Lectures 5,6: Boltzmann kinetic equation

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Fall 2008 8.513 “Quantum Transport”

- Distribution function, Liouville equation
- Boltzmann collision integral, general properties
- Irreversibility, coarse graining, chaotic dynamics
- Relaxation of angular harmonics
- Example: Drude conductivity
- Diffusion equation
- Magnetotransport
- Quantizing fields: Shubnikov-de Haas oscillations
- Transport in a long-range disorder
**Scattering by randomly placed impurities**

Disorder potential $V(r) = \sum_j V(r - r_j)$. B.k.e. takes the form

$$\frac{df}{dt} \equiv Lf = \int w(p, p')(f(p') - f(p)) \frac{d^2p'}{(2\pi\hbar)^2}$$

where $L = \partial_t + v \nabla_r + F \nabla_p$ is the Liouville operator.

In the Born approximation $w(p, p') = 2\pi|V_{p-p'}|^2\delta(\epsilon_p - \epsilon_{p'})$. Writing $\int \frac{d^2p'}{(2\pi\hbar)^2} = \oint \frac{d\theta_{p'}}{2\pi} \int \nu d\epsilon_{p'}$ with the density of states $\nu = dN/d\epsilon = m/(2\pi\hbar^2)$ find

$$\frac{df}{dt} = \nu \int d\theta_{p'}|V_{p-p'}|^2(f(p') - f(p))$$

where $|p'| = |p|$.
**Relaxation of Angular Harmonics**

For spatially uniform system \((L = \partial_t)\) analyze the angular dependence of the collision integral in B.k.e.

\[
\frac{df}{dt} \equiv Lf = \nu \int \frac{d\theta p'}{2\pi} w(\theta_p - \theta_{p'})(f(p') - f(p))
\]

Use the Fourier series

\[
f(p) = \sum_m e^{im\theta} \tilde{f}_m, \quad \nu w(\theta_p - \theta_{p'}) = \sum_m \gamma_m e^{im(\theta_p - \theta_{p'})}
\]

where \(\tilde{f}_0 = \oint f(p') \frac{d\theta p'}{2\pi}\) is proportional to the total particle number, \(\tilde{f}_{\pm 1} = \oint e^{\mp i\theta p'} f(p') \frac{d\theta p'}{2\pi}\) are proportional to the particle current density components \(j_x \pm ij_y\), etc. For the collision integral we have

\[
St(\tilde{f}_m) = (\gamma_m - \gamma_0)\tilde{f}_m, \quad \tilde{f}_m(t) \propto e^{-(\gamma_0 - \gamma_m)t}
\]

Relaxation for \(m \neq 0\) because \(\gamma_m \neq 0 < \gamma_0\); no relaxation for \(\tilde{f}_0\) (particle number conservation)
**Example: Drude conductivity**

For a spatially uniform system the Boltzmann kinetic equation

\[(\partial_t + v \nabla_r + eE \nabla_p) f(r, p) = St(f)\]

becomes

\[eE \nabla_p f(p) = St(f)\]

Solve for the perturbation of the distribution function due to the \(E\) field:

\[f(p) = f_0(p) + f_1(p) + ..., \quad f_1 \propto \cos \theta, \sin \theta\]

where \(f_0\) is isotropic. To the lowest order in \(E\) find

\[f_1 = -\tau_{tr} eE \nabla_p f_0(p)\]

\[j = \int e v f_1(p) \frac{d^2p}{(2\pi \hbar)^2} = \frac{e^2 \tau_{tr} E}{m} \int f_0(p) \frac{d^2p}{(2\pi \hbar)^2} = \frac{e^2 \tau_{tr} n}{m} E\]

We integrated by parts assuming energy independent \(\tau_{tr}\), valid for degenerate Fermi gas \(T \ll E_F\). At finite temperatures, and for energy-dependent \(\tau_{tr}\), find \(\sigma = \frac{e^2 n}{m} \langle \tau_{tr}(E) \rangle_E\).
**Diffusion equation**

Solve B.k.e. for weakly nonuniform density distribution (and no external field!).

\[(\partial_t + \mathbf{v}\nabla_r) f(\mathbf{r}, \mathbf{p}) = S t(f)\]

First, integrate over angles \(\theta_p\) to obtain the continuity equation:

\[
\frac{\partial n}{\partial t} + \nabla \mathbf{j} = 0, \quad \mathbf{j} = \langle \mathbf{v} f \rangle_{\theta}, \quad n = \langle f \rangle_{\theta}
\]

Here \(\mathbf{j}\) and \(n\) is particle number current and density. Next, use angular harmonic decomposition \(f(\mathbf{p}) = f_0(\mathbf{p}) + f_1(\mathbf{p}) + ..., \ f_1 \propto \cos \theta, \ \sin \theta\) and relate \(f_1\) with a gradient of \(f_0\). Perturbation theory in small spatial gradients:

\[
\mathbf{v} \nabla_r f_0 = -\frac{1}{\tau_{tr}} f_1, \quad \frac{1}{\tau_{tr}} = \langle w(\theta)(1 - \cos \theta) \rangle_{\theta}
\]

Use \(f_1 = -\tau_{tr} \mathbf{v} \nabla_r f_0\) to find the current \(j_\alpha = \langle \mathbf{v}_\alpha f_1 \rangle = -\tau_{tr} \langle \mathbf{v}_\alpha \mathbf{v}_\beta \rangle \nabla_\beta f_0\).

From \(\langle \mathbf{v}_\alpha \mathbf{v}_\beta \rangle = \frac{1}{2} \delta_{\alpha\beta} v_F^2\) have

\[
\mathbf{j} = -\frac{1}{2} \tau_{tr} v_F^2 \nabla f_0 = -D \nabla f_0 = -D \nabla n
\]
Features

Diffusion constant

\[ D = \frac{1}{2} \tau_{tr} v_F^2 = \frac{1}{2} v_F \ell, \quad \ell = v_F \tau_{tr} \]

where \( \ell \) is the mean free path. From Einstein relation \( \sigma = e^2 \nu D \) find

\[ \sigma = e^2 \nu D = g_s g_v \frac{e^2}{h} k_F \ell = \frac{e^2 \tau_{tr} n}{m} \]

where \( g_s, g_v \) the spin and valley degeneracy factors.

Used the density of states \( \nu = g_s g_v \frac{2 \pi p dp}{(2 \pi h)^2 dE} = \frac{g_s g_v k_F}{2 \pi h v_F} \)

1) Temperature dependence due to \( \tau_{tr}(E) \), weak near degeneracy;

2) Boltzmann eqn. is a quasiclassical treatment valid for \( k_F \ell \gg 1 \). In this case \( \sigma \gg \frac{e^2}{h} \), metallic behavior;

3) At \( k_F \ell \sim 1 \), or \( \lambda_F \sim \ell \), onset of localization
**Another approach**

**Diffusion constant from velocity correlation:**

\[ D = \int_0^\infty dt \langle v_x(t)v_x(0) \rangle, \quad \text{ensemble averaging: } \theta, \text{ disorder} \]

**Derivation:**

\[ \langle (x(t) - x(0))^2 \rangle = \int_0^t \int_0^t dt' dt'' \langle v_x(t')v_x(t'') \rangle = 2Dt. \]

**Explanation \((T_2 \equiv \tau_{tr})\):**

Exponentially decreasing correlations \( \langle v_x(t)v_x(0) \rangle = e^{-t/\tau_{tr}} \langle v_x^2(0) \rangle = \frac{1}{2}v_F^2e^{-t/\tau_{tr}} \), yield \( D = \frac{1}{2}v_F^2\tau_{tr}. \)
MAGNETOTRANSPORT

Finite $B$ field, Lorentz force, current not along $E$. Thus conductivity $\sigma$ not a scalar but a 2x2 tensor.

Einstein relation $\sigma_{\alpha\beta} = e^2 \nu D_{\alpha\beta}$ for the diffusion tensor

$$D_{\alpha\beta} = \int_0^\infty dt \langle v_\alpha(t)v_\beta(0) \rangle, \quad \alpha, \beta = 1, 2$$

Between scattering events circular orbits $\omega_c = eB/m$, $R_c = mv_F/eB$. Complex number notation $\tilde{v}(t) = v_x(t) + iv_y(t) = v_F e^{i\theta + i\omega_c t}$. Find $D$ from

$$D_{xx} + iD_{yx} = \int_0^t dt \langle \tilde{v}(t) \cos \theta v_F \rangle \theta e^{-t/\tau_{tr}} = \frac{D}{1 + (\omega_c \tau)^2} (1 - i\omega \tau)$$

$$D_{yy} = D_{xx}, \quad D_{xy} = -D_{yx}.$$
Conductivity and resistivity tensors

\[ \hat{\sigma} = \frac{\sigma}{1 + (\omega_c \tau)^2} \begin{pmatrix} 1 & -\omega_c \tau \\ \omega_c \tau & 1 \end{pmatrix}, \quad \hat{\rho} = \hat{\sigma}^{-1} = \rho \begin{pmatrix} 1 & \omega_c \tau \\ -\omega_c \tau & 1 \end{pmatrix} \]

The off-diagonal element:

\[ \rho_{xy} \equiv R_H = \frac{B}{en} = \frac{1}{g_{s}g_{v}} \frac{h}{e^2} \frac{\hbar \omega_c}{E_F} \]

Features:

(i) Classical effects of \( B \) field important when \( \omega_c \tau \gtrsim 1 \), these field can be weak in high mobility samples;

(ii) Recover classical Hall resistivity;

(iii) Zero magnetoresistance in this model: \( \rho_{xx}(B) - \rho_{xx}(0) = 0 \). Generic for short-range scattering.

(iv) The behavior (i), (ii) is fairly robust in the classical model, but not in the presence of quantum effects.
Quantum effects

We’ve used $\sigma = e^2 \nu D$ with the zero-field density of states; assumed that $\tau_{tr}$ is independent of $B$.

From Born approximation for delta function impurities $U(r) = \sum_j u \delta(r - r_j)$ we have (see above):

$$\tau^{-1} = \frac{\pi}{\hbar} \nu(E_F) u^2 c_i$$

with $c_i$ the impurity concentration. For $\nu(E_F)$ modulated by Landau levels

$$\nu(\epsilon) = \sum_{n>0} n_{LL} \delta(\epsilon - n \hbar \omega_c), \quad n_{LL} = B/\Phi_0 = eB/\hbar$$

find Shubnikov-de Haas (SdH) oscillations periodic in $1/B$.

Period found from particle density on one Landau level $n_{LL} = eB/\hbar$, giving $\Delta(1/B) = \frac{e g_s g_v}{\hbar n_{el}}$. Can be used to determine electron density.

Plateaus in $R_H$ at $R_H = \frac{1}{g_s g_v e^2 N}$, with $N = 1, 2, \ldots$: the integer Quantum Hall effect.
Figure 1: Schematic dependence of the longitudinal resistivity $\rho_{xx}$ (normalized to the zero-field resistivity) and of the Hall resistivity $\rho_{xy} = R_H$ (normalized to $h/2e^2$) on the reciprocal filling factor $\nu^{-1} = 2eB/hn_{el}$ (for $g_s = 2$ and $g_v = 1$). Deviations from the quasiclassical result occur in strong $B$ field, in the form of Shubnikov-de Haas oscillations in $\rho_{xx}$ and quantized plateaus in $\rho_{xy}$. 
Applications of the SdH effect

SdH oscillations in D=3 are sensitive to the extramal crosssections of Fermi surface, which depend on the orientation of magnetic field w.r.p.t. crystal axes

Thus SdH can, and indeed are, used to map out the Fermi surface 3D shapes.
**Fermi surface splitting from SdH oscillations**

![Graph showing gate voltage dependence of SdH oscillations. The graph displays oscillations at different gate voltages, with a clear indication of beating patterns due to spin-orbit interaction.](image)

Classical transport in a long-range disorder

Relevant e.g. for high mobility semiconductor systems in which charge donors are placed in a layer at a large distance $d$ from the two-dimensional electron gas (2DEG), $k_F d \approx 10$. Also of pedagogical interest, as an illustration of nonzero magnetoresistance arising from classical transport.

Random potential with long-range correlations, $W(r-r') = \langle V(r)V(r') \rangle$ decays at $|r-r'| \sim d \gg \lambda_F$. As a model we take $\tilde{W}(q) = \int e^{iqr} W(r) d^3r = (\pi \hbar^2/m)^2 n_i e^{-2|q|d}$ (the prefactor $(\pi \hbar^2/m)^2$ is due to correlations in impurity positions and/or charge states).

Slight bending of the classical trajectory (which is a straight line for $V = 0$):

$$\frac{dp}{dt} = -\nabla V, \quad \frac{d\theta}{dt} = (mv_F)^{-1} \mathbf{n} \times \nabla V$$

where $\mathbf{n} = \mathbf{v}/|\mathbf{v}|$. Diffusion along the Fermi surface:

$$(\partial_t + \mathbf{v} \nabla_r + e\mathbf{E} \nabla_p) f(r,p) = D_\theta \frac{\partial^2 f}{\partial \theta^2}$$

(instead of $St(f)$)

$$D_\theta = \int_0^\infty dt \langle \dot{\theta}(t) \dot{\theta}(0) \rangle = (mv_F)^{-2} \int_0^\infty \langle \partial_y V(x=v_F t) \partial_y V(x=0) \rangle = \frac{1}{2m^2v_F^3} \sum_{q_y} q_y^2 \tilde{W}(q_y)$$

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**Transport time**

**From diffusion eqn:** For spatially uniform system write $\partial_t f = D_\theta \frac{\partial^2 f}{\partial \theta^2}$; for the harmonics $\delta f(\theta) \propto \cos \theta, \sin \theta$ have $\delta f(t) \propto e^{-D_\theta t}$. Thus

$$\tau_{tr}^{-1} = D_\theta = \frac{1}{2\pi m^2 v_F^3} \int_0^\infty q^2 \tilde{W}(q) dq$$

**From Fermi’s GR:** The scattering rate $w_{pp'} = 2\pi |V_{p-p'}|^2 \delta(\epsilon_{p'} - \epsilon_p) n_i$ yields

$$\tau_{tr}^{-1} = \int (1 - \cos \theta') w_{pp'} \frac{d^2 p'}{(2\pi \hbar)^2}$$

Using $\int ... \delta(\epsilon_{p'} - \epsilon_p) \frac{d^2 p'}{(2\pi \hbar)^2} = \int_{-\pi}^\pi \nu \frac{d\theta'}{2\pi}$, expanding $1 - \cos \theta \approx \frac{1}{2} \theta^2$ and replacing $\int_{-\pi}^\pi d\theta \rightarrow \int_{-\infty}^\infty d\theta$, find

$$\tau_{tr}^{-1} = \frac{n_i \nu}{2} \int_{-\infty}^\infty |V_{p-p'}|^2 \theta^2 d\theta = \frac{n_i \nu \hbar^2}{(mv_F)^3} \int_0^\infty \tilde{W}(q) q^2 dq$$

with $\nu = m/(2\pi \hbar^2)$, coincides with $\tau_{tr}$ found from the $\theta$-diffusion equation.
**Magnetotransport problem: memory effects**

The relaxation-time approximation: collisions with impurities described by Poisson statistics (no memory about previous collisions):  \( \langle v_\alpha(t)v_\beta(0) \rangle = e^{-t/\tau} \langle v_\alpha(0)v_\beta(0) \rangle \).

Generalize to a memory function \( f(t) = e^{-t/\tau} (1 + \sum_{n=1}^{\infty} c_n (t/\tau)^n / n!) \). Then the response to a dc electric field \( E \parallel \hat{x} \) will be

\[
j_x + i j_y = \frac{ne^2}{m} \int_0^\infty f(t) e^{i\omega_c t} E dt = \frac{\sigma_0 E}{1 - i\omega_c \tau} \left( 1 + \sum_{n=1}^{\infty} \frac{c_n}{(1 - i\omega_c \tau)^n} \right)
\]

where \( \sigma_0 = ne^2 \tau / m \) the Drude conductivity. For \( c_n = 0 \) recover zero magnetoresistance \( \Delta \rho_{xx} = \rho_{xx}(B) - \rho_{xx}(0) = 0 \) and classical Hall resistivity \( \rho_{xy} = B / ne \). However, for a non-Poissonian memory function \( f(t) \) the magnetoresistance does not vanish. Thus \( \Delta \rho_{xx}(B) \) is a natural probe of the memory effects in transport.

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