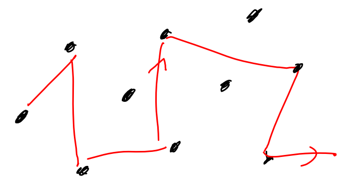
Dis 1

Disordered Systems (Rickayzen, Chapter 4)

"disordered metal": static impurities, from which electrons scatter elastically



- momentum is not conserved, energy is.

Goal: calculate $\mathcal{G}(1,2)$, current, etc.

$$\hat{H} = \hat{H}_{kin} + \hat{H}_{imp} \qquad (\text{no interactions}) \tag{1}$$

$$\hat{H}_{kin} = \sum_{\sigma} \int d\vec{r}\, \psi^{\dagger}_{\sigma}(\vec{r})\, h_0(\vec{r})\, \psi_{\sigma}(\vec{r}) = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} \tag{2}$$

spin [fermions, $\zeta = -1$ from now on]

usual assumption: $\varepsilon_k = \frac{k^2}{2m} - \mu$ (free electrons) (3)

more generally: Bloch bands.

Dis 2

Impurities: (non-magnetic)

$$\hat{H}_{imp} = \sum_{\sigma} \int d\vec{r}\, \hat{\psi}^{\dagger}_{\sigma}(\vec{r})\, \hat{\psi}_{\sigma}(\vec{r})\, U_{imp}(\vec{r}) \tag{1}$$

spin conserved

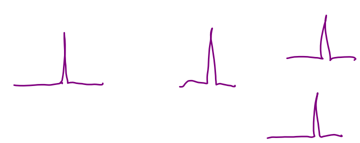
Impurity potential:

$$U_{imp}(\vec{r}) \overset{(2a)}{=} \sum_i U(\vec{r} - \vec{R}_i) \overset{(2b)}{=} \sum_i \frac{1}{Vol} \sum_{\vec{p}} e^{i\vec{p}\cdot(\vec{r}-\vec{R}_i)}\, \tilde{U}(\vec{p}) \tag{2}$$

sum over all impurities; impurity position

$U(\vec{r})$ is impurity scattering potential, typically short-ranged:

e.g. $U(\vec{r}) = U_0\, \delta(\vec{r})$ (3)



then $\tilde{U}(\vec{p}) = U_0$ units: $[U_0]$ = energy per volume (4)

or: broadened δ-function:

Expand $\hat{\psi}_\sigma(\vec{r})$ in basis of plain waves : **Dis 3**

$$\hat{\psi}_\sigma(\vec{r}) = \frac{1}{Vol^{1/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \, c_{\vec{k}\sigma}(t) \qquad (1)$$

wave function is known, simple

time evolution is complicated, since momentum states are not eigenstates of $\hat{H}$.

Comment: alternatively, we could use exact eigenbasis of $\hat{H}$:

$$\hat{H}|\psi_\lambda\rangle = E_\lambda |\psi_\lambda\rangle \quad , \quad \langle \vec{r}|\psi_\lambda\rangle = \psi_\lambda(\vec{r}) \qquad (2a)$$

$$\hat{\psi}_\sigma(\vec{r},t) = \sum_\lambda \psi_\lambda(\vec{r},\sigma) \; c_\lambda(t) \qquad (2b)$$

time evolution known : $e^{-i\xi_\lambda t} c_\lambda$

wave-function unknown

(1) is useful for explicit calculations involving "impurity averaging"

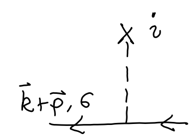
(2) " " " deriving exact relations, valid before impurity averaging.

$\hat{H}_{imp}$ in momentum representation: **Dis 4**

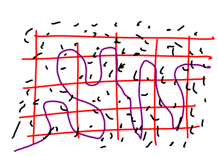
$$\hat{H}_{imp} \overset{(2.1)}{=} \sum_\sigma \int d\vec{r} \left(\frac{1}{Vol} \sum_{\vec{k}\vec{k}'} e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}} \, c^\dagger_{\vec{k}'\sigma} c_{\vec{k}\sigma} \right) \left(\sum_i \frac{1}{Vol} \sum_{\vec{p}} e^{i\vec{p}\cdot(\vec{r}-\vec{R}_i)} \, \hat{u}(\vec{p}) \right) \qquad (1)$$

$$= \delta_{\vec{k}'-\vec{k},\,\vec{p}}$$

$$= \sum_\sigma \sum_{\vec{k},\vec{p}} \frac{1}{Vol} \sum_i e^{-i\vec{p}\cdot\vec{R}_i} \, \tilde{u}(\vec{p}) \; c^\dagger_{\vec{k}+\vec{p},\sigma} c_{\vec{k}\sigma} \qquad (2)$$

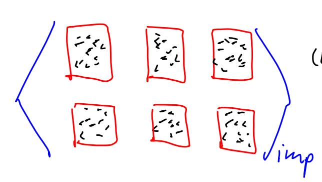


"Impurity averaging": Physical assumption: macroscopic observables (e.g. current) are determined by large regions with very many impurities. Thus, an electron diffusing through the sample "performs an average over impurity positions", because it visit many different regions, in each of which the microscopic placement of impurity positions is different. Thus the system is "self-averaging".



(3)

To model this situation: construct an <u>ensemble</u> of systems that differ only in the placement of their impurity positions, then perform an <u>ensemble average over all impurity positions</u>.



(4)

Dis5

Concretely: $\left\langle f(\vec{R}_i)\right\rangle_{imp} \equiv \frac{1}{Vol}\int d\vec{R}_i \; f(\vec{R}_i) \equiv \left\langle f(\vec{R})\right\rangle_{\vec{R}}$ (1)

$$\left\langle U_{imp}(\vec{r})\right\rangle_{imp} \overset{(2.2a)}{=} \sum_i \left\langle U(\vec{r}-\vec{R}_i)\right\rangle_{imp} = \sum_i \overline{U} = \underbrace{N_{imp}}_{\text{total number of impurities}} \overline{U} \qquad (2)$$

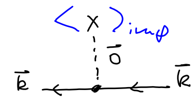
bar denotes imp. average

$$\text{or} \overset{(2.2b)}{=} \sum_i \frac{1}{Vol}\sum_{\vec{p}} \underbrace{\left\langle e^{i\vec{p}\cdot(\vec{r}-\vec{R}_i)}\right\rangle_{imp}}_{\delta_{\vec{p},0}} \tilde{U}(\vec{p}) = \frac{N_{imp}}{Vol}\tilde{U}(0) \underset{(2.4)}{=} C_{imp}\,\tilde{U}(0) \qquad (3)$$

impurity concentration

$$\left\langle \hat{H}_{imp}\right\rangle_{imp} \overset{(4.2)}{=} \sum_\sigma \sum_{\vec{k},\vec{p}} \overbrace{\frac{1}{Vol}\sum_i}^{C_{imp}} \overbrace{\left\langle e^{-i\vec{p}\cdot\vec{R}_i}\right\rangle_{imp}}^{\delta_{\vec{p},0}} \tilde{U}(\vec{p})\, c^\dagger_{\vec{k}+\vec{p},\sigma} c_{\vec{k}\sigma} \qquad (4)$$

$$= \sum_{\vec{k}\sigma} \underbrace{U_0\, C_{imp}}\, c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \qquad (5)$$



Note: momentum conservation after imp. averaging!!

Can be absorbed into $\varepsilon(k)$ by constant shift of chemical potential: $\mu \to \mu - \tilde{U}(0)\,C_{imp}$

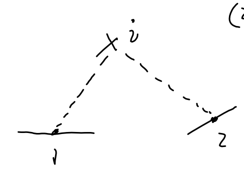
So, set $\left\langle U_{imp}(\vec{r})\right\rangle_{imp} = C_{imp}\,U_0 \equiv 0$ without loss of generality. (6)

Dis6

$$\left\langle U_{imp}(\vec{r}_1)\,U_{imp}(\vec{r}_2)\right\rangle_{imp} = \sum_{i_1,i_2}\left\langle U(\vec{r}_1-\vec{R}_{i_1})\,U(\vec{r}_2-\vec{R}_{i_2})\right\rangle_{imp} \qquad (1)$$

$$= \sum_{i_1\neq i_2}\left\langle U(\vec{r}_1-\vec{R}_{i_1})\right\rangle_{imp}\left\langle U(\vec{r}_2-\vec{R}_{i_2})\right\rangle_{imp} \overset{(5.6)}{=} 0 \qquad (2a)$$

$$+ \sum_{i_1}\left\langle U(\vec{r}_1-\vec{R}_i)\;U(\vec{r}_2-\vec{R}_i)\right\rangle_{imp} \qquad (2b)$$



two scattering off same impurity.

$$= \sum_i \overbrace{\frac{1}{Vol}\int d\vec{R}_i\; U(\vec{r}_1-R_i)\,U(\vec{r}_2-R_i)}^{\equiv\ \left\langle U(\vec{r}_1)U(\vec{r}_2)\right\rangle_{\vec{R}}\ (3a)} \qquad (3)$$

$$= \underbrace{N_{imp}\frac{1}{Vol}}_{C_{imp}}\frac{1}{Vol}\sum_{\vec{p}_1\vec{p}_2}\tilde{U}(\vec{p}_1)\,\tilde{U}(\vec{p}_2)\; e^{i(\vec{p}_1\cdot\vec{r}_1+\vec{p}_2\cdot\vec{r}_2)}\;\underbrace{\frac{1}{Vol}\int d\vec{R}_i\; e^{-i(\vec{p}_1+\vec{p}_2)\cdot\vec{R}_i}}_{\delta_{\vec{p}_1,-\vec{p}_2}} \qquad (4)$$

$$= C_{imp}\frac{1}{Vol}\sum_{\vec{p}_1} e^{i\vec{p}_1\cdot(\vec{r}_1-\vec{r}_2)}\;|\tilde{U}(\vec{p}_1)|^2 \qquad (5)$$

we used $\tilde{U}(-\vec{p}) = \tilde{U}^*(\vec{p})$, which follows from $U(\vec{r}) = U^*(\vec{r})$. (6)

Note: impurity averaging has restored translational invariance!

Dis 7

$\tau_1 \quad \tau_2$

$$\langle \hat H_{imp} \hat H_{imp} \rangle = \sum_{\sigma_1\sigma_2} \int d\vec r_1 \int d\vec r_2 \left(\psi^{\dagger\, k_1'}_{\sigma_1}(\vec r_1)\, \psi^{k_1}_{\sigma_1}(\vec r_1)\right) \left(\psi^{\dagger\, k_2'}_{\sigma_2}(\vec r_2)\, \psi^{k_2}_{\sigma_2}(\vec r_2)\right)_{(\tau_2)} \quad (1)$$

(3.1) $\frac{1}{Vol}\, e^{-i(\vec k_1' - \vec k_1)\vec r_1} \quad \frac{1}{Vol} e^{-i(\vec k_2' - \vec k_2)\cdot \vec r_2}$

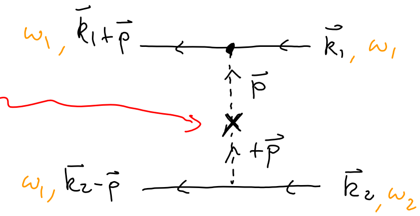
(6.5) $e^{i\vec p\cdot(\vec r_1 - \vec r_2)}$

$\vec k_1' = \vec k_1 + \vec p \,, \quad \vec k_2' = \vec k_2 - \vec p$

$$\times\; N_{imp} \overset{(6.3)}{\langle U(\vec r_1 - \vec R)\, U(\vec r_2 - \vec R)\rangle_{\vec R}}$$

$$= \sum_{\vec k_1 \sigma_1} \sum_{\vec k_2 \sigma_2} \frac{1}{Vol} \sum_{\vec p} C_{imp} |\hat u(\vec p)|^2 \left(c^\dagger_{\vec k_1 + \vec p, \sigma_1}\, c_{\vec k_1, \sigma_1}\right)(\tau_1) \left(c^\dagger_{\vec k_2 - \vec p, \sigma_2}\, c_{\vec k_2, \sigma_2}\right)(\tau_2) \quad (2)$$

- momentum conservation after impurity averaging (3)



- total momentum flowing out of impurity $= \vec 0$ (4)

- no frequency change, since impurity is static! (5)

Dis 8

$$\langle U_{imp}(\vec r_1)\, U_{imp}(\vec r_2)\, U_{imp}(\vec r_3)\rangle_{imp} \quad (1)$$

$$= \sum_{i_1} \sum_{i_2 \neq i_1} \sum_{i_3 \neq i_2, i_1} \langle U(\vec r_1 - R_{i_1})\rangle_{R_{i_1}} \langle U(\vec r_2 - \vec R_{i_2})\rangle_{\vec R_{i_2}} \langle U(\vec r_3 - \vec R_{i_3})\rangle_{\vec R_{i_3}} \quad (2)$$

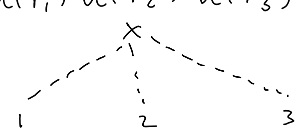
(5.6) $= 0$

$$+ \sum_{i_1} \Big(\sum_{i_2 = i_3 \neq i_1} \Big) \langle U(\vec r_1 - R_{i_1})\rangle_{\vec R_{i_1}} \langle U(\vec r_2 - R_{i_2})\; U(\vec r_2 - R_{i_2})\rangle_{\vec R_{i_2}} \quad (3)$$

$$+ \sum_{i_1 = i_2 = i_3} \langle U(\vec r_1 - R_{i_1})\, U(\vec r_2 - \vec R_{i_1})\; U(\vec r_3 - \vec R_{i_1})\rangle_{\vec R_i}. \quad (4)$$

$$= N_{imp} \langle U(\vec r_1)\, U(\vec r_2)\, U(\vec r_3)\rangle_{\vec R} \quad (5)$$

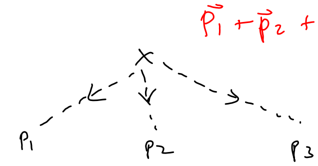
(notation analogous to 7.3a)



$\frac{1}{Vol} \int d\vec R\; e^{i\vec p_1(\vec r_1 - \vec R)}\, e^{i\vec p_2(\vec r_2 - \vec R)}\, e^{i\vec p_3(\vec r_3 - \vec R)}$

after Fourier transforming, this will yield

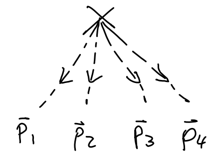
$\vec p_1 + \vec p_2 + \vec p_3 = 0$



Dis9

$$\langle U_{imp}(\vec{r}_1)\, U_{imp}(\vec{r}_2)\, U_{imp}(\vec{r}_3)\, U_{imp}(\vec{r}_4)\rangle_{imp} \qquad (1)$$

$$= N_{imp} \langle u(\vec{r}_1)\, u(\vec{r}_2)\, u(\vec{r}_3)\, u(\vec{r}_4)\rangle \implies \sum_{i=1}^{4} \vec{p}_i = 0$$



multiple scatterings off single impurity

(2)

$$+ N_{imp}^2 \left\{ \begin{array}{l} \langle u(\vec{r}_1)\, u(\vec{r}_2)\rangle \langle u(\vec{r}_3)\, u(\vec{r}_4)\rangle \\ + \quad 1 \quad 3 \qquad 2 \quad 4 \\ + \quad 1 \quad 4 \qquad 2 \quad 3 \end{array} \right\} \qquad (3)$$

in general: sum over all possible pairings

$\vec{p}_1$	$\vec{p}_2$	$\vec{p}_3$	$\vec{p}_4$
1	3	2	4
1	4	2	3

double scattering off two separate impurities

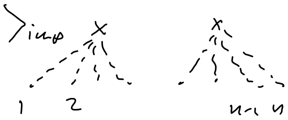
Dis10

Generally: $\langle U_{imp}(\vec{r}_1) \;\ldots\; U_{imp}(\vec{r}_n)\rangle_{imp}$

$$= N_{imp} \langle u(\vec{r}_1) \ldots\ldots u(\vec{r}_n)\rangle_{imp}$$

$$+ N_{imp}^2 \sum \langle u(\vec{r}_1)\, u(\vec{r}_2) \ldots\rangle_{imp} \langle \ldots\ldots u(\vec{r}_{n-1})\, u(\vec{r}_n)\rangle_{imp}$$

all possible pairings of indices involving two averages



$$+ N_{imp}^3 \sum_{3\text{ averages}} \langle \quad \rangle_{imp} \langle \quad \rangle_{imp} \langle \quad \rangle_{imp}$$

$+ \ldots$

But: $u(\vec{r}) = \frac{1}{Vol} \sum_{\vec{p}} e^{i\vec{p}\cdot\vec{r}}\, \hat{u}(\vec{p})$ (1)

and each $\langle \quad \rangle_{imp}$ yields a Kronecker $\delta_{\vec{p}_1+\ldots+\vec{p}',0}$

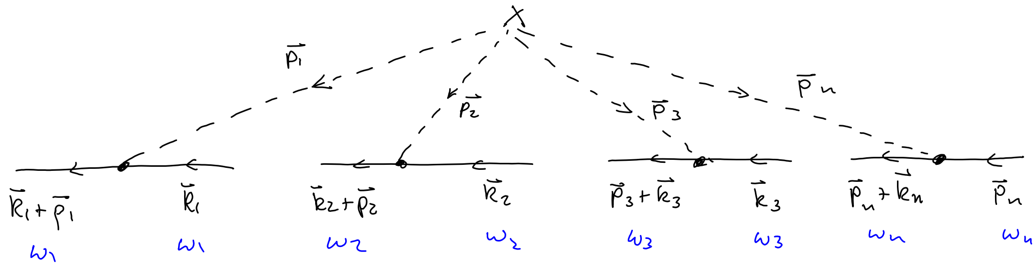
which kills one momentum sum, leaving a left-over factor $\frac{1}{Vol}$.

So, we get $\frac{(N_{imp})^m}{(Vol)^m} \left(\sum_{\vec{p}} \delta_{\vec{p}+\ldots,0}\right)^m \sim (c_{imp})^m$ (2)

Dis 11

For "weak disorder", c_{imp} is small, and we can <u>neglect</u> all contributions $(c_{imp})^m$ with $m \geq 2$

<u>Feynman rule for contribution linear in c_{imp}</u>



$$N_{imp} \frac{1}{(Vol)^n} \sum_{\vec{p}_1 \ldots \vec{p}_n} \hat{u}(\vec{p}_1) \ldots \hat{u}(\vec{p}_n) \quad \delta_{\vec{p}_1 + \ldots + \vec{p}_n,\, \vec{0}} \qquad (1)$$

Overall $(-)^n$ is absorbed in $(\mathcal{G})^n = (-\langle\ \rangle)^n$ (2)

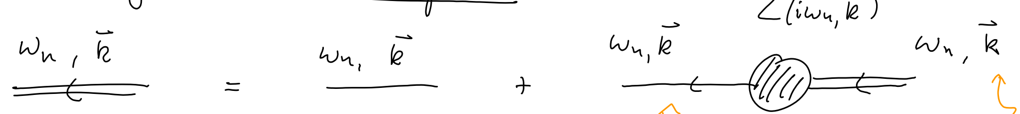
from $(-H_{imp})^n$

each inserting of impurity line changes

$\mathcal{G} \sim -\langle \psi_1 \psi_2^+ \rangle \to -\langle \psi_1 (-\psi_i^+ \psi_i) \psi_2 \rangle \sim (\mathcal{G})^2$

Dis 12

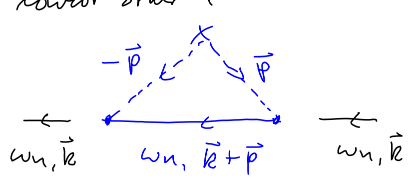
<u>1-Particle GF for disordered system</u>



(1)

due to momentum conservation at each impurity, $\vec{k}_{in} = \vec{k}_{out}$.

Self-energy to lowest order $(n=2)$ (2)

$\Sigma(i\omega_n, \vec{k}) =$ 

$= \frac{N_{imp}}{(Vol)^2} \sum_{\vec{p}} \tilde{u}(\vec{p}) \tilde{u}(-\vec{p})\, \mathcal{G}^{(0)}(i\omega_n, \vec{k}+\vec{p})$

$\vec{p}\,' = \vec{k} + \vec{p}$

$$= c_{imp} \int d\varepsilon_{p'}\, \mathcal{N}(\varepsilon_{p'}) \int \frac{d\Omega_{p'}}{4\pi} |\tilde{u}(\vec{k} - \vec{p}\,')|^2 \frac{1}{i\omega_n - \varepsilon_{\vec{p}\,'}} \qquad (3)$$

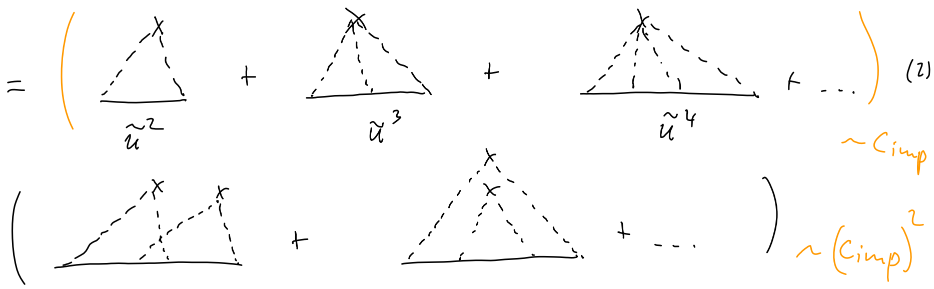
Life-time: $$\frac{1}{2\tau_k(\omega)} \equiv -\mathrm{Im}\, \Sigma_1(\omega + i0^+, \vec{k}) \qquad (4)$$

$$= c_{imp}\, \mathrm{Im} \Big\{ (-i\pi)\, \mathcal{N}(\varepsilon_F) \underbrace{\int d\varepsilon_{p'} \int \frac{d\Omega_{p'}}{4\pi} |\tilde{u}(\vec{k} - \vec{p}\,')|^2 \delta(\omega - \varepsilon_{p'})}_{\equiv\, \overline{|\tilde{u}_{\vec{k}}|^2}} \Big\} = 2\pi\, c_{imp}\, \mathcal{N}(\varepsilon_F)\, \overline{|\tilde{u}_{\vec{k}}|^2}$$

average over all directions (5)

More generally: $\boxed{\text{Dis 13}}$

$\Sigma(i\omega_n, \vec{k}) =$



+

for "weak scattering potential", assume "$\tilde{u}$ is small",

keep only $\tilde{u}^2$ terms, which yields (12.2)