Electronic Spin Susceptibility Enhancement in Pauli Limited Unconventional Superconductors

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HAMILTONIAN

The matrix representation($\mathcal{H} = \bar{\Psi}\hat{\mathcal{H}}\Psi$) of the Hamiltonian of interest is:

$$\hat{\mathcal{H}} = \begin{pmatrix} \xi_{\mathbf{k}-}\boldsymbol{\sigma}^0 - e_z\boldsymbol{\sigma}^z & \Delta_{\mathbf{k}-}(i\boldsymbol{\sigma}^y) & m^*_{\mathbf{q}}(\boldsymbol{\sigma}^m)^\dagger & 0 \\ -\Delta^*_{\mathbf{k}-}(i\boldsymbol{\sigma}^y) & -(\xi_{-\mathbf{k}-}\boldsymbol{\sigma}^0 - e_z\boldsymbol{\sigma}^z) & 0 & -m^*_{\mathbf{q}}\big((\boldsymbol{\sigma}^m)^T\big)^\dagger \\ m_{\mathbf{q}}\boldsymbol{\sigma}^m & 0 & \xi_{\mathbf{k}+}\boldsymbol{\sigma}^0 - e_z\boldsymbol{\sigma}^z & \Delta_{\mathbf{k}+}(i\boldsymbol{\sigma}^y) \\ 0 & -m_{\mathbf{q}}(\boldsymbol{\sigma}^m)^T & -\Delta^*_{\mathbf{k}+}(i\boldsymbol{\sigma}^y) & -(\xi_{-\mathbf{k}+}\boldsymbol{\sigma}^0 - e_z\boldsymbol{\sigma}^z) \end{pmatrix} \tag{1}$$

$$\Psi^\dagger = \left[\; c^\dagger_{\mathbf{k}-\uparrow},\; c^\dagger_{\mathbf{k}-\downarrow},\; c_{-\mathbf{k}-\uparrow},\; c_{-\mathbf{k}-\downarrow},\; c^\dagger_{\mathbf{k}+\uparrow},\; c^\dagger_{\mathbf{k}+\downarrow},\; c_{-\mathbf{k}+\uparrow},\; c_{-\mathbf{k}+\downarrow} \;\right] \tag{2}$$

Where $\mathbf{k}\pm = \mathbf{k} \pm \mathbf{q}/2$, and $\boldsymbol{\sigma}^i$ are the pauli spin matricies with $\boldsymbol{\sigma}^0 = \mathcal{I}$ and $\boldsymbol{\sigma}^m = \boldsymbol{\sigma}\cdot\hat{m}$. The Zeeman energy splitting for electons is $e_z = \mu_e H_0$, with a resulting spectral gap of $2e_z$. Now we fix the magnetic response to be transverse to the large applied field H_0, so that $\boldsymbol{\sigma}^m = \boldsymbol{\sigma}^x$, which is degenerate with $\boldsymbol{\sigma}^m = \boldsymbol{\sigma}^y$. The eigenvalues of this matrix can be found by finding the roots of the characteristic polynomial:

$$\lambda^4 + p\lambda^2 + q\lambda + r = 0 \tag{3}$$

where we have used the following definitions

$$p = -(\Sigma^2_{\mathbf{k}-} + \Sigma^2_{\mathbf{k}+}) \tag{4}$$

$$q = \pm 2e_z(E^2_{\mathbf{k}-} - E^2_{\mathbf{k}+}) \tag{5}$$

$$r = E^2_{\mathbf{k}-}E^2_{\mathbf{k}+} - 2m^2E^2_q + m^4 \tag{6}$$

$$\Sigma^2_{\mathbf{k}} = \xi^2 + \Delta^2_{\mathbf{k}} + e^2_z + m^2_q \tag{7}$$

$$E^2_{\mathbf{k}} = \xi^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}} - e^2_z \tag{8}$$

$$E^2_{\mathbf{q}} = \xi_{\mathbf{k}-}\xi_{\mathbf{k}+} + \Delta_{\mathbf{k}-}\Delta_{\mathbf{k}+} - e^2_z \tag{9}$$

The corresponding eigenvectors are:

$$\Psi^+ = \begin{bmatrix} \Delta_{\mathbf{k}+} + \frac{(-(\Delta_{\mathbf{k}-}\Delta_{\mathbf{k}+} - m^2_{\mathbf{q}}) - (-e_z - \xi_{\mathbf{k}-} - \lambda)(e_z - \xi_{\mathbf{k}+} - \lambda))(e_z + \xi_{\mathbf{k}+} - \lambda)}{\Delta_{\mathbf{k}+}(-e_z - \xi_{\mathbf{k}-} - \lambda) + \Delta_{\mathbf{k}-}(e_z + \xi_{\mathbf{k}+} - \lambda)} \\ 0 \\ 0 \\ -\frac{\Delta_{\mathbf{k}-}(-e^2_z + \Delta^2_{\mathbf{k}+} + \xi^2_{\mathbf{k}+} + 2e_z\lambda - \lambda^2) - \Delta_{\mathbf{k}+}m^2_{\mathbf{q}}}{\Delta_{\mathbf{k}+}(-e_z - \xi_{\mathbf{k}-} - \lambda) + \Delta_{\mathbf{k}-}(e_z + \xi_{\mathbf{k}+} - \lambda)} \\ 0 \\ \frac{m_{\mathbf{q}}\left[(\Delta_{\mathbf{k}-}\Delta_{\mathbf{k}+} - m^2_{\mathbf{q}}) + (-e_z - \xi_{\mathbf{k}-} - \lambda)(e_z - \xi_{\mathbf{k}+} - \lambda)\right]}{\Delta_{\mathbf{k}+}(-e_z - \xi_{\mathbf{k}-} - \lambda) + \Delta_{\mathbf{k}-}(e_z + \xi_{\mathbf{k}+} - \lambda)} \\ m_{\mathbf{q}} \\ 0 \end{bmatrix} \tag{10}$$

$$\Psi^- = \begin{bmatrix} 0 \\ -\Delta_{\mathbf{k}+} - \frac{(-(\Delta_{\mathbf{k}-}\Delta_{\mathbf{k}+}-m_{\mathbf{q}}^2)-(e_z-\xi_{\mathbf{k}-}-\lambda)(-e_z-\xi_{\mathbf{k}+}-\lambda))(-e_z+\xi_{\mathbf{k}+}-\lambda)}{\Delta_{\mathbf{k}+}(e_z-\xi_{\mathbf{k}-}-\lambda)+\Delta_{\mathbf{k}-}(-e_z+\xi_{\mathbf{k}+}-\lambda)} \\ -\frac{\Delta_{\mathbf{k}-}(-e_z^2+\Delta_{\mathbf{k}+}^2+\xi_{\mathbf{k}+}^2-2e_z\lambda-\lambda^2)-\Delta_{\mathbf{k}+}m_{\mathbf{q}}^2}{\Delta_{\mathbf{k}+}(e_z-\xi_{\mathbf{k}-}-\lambda)+\Delta_{\mathbf{k}-}(-e_z+\xi_{\mathbf{k}+}-\lambda)} \\ 0 \\ \frac{-m_{\mathbf{q}}\left[(\Delta_{\mathbf{k}-}\Delta_{\mathbf{k}+}-m_{\mathbf{q}}^2)+(e_z-\xi_{\mathbf{k}-}-\lambda)(-e_z-\xi_{\mathbf{k}+}-\lambda)\right]}{\Delta_{\mathbf{k}+}(e_z-\xi_{\mathbf{k}-}-\lambda)+\Delta_{\mathbf{k}-}(-e_z+\xi_{\mathbf{k}+}-\lambda)} \\ 0 \\ 0 \\ m_{\mathbf{q}} \end{bmatrix} \tag{11}$$

For $q = 2e_z(E_{\mathbf{k}-}^2 - E_{\mathbf{k}+}^2)$ and $q = -2e_z(E_{\mathbf{k}-}^2 - E_{\mathbf{k}+}^2)$ respectively, where λ_i is a root of the corresponding polynomial from (**??**).

$$\psi_i^+ = \begin{bmatrix} \Delta_{\mathbf{k}+} - \frac{(E_{\mathbf{q}}^2-m_{\mathbf{q}}^2+e_z(\xi_{\mathbf{k}+}-\xi_{\mathbf{k}-})+\lambda_i(\xi_{\mathbf{k}+}+\xi_{\mathbf{k}-})+\lambda_i^2)(\xi_{\mathbf{k}+}+e_z-\lambda_i)}{\Delta_{\mathbf{k}-}(\xi_{\mathbf{k}+}+e_z-\lambda_i)-\Delta_{\mathbf{k}+}(\xi_{\mathbf{k}-}+e_z+\lambda_i)} \\ -\frac{\Delta_{\mathbf{k}-}(E_{\mathbf{k}+}^2+2e_z\lambda_i-\lambda_i^2)-\Delta_{\mathbf{k}+}m_{\mathbf{q}}^2}{\Delta_{\mathbf{k}-}(\xi_{\mathbf{k}+}+e_z-\lambda_i)-\Delta_{\mathbf{k}+}(\xi_{\mathbf{k}-}+e_z+\lambda_i)} \\ \frac{m_{\mathbf{q}}\left[E_{\mathbf{q}}^2-m_{\mathbf{q}}^2+e_z(\xi_{\mathbf{k}+}-\xi_{\mathbf{k}-})+\lambda_i(\xi_{\mathbf{k}+}+\xi_{\mathbf{k}-})+\lambda_i^2\right]}{\Delta_{\mathbf{k}-}(\xi_{\mathbf{k}+}+e_z-\lambda_i)-\Delta_{\mathbf{k}+}(\xi_{\mathbf{k}-}+e_z+\lambda_i)} \\ m_{\mathbf{q}} \end{bmatrix} \tag{12}$$

$$\psi^- = \begin{bmatrix} -\Delta_{\mathbf{k}+} + \frac{(E_{\mathbf{q}}-m_{\mathbf{q}}^2-e_z(\xi_{\mathbf{k}+}-\xi_{\mathbf{k}-})+\lambda_i(\xi_{\mathbf{k}+}+\xi_{\mathbf{k}-})+\lambda_i^2))(\xi_{\mathbf{k}+}-e_z-\lambda_i)}{\Delta_{\mathbf{k}-}(\xi_{\mathbf{k}+}-e_z-\lambda_i)-\Delta_{\mathbf{k}+}(\xi_{\mathbf{k}-}-e_z+\lambda_i)} \\ -\frac{\Delta_{\mathbf{k}-}(E_{\mathbf{k}+}^2-2e_z\lambda_i-\lambda_i^2)-\Delta_{\mathbf{k}+}m_{\mathbf{q}}^2}{\Delta_{\mathbf{k}-}(\xi_{\mathbf{k}+}-e_z-\lambda_i)-\Delta_{\mathbf{k}+}(\xi_{\mathbf{k}-}-e_z+\lambda_i)} \\ -\frac{m_{\mathbf{q}}\left[E_{\mathbf{q}}^2-m_{\mathbf{q}}^2-e_z(\xi_{\mathbf{k}+}-\xi_{\mathbf{k}-})+\lambda_i(\xi_{\mathbf{k}+}+\xi_{\mathbf{k}-})+\lambda_i^2\right]}{\Delta_{\mathbf{k}-}(\xi_{\mathbf{k}+}-e_z-\lambda_i)-\Delta_{\mathbf{k}+}(\xi_{\mathbf{k}-}-e_z+\lambda_i)} \\ m_{\mathbf{q}} \end{bmatrix} \tag{13}$$

These vectors can be written as two different sets of four vectors corresponding to the basis states

$$\left[\; c_{\mathbf{k}-\uparrow}^{\dagger},\;\; c_{-\mathbf{k}-\downarrow},\;\; c_{\mathbf{k}+\downarrow}^{\dagger},\;\; c_{-\mathbf{k}+\uparrow} \;\right] \tag{14}$$

and

$$\left[\; c_{\mathbf{k}-\downarrow}^{\dagger},\;\; c_{-\mathbf{k}-\uparrow},\;\; c_{\mathbf{k}+\uparrow}^{\dagger},\;\; c_{-\mathbf{k}+\downarrow} \;\right] \tag{15}$$

Now we can write the matrix which transforms to these new basis states $\Gamma = \{\Psi_i^+, \Psi_i^-\}$, $\mathcal{D}\Psi = \Gamma$ with operators $\gamma_{\mathbf{k},i}^{\pm}$:

$$\mathcal{D}^+ = \begin{bmatrix} (\psi_1^+)^\dagger \\ (\psi_2^+)^\dagger \\ (\psi_3^+)^\dagger \\ (\psi_4^+)^\dagger \end{bmatrix} \quad , \qquad \mathcal{D}^- = \begin{bmatrix} (\psi_1^-)^\dagger \\ (\psi_2^-)^\dagger \\ (\psi_3^-)^\dagger \\ (\psi_4^-)^\dagger \end{bmatrix} \tag{16}$$

$$\left[\; \gamma_{\mathbf{k}-1}^{\dagger},\;\; \gamma_{-\mathbf{k}-2},\;\; \gamma_{\mathbf{k}+3}^{\dagger},\;\; \gamma_{-\mathbf{k}+4} \;\right] \tag{17}$$

and

$$\left[\; \gamma_{\mathbf{k}-1}^{\dagger},\;\; \gamma_{-\mathbf{k}-2},\;\; \gamma_{\mathbf{k}+3}^{\dagger},\;\; \gamma_{-\mathbf{k}+4} \;\right] \tag{18}$$

By computing the inverse of $\mathcal{D}$ we can find the old operators in terms of the new to use in the self consistent calculation for Δ and $m_{\mathbf{q}}$.

We also wish to calculate the free energy (F) in this new mixed state $F = -Tln(Z)$ where Z is the partition function for the diagnol Hamiltonian ($\mathcal{H} = \sum_i \lambda_i \gamma_i^\dagger \gamma_i$):

$$Z \quad = Tr\Big(e^{-\beta(\mathcal{H}-\mu N)}\Big) \tag{19}$$

$$\Pi_{\mathbf{k},i}\Big(1 + e^{-\beta\lambda_{\mathbf{k},i}}\Big) \tag{20}$$

$$F = -T\sum_{\mathbf{k},i} ln\big(1 + e^{-\beta\lambda_{\mathbf{k},i}}\big) \tag{21}$$

CHARACTERISTIC POLYNOMIAL

- Add and subtract $\lambda^2 u + u^2/4$

$$\lambda^4 + p\lambda^2 + q\lambda + r \tag{22}$$
$$= (\lambda^2 + \frac{u}{2})^2 - ((u-p)\lambda^2 - q\lambda + (\frac{u^2}{4} - r)) \tag{23}$$
$$= (\lambda^2 + \frac{u}{2})^2 - (u-p)\left(\lambda^2 - \frac{q}{u-p}\lambda + \frac{\frac{u^2}{4} - r}{u-p}\right) \tag{24}$$
$$= (\lambda^2 + \frac{u}{2})^2 - (u-p)\left(\lambda^2 - \frac{q}{u-p}\lambda + \frac{\frac{u^2}{4} - r}{u-p}\right) \tag{25}$$

$$P = (\lambda^2 + \frac{u}{2}) \tag{26}$$
$$Q = \sqrt{u-p}\left(\lambda - \frac{q}{2(u-p)}\right) \tag{27}$$

Which requires

$$\frac{q}{2(u-p)} = \sqrt{\frac{u^2/4 - r}{u-p}} \tag{28}$$
$$q^2/4 = (u-p)(u^2/4 - r) \tag{29}$$
$$q^2/4 = u^3/4 - pu^2/4 - ru + rp \tag{30}$$
$$0 = u^3 - pu^2 - 4ru + (4rp - q^2) \tag{31}$$

Now we get $\lambda^4 + p\lambda^2 + q\lambda + r = (P+Q)(P-Q) = P^2 - Q^2$ for a certain u which satisfies the resolvent cubic (above, only need one root) We can find the solutions to the cubic exactly by the following method:
1) write above as $u^3 + c_2 u^2 + c_1 u + c_0$
$c2 = -p$
$c1 = -4r$
$c0 = 4rp - q^2$
2) define $u = z - c_2/3$ to get $z^2 + a_1 z = a_0$
$a_1 = c_1 - c_2^2/3$
$a_0 = c_1 c_2/3 - c_0 - 2c_2^3/27$
3) define $z = w - a_1/(3w)$ to get $(w^3)^2 - a_0 w^3 - a_1^3/27 = 0$
The solutions to w are:

$$w = \sqrt[3]{\frac{a_0}{2} \pm \sqrt{\left(\frac{a_0}{2}\right)^2 + \frac{a_1^3}{27}}} \tag{32}$$

The corresponding solutions to u are:

$$u = w - a_1/(3w) - c_2/3 \tag{33}$$

Plug in u and solve for roots of $P \pm Q$:

$$\lambda^2 \pm \sqrt{u-p}\lambda + \frac{1}{2}\left(u \mp \sqrt{u^2 - 4r}\right) \tag{34}$$
$$\lambda = \pm\frac{\sqrt{u-p}}{2}\{\pm\}\sqrt{\frac{|u-p|}{4} - \frac{1}{2}\left(u \pm \sqrt{u^2 - 4r}\right)} \tag{35}$$