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Length scales and mesoscopic systems

L = length scale of device; system size

l_e = elastic mean free path = average distance between collisions

l_φ = phase coherence length = average distance traveled with well-defined QM phase; QM phase is randomized by inelastic scattering (electron-electron, electron-phonon scattering); l_φ decreases with increasing temperature T

$\lambda_F = 2\pi/k_F = 2\pi\hbar/p_F = h/\sqrt{2m^* E_F}$ = Fermi wavelength

In conventional devices: $L \gg l_e, l_\varphi, \lambda_F$

In mesoscopic devices: $L \lesssim l_e, l_\varphi, \lambda_F$ (meso: "in between")

$L < l_e$ (and $L < l_\varphi$): ballistic transport

$L < l_\varphi$: phase coherent transport (diffusive if $L > l_e$)

$L < \lambda_F$: quantization effects

$\frac{e^2}{C} > k_B T$: single electron charging effects; C = system capacitance

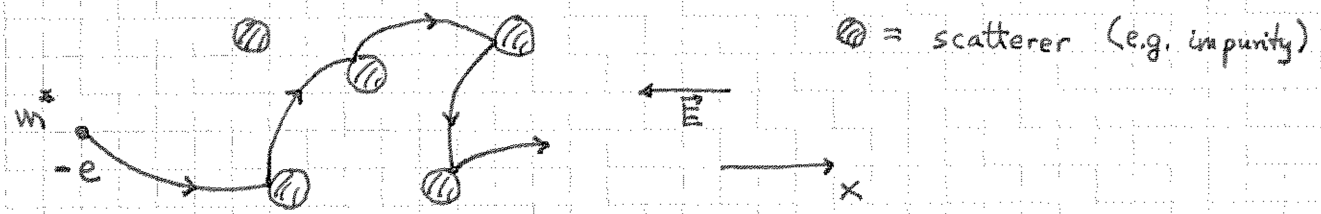
Typical mesoscopic devices: $L \lesssim 10 - 100$ nm

($l_e \approx 10^2 - 10^4$ nm, $l_\varphi \gtrsim 200$ nm, $\lambda_F \sim 40$ nm)

Transport theory

- elements of conventional transport theory: Drude conductivity, Boltzmann equation, Kubo formula
- conductance in terms of transmission: Landauer formula, Büttiker-Landauer formalism

Classical Drude theory



N2 : $m^* \frac{dv_x}{dt} = -eE_x$

Assume isotropic scattering $\Rightarrow$ $\langle \vec{v} \rangle = 0$ after each collision

$\Rightarrow \langle v_x \rangle = -\frac{e}{m^*} E_x \tau$; τ = average time between collisions

Mobility μ_e defined by $\langle \vec{v}_d \rangle = -\mu_e \vec{E}$

$\Rightarrow$

$\mu_e = e\tau / m^*$ (Drude mobility)

Current density: $\vec{j} = -en \langle \vec{v}_d \rangle$ (n = carrier density)

$= \frac{e^2 n \tau}{m^*} \vec{E}$

Ohms Law: $\vec{j} = \sigma \vec{E}$

$\Rightarrow$ $\boxed{\sigma = \frac{e^2 n \tau}{m^*}}$ Drude conductivity

Resistivity: $\rho = 1/\sigma = m^* / e^2 n \tau$

(Later: $\vec{B} \neq 0$, "magnetotransport")

Boltzmann transport equation

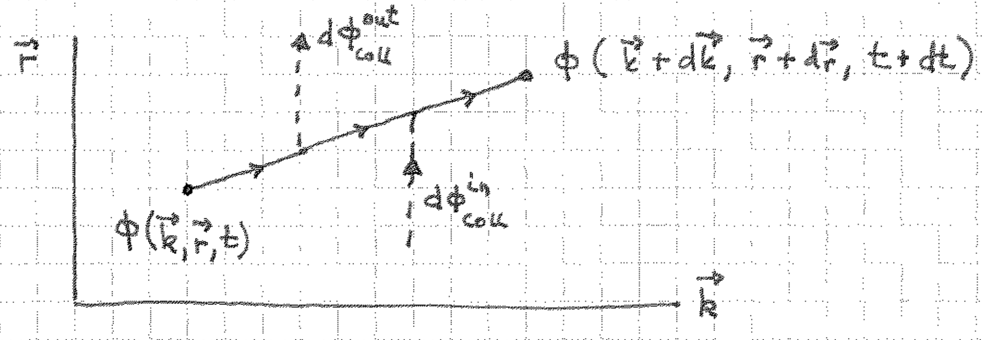
For electrons (fermions), Fermi-Dirac is the equilibrium distribution function:

$$f(E) = \left\{ \exp\left[\frac{E - E_F}{k_B T} \right] + 1 \right\}^{-1}$$

Presence of external fields $\vec{E}, \vec{B}$ and scattering mechanisms results in a nonequilibrium distr. function $\phi(\vec{k}, \vec{r}, t)$ in $2 \cdot D$ dimensional phase space $\{\vec{k}, \vec{r}\}$ (with $\vec{p} = \hbar \vec{k}$):

$\phi(\vec{k}, \vec{r}, t)$ = probability of finding electron with momentum $\hbar\vec{k}$ in position $\vec{r}$ at time t ("semiclassical" since both $\vec{p}$ and $\vec{r}$ are specified)

Evolution of ϕ by drift and scattering (collisions):



N2: $\frac{\hbar d\vec{k}}{dt} = \vec{F} \Rightarrow d\vec{k} = -\frac{e}{\hbar}\vec{E}\,dt$ (assume $\vec{B}=0$)

$$d\vec{r} = \vec{v}\,dt, \quad \vec{v} = \hbar^{-1} \nabla_k E(\vec{k})$$

$$d\phi_{coll} = d\phi_{coll}^{in} - d\phi_{coll}^{out} = \left(\frac{\partial \phi(\vec{k},\vec{r},t)}{\partial t} \right)_{coll} dt$$

= change in ϕ due to (random) collisions

If no collisions, $\phi(\vec{k},\vec{r},t) = \phi(\vec{k}+d\vec{k}, \vec{r}+d\vec{r}, t+dt)$ (particle conservation)

With collisions, $\phi(\vec{k}+d\vec{k}, \vec{r}+d\vec{r}, t+dt) - \phi(\vec{k},\vec{r},t) = d\phi_{coll} = \left(\frac{\partial\phi}{\partial t}\right)_{coll} \cdot dt$

To $\mathcal{O}(dt)$:

$$\phi(\vec{k}+d\vec{k}, \vec{r}+d\vec{r}, t+dt) = \phi(\vec{k},\vec{r},t) + d\vec{k}\cdot\nabla_k\phi(\vec{k},\vec{r},t) + d\vec{r}\cdot\nabla\phi(\vec{k},\vec{r},t) + dt\cdot\frac{\partial\phi(\vec{k},\vec{r},t)}{\partial t}$$

$$\Rightarrow \boxed{-\frac{e}{\hbar}\vec{E}\cdot\nabla_k\phi + \vec{v}\cdot\nabla\phi + \frac{\partial\phi}{\partial t} = \left(\frac{\partial\phi}{\partial t}\right)_{coll}}$$

B.T.E. (with $\vec{B}=0$)

Collision term: $\mathcal{P}\{|\vec{k}'\rangle \text{ occupied}\}$ $\mathcal{P}\{|\vec{k}\rangle \text{ empty}\}$

$$\left(\frac{\partial\phi_k}{\partial t}\right)_{coll} = \int\frac{d^3k'}{(2\pi)^3}\left\{\underbrace{\phi_{k'}(1-\phi_k)W(k',k)}_{\text{in (from }\vec{k}'\text{ to }\vec{k})} - \underbrace{\phi_k(1-\phi_{k'})W(k,k')}_{\text{out (from }\vec{k}\text{ to }\vec{k}')}\right\}$$

$\frac{d^3k'}{(2\pi)^3}\cdot W(\vec{k},\vec{k}')$ = rate of scattering from state $|\vec{k}\rangle$ to state $|\vec{k}'\rangle$

$\sim |\langle\vec{k}'|V|\vec{k}\rangle|^2$ (Fermi golden rule)

V = scattering potential (impurities, phonons etc.)

$\Rightarrow$ BTE is, in general, a complicated integro-differential equation!

Relaxation time approximation (RTA):

$$\left(\frac{\partial\phi}{\partial t}\right)_{coll} = -\frac{\phi-f}{\tau}$$

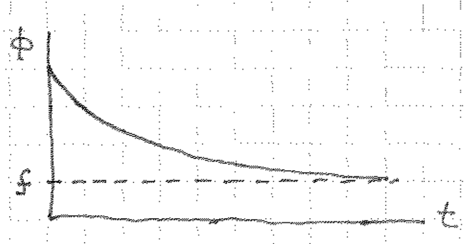
($\phi - f$ = deviation from equilibrium)

Assume spatially uniform system $\Rightarrow$ $\nabla\phi = 0$

1. What is $\phi(\vec{k},t)$ if $\vec{E}=0$ (for $t\geq 0$)?

$$\frac{\partial\phi}{\partial t} = \left(\frac{\partial\phi}{\partial t}\right)_{coll} = -\frac{\phi-f}{\tau}$$

$$\Rightarrow \phi(\vec{k},t) = f(\vec{k}) + [\phi(\vec{k},0) - f(\vec{k})]e^{-t/\tau}$$



$\Rightarrow$ exp. decay towards equilibrium

2. What is stationary state if $\vec{E} \neq 0$?

$$\frac{\partial \phi}{\partial t} = 0 \quad \Rightarrow \quad -\frac{e}{\hbar}\vec{E}\cdot\nabla_k \phi(\vec{k}) = -\frac{\phi(\vec{k}) - f(\vec{k})}{\tau}$$

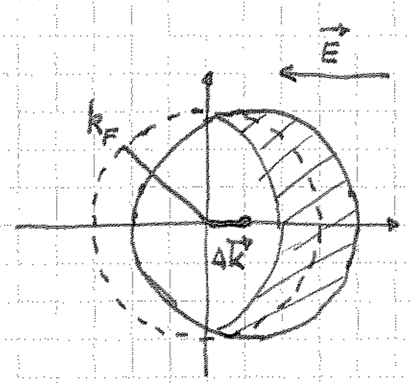
$$\Rightarrow \phi(\vec{k}) = f(\vec{k}) + \underbrace{\frac{e\tau}{\hbar}\vec{E}\cdot\nabla_k \phi(\vec{k})}$$

assume small deviation from $f \rightarrow \nabla_k \phi \approx \nabla_k f$

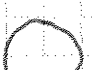
$$\Rightarrow \phi(\vec{k}) \approx f(\vec{k}) + \frac{e\tau}{\hbar}\vec{E}\cdot\nabla_k f(\vec{k}) \approx f\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right)$$

(Taylor expansion to $\mathcal{O}(E)$)

$\Rightarrow$ within RTA, effect of $\vec{E}$ is to displace Fermi sphere $f(\vec{k})$ by $\Delta\vec{k} = -e\tau\vec{E}/\hbar$



$E=0$: sphere, radius k_F, center at $k=0$



$E \neq 0$: sphere, radius k_F, center at $\Delta\vec{k} = -e\tau\vec{E}/\hbar$

if $\vec{E} = 0$: zero net current, pairs of electrons with momentum $\pm\hbar\vec{k}$ upto $k = k_F$

if $\vec{E} \neq 0$: nonzero current due to electrons in hatched region

3. What is RTA mobility and conductivity ?

Net shift in velocity: $\Delta\vec{v} = \hbar\Delta\vec{k}/m^* = (-e\tau/m^*)\vec{E}$

$\Rightarrow$ RTA mobility = Drude mobility: $\mu_e = e\tau/m^*$

Conductivity: $\vec{j} = \sigma\vec{E} \Rightarrow \sigma = \vec{j}\cdot\vec{E}/E^2$

$$\vec{j} = \int(-e)\vec{v}\,dn = \int(-e)(\hbar\vec{k}/m^*)(dN/V) \qquad dN = \phi(\vec{k})\cdot\underbrace{D(\vec{k})}_{=V/4\pi^3}\cdot d^3k$$

$$= (-e\hbar/4\pi^3 m^*)\int \vec{k}\, f(\vec{k} + e\tau\vec{E}/\hbar)\,d^3k$$

$\Rightarrow \sigma = \ldots\ldots$ Exercise 6 $\ldots\ldots = e^2\tau n/m^*$ = Drude conductivity !

Kubo formula

= transport coefficients in terms of auto-correlation functions

Example: diffusion constant D

Fick's law: $\vec{j} = -D\,\nabla n$ $\qquad \vec{j}$ = particle current density

n = particle density

Continuity eqn: $\frac{\partial n}{\partial t} + \nabla\cdot\vec{j} = 0$

$\Rightarrow \frac{\partial n}{\partial t} = D\,\nabla^2 n$ $\qquad$ (Diffusion equation)

Spatial average: $\langle g(t)\rangle = \int d^3r\; g(\vec{r},t)\,n(\vec{r},t)$

("Trick":)

Multiply diff. eqn. with $\int d^3r\;(\vec{r}(t)-\vec{r}(0))^2$ and use integration by parts twice on right hand side:

$$\int d^3r\;(\underbrace{\vec{r}(t)}_{=\vec{r}}-\underbrace{\vec{r}(0)}_{=\vec{r}_0})^2\,\nabla^2 n = \int dx\,dy\,dz\left\{\left[(x-x_0)^2\left(\frac{\partial^2 n}{\partial x^2}+\frac{\partial^2 n}{\partial y^2}+\frac{\partial^2 n}{\partial z^2}\right)+\dots\right\}\right.$$

- 3 terms are nonzero, each with factor of 2, from $\frac{\partial}{\partial x}(x-x_0)^2 = 2(x-x_0)$
- assume normalized n: $\int d^3r\; n(\vec{r},t) = 1$ $\qquad$ (probability distribution)
- assume n sufficiently localized $\Rightarrow$ surface terms $\left.\{\dots\}\right|_{-\infty}^{\infty} = 0$

$$\Rightarrow \frac{\partial}{\partial t}\underbrace{\langle(\vec{r}(t)-\vec{r}(0))^2\rangle}_{} = 6D$$

must be prop. with t to give const. value of D

$\Rightarrow$ may write

$$D = \lim_{t\to\infty}\frac{1}{6t}\left\langle\left(\vec{r}(t)-\vec{r}(0)\right)^2\right\rangle \qquad (\text{at least } t \gg 0)$$

$$\int_0^t d\vec{r} = \int_0^t \vec{v}(t')\,dt' \quad\Rightarrow\quad \vec{r}(t)-\vec{r}(0) = \int_0^t \vec{v}(t')\,dt'$$

$$\Rightarrow D = \lim_{t\to\infty} \frac{1}{6} \frac{\partial}{\partial t} \left\langle \left(\int_0^t \vec{v}(t')\,dt' \right)^2 \right\rangle$$

$$= \lim_{t\to\infty} \frac{1}{3} \left\langle \int_0^t \vec{v}(t')\,dt' \cdot \vec{v}(t) \right\rangle$$

$$= \frac{1}{3} \lim_{t\to\infty} \int_0^t dt' \underbrace{\langle \vec{v}(t)\,\vec{v}(t') \rangle}_{\text{velocity auto-correlation function}}$$

Linear response (Fick's law) is "equilibrium theory"

$\Rightarrow$ only time <u>difference</u> is relevant in correlation function

$\Rightarrow \langle \vec{v}(t)\,\vec{v}(t') \rangle = \langle \vec{v}(t-t')\,\vec{v}(0) \rangle$

Introduce $\tau = t - t' \Rightarrow d\tau = -dt'$

$$\Rightarrow \int_0^t dt' = -\int_t^0 d\tau = \int_0^t d\tau$$

$$\Rightarrow \boxed{D = \frac{1}{3} \int_0^\infty d\tau \, \langle \vec{v}(\tau)\,\vec{v}(0) \rangle}$$

Kubo formula for diffusion constant

Similar approach to Ohm's law ($\vec{j} = \sigma \vec{E} = -\sigma \nabla V$) and continuity eqn. for el. charge $\Rightarrow$ el. conductivity σ in terms of time correlation function

$\Rightarrow$ expect to find simple relation between D and σ:

$$D = \frac{k_B T}{n e^2}\,\sigma \qquad \text{(Einstein relation)}$$

End
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(May be derived from equilibrium statistical mechanics, e.g., by considering pn-junction and balance between <u>drift</u> current $\vec{j}_F = n \mu \vec{F} = -n e \mu \vec{E}$ and <u>diffusion</u> current $\vec{j}_D = -D \cdot \nabla n$)