P503

LECTURE 8

Effect of impurities on the thermodynamic properties of the electron gas.

Define finite-T (or Matsubara) GF for electrons:

$$\mathcal{G}(\vec{p}, \tau-\tau') = \langle T_\tau [\tilde{c}_p(\tau)\, \tilde{c}_p^+(\tau')] \rangle_\beta \qquad \tilde{c}_p(\tau) = e^{\tau H} c_p e^{-\tau H}$$

$$\mathcal{F}(\vec{p}, \vec{p}\,'; \tau-\tau') = \langle T_\tau [\tilde{c}_p(\tau)\, \tilde{c}_{p'}^+(\tau')] \rangle_\beta$$

As before, the change due to impurity potential in the thermodynamic potential can be written as

$$\boxed{\Omega_U - \Omega_0 = -\int_0^1 d\lambda \sum_{pp'} U(p-p') \lim_{\tau \to 0^+} \mathcal{F}(p, p'; \tau)}$$

We will now calculate $\mathcal{F}$ by setting up an eq of motion, as for phonons, in imaginary time.

Begin with calculation of UNPERTURBED GF

$$\mathcal{G}^0(\vec{p}, \tau) = \langle T_\tau [\tilde{c}_p(\tau)\, \tilde{c}_p^+(0)] \rangle_{\beta, 0}$$

average at $T = 1/\beta$ with respect to ~~the~~ $H_0 = \sum \varepsilon_p c_p^+ c_p$

$$\tilde{c}_p(\tau) = e^{\tau H_0} c_p e^{-\tau H_0} = e^{-\varepsilon_p \tau} c_p$$

obtained by expanding $e^{\tau H_0} = 1 + \tau H_0 + \ldots$ and performing commutators

$\underline{\tau < 0}$:

$$g^0(p,\tau) = -\langle \tilde{c}_p^+(0)\, \tilde{c}_p(\tau) \rangle_{\beta,0} = -e^{-\varepsilon_p \tau} \langle c_p^+ c_p \rangle_{\beta,0}$$

$$= -e^{-\varepsilon_p \tau} f_p \qquad f_p = \frac{1}{e^{\beta \varepsilon_p}+1}$$

Fermi function

$$g^0(\vec{p},\tau) = \begin{cases} e^{-\varepsilon_p \tau}(1-f_p) & \tau > 0 \\ -e^{-\varepsilon_p \tau} f_p & \tau < 0 \end{cases} \Bigg\} \; e^{-\varepsilon_p \tau}\left[\theta(\tau) - f_p\right]$$

- Antiperiodic property of $g(\vec{p},\tau)$: One can show

$$g(\vec{p},\tau+\beta) = -g(\vec{p},\tau)$$ for fermions. (Check!)

$\Rightarrow$ This implies that $g(\vec{p},\tau)$ is PERIODIC in τ with period 2β. We therefore take $\tau \in (-\beta,\beta)$ as a fundamental interval for computing F.T.:

$$g^0(\vec{p},\tau) = \sum_{\nu_n} e^{i\nu_n \tau} g^0(\vec{p},\nu_n) \qquad \tau \in (-\beta,\beta)$$

$$g^0(\vec{p},\nu_n) = \frac{1}{2\beta} \int_{-\beta}^{\beta} e^{-i\nu_n \tau} g^0(\vec{p},\tau) \qquad \boxed{\nu_n = \frac{2\pi n}{2\beta}}$$

$$= \frac{1}{2\beta}\left[(1-f_p) \int_0^\beta d\tau\, e^{-i\nu_n\tau} e^{-\varepsilon_p\tau} - f_p \int_{-\beta}^0 d\tau\, e^{-i\nu_n\tau} e^{-\varepsilon_p\tau} \right]$$

$$= \frac{1}{2\beta} \frac{1}{(-i\nu_n - \varepsilon_p)} \left[\frac{e^{-i\nu_n\beta} - e^{\beta\varepsilon_p}}{1+e^{+\beta\varepsilon_p}} - \frac{1 - e^{i\nu_n\beta} e^{\beta\varepsilon_p}}{e^{\beta\varepsilon_p}+1} \right]$$

- Note that this vanishes for n even $\left(e^{\pm i\nu_n\beta} = 1 \right)$

$$\boxed{ g^0(\vec{p}, \nu_n) = \frac{1/\beta}{i\nu_n + \varepsilon_p}, \qquad \nu_n = \frac{\pi n}{\beta}, \quad n = \pm 1, \pm 3, \dots }$$

fermionic Matsubara frequencies

Compare $\omega_n = \frac{2\pi n}{\beta}$, $n \in \mathbb{Z}$

$\nu_n = \frac{2\pi}{\beta}(n+\frac{1}{2})$, $n \in \mathbb{Z}$

- To find $\mathcal{F}(\vec{p}, \vec{p}\,'; \tau)$ we set up the same iterative solution as we did in $T=0$ case.

For short range potential $U(\vec{x}) = U\,\delta(\vec{x})$ we find

$$\mathcal{F}(p, p'; \nu_n) = \delta_{pp'}\, g^0(p, \nu_n) - g^0(p, \nu_n)\, \beta \frac{U}{V}\, g^0(p, \nu_n)$$

$$- \dots - g^0(p, \nu_n) \left[- \sum_{p_1} \frac{U}{V} \beta\, g^0(p_1, \nu_n) \right]^n g^0(p, \nu_n) + \dots$$

As before, define $g_0(\nu_n) = \frac{1}{V}\sum_{p_1} g^0(p_1,\nu_n)$

Then

$$\mathcal{F}(p,p';\nu_n) = g^0(p,\nu_n)\left[\delta_{pp'} - \frac{\beta U/V}{1+\beta U g_0(\nu_n)}\, g^0(p,\nu_n)\right]$$

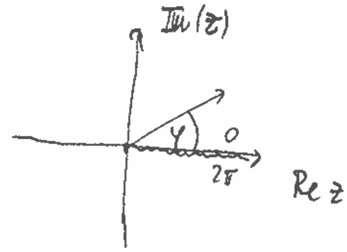
Finally

$$\Omega_U - \Omega_0 = -U\sum_n e^{i\nu_n 0^-} g_0(\nu_n)\left[1 - g_0(\nu_n)\int_0^1 d\lambda\, \frac{\beta\lambda U}{1+\beta\lambda U g_0(\nu_n)}\right]$$

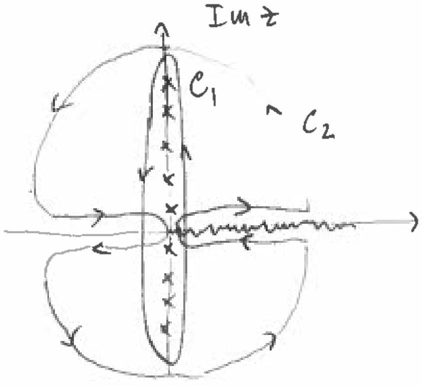
$$= -\frac{1}{\beta}\sum_n e^{i\nu_n 0^-} \ln\left[1+\beta U g_0(\nu_n)\right]$$

We now have to perform fermionic Matsubara sum involving a function with a branch cut $\ln(z)$

$z = re^{i\varphi} \rightarrow \ln z = \ln r + i\varphi$



$$\sum_n e^{i\nu_n 0^-} A(-i\nu_n) = -\frac{\beta}{2\pi i}\int_{C_1} dz\, \frac{e^{z0^-}}{e^{\beta z}+1} A(z)$$



poles at $e^{\beta z} = -1$

$z = \frac{2\pi}{\beta}(n+\frac{1}{2}) \quad n \in \mathbb{Z}$

$$= -\frac{\beta}{2\pi i}\int_{-\infty}^{\infty} d\varepsilon \, \frac{1}{e^{\beta\varepsilon}+1}\left[A(\varepsilon+i\delta) - A(\varepsilon-i\delta)\right]$$

$$\Omega_U - \Omega_0 = \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\varepsilon \, f(\varepsilon) \ln\left[\frac{1-U g_0(\varepsilon+i\delta)}{1-U g_0(\varepsilon-i\delta)}\right]$$

$$= \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\varepsilon \, f(\varepsilon) \ln \frac{T(\varepsilon-i\delta)}{T(\varepsilon+i\delta)} \quad \leftarrow \quad T\text{-matrix}$$

$$= -\frac{1}{\pi}\int_{-\infty}^{\infty} d\varepsilon \, f(\varepsilon)\, \delta_0(\varepsilon)$$

We can obtain change in entropy and specific heat through thermodynamic relations:

$$\Delta S = \frac{d(\Omega_U - \Omega_0)}{dT}$$

$$\frac{\Delta C_V}{T} = -\frac{d^2}{dT^2}(\Omega_U - \Omega_0)$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty} d\varepsilon \, \frac{\partial^2 f}{\partial T^2}\, \delta_0(\varepsilon) \quad \leftarrow$$ evaluate using standard Sommerfeld expansion (P502)

$$\simeq k_B^2 \, \frac{\delta_0'(\varepsilon_F)}{\pi}\left[-\int_{-\infty}^{\infty} dx\, x^2 f'(x)\right] + O(T^2)$$