Spin Susceptibility Calculation for the Inhomogeneous Superconducting state

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Spin Susceptibility

The presence of a magnetic field introduces a potential for particles with spin $V = -\vec{m} \cdot \vec{H}$. The magnetization due to this potential is given by $M_\alpha(t) = -i \int\limits_{-\infty}^{t} < [m_\alpha(t), V(t')] > dt'$, and the magnetic susceptibility is $\chi_{\alpha,\beta}(x,x',t) = i \int\limits_{-\infty}^{t} < [m_\alpha(x,t), m_\beta(x',t')] > dt'$. The magnetic moment is given by $m_\alpha(x,t) = \mu_e \sum\limits_{s,s'} \sigma^\alpha_{s,s'} \psi^\dagger_s(x,t)\psi_{s'}(x,t)$ (Mahan). Now we can proceed to calculate the susceptibitily. In the case of uniform time, we can assume that the product $m_\alpha(x,t), m_\beta(x',t')$ is a function of $\tau = t - t'$. In this limit we get:

$$
\begin{aligned}
\chi_{\alpha,\beta}(x,x',0) &= i \int\limits_{-\infty}^{0} < [m_\alpha(x,t), m_\beta(x',0)] > dt' \\
&= -i\mu_e^2 \sum_{s,s',t,t'} \sigma^\beta_{s,s'}\sigma^\alpha_{t,t'} \int\limits_{-\infty}^{t} dt < [\psi^\dagger_s(x',0)\psi_{s'}(x',0), \psi^\dagger_t(x,t)\psi_{t'}(x,t)] >
\end{aligned}
$$

From now on we will use the s and s' subscripts to denote the spin for the (x',0) coordinates while the t and t' subscripts denote the spin for the (x,t) coordinates so that $\psi^\dagger_s = \psi^\dagger_s(x',0)$ and $\psi^\dagger_t = \psi^\dagger_t(x,t)$. The correlation function inside the integral evaluates as follows.

$$
\begin{aligned}
< [\psi^\dagger_s\psi_{s'}, \psi^\dagger_t\psi_{t'}] > &= < \psi^\dagger_s\psi_{s'}\psi^\dagger_t\psi_{t'} > - < \psi^\dagger_t\psi_{t'}\psi^\dagger_s\psi_{s'} > \\
&= < \psi^\dagger_s\psi_{s'} >< \psi^\dagger_t\psi_{t'} > - < \psi^\dagger_s\psi^\dagger_t >< \psi_{s'}\psi_{t'} > \\
&\quad + < \psi^\dagger_s\psi_{t'} >< \psi_{s'}\psi^\dagger_t > - < \psi^\dagger_t\psi_{t'} >< \psi^\dagger_s\psi_{s'} > \\
&\quad + < \psi^\dagger_t\psi^\dagger_s >< \psi_{t'}\psi_{s'} > - < \psi^\dagger_t\psi_{s'} >< \psi_{t'}\psi^\dagger_s > \\
&= - < \psi^\dagger_s\psi^\dagger_t >< \psi_{s'}\psi_{t'} > + < \psi^\dagger_s\psi_{t'} >< \psi_{s'}\psi^\dagger_t > \\
&\quad + < \psi^\dagger_t\psi^\dagger_s >< \psi_{t'}\psi_{s'} > - < \psi^\dagger_t\psi_{s'} >< \psi_{t'}\psi^\dagger_s >
\end{aligned}
$$

To evaluate these various correlation functions we use the Bogoliubov representation for the field operators $\psi_s = \sum\limits_k \gamma_{sk}(t)u_k(x) - s\gamma^\dagger_{-sk}(t)v^*_k(x) = \sum\limits_k \Gamma_{sk}(x,t) - \Gamma^\dagger_{-sk}(x,t)$, where $s = \pm1$ (+ for spin up, - for spin down), $u_k(x)$ and $v_k(x)$ are complex functions and the γ's are operators. (NOTE: k$\neq$momentum as in the homogeneous case) We find the time dependence of the γ operators via the Heisenberg representation, $\frac{d}{dt}\gamma_{sk} = \frac{i}{\hbar}[H, \gamma_{sk}] = \frac{-i\epsilon_{sk}}{\hbar}\gamma_{sk}$ and $\frac{d}{dt}\gamma^\dagger_{sk} = \frac{i\epsilon_{sk}}{\hbar}\gamma^\dagger_{sk}$. The γ operators also obey fermionic anticommutation relations $\gamma^\dagger_{n\alpha}, \gamma_{m\beta} = \delta_{\alpha\beta}\delta nm$, $\gamma_{n\alpha}, \gamma_{m\beta} = 0$

$$\gamma_{sk}(t) = \gamma_{sk}e^{-i\omega_{sk}t} \qquad \gamma^\dagger_{sk}(t) = \gamma^\dagger_{sk}e^{i\omega_{sk}t}$$

Finally, we note that in the Bogoliubov representation the only operators are the γ's, so they are the only things that contribute to the correlations. The correlation relations for the γ's are:

$$< \gamma^\dagger_{\alpha k}\gamma_{\beta p} >= \delta_{pk}\delta_{\alpha\beta}f(\epsilon_{\alpha k}) \qquad < \gamma_{\alpha k}\gamma_{\beta p} >=< \gamma^\dagger_{\alpha k}\gamma^\dagger_{\beta p} >= 0$$

Where $f(\epsilon_{\alpha k}) = f_{\alpha k}$ is the fermi function(De Gennes). Using the definition of Γ and omitting the time bit, we can deduce the following rules:

$$< \Gamma^\dagger_{\alpha k}\Gamma_{\beta p} >= \delta_{pk}\delta_{\alpha\beta}f(\epsilon_{\alpha k})u^*_k u_p \quad < \Gamma^\dagger_{\alpha k}\Gamma_{-\beta p} >= \beta\delta_{pk}\delta_{\alpha\beta}f(\epsilon_{\alpha k})u^*_k v_p \quad < \Gamma^\dagger_{-\alpha k}\Gamma_{-\beta p} >= \alpha\beta\delta_{pk}\delta_{\alpha\beta}f(\epsilon_{\alpha k})v^*_k v_p$$

Going back to the sum of wick contractions, and dropping the quantum number subscript on the Γ's:

$$\begin{aligned}
< [\psi^\dagger_s\psi_{s'}, \psi^\dagger_t\psi_{t'}] >= &- (- < \Gamma^\dagger_s\Gamma_{-t} > - < \Gamma_{-s}\Gamma^\dagger_t >)(- < \Gamma_{s'}\Gamma^\dagger_{-t'} > - < \Gamma^\dagger_{-s'}\Gamma_{t'} >) \\
&+ (< \Gamma^\dagger_s\Gamma_{t'} > + < \Gamma_{-s}\Gamma^\dagger_{-t'} >)(< \Gamma_{s'}\Gamma^\dagger_t > + < \Gamma^\dagger_{-s'}\Gamma_{-t} >) \\
&+ (- < \Gamma^\dagger_t\Gamma_{-s} > - < \Gamma_{-t}\Gamma^\dagger_s >)(- < \Gamma_{t'}\Gamma^\dagger_{-s'} > - < \Gamma^\dagger_{-t'}\Gamma_{s'} >) \\
&- (< \Gamma^\dagger_t\Gamma_{s'} > + < \Gamma_{-t}\Gamma^\dagger_{-s'} >)(< \Gamma_{t'}\Gamma^\dagger_s > + < \Gamma^\dagger_{-t'}\Gamma_{-s} >)
\end{aligned}$$

$$\begin{aligned}
= \delta_{st'}\delta_{s't}\Big[&[T^*_{ks}f_{ks}u_k(x')u^*_k(x) + T_{k-s}(1 - f_{k-s})v^*_k(x')v_k(x)][T_{ps'}(1 - f_{ps'})u^*_p(x')u_p(x) + T^*_{p-s'}f_{p-s'}v_p(x')v^*_p(x)] \\
&- [T_{ks'}f_{ks'}u_k(x)u^*_k(x') + T^*_{k-s'}(1 - f_{k-s'})v^*_k(x)v_k(x')][T^*_{ks}(1 - f_{ps})u^*_p(x)u_p(x') + T_{p-s}f_{p-s}v_p(x)v^*_p(x')]\Big] \\
+ss'\delta_{s-t}\delta_{s'-t'}\Big[&[T_{k-s}(1 - f_{k-s})u^*_k(x')v_k(x) - T^*_{ks}f_{ks}v_k(x')u^*_k(x)][T_{ps'}(1 - f_{ps'})v^*_p(x')u_p(x) - T^*_{p-s'}f_{p-s'}u_p(x')v^*_p(x)] \\
&+ [T_{k-s}f_{k-s}v_k(x)u^*_k(x') - T^*_{ks}(1 - f_{ks})u^*_k(x)v_k(x')][T^*_{p-s'}(1 - f_{p-s'})v^*_p(x)u_p(x') - T_{ps'}f_{ps'}u_p(x)v^*_p(x')]\Big]
\end{aligned}$$

Where $T_{ks} = e^{-i\omega_{ks}t}$ which carries the time dependence from the γ operators. Now we can carry out the time integration. When doing so, one must multiply the integrand by $e^{\delta t}$ to ensure convergence of the integral, then take the limit $\delta \to \infty$. The result is that the terms appearing in the denominator have an additional $+\delta$ which we will omit for now.

$$\begin{aligned}
\delta_{st'}\delta_{s't}\Big[&\frac{(f_{ks} - f_{ps'})u^*_p(x')u_p(x)u_k(x')u^*_k(x)}{i\omega_{ks} - i\omega_{ps'}} + \frac{(1 - f_{ps'} - f_{k-s})u^*_p(x')u_p(x)v^*_k(x')v_k(x)}{-i\omega_{ps'} - i\omega_{k-s}} \\
&+ \frac{(-1 + f_{p-s'} + f_{ks})v_p(x')v^*_p(x)u_k(x')u^*_k(x)}{i\omega_{p-s'} + i\omega_{ks}} + \frac{(f_{p-s'} - f_{k-s})v_p(x')v^*_p(x)v^*_k(x')v_k(x)}{i\omega_{p-s'} - i\omega_{k-s}}\Big] \\
+ss'\delta_{s-t}\delta_{s'-t'}\Big[&\frac{(1 - f_{k-s} - f_{ps'})u^*_k(x')v_k(x)v^*_p(x')u_p(x)}{-i\omega_{ps'} - i\omega_{k-s}} + \frac{(f_{k-s} - f_{p-s'})u^*_k(x')v_k(x)v^*_p(x)u_p(x')}{i\omega_{p-s'} - i\omega_{k-s}} \\
&+ \frac{(f_{ps'} - f_{ks})u^*_k(x)v_k(x')v^*_p(x')u_p(x)}{i\omega_{ks} - i\omega_{ps'}} + \frac{(-1 + f_{ks} + f_{p-s'})u^*_k(x)v_k(x')v^*_p(x)u_p(x')}{i\omega_{ks} + i\omega_{p-s'}}\Big]
\end{aligned}$$

The susceptibility is then:

$$
\begin{aligned}
\chi_{\alpha\beta}(x,x') = -\mu_e \sum_{s,s',p,k} \sigma^{\beta}_{ss'}\sigma^{\alpha}_{s's}\Bigg[& \frac{(f_{ks}-f_{ps'})u^*_p(x')u_p(x)u_k(x')u^*_k(x)}{\omega_{ks}-\omega_{ps'}-i\delta} \\
& - \frac{(1-f_{ps'}-f_{k-s})u^*_p(x')u_p(x)v^*_k(x')v_k(x)}{\omega_{ps'}+\omega_{k-s}+i\delta} \\
& + \frac{(-1+f_{p-s'}+f_{ks})v_p(x')v^*_p(x)u_k(x')u^*_k(x)}{\omega_{p-s'}+\omega_{ks}-i\delta} \\
& + \frac{(f_{p-s'}-f_{k-s})v_p(x')v^*_p(x)v^*_k(x')v_k(x)}{\omega_{p-s'}-\omega_{k-s}-i\delta}\Bigg] \\
+ss'\sigma^{\beta}_{ss'}\sigma^{\alpha}_{-s-s'}\Bigg[& - \frac{(1-f_{k-s}-f_{ps'})u^*_k(x')v_k(x)v^*_p(x')u_p(x)}{\omega_{ps'}+\omega_{k-s}+i\delta} \\
& + \frac{(f_{k-s}-f_{p-s'})u^*_k(x')v_k(x)v^*_p(x)u_p(x')}{\omega_{p-s'}-\omega_{k-s}-i\delta} \\
& + \frac{(f_{ps'}-f_{ks})u^*_k(x)v_k(x')v^*_p(x')u_p(x)}{\omega_{ks}-\omega_{ps'}-i\delta} \\
& + \frac{(-1+f_{ks}+f_{p-s'})u^*_k(x)v_k(x')v^*_p(x)u_p(x')}{\omega_{ks}+\omega_{p-s'}-i\delta}\Bigg]
\end{aligned}
$$

Bogoliubov-De Gennes Equations

We have calculated the magnetic spin susceptibitily in the Bogoliubov representation which involves the γ operators and complex functions of space $u(x)$ and $v(x)$. Becuase this choice diagonalizes the Hamiltonian the γ's consipire to give Fermi distribution functions and their time integration results in the energy's in denominator. We are left to find the explicit form of the u's and v's which we can calculate self consistently along with the superconducting order parameter(De Gennes).

To proceed we start with the electronic superconducting Hamiltonian (without the presence of a magnetic field).

$$
\mathcal{H} = \sum_{\alpha}\int d^3x\psi^{\dagger}_{\alpha}\Bigg[\frac{\vec{p}^2}{2m}+U(x)\Bigg]\psi_{\alpha} - \frac{1}{2}\sum_{\alpha\beta}\int d^3xd^3x'\psi^{\dagger}_{\alpha}(x)\psi^{\dagger}_{\beta}(x')V(x,x')\psi_{\beta}(x')\psi_{\alpha}(x)
$$

The term $U(x)$ is some potential which could discribe a contact potential at the interface, or a band mismatch on either side of the interface. From here we can rewrite the second term in the mean field limit.

$$
\begin{aligned}
\mathcal{H}_{eff} &= \mathcal{H}_0 + \mathcal{H}_1 \\
\mathcal{H}_0 &= \sum_{\alpha}\int d^3x\psi^{\dagger}_{\alpha}\Bigg[\mathcal{H}_e + U(x)\Bigg]\psi_{\alpha} \\
\mathcal{H}_1 &= \int d^3xd^3x'[\Delta(x,x')\psi^{\dagger}_{1}(x)\psi^{\dagger}_{-1}(x') + \Delta(x,x')^*\psi_{-1}(x')\psi_1(x)]
\end{aligned}
$$

Where we have introduced the superconducting order parameter $\Delta(x,x')$. Now we compute the commutator $[\mathcal{H}_{eff},\psi]$ using the anticommutation relations for ψ.

$$[\psi_1(x), \mathcal{H}_{eff}] = (\mathcal{H}_e + U(x))\psi_1 + \int d^3x' \Delta(x,x')\psi^\dagger_{-1}(x')$$
$$[\psi_{-1}(x), \mathcal{H}_{eff}] = (\mathcal{H}_e + U(x))\psi_{-1} - \int d^3x' \Delta(x,x')\psi^\dagger_{1}(x')$$

Now we use the definition of ψ in the Bogoliubov representation and the commutation relations for γ with $\mathcal{H}_{eff}$ to find the left hand side of the previous equations. We get, for each mode k:

$$\epsilon\gamma_1(t)u(x) + \epsilon\gamma^\dagger_{-1}v^*(x) = (\mathcal{H}_e + U(x))(\gamma_1(t)u(x) - \gamma^\dagger_{-1}(t)v^*(x)) + \int d^3x'\Delta(x,x')(\gamma^\dagger_{-1}(t)u^*(x') + \gamma_1(t)v(x'))$$
$$\epsilon\gamma_{-1}(t)u(x) - \epsilon\gamma^\dagger_{1}v^*(x) = (\mathcal{H}_e + U(x))(\gamma_{-1}(t)u(x) + \gamma^\dagger_{1}(t)v^*(x)) - \int d^3x'\Delta(x,x')(\gamma^\dagger_{1}(t)u^*(x') - \gamma_{-1}(t)v(x))$$

Since γ and $\gamma^\dagger$ are linearly independent we can equate like terms to get two equations from each of the two previous expressions. They turn out to be equivalent:

$$\epsilon_k u_k(x) = (\mathcal{H}_e + U(x))u_k(x) + \int d^3x'\Delta(x,x')v_k(x')$$
$$\epsilon_k v_k(x) = -(\mathcal{H}^*_e + U(x))v_k(x) + \int d^3x'\Delta^*(x,x')u_k(x')$$

Here we note that $\mathcal{H}^*_e = \mathcal{H}_e$ as long as there is no applied field. These are the Bogoliubov-De Genne equations for an inhomogenious superconductor and are equivalent to an integral eigen-equation $\epsilon_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \hat{\Omega} \begin{pmatrix} u_k \\ v_k \end{pmatrix}$. We can use these to calculate Δ and $U(x)$ self consistently.