Temperature GF

At $T=0$ we defined the order parameter as

$$\Delta = \lambda \langle \psi_\uparrow(x)\psi_\downarrow(x)\rangle$$

where the averaging is by the ground state.

At $T\neq 0$ we should take the statistical average

$$\Delta = \lambda\, \mathrm{Tr}\left(\hat{\rho}\, \psi_\uparrow(x)\psi_\downarrow(x)\right),$$

where $\hat{\rho} = \exp((\Omega - \tilde{H})\beta)$ and $e^{-\Omega\beta} = \mathrm{Tr}(e^{-\beta\tilde{H}})$

In order to calculate such statistical averages let's introduce the temperature GF.

We will use the analog of Heisenberg representation in imaginary time $i\tau$.

Matsubara operators

$$\psi^M(r,\tau) = e^{(H-\mu N)\tau}\,\psi(r)\,e^{-(H-\mu N)\tau}$$

$$\bar{\psi}^M(r,\tau) = e^{(H-\mu N)\tau}\,\psi^+(r)\,e^{-(H-\mu N)\tau}$$ – not the h.c.!

They satisfy equations of motion which are the analytic continuations of the Heisenberg equations at imaginary time

$$\frac{\partial}{\partial\tau}\psi^M(r,\tau) = [H, \psi^M(r,\tau)]$$

$$\frac{\partial}{\partial\tau}\bar{\psi}^M(r,\tau) = [H, \bar{\psi}^M(r,\tau)]$$

Temperature GF is defined through Matsubara operators using the temperature ordering operation which orders operators according to τ

$$G^M_{\alpha\beta}(r_1\tau_1, r_2\tau_2) = +\mathrm{Tr}\langle \rho\, T_\tau\, \psi_\alpha^M(r_1\tau_1)\,\bar{\psi}_\beta^M(r_2\tau_2)\rangle$$

where $|\tau_1 - \tau_2| < \beta$

1) Since the Hamiltonian is τ-independent,

$$G(\tau_1, \tau_2) = G(\tau_1 - \tau_2)$$

Indeed, take example $\tau_1 > \tau_2$

$$G(\tau_1\tau_2) = +\mathrm{Tr}\,\rho\,\psi^M(\tau_1)\,\bar{\psi}^M(\tau_2) =$$

$$e^{\beta\Omega}\mathrm{Tr}\left(e^{-\hat{H}\beta} e^{\hat{H}\tau_1}\psi(r_1)e^{-\hat{H}\tau_1}e^{\hat{H}\tau_2}\psi^+(r_2)e^{-\hat{H}\tau_2}\right) = +\mathrm{Tr}\left(\rho\, e^{\hat{H}\tau}\psi(r_1)e^{-\hat{H}\tau}\psi^+(r_2)\right)$$

2) $G(\tau<0) = \mp G(\tau+\beta)$ for fermions / bosons

Set for example $\tau<0$, but $\tau>-\beta$

$$-G(\tau) = \pm \mathrm{Tr}\left(e^{\beta(\Omega-\hat H)}\psi^+ e^{\hat H\tau}\psi e^{-\hat H\tau}\right) = \pm e^{\beta\Omega}\mathrm{Tr}\left(e^{-(\beta+\tau)\hat H}\psi^+_{(r_2)} e^{\hat H\tau}\psi_{(r_1)}\right)$$

$$-G(\tau+\beta) = -e^{\beta\Omega}\mathrm{Tr}\left(e^{-\beta\hat H} e^{\hat H(\tau+\beta)}\psi(r_1)\, e^{-\hat H(\tau+\beta)}\psi^+(r_2)\right) =$$

$$= e^{-\beta\Omega}\mathrm{Tr}\left(e^{\hat H\tau}\psi(r_1)\, e^{-\hat H(\tau+\beta)}\psi^+(r_2)\right) = e^{-\beta\Omega}\mathrm{Tr}\left(e^{-(\beta+\tau)\hat H}\psi^+(r_2)\, e^{-\hat H\tau}\psi(r_1)\right)$$

Sice $G^M(\tau)$ is defined at $|\tau|<\beta$

3) Fourier transform runs over discrete frequencies

$$G^M(\tau) = \overset{=1/\beta}{T}\sum_n e^{-i\omega_n\tau}\, G^M(\omega_n)$$

Due to the periodicity it is nonzero only Matsubara frequencies

$$G^M(\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} e^{i\omega_n\tau}\, G^M(\tau)\, d\tau,$$

$\omega_n = (2n+1)\pi T$ Fermion

$2n\pi T$ Boson

4) Due to the presence of T-ordering one can develop the diagrammatic technique which is quite similar to $T=0$ case

Feynman rules in momentum space

$\underset{p,\omega_n}{\Longrightarrow}$ $+\,G^M(p,\omega_n)$ $\quad$ $\underset{p,\omega_n}{\longrightarrow}$ $+\,G_0^M(p,\omega_n)$ $\quad$ $\underset{p}{\bullet\!-\!-\!-\!\bullet}$ $-\,V(p)$ $\quad$ $\circlearrowright$ n_0

The integration over internal momenta, summation by Matsubara frequencies, and spin is implied taking into account frequency / momentum conservation at every vertex

5) $G^M(\omega_n)$ is analitic continuation of $G^{R,A}$ to upper/lower ½ plane

$$G^M(\omega_n) = G^R(i\omega_n) \quad \omega_n>0$$

$$G^M(\omega_n) = G^A(i\omega_n) \quad \omega_n<0$$

Can be easily shown using the Källen – Lehman represent.

6) From G^M we can calculate observables.

Consider some physical operator $\hat A = \int \hat\psi^+(r)\,\hat a(r)\,\hat\psi(r)\, d^3r$

Then the average

$$\bar A = \mathrm{Tr}(\rho A) = \int \mathrm{Tr}\left(\rho\,\psi^+(r)\,\hat a(r)\,\psi(r)\right) d^3r = \overset{\text{Fermions}}{\mp}\int \hat a(r_2)\, G^M(r_1,r_2,\tau)\Big|_{\substack{r_1=r_2\\ \tau=-0}} d^3r_1$$

On the other hand the same average can be expressed throug the causal GF

$$\bar{A} = \mp i \int \hat{a}(r_2)\, G(r_1, r_2, t)\big|_{r_1=r_2,\, t=-0} d^3 r_2$$

Thus instead of the causal GF we can use the temperature one

Since we have $\tau=-0$ then we get summation by frequencies

$$\bar{A} = \mp T \sum_n \int \hat{a}(r_2)\, G(r_1, r_2, \omega_n)\big|_{r_1=r_2} d^3 r_1$$

Temperature dependence of the order parameter

Temperature GM in superconductor

$$G^M = + \mathrm{Tr}(\rho\, T\, \psi^M(r_1,\tau)\, \bar{\psi}^M(r_2,0))$$
$$F^M = + \mathrm{Tr}(\rho\, T\, \psi^M(r_1,\tau)\, \psi^M(r_2,0))$$
$$F^{M+} = + \mathrm{Tr}(\rho\, T\, \bar{\psi}^M(r_1,\tau), \bar{\psi}^M(r_2,0))$$

Order parameter $\Delta(r) = \lambda\, F^M(\tau=+0, r_1=r_2) = \lambda T \sum_n F(\omega_n, r_1=r_2)$

Will omit M superscript

Gorkov Eqs.

$$\begin{cases} \left(\frac{\partial}{\partial\tau_1} + H_0\right) G(x_1 x_2) + \Delta(x_1)\, F^+(x_1 x_2) = \delta(x_1 - x_2) \\ \left(\frac{\partial}{\partial\tau_1} - H_0\right) F^+(x_1 x_2) + \Delta^*(x_1)\, G(x_1 x_2) = 0 \end{cases}$$

$$H_0 = \frac{\hat{p}^2}{2m} - \mu = \xi_p$$

In the frequency domain

$$\begin{cases} (-i\omega_n + \xi_p)\, G + \Delta F^+ = 1 \\ (-i\omega_n - \xi_p)\, F^+ + \Delta^* G = 0 \end{cases} \Rightarrow \quad G = \frac{\xi_p + i\omega_n}{\xi_p^2 + \omega_n^2 + |\Delta|^2}$$

$$F^+ = \frac{\Delta^*}{\xi_p^2 + \omega_n^2 + |\Delta|^2}$$

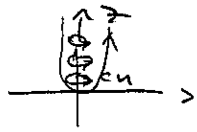
From the self-consistency Eq.

$$\Delta = \lambda T \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{\Delta}{\xi_p^2 + \omega_n^2 + \Delta^2} \qquad \int \frac{d^3p}{(2\pi)^3} = \nu_0 \int d\xi_p$$

$$1 = \nu_0 \lambda T \sum_n \int \frac{d\xi_p}{\xi_p^2 + \omega_n^2 + \Delta^2} = 2\pi \nu_0 \lambda T \sum_{n\geq 0}^{\omega^*} \frac{1}{\sqrt{\omega_n^2 + \Delta^2}}$$

The cutoff $\omega^* = \omega_d / 2\pi T$

Equivalently we could sum over ω_n first



$$\sum_{\omega>0}\frac{1}{\xi_p^2+\Delta^2+\omega_n^2} = \frac{1}{2\pi i}\sum_n \int_{C_n}\frac{dz}{\xi_p^2+\Delta^2+z^2}\,\mathrm{th}\left(\frac{z}{2T}\right) =$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\mathrm{th}(z/2T)}{\xi_p^2+\Delta^2+z^2}\,dz = \frac{\mathrm{th}\left(\sqrt{\xi_p^2+\Delta^2}\right)}{\sqrt{\xi_p^2+\Delta^2}}$$

$$\varepsilon = \sqrt{\xi_p^2+\Delta^2}-\Delta \qquad d\varepsilon = \frac{d\xi_p\,\xi_p}{\sqrt{\xi_p^2+\Delta^2}} = \frac{d\xi_p\,(\varepsilon^2+2\varepsilon\Delta)}{\sqrt{\xi_p^2+\Delta^2}}$$

$$\xi_p^2 = (\varepsilon+\Delta)^2-\Delta^2 = \varepsilon^2+2\varepsilon\Delta$$

$$1 = \nu_0\lambda \int_0^{\Omega_d}\mathrm{th}\left(\frac{\varepsilon+\Delta}{2T}\right)\frac{d\varepsilon}{\sqrt{\varepsilon^2+2\Delta\varepsilon}}$$

Let's determine T_c. Put $\Delta=0$

$$1 = 2\pi T\nu_0\lambda\sum_{n=0}^{N_{max}}\frac{1}{\omega_n} = 2\nu_0\lambda\sum_{n=0}^{N_{max}}\frac{1}{2n+1} = \nu_0\lambda\left(\ln\frac{\Omega_d}{2\pi T_c}+2\ln 2+C\right)$$

$C=0.577$ – Euler constant

$$T_c = \frac{2\Omega_d}{\pi}\gamma\, e^{-1/\nu_0\lambda} \qquad \gamma \simeq 1.78 = e^C$$

$T\to 0$

$$1 = 2\pi T\nu_0\lambda\sum_{n\ge 0}^{N_0 T_c/T}\frac{1}{\sqrt{\omega_n^2+\Delta^2}} = \int_0^{N_0 T_c/T}\frac{dn\,2\pi T}{\left((2n+1)^2\pi^2 T^2+\Delta^2\right)^{1/2}}\times\nu_0\lambda =$$

$$=\nu_0\lambda\int_0^{\Omega_d}\frac{dx}{(x^2+\Delta^2)^{1/2}} = \nu_0\lambda\,\mathrm{sh}^{-1}\frac{\Omega_d}{\Delta} \Rightarrow \Delta = \Omega_d\Big/\mathrm{sh}\frac{1}{\lambda\nu_0}$$

For small $\nu_0\lambda$

$$\Delta = 2\Omega_d\, e^{-1/\lambda\nu_0} \qquad \text{– BCS GAP}$$

GL. Theory

$$1-T/T_c = \frac{\Delta^2}{T_c^2}\frac{7\zeta(3)}{8\pi^2} \Rightarrow \Delta^2 = \frac{8\pi^2}{7\zeta(3)} T_c(T_c - T)$$

This result can be obtained also from the phenomenological GL theory. $F = \alpha(T-T_c)\Delta^2 + b\frac{\Delta^4}{2}$

$$(i\omega_n+\varepsilon)\left(1+\xi/\varepsilon\right)+(i\omega_n-\varepsilon)\left(1-\xi/\varepsilon\right) = \frac{2i\omega_n+2\xi}{\omega_n^2+\varepsilon^2}$$

$$\frac{1}{i\omega_n-\varepsilon-pv_s}$$

$$\frac{1}{i\omega_n+\varepsilon-pv_s}$$

$$-(\varepsilon \mp p v_s)$$