Greens

Problem: single particle, QM, disorder

$$\hat{H} = \hat{H}_0 + \hat{V} \qquad , \qquad i\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

Starting from the almost free particle approximation

$$\hat{H}_0 = \frac{p^2}{2m^*} \text{ effective}$$

If V is stationary: $\hat{H}\psi = \varepsilon\psi$ and we can introduce R/A Green's functions which obey

$$(\varepsilon - \hat{H} \pm i0)\,\hat{G}^{R/A} = \mathbb{1} \text{ operator } 1,$$

for example, $\delta(r-r')$ in coord. repr.

Formally $\hat{G}^{R/A} = \frac{1}{\varepsilon - \hat{H} \pm i0}$) inverse operator

resolution (in math)

Calculating the FT

$$\hat{G}^{R/A}(t) = \underbrace{\int \frac{d\varepsilon}{2\pi}\, e^{-i\varepsilon t}\, \hat{G}^{R/A}(\varepsilon)}_{\text{pole integral}} = \underbrace{\mp\theta(\pm t)}_{\text{retardation}}\, e^{-i\hat{H}t}$$

Calculating matrix elements in coord. repr:

$$\hat{G}^{R/A}(\vec{r}, \vec{r}\,'; t) = \mp i\theta(\pm t)\, \underbrace{\langle \vec{r}\,' | e^{-i\hat{H}t} | \vec{r} \rangle}_{\text{change to } \sum_{\text{eigen states}} : 1 = \sum_n |n\rangle\langle n|} =$$

$$= \mp i\theta(\pm t) \sum_n \varphi_n^*(\vec{r}\,')\, e^{-i\varepsilon_n t}\, \varphi_n(\vec{r})$$

and going back to the energy space

$$\boxed{G^{R/A}(\vec{r}, \vec{r}\,'; \varepsilon) = \sum_n \frac{\varphi_n^*(\vec{r}\,')\,\varphi_n(\vec{r})}{\varepsilon - \varepsilon_n \pm i0}}$$ — the Lehmann repr.

Important: GFs know about spectral properties & properties of w/f. - we can extract them from GFs by proper projecting:

Example DoS $\nu(\varepsilon) \equiv \sum_n \delta(\varepsilon - \varepsilon_n)$; $\rho(\varepsilon) \equiv \nu/Vol$

LDoS $\rho(\vec{r}, \varepsilon) = \sum_n |\varphi_n(\vec{r})|^2 \delta(\varepsilon - \varepsilon_n)$; $\nu = \int d\varepsilon\, \rho$

Consider the difference

$$G^R(\vec{r}, \vec{r}; \varepsilon) - G^A(\vec{r}, \vec{r}; \varepsilon) \overset{\text{Lehmann}}{=\!=} \sum_n |\varphi_n(\vec{r})|^2 \times$$

$$\overbrace{\left(\frac{1}{\varepsilon - \varepsilon_n + i0} - \frac{1}{\varepsilon - \varepsilon_n - i0} \right)}^{-2\pi i \delta(\varepsilon - \varepsilon_n)} = -2\pi i \underbrace{\sum_n |\varphi_n(\vec{r})|^2 \delta(\varepsilon - \varepsilon_n)}_{\rho(\vec{r}, \varepsilon)}$$

$$\Rightarrow \rho(\vec{r}, \varepsilon) = \frac{i}{2\pi} (G^R - G^A)_{r, r; \varepsilon}$$

Note that $G^R(x, y; \varepsilon) = [G^A(y, x; \varepsilon)]^*$

$$\Rightarrow \boxed{\rho(\vec{r}, \varepsilon) = -\frac{1}{\pi} \mathrm{Im}\, G^R(\vec{r}, \vec{r}; \varepsilon)}$$

&

$$\boxed{\rho(\varepsilon) = \frac{1}{Vol} \int d\vec{r}\, \rho(\vec{r}, \varepsilon) = -\frac{1}{\pi Vol} \mathrm{Im} \int d\vec{r}\, G^R(\vec{r}, \vec{r}; \varepsilon)}$$

Returning to operator repr

$$\int d\vec{r}\, G^R(\vec{r}, \vec{r}; \varepsilon) \to \mathrm{Tr}\, \hat{G}^R(\varepsilon)$$

$$\Rightarrow \boxed{\rho = -\frac{1}{\pi Vol} \mathrm{Im}\, \mathrm{Tr}\, \hat{G}^R(\varepsilon)}$$. which is repr. independent.

Now account for V which is random. Let's start (G-3) with the Dyson eq. ||omit $\pm i0$||

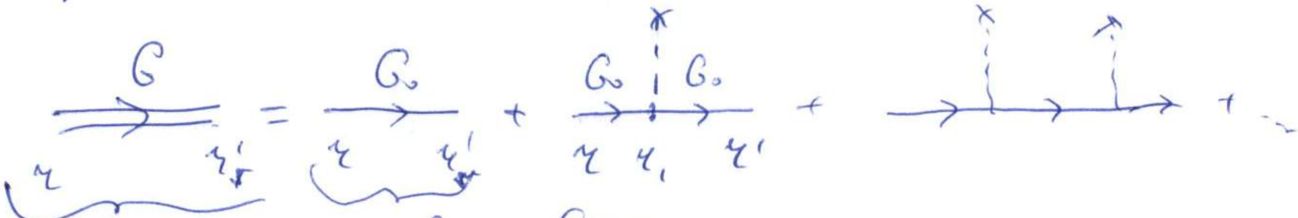
$$(\varepsilon-\hat H)\hat G = (\underbrace{\varepsilon-\hat H_0}_{\hat G_0^{-1}}-\hat V)\hat G = (\hat G_0^{-1}-\hat V)\hat G = \mathbb{1} \quad \times \hat G_0 \text{ from left}$$

$$\Rightarrow \hat G - \hat G_0\hat V\hat G = \hat G_0 \quad \text{or}$$

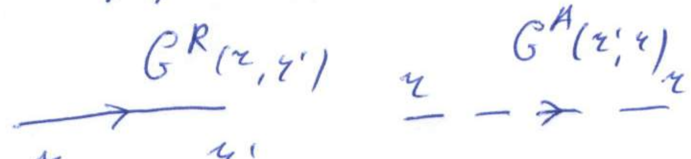
$$\boxed{\hat G = \hat G_0 + \hat G_0\hat V\hat G}$$

Now we can iterate:

$$\hat G = \hat G_0 + \hat G_0\hat V\hat G_0 + \hat G_0 V\hat G_0 V\hat G_0 + \dots$$ - interaction of a particle with the scalar potential V. Diagrams

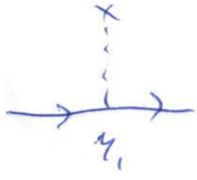


- impurity potential at r_1

Note: 

since $G^A(r';r) = G^R(r,r')^*$

Each matrix product is transformed to $\int d\vec r_i$:



$$= \int d\vec r_1\, G^R_\varepsilon(\vec r,\vec r_1)\, V(\vec r_1)\, G^R_\varepsilon(\vec r_1,\vec r')$$

the same energy since impurity is static and the energy cannot be changed.

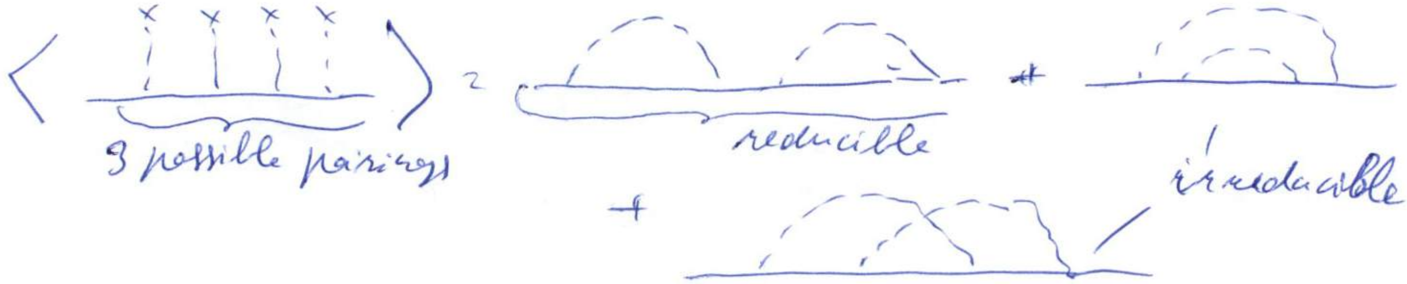
Now one can calculate $\langle G\rangle_{dis}$ for the model of the Gaussian white-noise V by using the Wick theorem

$\langle V \rangle_{dis} = 0$, $\langle VV \rangle_{dis} \neq 0$ – known

$\langle V(1)V(2)V(3)\rangle_{dis} = 0$; $\langle 1234 \rangle = \langle 12\rangle\langle 34\rangle + \langle 13\rangle\langle 24\rangle + \langle 14\rangle\langle 23\rangle$

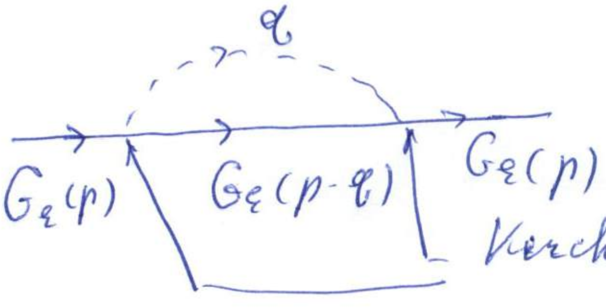
etc.

Graphically



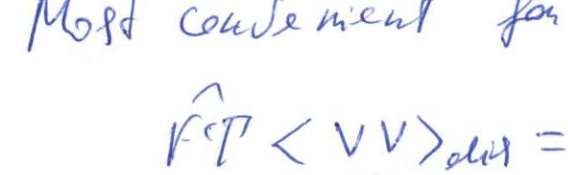
Most convenient for calculations is p-repr.

$\hat{FT}\langle VV\rangle_{dis} = \text{const} \Rightarrow$



Kirchoff's law at each vertex

Reducible diag. can be factorized, for example,



$$\Rightarrow G_0(\varepsilon,\vec{p})\Big[\overbrace{\int \frac{d\vec{q}}{2\pi}\langle VV\rangle G_0(\varepsilon,\vec{p}-\vec{q}) \times}^{\Sigma} G_0(\varepsilon,\vec{p})\Big]^2$$

the same block is repeated

Collecting the series of similar reducible diagrams we obtain the geometric series: the self-energy

$$\langle G\rangle_{dis} = G_0(\varepsilon,\vec{p})\Big(1+\sum_{n=1}^{\infty}\big[\Sigma(\varepsilon,\vec{p})\,G_0(\varepsilon,\vec{p})\big]^n\Big)$$

$\Sigma =$ 

$\Sigma_1 \qquad \Sigma_2^{(1)} \qquad \Sigma_2^{(2)} \qquad + \dots$

The geometric series solves the Dyson equation

$$\langle G \rangle = \cancel{\langle} G_0 \cancel{\rangle} + G_0 \Sigma \langle G \rangle \quad \text{|| the same } (\varepsilon, \vec{p}) \text{ ||}$$

$$\Rightarrow \quad \langle G^{R/A}(\varepsilon, \vec{p}) \rangle_{dis} = \frac{1}{\varepsilon - \varepsilon(\vec{p}) - \Sigma^{R/A}(\varepsilon, \vec{p})}$$

when $\varepsilon - \varepsilon(\vec{p}) \to G_0^{-1}(\varepsilon, \vec{p})$ and $\Sigma^{R/A}$ respects the retardation, i.e.

$\operatorname{Im} \Sigma^R < 0$; $\operatorname{Im} \Sigma^A > 0$ that's why $\pm i0$ is not needed any longer.

$\operatorname{Re} \Sigma$ - yields a shift of the μ (recall $\varepsilon : \varepsilon - \mu$) and is not important. Let's study $\operatorname{Im} \Sigma$: general calculations are impossible, take only Σ_1:

shift the variable

$\Sigma_1^{R/A} =$ 

$$= \underbrace{\frac{n_{imp} U_0^2}{2\pi}}_{\text{from FT}} \times \int \frac{d^d \vec{q}}{(2\pi)^d} G^{R/A}(\varepsilon, \vec{p} - \vec{q}) =$$

$$= \frac{n_{imp} U_0^2}{2\pi} \int \frac{d^d \vec{q}}{(2\pi)^d} \frac{1}{\varepsilon - \varepsilon(\vec{q}) \pm i0}$$

$\hookrightarrow$ change to $\underbrace{\int \frac{d\Omega_d}{\Omega_d}}_{1} \int \frac{d\xi}{2\pi} \nu(\xi)$

We study only a small vicinity of $\varepsilon_F \Rightarrow$

$$\nu(\xi) \to \nu(\varepsilon_F) \text{ - const}$$

$\Rightarrow$ Neglecting $\mathrm{Re}\,\Sigma_1$:

$$\Sigma_1^{R/A} \simeq \frac{n_{imp} V_0^2}{2\pi} \frac{\nu(\varepsilon_F)}{2\pi} \underbrace{\int \frac{d\xi}{\varepsilon - \xi \pm i0}}_{\mp i\pi \text{ (pole integral)}}$$

$$\mathrm{Im}\left(\Sigma_1^{R/A}\right) \simeq \mp \frac{1}{2} \frac{n_{imp} V_0^2 \nu(\varepsilon_F)}{2\pi}$$

Define $\dfrac{n_{imp} V_0^2 \nu(\varepsilon_F)}{2\pi} \equiv \dfrac{1}{\tau}$ — ellastic collision time (recall the Drude model)

Rewrite $\underbrace{n_{imp} V_0^2}_{\text{const in } \langle VV \rangle} = \dfrac{2\pi}{\nu(\varepsilon_F)\,\tau}$

Finally: $$\boxed{\left\langle G^{R/A}(\varepsilon, \vec{p}) \right\rangle_{dis} \simeq \frac{1}{\varepsilon - \varepsilon(\vec{p}) \pm \frac{i}{2\tau}}}$$ — transl. invariance has been restored!

Start of L4

Note: Σ_2, Σ_3, etc. will change $\tau(n_{imp} V_0^2)$ but the eq. itself will remain

Meaning of the self-energy: consider 3d case, $\varepsilon(\vec{p}) = \frac{p^2}{2m}$

$$G^{R/A}(\varepsilon, \underset{\vec{r}-\vec{r}'}{\vec{R}}) = \int \frac{d^3k}{(2\pi)^3} \frac{e^{i\vec{k}\vec{R}}}{\varepsilon - \frac{k^2}{2m} \pm \frac{i}{2\tau}} =$$

$$= \frac{2m}{(2\pi)^3} \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} k^2\, dk \frac{e^{ikR\cos\theta}}{\underset{2m\varepsilon}{p_\varepsilon^2} - k^2 \pm \frac{im}{\cancel{2}\tau}} =$$

$$= \frac{m}{2\pi^2} \int_0^{\infty} \frac{k^{\cancel{2}}\, dk}{i\cancel{k}R} \frac{e^{ikR} - e^{-ikR}}{p_\varepsilon^2 - k^2 \pm \frac{im}{\cancel{2}\tau}} =$$ change $k \to -k$

$$= \frac{m}{2\pi^2} \frac{1}{iR} \int_{-\infty}^{\infty} dk \frac{k\, e^{ikR}}{p_\varepsilon^2 - k^2 \pm \frac{im}{\cancel{2}\tau}}$$

Poles $k_p = p_\varepsilon \sqrt{1 \pm i \frac{1}{\tau} \frac{m}{\cancel{2} p_\varepsilon^2}}$

For $\varepsilon \sim \varepsilon_F$ $\frac{1}{\tau}\frac{m}{p_\varepsilon^2} \sim \frac{1}{\varepsilon_F \tau} \ll 1$ - the weak disorder limit

$$\Rightarrow K_p \simeq p_\varepsilon\left(1 \pm i\frac{1}{2\tau}\frac{m}{p_\varepsilon^2}\right) = p_\varepsilon \pm i\frac{1}{2\tau}\underbrace{\left(\frac{m}{p_\varepsilon}\right)}_{\to v_\varepsilon} = p_\varepsilon \pm \frac{i}{2}\frac{1}{l_\varepsilon}$$

Note that $l_\varepsilon = l$ at $\varepsilon = \varepsilon_F$.

Calculating the pole integral:

$$G^{R/A}(\varepsilon, \vec{R}) = \frac{m}{2\pi^2 i}\frac{1}{R}\cancel{2\pi i}\left.\frac{\cancel{K} e^{iKR}}{\cancel{2}\cancel{K}}\right|_{K=K_p^{(+)}} \Rightarrow$$

$$G^{R/A}(\varepsilon, \vec{R}) \simeq \underbrace{\frac{m}{2\pi R} e^{\pm i p_\varepsilon R}}_{G_0^{R/A}(\varepsilon, \vec{R}) \text{ at } l_\varepsilon \to \infty} e^{-R/2l_\varepsilon}$$

$$\Rightarrow \boxed{G^{R/A}(\varepsilon \vec{R}) = G_0^{R/A}(\varepsilon R)\, e^{-R/2l_\varepsilon}} \; -$$

due to the disordered potential the Green's function is cut at $|\vec{R}| > l_\varepsilon$. This is because $\vec{R}$ is not a good q-number and the state $|k\rangle$ decays.

Disorder averaged DoS

$$\rho = -\frac{1}{\pi \mathrm{Vol}} \mathrm{Im}\, \mathrm{Tr}\, \hat{G}^R(\varepsilon) = \frac{1}{\pi \mathrm{Vol}} \sum_{\vec{k}} \frac{1/2\tau}{(\varepsilon - \varepsilon_k)^2 + (1/2\tau)^2} \to$$

change to angles - trivial and $\nu_0(\xi)\, d\xi$

$$\frac{1}{2\pi \tau}\int_0^\infty d\xi \frac{\overbrace{\nu_d(\xi)/\mathrm{Vol}}^{\rho_0(\xi)}}{(\xi - \varepsilon)^2 + (1/2\tau)^2}$$

Example: $d = 2$, $\rho_0(\xi) = \rho_0 = \mathrm{const}$

$$\Rightarrow \rho = \frac{\rho_0}{2\pi\tau}\int_0^\infty d\xi \frac{1}{(\xi - \varepsilon)^2 + \frac{1}{(2\tau)^2}} = \frac{\rho_0}{2\pi}\cancel{\frac{1}{2}}\cancel{\tau}\left(\pi + 2\operatorname{atan}(2\varepsilon\tau)\right)$$

$= \frac{\rho_0}{2}\left(\frac{1}{2}+\frac{1}{\pi}\,\mathrm{atang}(2\varepsilon\tau)\right)$

For $\varepsilon \sim \varepsilon_F$ $\varepsilon\tau \gg \tau \Rightarrow \frac{1}{\pi}\,\mathrm{atang}(2\varepsilon\tau) \approx \frac{1}{2} - \frac{1}{2\pi\varepsilon\tau}$

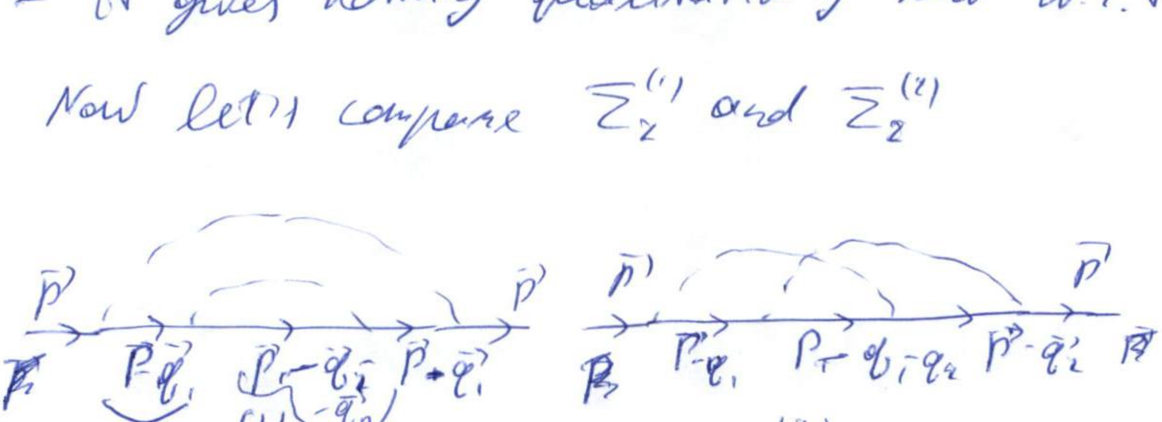
$\Rightarrow \rho \simeq \rho_0\left(1 - \frac{1}{2\pi}\frac{1}{\varepsilon\tau}\right)$ only small deviations from ρ_0 in pure systems.

Shall we go beyond the simplest (Born) approximation?

 can be taken into account as 

– it gives nothing qualitatively new w.r.t. Σ_1

Now let's compare $\Sigma_2^{(1)}$ and $\Sigma_2^{(2)}$



$$(1) \sim \int \frac{d\vec q_{1,2}}{(2\pi)^{2d}}\left(\frac{1}{\varepsilon - \varepsilon(\vec p - \vec q_1) + i/2\tau}\right)^2 \frac{1}{\varepsilon - \varepsilon(\vec p - \vec q_1 - \vec q_2) + i/2\tau}$$

$$= \int \frac{d\vec k_{1,2}}{(2\pi)^{2d}}\left(\frac{1}{\varepsilon - \varepsilon(k_1) + i/2\tau}\right)^2 \frac{1}{\varepsilon - \varepsilon(k_2) + i/2\tau}$$

Similarly

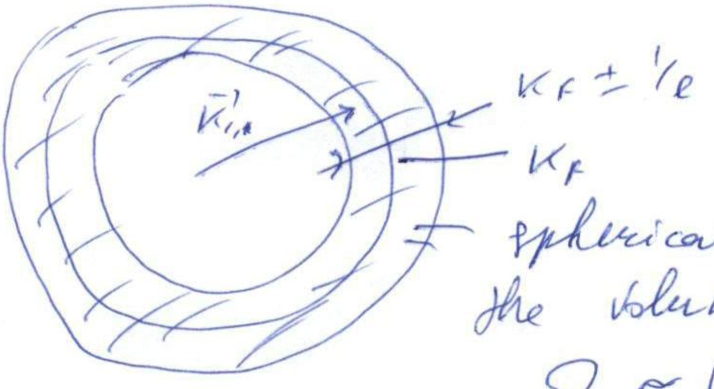
$$(2) \sim \int \frac{d\vec k_{1,2}}{(2\pi)^{2d}} \frac{1}{\varepsilon - \varepsilon(k_1) + i/2\tau}\,\frac{1}{\varepsilon - \varepsilon(k_2) + i/2\tau}\,\frac{1}{\varepsilon - \varepsilon(k_2 - k_1 + \vec p) + i/2\tau}$$

(6-9)

We expect that main contributions come from poles

$\Rightarrow$ $k_F - 1/\ell < |k_{1,2}| < k_F + 1/\ell$ due to broadening by $1/\tau$

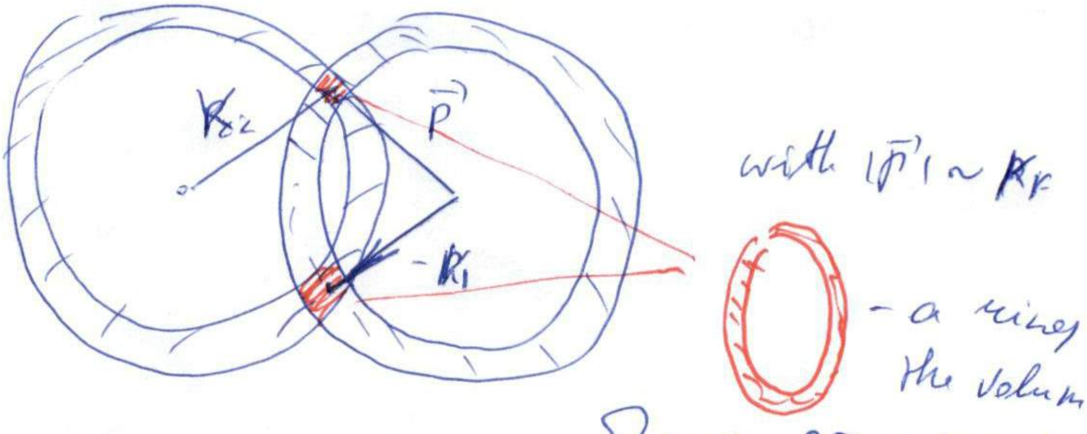
Consider 3d



$\Omega_\ell \simeq (4\pi k_F^2 \Delta k)$ $1/\ell$

But $\Sigma_2^{(2)}$ involves an additional constraint due to

$|k_2 - k_1 + \vec{p}| \simeq k_F$



$\Omega_r \simeq 2\pi k_F (\Delta k)^2$

The ratio of phase spaces:

$$\frac{(\Omega_\ell)^2}{\Omega_\ell \cdot \Omega_r} \sim \frac{\Omega_\ell}{\Omega_r} \propto \frac{k_F^2 \Delta k}{k_F (\Delta k)^2} \sim \boxed{k_F \ell}$$ - i.e., the

$\Rightarrow$ we conclude that

$$\frac{\Sigma_2^{(2)}}{\Sigma_2^{(1)}} \sim \frac{1}{k_F \ell} \sim \frac{a}{\ell} \ll$$ if we consider the limit of weak disorder,

i.e., the diagrams with „crossed-lines" are subleading, $\Sigma_2^{(2)}$ is not needed in our approach!