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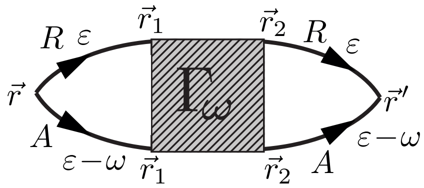
Sheet 5: Diffuson and conductivity

Exercise 1: Diffuson in reciprocal space

In reciprocal space, the two-particle vertex function Γ_ω can be expressed in terms of a geometric series, which can be used to derive a particularly simple expression for the probability P_d.

The probability $P_d(\vec{r}, \vec{r}\,', \omega)$ has the following diagrammatic representation

$P_d(\vec{r}, \vec{r}\,', \omega) =$



$$= \frac{1}{2\pi\rho_0} \int d\vec{r}_1 d\vec{r}_2 \; G^R_\varepsilon(\vec{r}, \vec{r}_1) G^R_\varepsilon(\vec{r}_1, \vec{r}\,') G^A_{\varepsilon-\omega}(\vec{r}, \vec{r}_1) G^A_{\varepsilon-\omega}(\vec{r}_2, \vec{r}\,') \Gamma_\omega(\vec{r}_1, \vec{r}_2), \tag{1}$$

where the two-particle vertex function Γ_ω can be obtained by summing up all orders of elementary collision processes of amplitude $\gamma = 1/(2\pi\rho_0\tau_e)$:

$$\begin{aligned} \Gamma_\omega(\vec{r}_1, \vec{r}_2) &= \gamma \; \delta(\vec{r}_1 - \vec{r}_2) + \gamma \int d\vec{r}\,'' \; \Gamma_\omega(\vec{r}_1, \vec{r}\,'') G^R_\varepsilon(\vec{r}\,'', \vec{r}_2) G^A_{\varepsilon-\omega}(\vec{r}_2, \vec{r}\,'') \\ &= \gamma \; \delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{\tau_e} \int d\vec{r}\,'' \; \Gamma_\omega(\vec{r}_1, \vec{r}\,'') P_0(\vec{r}\,'', \vec{r}_2, \omega). \end{aligned}$$

Here, $P_0(\vec{r}, \vec{r}\,', \omega) = \gamma\tau_e G^R_\varepsilon(\vec{r}, \vec{r}\,') G^A_{\varepsilon-\omega}(\vec{r}\,', \vec{r})$ is the probability, that a particle at $\vec{r}$ arrives at $\vec{r}\,'$ without *any* collision.
Show that, for a translation invariant system (i.e. after disorder averaging), the Fourier transform of the vertex function factorizes and is given by (Ω is the system's volume)

$$\Gamma_\omega(\vec{q}) = \gamma + \frac{1}{\tau_e} \Gamma_\omega(\vec{q}) \overbrace{\frac{\gamma\tau_e}{\Omega} \sum_{\vec{k}} G^R_\varepsilon(\vec{k}) G^A_{\varepsilon-\omega}(\vec{k} - \vec{q})}^{P_0(\vec{q}, \omega)}$$

and that the vertex is given by the geometric series

$$\Gamma_\omega(\vec{q}) = \frac{\gamma}{1 - P_0(\vec{q}, \omega)/\tau_e}.$$

Similarly, one can show that the Fourier transform of Eq.(1) factorizes as well

$$P_d(\vec{q}, \omega) = 2\pi\rho_0 P_0(\vec{q}, \omega)^2 \Gamma_\omega(\vec{q}) = P_0(\vec{q}, \omega) \frac{P_0(\vec{q}, \omega)/\tau_e}{1 - P_0(\vec{q}, \omega)/\tau_e}. \tag{2}$$

Use the explicit expressions for the disorder averaged single-particle Green's functions,

$$G_\varepsilon^{R/A}(\vec{k}) = \frac{1}{\varepsilon - \varepsilon(\vec{k}) \pm \frac{i}{2\tau_e}},$$

and linearize the dispersion $\varepsilon(\vec{k}-\vec{q}) \simeq \varepsilon(k) - \vec{v}\cdot\vec{q}$ (where $\vec{v} = \nabla_{\vec{k}}\,\varepsilon$ is the group velocity) to show that $P_0(\vec{q},k)$ can be written as (for $|k| \ll |q|$)

$$P_0(\vec{q},k) = \tau_e \int d\Omega_d \frac{1}{1 - i\omega\tau_e + i\vec{v}\vec{q}\tau_e},$$

where Ω_d is the solid angle in d dimensions.

Exercise 2: Conductivity

The goal of this exercise is to derive the Kubo formula for the linear response electric conductivity of a disordered metal.

Switching on an infinitesimal electrical field $\vec{E}$ in a metal induces a current density $\vec{j} = \sigma\vec{E}$, where the tensor σ is called the conductivity. The corresponding Hamiltonian can be written as

$$\mathcal{H} = \frac{[\vec{p} + e\vec{A}(t)]^2}{2m} + V(\vec{r}), \tag{3}$$

where the irrotational vector potential $\vec{A}$ generates an electric field:

$$\vec{E} = -\frac{\partial\vec{A}}{\partial t}\ , \ \nabla\times\vec{A} = \vec{H} = 0. \tag{4}$$

The current density is then given by $\vec{j} = Tr\{\rho\hat{j}\}$, where $\hat{j}$ is the current density operator and $Tr\{\}$ denotes the trace over all states. The single-particle density operator ρ obeys the Heisenberg equation of motion

$$i\hbar\frac{\partial\rho}{\partial t} = [\mathcal{H},\rho]. \tag{5}$$

We write the density operator as $\rho = \rho_0 + \delta\rho$, where ρ_0 corrsponds to $\vec{A} = 0$, and regularize the long time evolution by adding $-i\gamma(\rho - \rho_{\rm eq})$. Hence, the time evolution now reads

$$i\hbar\frac{\partial\rho}{\partial t} = [\mathcal{H},\rho] - i\gamma(\rho - \rho_{\rm eq}). \tag{6}$$

Furthermore, we introduce $\delta\rho_{\rm eq} = \rho_{\rm eq} - \rho_0$ and approximate the Hamiltonian in linear response by $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, with $\mathcal{H}_1$ being linear in $\vec{A}$. Show that in linear order of $\vec{A}$ the equation of motion reads

$$i\hbar\frac{\partial\delta\rho}{\partial t} = [\mathcal{H}_0,\delta\rho] + [\mathcal{H}_1,\rho_0] - i\gamma(\delta\rho - \delta\rho_{\rm eq}) \tag{7}$$

and that the current density operator can be written similar to the Hamiltonian as $\hat{j} = \hat{j}_0 + \hat{j}_1$ with

$$\hat{j}_0 = -\frac{e}{2m}\left(\hat{n}(\vec{r})\vec{p} + \vec{p}\,\hat{n}(\vec{r})\right),$$
$$\hat{j}_1 = -\frac{e^2}{2m}\left(\hat{n}(\vec{r})\vec{A} + \vec{A}\,\hat{n}(\vec{r})\right), \tag{8}$$

which implies, that the current in linear response becomes

$$\vec{j} = Tr\{\rho(t)\hat{j}\} \simeq Tr\{\rho_0\hat{j}_1\} + Tr\{\delta\rho(t)\hat{j}_0\}. \tag{9}$$

Suppose, that you know the full set $\{|\alpha\rangle, \varepsilon_\alpha\}$ of eigenstates and eigenenergies of the unperturbed many-body Hamiltonian $\mathcal{H}_0$. Furthermore Fourier transform Eq.(7) and use the invariance of the trace under basis change to get (for an electric field applied in x-direction)

$$\sigma_{xx} = \frac{i}{\omega}\left[\frac{ne^2}{m} + \frac{e^2}{m^2\Omega}\sum_{\alpha\beta}\frac{f(\varepsilon_\alpha) - f(\varepsilon_\beta)}{\varepsilon_\alpha - \varepsilon_\beta}\frac{\varepsilon_\alpha - \varepsilon_\beta - i\gamma}{\varepsilon_\alpha - \varepsilon_\beta - \hbar\omega - i\gamma}|\langle\alpha|p_x|\beta\rangle|^2\right]. \tag{10}$$

Use the so called f-sum rule

$$n + \frac{1}{m\Omega}\sum_{\alpha\beta}\frac{f(\varepsilon_\alpha) - f(\varepsilon_\beta)}{\varepsilon_\alpha - \varepsilon_\beta}|\langle\alpha|p_x|\beta\rangle|^2 = 0 \tag{11}$$

to rewrite the conductivity as

$$\sigma_{xx}(\omega) = -s\frac{\pi\hbar}{\Omega}\sum_{\alpha\beta}\frac{f(\varepsilon_\alpha) - f(\varepsilon_\beta)}{\varepsilon_\alpha - \varepsilon_\beta}\frac{\frac{e^2}{m^2}|\langle\alpha|p_x|\beta\rangle|^2}{\varepsilon_\alpha - \varepsilon_\beta - \hbar\omega - i\gamma} \tag{12}$$

with spin s. Shop that in the zero temperature limit this can be written as

$$\mathrm{Re}\,\sigma_{xx}(\varepsilon_F, \omega) = s\frac{\hbar}{\pi\Omega}Tr\left[\hat{j}_x\ \mathrm{Im}G^R_{\varepsilon_f}\ \hat{j}_x\ \mathrm{Im}G^R_{\varepsilon_F - \hbar\omega}\right], \tag{13}$$

which is the well known Kubo formula for conductivity.