & -\sin^2 \frac{\theta_{\tilde{\mathbf{k}}}}{2} \sin \theta_{\tilde{\mathbf{k}}} e^{+i\varphi_{\tilde{\mathbf{k}}}} \end{pmatrix}. \end{aligned} \quad (3.7)$$

Here, due to the nontrivial spin texture from the Weyl spin-orbit coupling in the band Hamiltonians, there are contributions from the $s_z = \pm 1$ spin-triplet channels. Specifically, there is a local $(p_x + ip_y)|\downarrow\downarrow\rangle$ and $(p_x - ip_y)|\uparrow\uparrow\rangle$ pairing for which the effective magnitude varies over the Fermi surface. Near the north pole, the $(p_x - ip_y)|\downarrow\downarrow\rangle$ pairing is more heavily weighted while the $(p_x - ip_y)|\downarrow\downarrow\rangle$ is suppressed, while the opposite holds near the south pole. The spin-singlet channel survives but likewise has momentum-dependence from the Weyl spin-orbit interaction in the band Hamiltonian. Moreover, the total angular momentum $j_z = l_z + s_z = 0$ is conserved. This description is consistent with the effective pairing in the helical band basis, $\Delta_{\text{MSC}}^{(q_p=-1, l_z=0)}$, which globally transforms according to conserved angular momentum $l_{z,\text{glob}} = 0$ but locally has features of a chiral p -wave superconductor, with $l_{z,\text{loc}} = \pm 1$, which arise from the induced spin-triplet channels.

3.2 Anomalous Green's function in projected basis

We consider the case that the band Hamiltonian has spin dependence. In this case, we first write down the anomalous Green's function in a band-diagonal representation via a unitary transformation. In this representation, the transformed anomalous Green's functions take an analogous form,

$$\begin{aligned} \mathcal{F}_{\alpha}^{(b)}(\mathbf{k}, ip_n) &= U_{\alpha}^{-1}(\mathbf{k}) \mathcal{F}_{\alpha}(\mathbf{k}, ip_n) [U_{\alpha}^{-1}]^T(-\mathbf{k}) \\ &= -\mathcal{G}_{\text{kin}, \alpha}^{(b)}(\mathbf{k}, ip_n) \Delta_{\alpha}^{(b)}(\mathbf{k}) e^{i\phi_{\alpha}} \left[1 + \mathcal{G}_{\text{kin}, \alpha}^{(b)\text{T}}(-\mathbf{k}, -ip_n) \Delta_{\alpha}^{(b)\dagger}(\mathbf{k}) \mathcal{G}_{\text{kin}, \alpha}^{(b)}(\mathbf{k}, ip_n) \Delta_{\alpha}^{(b)}(\mathbf{k}) \right]^{-1} \mathcal{G}_{\text{kin}, \alpha}^{(b)\text{T}}(-\mathbf{k}, -ip_n). \end{aligned} \quad (3.8)$$

Here, the unitary transformation diagonalizes the kinetic Hamiltonian, $H(\mathbf{k}) \rightarrow U^{-1}(\mathbf{k}) H(\mathbf{k}) U(\mathbf{k}) = H^{(b)}(\mathbf{k}) = \Lambda_1(\mathbf{k})$. Similarly, $i\omega - H(\mathbf{k}) \rightarrow U^{-1}(\mathbf{k})(i\omega - H(\mathbf{k}))U(\mathbf{k}) = i\omega - \Lambda_1(\mathbf{k})$ and $(i\omega - H(\mathbf{k}))^{-1} \rightarrow U^{-1}(\mathbf{k})(i\omega - H(\mathbf{k}))^{-1}U(\mathbf{k}) = (i\omega - \Lambda_1(\mathbf{k}))^{-1}$. Hence, $\mathcal{G}_{\text{kin}, \alpha}^{(b)}(\mathbf{k}, ip_n) = U_{\alpha}^{-1}(\mathbf{k}) \mathcal{G}_{\alpha}(\mathbf{k}, ip_n) U_{\alpha}(\mathbf{k}) = (ip_n - \Lambda_1(\mathbf{k}))^{-1}$ is the Green's function for the band Hamiltonian $H_{\text{kin}, 1}(\mathbf{k})$ evaluated in the band-diagonal representation.

Next, we project the anomalous Green's function to the Fermi surface of interest. As pairing only occurs between states near the Fermi surface(s) in the weak coupling regime, the band projected anomalous Green's function, $\mathcal{F}_{\alpha}^{(bp)}(\mathbf{k}, ip_n)$, is a good approximation of the one in band-diagonal rep and includes key physics ingredients pertinent to the pairing we are considering.

$$\begin{aligned} \mathcal{F}_{\alpha}^{(bp)}(\mathbf{k}, ip_n) &= -\mathcal{G}_{\text{kin}, \alpha}^{(bp)}(\mathbf{k}, ip_n) \Delta_{\alpha}^{(bp)}(\mathbf{k}) e^{i\phi_{\alpha}} \left[1 + \mathcal{G}_{\text{kin}, \alpha}^{(bp)\text{T}}(-\mathbf{k}, -ip_n) \Delta_{\alpha}^{(bp)\dagger}(\mathbf{k}) \mathcal{G}_{\text{kin}, \alpha}^{(bp)}(\mathbf{k}, ip_n) \Delta_{\alpha}^{(bp)}(\mathbf{k}) \right]^{-1} \mathcal{G}_{\text{kin}, \alpha}^{(bp)\text{T}}(-\mathbf{k}, -ip_n) \\ &= -\frac{e^{i\phi_{\alpha}} \Delta_{\alpha}^{(b)}(\mathbf{k})}{p_n^2 + E_{\alpha, \mathbf{k}}^2}. \end{aligned} \quad (3.9)$$

Here, $\mathcal{G}_{\text{kin}, \alpha}^{(b)}(\mathbf{k}, ip_n) = P_+(ip_n - \Lambda_1(\mathbf{k}))^{-1}P_+$ is the Green's function for the band Hamiltonian $H_{\text{kin}, 1}(\mathbf{k})$ evaluated in the band-diagonal representation and projected to FS_1 corresponding to its first band of $H_{\text{kin}, 1}(\mathbf{k})$. Here, $P_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ is the projection operator and $\Lambda_1(\mathbf{k}) = \text{diag}(\lambda_{1;1}(\mathbf{k}), \lambda_{1;2}(\mathbf{k}))$ which is the diagonal matrix of the two eigenvalues of $H_{\text{kin}, 1}(\mathbf{k})$. $\Delta_{\alpha}^{(bp)}(\mathbf{k}) = \begin{pmatrix} \Delta_{\text{proj}}(\mathbf{k}) & 0 \\ 0 & 0 \end{pmatrix}$ is the effective pairing matrix in the projected band basis, as introduced in Sec. 3.1, and $\xi_{\alpha, \mathbf{k}}$ is the band dispersion of the eigenstate at the Fermi level.

We show the above form of the anomalous Green's function explicitly below (dropping \mathbf{k} and α and absorbing the U(1) phase for convenience of notation):

$$\begin{aligned}\mathcal{F}^{(b)}(i\omega) &\approx \mathcal{F}^{(bp)}(i\omega) \\ &= -\mathcal{G}_{\text{kin},1}^{(bp)}(\mathbf{k}, i\omega)\Delta^{(bp)}\left[1 + \mathcal{G}_{\text{kin},2}^{(bp)\text{T}}(-\mathbf{k}, -i\omega)\Delta^{(bp)\dagger}\mathcal{G}_{\text{kin},1}^{(bp)}(\mathbf{k}, i\omega)\Delta^{(bp)}\right]^{-1}\mathcal{G}_{\text{kin},2}^{(bp)\text{T}}(-\mathbf{k}, -i\omega) \\ &= -\begin{pmatrix} \frac{1}{i\omega - \lambda_{1;1}(\mathbf{k})} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta_{\text{proj}}(\mathbf{k}) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 + \frac{|\Delta_{\text{proj}}|^2}{(i\omega - \lambda_{1;1}(\mathbf{k}))(-i\omega - \lambda_{2;1}(-\mathbf{k}))} & 0 \\ 0 & 1 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{-i\omega - \lambda_{2;1}(-\mathbf{k})} & 0 \\ 0 & 0 \end{pmatrix}\end{aligned}\quad (3.10)$$

Now, suppose that $\lambda_{1;1}(\mathbf{k}) = \lambda_{2;1}(-\mathbf{k}) = \xi_{\mathbf{k}}$. This may be achieved, for example, when the two Fermi surfaces are related by parity.

$$\begin{aligned}&= -\begin{pmatrix} \frac{1}{i\omega - \xi_{\mathbf{k}}} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta_{\text{proj}}(\mathbf{k}) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 + \frac{|\Delta_{\text{proj}}|^2}{\omega^2 + \xi_{\mathbf{k}}^2} & 0 \\ 0 & 1 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{-i\omega - \xi_{\mathbf{k}}} & 0 \\ 0 & 0 \end{pmatrix} \\ &= -\begin{pmatrix} \frac{1}{i\omega - \xi_{\mathbf{k}}} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta_{\text{proj}}(\mathbf{k}) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{\omega^2 + \xi_{\mathbf{k}}^2}{\omega^2 + \xi_{\mathbf{k}}^2 + |\Delta_{\text{proj}}|^2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{-i\omega - \xi_{\mathbf{k}}} & 0 \\ 0 & 0 \end{pmatrix} \\ &= -\begin{pmatrix} \frac{\Delta_{\text{proj}}}{\omega^2 + \xi_{\mathbf{k}}^2 + |\Delta_{\text{proj}}|^2} & 0 \\ 0 & 0 \end{pmatrix} \\ &= -\frac{\Delta^{(bp)}}{\omega^2 + E_{\mathbf{k}}^2}\end{aligned}\quad (3.11)$$

in which $|\Delta_{\text{proj}}|^2 \equiv \text{Tr}[\Delta^{(bp)\dagger}\Delta^{(bp)}]$, which does not have the factor of 1/2 (because we are effectively projecting to a 1D representation).

Note: Here, we briefly cover the Green's function in a band-diagonal basis. Without loss of generalization, consider a 2×2 Hamiltonian kernel. The projected Green's function in the band-diagonal basis may generally be expressed as

$$\begin{aligned}\mathcal{G}_{\text{kin}}^{(b)}(ip_n) &= P_+(ip_n - \alpha\sigma_0 - \beta\sigma_z)^{-1}P_+ \\ &= P_+\frac{(ip_n - \alpha)\sigma_0 + \beta\sigma_z}{(ip_n - \alpha)^2 - \beta^2}P_+ \\ &= \frac{1}{(ip_n - \alpha)^2 - \beta^2} \begin{pmatrix} (ip_n - \alpha) + \beta & 0 \\ 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} [ip_n - \alpha - \beta]^{-1} & 0 \\ 0 & 0 \end{pmatrix} \\ &\simeq \begin{pmatrix} [ip_n - [\Lambda]_{1,1}]^{-1} & 0 \\ 0 & 0 \end{pmatrix}\end{aligned}\quad (3.12)$$

This is generally true, as $P_+ = \text{diag}(1, 0, 0, \dots)$ commutes with any diagonal matrix.

A Refresher: Inverse of block matrix and Schur complement

We present a quick math refresher to find the inverse of a square matrix. Consider the matrix

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad (\text{A.1})$$

where A , B , C , and D are matrices. We compute the inverse by Gauss-Jordan elimination

$$\begin{aligned} M &= \mathbb{1}M \\ \begin{pmatrix} A & B \\ C & D \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} M \\ \begin{pmatrix} 1 & A^{-1}B \\ C & D \end{pmatrix} &= \begin{pmatrix} A^{-1} & 0 \\ 0 & 1 \end{pmatrix} M \\ \begin{pmatrix} 1 & A^{-1}B \\ 0 & D - CA^{-1}B \end{pmatrix} &= \begin{pmatrix} A^{-1} & 0 \\ -CA^{-1} & 1 \end{pmatrix} M \\ \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix} &= \begin{pmatrix} A^{-1} & 0 \\ -[D - CA^{-1}B]^{-1}CA^{-1} & [D - CA^{-1}B]^{-1} \end{pmatrix} M \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} &= \begin{pmatrix} A^{-1} + A^{-1}B[D - CA^{-1}B]^{-1}CA^{-1} & -A^{-1}B[D - CA^{-1}B]^{-1} \\ -[D - CA^{-1}B]^{-1}CA^{-1} & [D - CA^{-1}B]^{-1} \end{pmatrix} M \end{aligned} \quad (\text{A.2})$$

If one were to instead start with the bottom row, then the top left matrix element would read $M_{11}^{-1} = [A - BD^{-1}C]^{-1}$. We show this equality below:

$$\begin{aligned} M_{11}^{-1} &= A^{-1} + A^{-1}B[D - CA^{-1}B]^{-1}CA^{-1} \\ &= A^{-1}(1 + B[D - CA^{-1}B]^{-1}CA^{-1}) \\ &= A^{-1}\left(1 + B\left\{D[1 - D^{-1}CA^{-1}B]\right\}^{-1}CA^{-1}\right) \\ &= A^{-1}\left(1 + B\left[1 - \underbrace{D^{-1}CA^{-1}B}_{\equiv \Delta}\right]^{-1}D^{-1}CA^{-1}\right) \\ &= A^{-1}\left(1 + B\left[1 + \Delta + \Delta^2 + \Delta^3 + \dots\right]D^{-1}CA^{-1}\right) \\ &= A^{-1}\left(1 + \underbrace{BD^{-1}CA^{-1}}_{\equiv \Delta'} - BD^{-1}CA^{-1}BD^{-1}CA^{-1} + \dots\right) \\ &= A^{-1}\left(1 + \Delta' + \Delta'^2 + \Delta'^3 + \dots\right) = A^{-1}(1 - \Delta')^{-1} \\ &= A^{-1}\left(1 - BD^{-1}CA^{-1}\right)^{-1} \\ &= \left[\left(1 - BD^{-1}CA^{-1}\right)A\right]^{-1} \\ &= \left(A - BD^{-1}C\right)^{-1}. \end{aligned} \quad (\text{A.3})$$

This element is defined as the [Schur complement](#) of D .

B Equation of motion theory

Here, we give a brief recap of the equation of motion theory to find the Green's function. Recall that for the time derivative of the time-evolved operator A is

$$\partial_\tau A(\tau) = \partial_\tau (e^{\tau H} A e^{-\tau H}) = e^{\tau H} [H, A] e^{-\tau H} \equiv [H, A](\tau). \quad (\text{B.1})$$

Consider the correlation function

$$\begin{aligned} C_{AB} &= -\langle \mathcal{T}_\tau A(\tau)B(0) \rangle \\ &= -\Theta(\tau)\langle A(\tau)B(0) \rangle - \chi\Theta(-\tau)\langle B(0)A(\tau) \rangle \end{aligned} \quad (\text{B.2})$$

in which $\chi = +$ for bosonic operators and $\chi = -$ for fermionic. The above is a thermal average, $\langle \cdots \rangle = \frac{1}{Z} \text{Tr}(e^{-\beta H} \cdots)$ in which $Z = e^{-\beta H}$. Then, the time derivative is given by

$$-\partial_\tau C_{AB}(\tau) = \partial_\tau \langle \mathcal{T}_\tau A(\tau)B(0) \rangle = 0 + \left\langle \partial_\tau (\mathcal{T}_\tau A(\tau)B(0)) \right\rangle \quad (\text{B.3})$$

$$\begin{aligned} &= \partial_\tau[\Theta(\tau)]\langle A(\tau)B(0) \rangle + \chi\partial_\tau[\Theta(\tau)]\langle B(0)A(\tau) \rangle \\ &\quad + \Theta(\tau)\left\langle \partial_\tau A(\tau)B(0) \right\rangle + \chi\Theta(-\tau)\left\langle B(0)\partial_\tau A(\tau) \right\rangle \\ &= \boxed{\delta(\tau)\left\langle A(0)B(0) - \chi B(0)A(0) \right\rangle + \left\langle \mathcal{T}_\tau[H, A](\tau)B(0) \right\rangle} \quad (\text{B.4}) \end{aligned}$$

It is useful to have the commutation for the non-interacting Hamiltonians, which may be expressed as

$$H = \sum_{\nu, \nu'} \mathcal{H}_{\nu, \nu'} c_\nu^\dagger c_{\nu'}. \quad (\text{B.5})$$

In this case,

$$\begin{aligned} [H, c_\sigma] &= \sum_{\nu, \nu'} \mathcal{H}_{\nu, \nu'} [c_\nu^\dagger c_{\nu'}, c_\sigma] \\ &= \sum_{\nu, \nu'} \mathcal{H}_{\nu, \nu'} \left(c_\nu^\dagger [c_{\nu'}, c_\sigma] + [c_\nu^\dagger, c_\sigma] c_{\nu'} \right) \\ &= \sum_{\nu, \nu'} \mathcal{H}_{\nu, \nu'} \left((1 - \chi)c_\nu^\dagger c_{\nu'} c_\sigma + (1 - \chi)c_\nu^\dagger c_\sigma c_{\nu'} - \delta_{\sigma, \nu} c_{\nu'} \right) \\ &= \sum_{\nu, \nu'} \mathcal{H}_{\nu, \nu'} \left((1 - \chi)c_\nu^\dagger c_{\nu'} c_\sigma + \underbrace{\chi(1 - \chi)}_{=\chi-1} c_\nu^\dagger c_{\nu'} c_\sigma - \delta_{\sigma, \nu} c_{\nu'} \right) \\ &\implies [H, c_\sigma] = - \sum_{\nu'} \mathcal{H}_{\sigma, \nu'} c_{\nu'} \end{aligned} \quad (\text{B.6})$$

Above, we have used the following relations:

$$\begin{aligned} [c_\nu^\dagger, c_\sigma] &= c_\nu^\dagger c_\sigma - c_\sigma c_{\nu'}^\dagger \\ &= c_\nu^\dagger c_\sigma - \left(\chi c_{\nu'}^\dagger c_\sigma + \delta_{\sigma, \nu} \right) \\ &= (1 - \chi)c_\nu^\dagger c_\sigma - \delta_{\sigma, \nu} \end{aligned} \quad (\text{B.7})$$

$$\begin{aligned} [c_\nu, c_\sigma] &= c_\nu c_\sigma - c_\sigma c_\nu \\ &= c_\nu c_\sigma - \chi c_\nu c_\sigma \\ &= (1 - \chi)c_\nu c_\sigma \end{aligned} \quad (\text{B.8})$$

$$\begin{aligned} [AB, C] &= ABC - ACB + ACB - CAB \\ &= A[B, C] + [A, C]B \end{aligned} \quad (\text{B.9})$$

Note in the above we have used discrete values, but it can easily be generalized to the continuum case.

The equation of motion for the Green's function $G_{\sigma,\sigma'}(\tau) = -\langle \mathcal{T}_\tau c_\sigma(\tau) c_{\sigma'}^\dagger(0) \rangle$ may be expressed as

$$\begin{aligned} -\partial_\tau G_{\sigma,\sigma'}(\tau) &= \delta(\tau) \langle c_\sigma(0) c_{\sigma'}^\dagger(0) - \chi c_{\sigma'}^\dagger(0) c_\sigma(0) \rangle + \langle \mathcal{T}_\tau [H, c_\sigma](\tau) c_{\sigma'}^\dagger(0) \rangle \\ &= \delta(\tau) \left\langle \chi c_{\sigma'}^\dagger(0) c_\sigma(0) + \delta_{\sigma,\sigma'} - \chi c_{\sigma'}^\dagger(0) c_\sigma(0) \right\rangle + \langle \mathcal{T}_\tau [H, c_\sigma](\tau) c_{\sigma'}^\dagger(0) \rangle \\ &= \delta(\tau) \delta_{\sigma,\sigma'} + \left\langle \mathcal{T}_\tau e^{\tau H} \left(- \sum_{\nu'} \mathcal{H}_{\sigma,\nu'} c_{\nu'} \right) e^{-\tau H} c_{\sigma'}^\dagger(0) \right\rangle \\ &= \delta(\tau) \delta_{\sigma,\sigma'} - \sum_{\nu} \mathcal{H}_{\sigma,\nu} \left\langle \mathcal{T}_\tau c_\nu(\tau) c_{\sigma'}^\dagger(0) \right\rangle \end{aligned} \quad (\text{B.10})$$

$\implies -\partial_\tau G_{\sigma,\sigma'}(\tau) = \delta(\tau) \delta_{\sigma,\sigma'} + \sum_{\nu} \mathcal{H}_{\sigma,\nu} G_{\nu,\sigma'}(\tau)$

(B.11)

Again, we reiterate that σ, σ', ν sum over all degrees of freedom of the system (position, orbital, spin, particle-hole, etc.). If one expresses in matrix form, with $\mathcal{G}^{-1}\mathcal{G} = \mathbb{1}$, then

$\mathcal{G}_0^{-1} = -\partial_\tau - H$

(B.12)

The Green's function is solved and should satisfy the periodic boundary conditions, $\mathcal{G} = \chi \mathcal{G}(\tau + \beta)$. To see this periodic boundary condition, consider (first for the case $\tau < 0$ and $\tau < \beta$)

$$\begin{aligned} C_{AB}(\tau + \beta) &= -\langle \mathcal{T}_\tau A(\tau + \beta) B(0) \rangle \\ &= -\frac{1}{Z} \text{Tr} \left[e^{-\beta H} e^{(\tau+\beta)H} A e^{-(\tau+\beta)H} B(0) \right] \\ &= -\frac{1}{Z} \text{Tr} \left[e^{\tau H} A e^{-\tau H} e^{-\beta H} B(0) \right] \\ &= -\frac{1}{Z} \text{Tr} \left[e^{-\beta H} B(0) e^{\tau H} A e^{-\tau H} \right] \\ &= -\frac{1}{Z} \text{Tr} \left[e^{-\beta H} B(0) A(\tau) \right] \\ &= -\chi \frac{1}{Z} \text{Tr} \left[e^{-\beta H} \mathcal{T}_\tau (A(\tau) B(0)) \right] \\ &= \chi C_{AB}(\tau + \beta) \end{aligned} \quad (\text{B.13})$$

in which $Z = \exp(-\beta H)$.

For an interacting system, one employs Wick's theorem to reduce the n -particle correlation functions to many 2-body correlation functions. The theorem may be proved using the equation of motion theory.

Often, one works in the imaginary frequency space, which is defined by the Fourier transforms:

$$\mathcal{G}(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \mathcal{G}(\tau) \quad (\text{B.14a})$$

$$\mathcal{G}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} \mathcal{G}(i\omega_n) \quad (\text{B.14b})$$

given that the Green's function is defined on the interval $0 < \tau < \beta$, over which it is periodic. Above,

$$i\omega_n = \begin{cases} \frac{2\pi n}{\beta} & (\text{bosons}) \\ \frac{\pi(2n+1)}{\beta} & (\text{fermions}) \end{cases} \quad (\text{B.15})$$

for integers n . Substituting the Fourier transform into $\mathcal{G}^{-1}(\tau)$, one recovers

$$\mathcal{G}^{-1} = i\omega_n - \mathcal{H} \quad (\text{B.16})$$

as expected.

C Matsubara frequency summation

We provide a brief recap of the Matsubara frequency summation. Generally, after Fourier transforming from the τ -domain to imaginary frequency, one ends up with a function of the form $\frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n)$, where the summation is over Matsubara frequencies.

Here, we employ the Cauchy residue theorem, in which

$$\frac{1}{2\pi i} \oint_S dz f(z) = \sum_{z_n} \text{Res}[f(z_n)], \quad (\text{C.1})$$

in which the summation is over the poles in the complex plane. In this case, it is convenient to express $f(z)$ as the product of two functions $f(z) = g(z)n(z)$ in which $n(z)$ has poles at the Matsubara frequencies with residue $\pm\beta$. In that case,

$$\begin{aligned} \frac{1}{2\pi i} \oint dz f(z) &= \sum_{z'_n} \text{Res}[g(z'_n)] n(z'_n) + \sum_{i\omega_n} \text{Res}[n(i\omega_n)] g(i\omega_n) \\ &= \sum_{z'_n} \text{Res}[g(z'_n)] n(z'_n) \pm \frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) \end{aligned} \quad (\text{C.2})$$

in which we have split the summation between the poles of $g(z)$ and the poles of $n(z)$ corresponding to the Matsubara frequencies.

It is apparent that the Fermi-Dirac and Bose-Einstein distributions satisfy the requirements. Recall that $i\omega_n = 2\pi n/\beta$ and $\pi(n+1)/\beta$ for bosons and fermions respectively. Near a pole $z_n = \delta z + i\omega_n$, $n(z)$ may be expressed as

$$\begin{aligned} n_\chi(\delta z + i\omega_n) &= \frac{1}{e^{\beta(i\omega_n + \delta z)} - \chi} \\ &= \frac{1}{\chi(1 + \beta\delta z + \dots) - \chi} \\ &= \frac{1}{\chi\beta\delta z} \end{aligned} \quad (\text{C.3})$$

in which $\chi = +1$ refers to the boson case and $\chi = -1$ the fermion case. As such,

$$\text{Res}[n_\chi(i\omega_n)] = \chi \frac{1}{\beta} \quad (\text{C.4})$$

Therefore, one may reexpress the sum as

$$\frac{1}{\beta} \sum_{i\omega_n} g(i\omega_n) = -\chi \frac{1}{2\pi i} \underbrace{\oint dz f(z)}_{\rightarrow 0} - \chi \sum_{z_n} \text{Res}[g(z_n)] n_\chi(z_n) \quad (\text{C.5})$$

in which the integral vanishes as the contour is taken to infinity (which is true if $f(z)$ decays faster than $1/z$).

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