Thermodynamics of a 2-band superconductor with impurities

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1 A clean 2-band Superconductor

In a clean 2-band superconductor, the Hamiltonian is

$$H_0 = \sum_{k,\alpha,\sigma} \varepsilon(k) c^\dagger_{k,\mu,\sigma} c_{k,\mu,\sigma} + \sum_{k,k',\alpha,\beta} V_{\alpha\beta} c^\dagger_{k,\alpha,\uparrow} c^\dagger_{-k,\alpha,\downarrow} c_{k,\beta,\uparrow} c_{-k,\beta,\downarrow}$$

where $V_{\alpha\beta}$ and the OP are scalars.

Mean field approximation:

$$H_0 = \sum_{\alpha,\mathbf{k}} \psi^\dagger_{\alpha,\mathbf{k}} (\vec{h}_{\alpha,\mathbf{k}} \cdot \vec{\tau}_\alpha) \psi_{\alpha,\mathbf{k}} - \sum_{\alpha,\beta} V_{\alpha\beta} A^*_\alpha A_\beta,$$

where α is the band index, $\vec{\tau}$ is the Pauli tensor in isospin space, $\psi_{\alpha,\mathbf{k}} = (c_{\mathbf{k},\uparrow,\alpha}, c^\dagger_{-\mathbf{k},\downarrow,\alpha})^{\mathrm{T}}$ is the Numbu spinor, $A_\alpha = \sum_{\mathbf{k}} < c_{\mathbf{k},\uparrow,\alpha} c_{-\mathbf{k},\downarrow,\alpha} >$ contributes to the order parameter, $\Delta_\alpha = \sum_\beta V_{\alpha\beta} A_\beta$ is the order parameter, and $\vec{h}_\alpha = (\mathrm{Re}(\Delta), -\mathrm{Im}(\Delta), \varepsilon_{\mathbf{k},\alpha})$

The first term is a simple sum over the one-band free energy.The second term can be rewritten using SC order parameter.

$$\sum_{\alpha,\beta} V_{\alpha\beta} A^*_\alpha A_\beta = \frac{1}{\det(V)} [V_{11}|\Delta_2|^2 + V_{22}|\Delta_1|^2 - 2V_{12}\mathrm{Re}(\Delta^*_1 \Delta_2)],$$

To obtain the free energy, we write down the mean-field action

$$S = \int_0^\beta d\tau \left(\sum_{\alpha,\mathbf{k}} \psi^\dagger_{\alpha,\mathbf{k}} \partial_\tau \psi_{\alpha,\mathbf{k}} + H \right) = \int_0^\beta d\tau \left[\sum_{\alpha,\mathbf{k}} \psi^\dagger_{\alpha,\mathbf{k}} (\partial_\tau + \mathcal{H}_{\alpha,\mathbf{k}}) \psi_{\alpha,\mathbf{k}} - \sum_{\alpha,\beta} V_{\alpha\beta} A^*_\alpha A_\beta, \right]$$

where $\mathcal{H}_{\alpha,\mathbf{k}} = \vec{h}_{\alpha,\mathbf{k}} \cdot \vec{\tau}_\alpha$. Integrating the second term (scalar) is straightforward whereas the first term is a standard Gaussian integral in the Matsubara space

$$S_{MF} = \sum_{\alpha,\mathbf{k},\omega_n} \ln\det(-i\omega_n + \mathcal{H}_{\alpha,\mathbf{k}}) + \sum_{\alpha,\beta} V_{\alpha\beta} A^*_\alpha A_\beta,$$

where the amplitude of fluctuation (i.e. the Green's function) is also given by

$$\psi^\dagger_{\alpha,\mathbf{k},\omega_n} \psi_{\alpha,\mathbf{k},\omega_n} = -\mathcal{G}_\alpha(\mathbf{k}, i\omega_n) = (-i\omega_n + \mathcal{H}_{\alpha,\mathbf{k}})^{-1}.$$

In the saddle-point approximation, $Z \approx \exp(-S_{MF})$, then the free energy is related to the single-particle Nambu-Gorkov Green's function via

$$F = \beta^{-1} \left(\sum_{\alpha,\mathbf{k},\omega_n} \ln \mathcal{G}^{-1}_\alpha(\mathbf{k}, i\omega_n) + \sum_{\alpha,\beta} V_{\alpha\beta} A^*_\alpha A_\beta \right).$$

This can be evaluated as a Matsubara sum

$$F = -T \sum_{\alpha} N_\alpha(0) \int_{-\omega_{AFM}}^{\omega_{AFM}} \mathrm{d}\varepsilon \sum_{i\omega_n} \ln\left[\omega_n^2 + \Delta_\alpha^2 + \varepsilon^2\right] + \sum_{\alpha,\beta} V_{\alpha,\beta} \bar{A}_\alpha A_\beta,$$

subjected to the regularisation

$$\sum_{i\omega_n} \ln(\omega_n^2 + \Delta_n^2 + \varepsilon^2) = 2\ln(2\cosh(\beta\sqrt{\Delta^2+\varepsilon^2}/2)).$$

2 T-matrix approximation

At a finite impurity concentration,

$$H = \sum_{\alpha,k} \psi^\dagger_{\alpha,k}(\varepsilon_{\alpha,k}\tau^3 + \Delta_\alpha \tau^1)\psi_{\alpha,k} + \sum_{\alpha,\beta} V_{\alpha,\beta}\bar{A}_\alpha A_\beta + \sum_{\alpha,\beta,k,k'} \psi^\dagger_{\alpha,k}(U_{\alpha,\beta,k,k'}\tau^3)\psi_{\beta,k'},$$

where I would assume $U_{\alpha,\beta,k,k'} = \sum_{i,\alpha,\beta} U_{\alpha,\beta}\exp(i(k-k')R_i)$. The dressed single-particle Green's function can be renormalised from the impurity T matrix in the single-site approximation (low concentration) as

$$G_\alpha^{-1}(k, i\omega_n) = i\tilde{\omega}_n\tau^0 - \tilde{\varepsilon}_{\alpha,k}\tau^3 - \tilde{\Delta}_\alpha\tau^1,$$

with renormalisation given by Eq.(11) - Eq.(17) in Bang2017. (?) Why do the renormalisation have contribution from both bands?

Are we, then, able to infer that the Hamiltonian can be rewritten as

$$H = \sum_{\alpha,k} \psi^\dagger_{\alpha,k}(\tilde{\varepsilon}_{\alpha,k}\tau^3 + \tilde{\Delta}_\alpha\tau^1)\psi_{\alpha,k} + \sum_{\alpha,\beta} V_{\alpha,\beta}\bar{A}_\alpha A_\beta,$$

with the scalar term NOT renormalised (because it is not sandwiched between two fields).

Then, by a similar argument, the free energy is given by

$$F = -T \sum_{\alpha} N_\alpha(0) \int_{-\omega_{AFM}}^{\omega_{AFM}} \mathrm{d}\varepsilon \sum_{i\omega_n} \ln\left[\tilde{\omega}_n^2 + \tilde{\Delta}_\alpha^2 + \varepsilon^2\right] + \sum_{\alpha,\beta} V_{\alpha,\beta}\bar{A}_\alpha A_\beta$$

which we calculate from Taylor expansion (not satisfactory)

$$\sum_{i\omega_n} \ln(\tilde{\omega}_n^2 + \tilde{\Delta}_n^2 + \varepsilon^2) = \sum_{i\omega_n} \ln(\omega_n^2 + \Delta_n^2 + \varepsilon^2) + \sum_{\omega_n} \frac{2(\Delta(\delta\omega_n) + \omega_n(\delta\Delta))}{\Delta^2 + \omega_n^2 + \varepsilon^2} +$$

$$\sum_{\omega_n} \frac{1}{(\omega_n^2 + \varepsilon^2 + \Delta^2)^2}\left[(\Delta^2 + \varepsilon^2 - \omega_n^2)\delta\omega_n^2 + (-\Delta^2 + \varepsilon^2 + \omega_n^2)\delta\Delta^2 - (4\Delta\omega_n)\delta\omega_n\delta\Delta\right] + \mathcal{O}(\delta^3).$$

3 Challenges

- Not satisfied by the Taylor expansion
- Does the theory break down at high Γ? If so, is there an easy replacement/extention?
- How to do T-matrix for a two-band superconductor? Why do, say Δ_1, get corrections from both bands?