Conductivity: Response to an applied field (Rickayzen, § 4.3)

$\boxed{\text{Dis 26}}$

Electric field: $\vec{E}(\vec{r},t) = -\vec{\nabla} V - \partial_t \vec{A}$ (1)

We choose gauge for which $V(\vec{r},t) = 0$ (2)

For free electrons, $\varepsilon_k = \frac{k^2}{2m} - \mu$, we then have:

$$\hat{H} = \sum_\sigma \int d\vec{r} \; \psi^\dagger_\sigma(\vec{r}) \Big[\frac{1}{2m} \big(\underbrace{-i\vec{\nabla}\hbar - e\vec{A}}_{} \big)^2 + U_{imp}(\vec{r}) \Big] \hat{\psi}_\sigma(\vec{r}) \quad (3)$$

"minimal coupling", ensures gauge invariance under

$$\psi \to e^{i\phi}\psi, \quad \vec{A} \to \vec{A} + \frac{1}{e}\vec{\nabla}\phi \quad (4)$$

$\vec{A}$-independent

$$= H_0 + H'(t) \quad (5)$$

$\boxed{\text{Dis 27}}$

$$H'(t) = \frac{ie\hbar}{2m} \sum_\sigma \int d\vec{r} \; \psi^\dagger_\sigma(\vec{r}) \big(\vec{A}\cdot\vec{\nabla} + \underbrace{\vec{\nabla}\cdot\vec{A}}_{= -\overleftarrow{\nabla}\cdot\vec{A} \text{ after int. by parts}} \big) \psi_\sigma(\vec{r}) \quad (1)$$

$$= -\sum_\sigma \int d\vec{r}_2 \; \vec{A}(2) \cdot \underbrace{\vec{j}_{22'} \psi^\dagger_\sigma(\vec{r}_{2'}) \psi_\sigma(\vec{r}_2) \Big|_{\vec{r}_{2'} = \vec{r}_2,\; t_{2'} = t_2 + 0^+}}_{\hat{\vec{j}}_\sigma(\vec{r}_2)} \equiv -\sum_\sigma \int d\vec{r}_2 \; \vec{A}(2) \cdot \hat{\vec{j}}(\vec{r}_2) \quad (2)$$

where $\vec{j}_{22'} \equiv -\frac{ie\hbar}{2m} \big(\vec{\nabla}_2 - \vec{\nabla}_{2'} \big)$ (3)

Now, velocity in presence of vector potential is classically defined as

$$\vec{v} = (\vec{p} - e\vec{A})/m, \quad \text{and current is} \quad \vec{j} = e\vec{v}\cdot n \quad (4)$$

Hence, current operator describing total current density is:

$$\hat{\vec{J}}_{tot}(\vec{r}_1) = \sum_{\sigma_1} \Big(\overset{(a)}{\vec{j}_{11'}} - \overset{(b)}{\frac{e^2}{m} \vec{A}(1)} \Big) \underbrace{\psi^\dagger_\sigma(\vec{r}_{1'}) \psi_\sigma(\vec{r}_1)}_{\equiv \hat{n}_{\sigma,11'}} \Big|_{\vec{r}_1' = \vec{r}_1} \quad (5)$$

DIS 28

Linear (in $\vec{A}$) response of $\hat{J}_{tot}$ to $\hat{H}'(t)$ is :

$\in (x,y,z)$ (b)   gives factor 2   "diamagnetic term" [current is induced that opposes external B-field]

$$\langle \delta \hat{J}^{\alpha}_{tot}(t_1,\vec{r}_1) \rangle = - \frac{e^2}{m} A^{\alpha}(1) \sum_{\sigma_1} \underbrace{\langle \hat{n}_{\sigma,1'1} \rangle}_{= \bar{n}_{\sigma_1} = \text{average density per spin}} \tag{1}$$

(a), Kubo   (27.5)   (27.2)

$$+ \int_{-\infty}^{\infty} dt_2 \, (-i)\,\theta(t_1 - t_2) \, \langle [J^{\alpha}_{tot}(t_1,\vec{r}_1) , H'(t_2)] \rangle \tag{2}$$

average over spin

$$= -2 \int_{-\infty}^{\infty} dt_2 \int d\vec{r}_2 \sum_{\beta = x,y,z} A^{\beta}(2) \underbrace{j^{\alpha}_{1''} \, j^{\beta}_{22'} \, (-i)\,\theta(t_1-t_2) \frac{1}{2}\sum_{\sigma_1\sigma_2} \langle [\psi^{\dagger}_{\sigma_1}(1')\psi_{\sigma_1}(1) , \psi^{\dagger}_{\sigma_2}(2')\psi_{\sigma_2}(2)] \rangle}_{\overset{(4')}{=}\, \mathcal{G}^R_{\alpha\beta}(t_1-t_2,\, \vec{r}_1-\vec{r}_2)} \tag{3}$$

gives factor 2

$$= \left[-\frac{2e^2}{m} \bar{n}_{\sigma_1} A(1) - 2 \int_{-\infty}^{\infty} dt_2 \int d\vec{r}_2 \sum_{\beta} A^{\beta}(2) \, \mathcal{G}^R_{\alpha\beta}(t_1 - t_2, \vec{r}_1 - \vec{r}_2) \right] \tag{4}$$

transl. invariant after impurity averaging

to disentangle the convolution, Fourier transform!

DIS 29

$$\vec{E}(t_2,\vec{r}_2) = \int \frac{d\omega}{2\pi} e^{-i\omega t_2} \, e^{i\vec{q}\cdot\vec{r}_2} \, \vec{E}(\omega,\vec{q}) \tag{1}$$

Analogously for $\vec{A}(2)$, with $A^{\alpha}(\omega,\vec{q}) = \dfrac{E^{\alpha}(\omega,\vec{q})}{i\omega}$ (since $\vec{E} \overset{(26.1)}{=} -\partial_t \vec{A}$)   (2)

$$\Rightarrow \quad \delta J^{\alpha}(\omega,q) \overset{(28.4)}{=} \sum_{\beta} \sigma_{\alpha\beta}(\omega,q) \, E^{\beta}(\omega,q) \tag{3}$$

by definition, this is the "conductivity"

$$\text{with} \quad \sigma_{\alpha\beta}(\omega,q) = -2 \left[\mathcal{G}^R_{\alpha\beta,\sigma_1}(\omega,\vec{q}) + \delta_{\alpha\beta} \frac{e^2}{m} \bar{n}_{\sigma_1} \right] \frac{1}{i\omega} \tag{4}$$

"conductivity tensor"   can be calculated via Matsubara $\bar{\mathcal{G}}_{\alpha\beta}(i\omega_n,\vec{q})$ "diamagnetic term"

Dis 30

We need the Matsubara transform of:

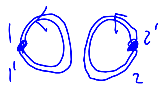
$$\mathcal{G}_{\alpha\beta}(1,2) \overset{(28.3)}{\equiv} - j^{\alpha}_{11'} j^{\beta}_{22'} \; \frac{1}{2}\sum_{\sigma_1\sigma_2} \underbrace{\langle T_\tau \psi^\dagger_{\sigma_1}(1') \psi_{\sigma_1}(1) \psi^\dagger_{\sigma_2}(2') \psi_{\sigma_2}(2) \rangle}_{\text{quantum and thermal averaging (not yet imp. ave.)}} \tag{1}$$

(a) (b)

Wick's theorem applies, since $H_0 = H_{kin} + H_{imp}$ is quadratic.

$$= -\frac{1}{2}\sum_{\sigma_1\sigma_2} \langle \underset{= 0}{\hat{j}^{\alpha}(1)} \rangle \langle \underset{= 0}{\hat{j}^{\beta}(2)} \rangle + j^{\alpha}_{11'} j^{\beta}_{22'} \underbrace{\frac{1}{2}\sum_{\sigma_1\sigma_2} \mathcal{G}(1,2')\,\mathcal{G}(2,1')}_{\equiv\, \mathcal{G}\mathcal{G}(\tau_1-\tau_2;\, r_1, r_2';\, r_2, r_1')} \tag{2}$$

(a) (b) spin dependence is averaged out; drop σ-index from now on.



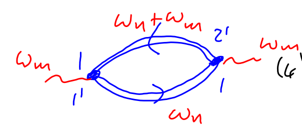
since no current flows if $\vec{E} = 0$

Matsubara-transform:

$$\overline{\mathcal{G}\mathcal{G}}(i\omega_m, r_1, r_2'; r_2, r_1') = \int d\tau_{12}\, e^{i\omega_m \tau_{12}} \frac{1}{\beta^2} \sum_{\omega_m \omega_\ell} e^{-i(\omega_\ell - \omega_n)\tau_{12}} \times \bar{\mathcal{G}}(i\omega_\ell, r_1, r_2')\, \bar{\mathcal{G}}(i\omega_n, r_2, r_1') \tag{3}$$

↑ Bose frequency; $\beta\,\delta_{\omega_\ell, \omega_n+\omega_m}$; Fermi

$$= \frac{1}{\beta}\sum_{\omega_n} \bar{\mathcal{G}}(i\omega_m + i\omega_n;\, 1, 2')\, \bar{\mathcal{G}}(i\omega_n, 2, 1') \tag{4}$$



Dis 31

To perform the Matsubara sum with specific knowledge of correlators (whose real-space form in presence of disorder is complicated!), use spectral representation:

$$\overline{\mathcal{G}\mathcal{G}}(i\omega_m, r_1, r_2'; r_2, r_1') \overset{(17.4)}{=} \int d\bar\omega \int d\bar\omega'\, \mathcal{A}(\bar\omega'; 1,2')\, \mathcal{A}(\bar\omega; 2,1') \underbrace{\frac{1}{\beta}\sum_{\omega_n} \frac{1}{i\omega_m + i\omega_n - \bar\omega'} \frac{1}{i\omega_n - \bar\omega}}_{\frac{n_F(\bar\omega) - n_F(\bar\omega')}{i\omega_m - \bar\omega' + \bar\omega} \;=\; S(i\omega_m) \text{ from (GF68.2)}} \tag{1}$$

(GF68.6)

analytically continue: $i\omega_m \to \omega + i0^+$;

$$\mathcal{G}\mathcal{G}^R(\omega; r_1, r_2'; r_2, r_1') = \int d\bar\omega \int d\bar\omega'\, \overset{(a)}{\mathcal{A}(\bar\omega'; 1,2')}\, \overset{(b)}{\mathcal{A}(\bar\omega; 2,1')} \frac{n_F(\bar\omega)}{\omega + i0^+ + \bar\omega - \bar\omega'} \tag{2}$$

($\bar\omega \leftrightarrow \bar\omega'$ in 2nd term):

$$+ \int d\bar\omega' \int d\bar\omega\, \overset{(c)}{\mathcal{A}(\bar\omega; 1,2')}\, \overset{(d)}{\mathcal{A}(\bar\omega'; 2,1')} \frac{n_F(\bar\omega)}{\bar\omega - \omega - i0^+ - \bar\omega'}$$

Insert $\mathcal{A} = \frac{i}{2\pi}(\mathcal{G}^R - \mathcal{G}^A)$ (3)

$$= \frac{i}{2\pi} \int d\bar\omega\, n_F(\bar\omega) \left\{ \overset{(a)}{\mathcal{G}^R(\omega+\bar\omega; 1,2')} \overset{(b)}{\left[\mathcal{G}^R - \mathcal{G}^A\right](\bar\omega; 2,1')} + \overset{(c)}{\left[\mathcal{G}^R - \mathcal{G}^A\right](\bar\omega; 1,2')} \overset{(d)}{\mathcal{G}^A(\bar\omega - \omega; 2,1')} \right\} \tag{4}$$

$\boxed{\text{Dis32}}$

$$\mathcal{G}\mathcal{G}^R(\omega; r_1, r_2'; r_2, r_1') = \mathcal{G}\mathcal{G}^{RA} + \mathcal{G}\mathcal{G}^{RR+AA} \qquad (0)$$

$\bar\omega - \omega \to \bar\omega$ in 2nd term

$$\mathcal{G}\mathcal{G}^{RA}(\omega; r_1, r_2'; r_2, r_1') = -\frac{i}{2\pi}\int d\bar\omega \left\{ n_F(\bar\omega) - n_F(\omega+\bar\omega) \right\} \mathcal{G}^R(\omega+\bar\omega; 1, 2')\, \mathcal{G}^A(\bar\omega; 2, 1') \qquad (1)$$

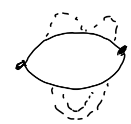
$$\mathcal{G}^{RR+AA}(\omega; r_1, r_2'; r_2, r_1') = \frac{i}{2\pi}\int d\bar\omega \Big\{ n_F(\bar\omega)\, \mathcal{G}^R(\omega+\bar\omega; 1, 2')\, \mathcal{G}^R(\bar\omega; 2, 1') - n_F(\omega+\bar\omega)\, \mathcal{G}^A(\omega+\bar\omega; 1, 2')\, \mathcal{G}^A(\bar\omega; 2, 1') \Big\} \qquad (2)$$

We'll consider first $\mathcal{G}\mathcal{G}^{RA}$ (yields Drude conductivity),

then $\mathcal{G}\mathcal{G}^{RR+AA}$ (cancels diamagnetic contribution)

Now perform disorder average, in the approximation

$$\langle \mathcal{G}^X \mathcal{G}^Y \rangle_{imp} \simeq \langle \mathcal{G}^X \rangle_{imp} \langle \mathcal{G}^Y \rangle_{imp} \qquad (3)$$



(included)

thus neglecting impurity lines that connect $\mathcal{G}^X$ and $\mathcal{G}^Y$, such as

(neglected)
(will be considered later)