Physics of disorder

8.512 Theory of solids II (Spring 2022)

Topics:

- Kinetic theory for electrons
- Fluctuation-dissipation theorem
- Landau Fermi-liquids
- Quantum disordered systems: Anderson localization
- Kubo formula for conductivity
- Thouless conductance and sensitivity to boundary conditions
- Scaling theory of localization
- Mott variable range hopping
- Quantum Hall effect revisited

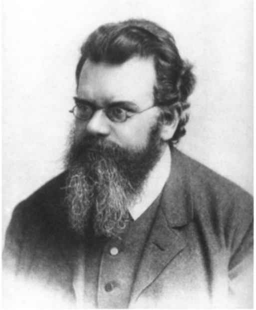
Today:

- From kinetic theory to hydrodynamics;
- Einstein relation for diffusivity D;
- Irreversibility and coarse graining
- Cluster expansion: divergences, tails, memory effects

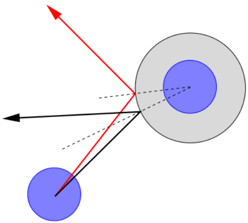
Boltzmann's statistical mechanics

Boltzmann proposed to explain the motion of a gas cloud by using the dynamics of microscopic particles—atoms and molecules, whose existence was highly disputed during Boltzmann's lifetime.

In his 1872 paper, Boltzmann derived the famous nonlinear *Boltzmann equation* in the limit of low particle densities, assuming that the dynamics of the colliding gas molecules is chaotic.



Ludwig Boltzmann (1844-1906)



- The Boltzmann gas: sensitivity to initial conditions in two-particle collisions
- Chaotic behavior at microscales
- Memory of the microstate erased through collisions
- Conserved quantities, e.g. P or E, quickly shared among different particles
- Separation of time scales: short memory times for nonconserved quantities, long memory times for conserved quantities
- Orderly behavior at macroscales (=hydrodynamics)

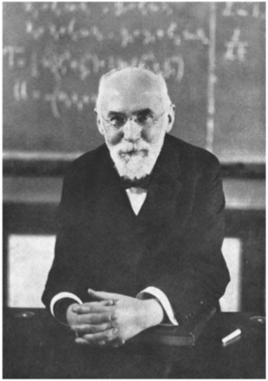
General remarks

- Boltzmann's great insight was that the arrow of time is essential for understanding the dynamics
- Applicable to systems with unbroken time reversal symmetry. In a Boltzmann gas the Hamiltonian is invariant under time reversal, but the dynamics is not
- The arrow of time originates from stochastic/chaotic dynamics on the microscales
- The fundamental relation between orderly behavior at macroscales (=hydrodynamics) and conservation laws
- Hydrodynamic modes: (a new type of) collective modes arising from the conservation laws and not from symmetry breaking
- Hydrodynamic modes: soft modes in the long-wavelength limit, $\omega(k) \to 0$ when $k \to 0$ (sometimes called "zero modes")
- This is a very general framework: similar behavior in other transport problems, classical and quantum

The Lorentz gas

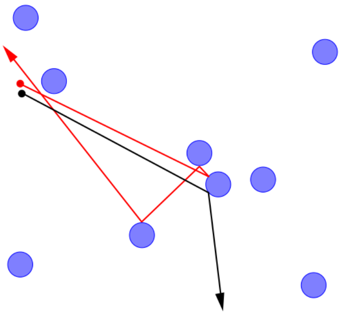
In an attempt to describe the evolution of a dilute electron gas in a metal, Lorentz proposed in 1905 a model, where the heavier atoms are assumed to be fixed, whereas the electrons are interacting with the atoms but not with each other. For simplicity, Lorentz assumed like Boltzmann that the atoms can be modeled by elastic spheres.

The Lorentz gas is still one of the iconic models for chaotic diffusion, both in a random and periodic configuration of scatterers.



Hendrik Lorentz (1853-1928)

A toy model for transport to illustrate Boltzmann's ideas



The Lorentz gas with randomly positioned scatterers.

In Lorentz models classical point particles without mutual interaction move in a random array of stationary scatterers. Lorentz models are glorified pin-ball machines! The shape of the scatterers, and the dimensionality of space can be chosen freely.

Later: quantum particles, quantum scatterers

From kinetic theory to hydrodynamics

Assume a small number density of scatterers n_s. First discuss $n_s \to 0$ limit, consider corrections afterwards.
Boltzmann equation is the equation of motion for the one-particle distribution $f(\mathrm{r}, \mathrm{v}, t)$ of the moving particles. For infinite space and with no external forces, the equation reads

$$(\partial_t + \mathrm{v} \cdot \nabla_r)\, f(\mathrm{r}, \mathrm{v}, t) = B\, f(\mathrm{r}, \mathrm{v}, t) \tag{1}$$

where B is the collision operator.
The LHS describes the Liouville (time-reversible, unitary) evolution in phase space $\partial_t f + \{H, g\} = 0$. The RHS describes collisions, breaks time reversal symmetry.
Collision operator particularly simple in 3D for spherical scatterers due to the isotropy of classical scattering off a sphere (not true in $D \neq 3$)

$$B\, f(\mathrm{r}, \mathrm{v}, t) = \frac{1}{4} n_s v a^2 \int d\Omega_{\mathrm{v}'} \left[f(\mathrm{r}, \mathrm{v}', t) - f(\mathrm{r}, \mathrm{v}, t) \right] = (\text{incoming}) - (\text{outgoing})$$

Kinetic eqn (1) is a linear equation in f, can be written in terms of a projection operator

$$B\, f = \frac{1}{\tau} (P - 1)\, f, \quad P\, f = \frac{1}{4\pi} \int d\Omega_{\mathrm{v}'} f(\mathrm{r}, \mathrm{v}', t), \quad P^2 = P!$$

with $\tau = (n_s v \pi a^2)^{-1}$ the mean free scattering time, i.e. the average time between successive collisions.

Exact solution, separation of time scales.

Taking Fourier transforms in space and time

$$f_{k,\omega}(\mathrm{v}) = \int d^3r \int dt e^{i\omega t - i\mathrm{kr}} f(\mathrm{r}, \mathrm{v}, t)$$

we obtain the following form of the Boltzmann equation

$$(-i\omega + i\mathrm{v}\cdot\mathrm{k}) f_{k,\omega}(\mathrm{v}) = \frac{1}{\tau}\left(P - 1\right) f_{k,\omega}(\mathrm{v}) + f_k(t=0)$$

The last term describes the initial conditions (an arbitrary $f(\mathrm{r}, \mathrm{v})_{t=0}$).
The beauty of this problem is that it can be explicitly solved.
Solution demonstrates that memory is erased at a different rate for different degrees of freedom. An executive summary of the results:

- Non-conserved modes decay quickly: $\delta f(\mathrm{v}) \sim e^{-t/\tau}$;
- Conserved particle #, a zero mode with a slow decay: $\delta f_0 \sim e^{-\Lambda_k t}$, $\Lambda_k \to 0$ as $k \to 0$
- The zero mode δf_0: $\Lambda_k = Dk^2 \to 0$ at small k ($D =$ diffusivity)
- P projects the general solution δf on the zero mode δf_0
- A similar separation of time scales for other conserved quantities, should there be any (5 modes in Boltzmann gases!)

We will now prove it, and compute D.

Projecting on the hydrodynamic mode

$$(-i\omega + i\mathrm{v}\cdot\mathrm{k})f_{k,\omega}(\mathrm{v}) = \frac{1}{\tau}\left(P-1\right)f_{k,\omega}(\mathrm{v}) + f_k(t=0)$$

$$f_{k,\omega}(\mathrm{v}) = \frac{\tau^{-1}}{-i\omega + \tau^{-1} + ik\mathrm{v}} P f_{k,\omega}(\mathrm{v}) + \frac{f_k(\mathrm{v})_{t=0}}{-i\omega + \tau^{-1} + ik\mathrm{v}}$$

Act on this with $P = \frac{1}{4\pi}\int d\Omega_{\mathrm{v}}\ldots$:

$$P\frac{\tau^{-1}}{-i\omega + \tau^{-1} + ik\mathrm{v}} = \frac{1}{2}\int_{-1}^{1} dx \frac{\tau^{-1}}{-i\omega + \tau^{-1} + ik\mathrm{v}x} = \frac{1}{k\mathrm{v}\tau}\tan^{-1}\frac{k\mathrm{v}\tau}{1 - i\omega\tau}$$

$$Pf_{k,\omega}(\mathrm{v}) = \frac{1}{1 - \frac{1}{k\mathrm{v}\tau}\tan^{-1}\frac{k\mathrm{v}\tau}{1-i\omega\tau}} P\frac{f_k(\mathrm{v})_{t=0}}{-i\omega + \tau^{-1} + ik\mathrm{v}}$$

Expand in small ω and k:

$$1 - \frac{1}{k\mathrm{v}\tau}\tan^{-1}\frac{k\mathrm{v}\tau}{1-i\omega\tau} \approx 1 - \frac{1}{1-i\omega\tau} + \frac{1}{3}(k\mathrm{v}\tau)^2 = i\omega\tau + Dk^2\tau + O(\omega^2, k^4),$$

$D = \frac{\mathrm{v}^2\tau}{3}$ (using $\tan^{-1} y = y - \frac{1}{3}y^3 + O(y^5)$). Consider the pole:

$$Pf_{k,\omega}(\mathrm{v}) \sim \frac{1}{i\omega + Dk^2} = \int_{-\infty}^{\infty} dt e^{i\omega t} e^{-Dk^2 t}\Theta(t)$$

Describes relaxation at a rate that becomes vanishingly small at $k \to 0$.

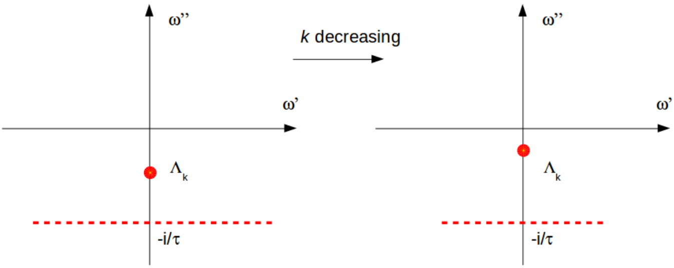
Identify $Pf_{k,\omega}(\mathrm{v})$ with a zero mode for particle number, and D with the diffusivity

Spectrum, separation of time scales.

The rates for all modes, conserved and nonconserved, can be seen in the general solution:

$$f_{k,\omega}(\mathrm{v}) = \frac{\tau^{-1}}{-i\omega+\tau^{-1}+ik\mathrm{v}} \frac{1}{1-\frac{1}{kv\tau}\tan^{-1}\frac{kv\tau}{1-i\omega\tau}} P\frac{f_k(\mathrm{v})_{t=0}}{-i\omega+\tau^{-1}+ik\mathrm{v}} + \frac{f_k(\mathrm{v})_{t=0}}{-i\omega+\tau^{-1}+ik\mathrm{v}}$$

Spectrum of eigenvalues $(B - ik\mathrm{v})f = \lambda_k f$ (notation $\omega = i\lambda_k$):



- One discrete eigenvalue $\omega = -i\Lambda_k$, satisfying $1 = \frac{1}{kv\tau}\tan^{-1}\frac{kv\tau}{1-\Lambda_k\tau}$
- Continuous spectrum $\omega = -\frac{i}{\tau} + kvx$, $-1 < x < 1$.

A zero mode: eigenvalue $\Lambda_k = -iDk^2 \to 0$ as $k \to 0$.
Note: all eigenvalues are in the lower halfplane of complex ω (causality!)

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Hydrodynamics. Einstein relation.

Find zero modes. Here, the density mode: $\Lambda_k = -iDk^2 \to 0$ at $k \to 0$.
In a general case, identify conserved quantities. Introduce hydrodynamics (= conservation laws).
In our Lorentz gas

$$\partial_t n + \nabla \mathrm{j} = 0, \quad \mathrm{j} = -D\nabla n, \quad D = v^2\tau/3.$$

This gives diffusion equation: $(\partial_t + D\nabla^2)n(r,t) = 0$
However, in general, computing D is not an easy task.

Einstein relation!

Need a general formula for D, valid for all densities n_s of the scatterers.
Define the mean square displacement as $\Delta(t) = \langle(\mathrm{r}(t) - \mathrm{r}(0))^2\rangle$
According to the diffusion equation one has asymptotically $\Delta(t) \sim 2dDt$ (here d is space dimensionality).
Einstein theory relates D with velocity autocorrelation function as

$$D = \frac{1}{d}\lim_{t\to\infty}\int_0^t \langle \mathrm{v}(t')\mathrm{v}(0)\rangle dt'$$

For the other transport coefficients, the shear and bulk viscosities and the heat conductivity, such formulas are known as Green-Kubo formulas.

Proof

For a particle trajectory $r(t)$:

$$\frac{d\Delta(t)}{dt} = \frac{d}{dt}\langle(r(t)-r(0))^2\rangle = 2\langle v(t)\cdot(r(t)-r(0))\rangle = 2\int_0^t dt'\langle v(t)\cdot v(t')\rangle$$

But the equilibrium average $\langle ... \rangle$ depends only on the difference of time arguments $\tau = t - t'$; therefore

$$\frac{d\Delta(t)}{dt} = 2\int_0^t d\tau\langle v(\tau)\cdot v(0)\rangle =_{t\to\infty} = 2\int_0^\infty d\tau\langle v(\tau)\cdot v(0)\rangle$$

Therefore $\Delta(t) = 2t\int_0^\infty d\tau\langle v(\tau)\cdot v(0)\rangle$ at long times $t \gg \tau$.
On the other hand, for a distribution $n(r,t)$ obeying diffusion equation,

$$\partial_t \int d^d r r^2 n(r,t) = -D\int d^d r r^2 \nabla^2 n(r,t) =_{by\ parts} = 2dD\int d^d r n(r,t) = 2dD$$

Comparing to the linear dependence $\Delta(t)$ gives
$D = \frac{1}{d}\int_0^\infty d\tau\langle v(\tau)\cdot v(0)\rangle$
It is instructive to apply it to the Lorentz gas: for the autocorrelation function $\langle v(\tau)\cdot v(0)\rangle = v^2 e^{-t/\tau}$ obtain the familiar result $D = v^2\tau/d$.

Discussion

The beauty of the spherical Lorentz model is that all the general statements re the separation of time scales for the hydrodynamic and non-hydrodynamic quantities can be backed up by explicit calculation.

A mathematician would say that our spectral analysis of Lorentz gas shows that Boltzmann dynamics is Markovian, i.e. it depends on the present state and not on the states in the long past.

Finally, a grain of salt. The simple picture we have presented here is a little too good to be true. When higher density effects are included, the separation of time scales will no longer be quite as clean as the Boltzmann equation predicts. The reason is the long time tail in the velocity autocorrelation function. The tail is weaker in the Lorentz model than in a fluid, decaying as $t^{-5/2}$ (in 3 dimensions) rather than $t^{-3/2}$. But it is there.

Yet, some of the basic wisdom of the theory based on the separation of time scales as presented here may be expected to survive. The non-Markovian effects (nonlocality, or memory) are weak.

To compute D, all we need is the average of $\mathrm{v}(t)$, conditional on $\mathrm{v}(t=0)=\mathrm{v}_0$, i.e. we can restrict ourselves to the spatially homogeneous case and study

$$\partial_t f(\mathrm{v},t) = B\, f(\mathrm{v},t)$$

with a spatially uniform initial state $f(\mathrm{r},\mathrm{v})_{t=0}=\delta(\mathrm{v}-\mathrm{v}_0)$. The distribution at $t>0$ can be written as

$$f(\mathrm{v},t) = \tfrac{1}{\partial_t - B} f(\mathrm{r},\mathrm{v})_{t=0}$$

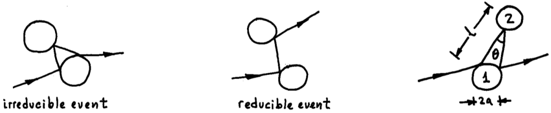
Then the diffusion constant is $D=\lim_{z\to 0}\frac{1}{d}\int d\mathrm{v}_0\mathrm{v}_0\cdot\int d\mathrm{v}\mathrm{v}\frac{1}{z-B}$ $\times\delta(\mathrm{v}-\mathrm{v}_0)/\int d\mathrm{v}_0=\lim_{z\to 0}\frac{1}{d}\mathrm{v}\frac{1}{z-B}\mathrm{v}$. Now, B is a scalar operator, so $B\mathrm{v}$ must be a vector (possibly negative) in the direction of v. Furthermore, the only eigenfunction of B with vanishing eigenvalue is 1, which is orthogonal to v. (Again a consequence of # conservation). So there is no problem with the inverse and we get

$$D^{-1} = \frac{d}{v^4}\lim_{z\to 0}\mathrm{v}(z-B)\mathrm{v} = -\frac{d}{v^4}\mathrm{v}B\mathrm{v}.$$

For $B=\frac{1}{\tau}(P-1)$, as above, we have $D^{-1}=\frac{3}{v^4}\mathrm{v}\left(-\frac{1}{\tau}\right)\mathrm{v}=\frac{3}{v^2\tau}$ which gives $D=\frac{1}{3}v^2\tau$ as before. This approach becomes extremely useful if we wish to consider the effects of repeated collisions ("recollisions"). In this case we must deal with B which is nonlocal in time (memory effects).

The breakdown of cluster expansion. Divergences, tails and memory effects.

For the density of scatterers which is not infinitesimally small, is there a power series expansion in n_s? Expect, naively, $D = \frac{a_1}{n_s} + a_2 + a_3 n_s + \dots$ Virial expansion? Perturbation series to compute a_i?



Divergences due to recollision events: $\delta B \sim \lim_{L\to\infty} a^{d-1} \int^L dl (a\theta)^{d-1} =$

$$= a^{3d-3} \int^L \frac{dl}{l^{d-1}} \sim \begin{cases} a^3 \lim_{L\to\infty} \log L & d=2 \\ a^5 \cdot const & d=3 \end{cases}$$

This looks pretty bad. Although the integral remains finite in $d = 3$ dimensions, it diverges logarithmically in $d = 2$. Of course, this is just an estimate of one term out of a sum of terms $O(n_s^2)$. On might still hope that the diverging terms would cooperate to destroy each other. But they won't. The simplicity of the Lorentz models makes a direct calculation feasible and the conclusion is that the divergence remains!

What to do about diverging terms?

Lorentz model is not only useful in diagnosing the ills, it also points to the cure. What is wrong with the cluster expansions is clearly that events with long straight trajectories are being overemphasized. A straight segment of the path should be weighted with the probability $e^{-l/\lambda}$ that it stays unbroken over a length l.
To lowest order in the density n_s the mean free path is $\lambda = (n_s \sigma)^{-1}$ where σ is the total cross section of the scatterers.
But adding such a damping on the straight trajectories changes the picture completely! Take the log divergence for $d = 2$:

$$\delta B \sim \lim_{L \to \infty} n_s^2 a^3 \int^L dl \frac{e^{-l/\lambda}}{l} \sim_{n_s a^2 \ll 1} n_s^2 a^3 \log(n_s a^2)$$

This gives terms order $n_s^2 \log(n_s)$ in the small-n_s expansion.
Further, recollision events with long excursions were found to give rise to power laws in velocity autocorrelation function of a tagged particle $\langle \mathrm{v}(t)\mathrm{v}(0)\rangle \sim t^{-d/2}$. In $d = 2$, this gives a log-diverging correction to D.
Dynamics non-Markovian: analysis predicts memory effects due to recollisions.

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The fluctuation-dissipation theorem

The fluctuation-dissipation theorem says that when there is a process that dissipates energy, turning it into heat (e.g. friction), there is a reverse process related to thermal fluctuations.

A general relation between linear response (susceptibility) and a pair correlation function (dynamical structure factor)

General proof (Callen, Welton)
Examples:
Brownian random walks, Einstein theory
Johnson-Nyquist noise, classical and quantum

Weak probes and Kubo susceptibility (reminder)

- The magic of the linear response: probing the system in its ground state through a non-equilibrium process
- The notion of linear susceptibility χ_{ji}: response of an observable O_j to the perturbation O_i
- System Hamiltonian $\mathcal{H} = \mathcal{H}_0 + O_i f_i(t)$; Susceptibility

$$\chi_{ji} = \frac{''\mathrm{response}''}{''\mathrm{force}''\ f_i}, \ \ \langle O_j(t) \rangle = \int_{-\infty}^{\infty} dt' \chi_{ji}(t-t') f_i(t')$$

- Relate χ_{ji} to the properties of the system in equilibrium:
  $\chi_{ji}(t-t') = \frac{i}{\hbar} \Theta(t-t') \langle G | [O_j(t), O_i(t')] | G \rangle$
- At $T > 0$ replace $\langle G | ... | G \rangle \to \frac{1}{Z} \sum_\alpha e^{-\beta E_\alpha} \langle \alpha | ... | \alpha \rangle$

Examples (reminder)

Perturb system by driving it out of equilibrium, then measure an observable O_i. E.g. particle density (compressibility), current (conductivity), or magnetization (χ_{spin}):

System Hamiltonian with a perturbation describing a weak probe.

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'(t), \quad \mathcal{H}'(t) = \sum_j O_j A_j(t)$$

E.g. for O_i being particle density:

$$\mathcal{H}' = \int \hat{\rho}(x,t) U(x,t) d^3x$$

with $\hat{\rho}(x,t) = \sum_i \delta(x - x_i(t))$ in 1st quantization and $\hat{\rho}(x,t) = \psi^\dagger(x)\psi(x)$ in 2nd quantization. Or, a magnetic coupling

$$\mathcal{H}' = -\int \hat{m}_z(x,t) H_z(x,t) d^3x, \quad \hat{m}_z = \mu(\hat{\rho}_\uparrow - \hat{\rho}_\downarrow)$$

Or, electric current coupled to the EM vector potential

$$\mathcal{H}' = -\int \frac{1}{c} \mathrm{j}(x,t) \mathrm{A}(x,t) d^3x, \quad \mathrm{E} = -\frac{1}{c}\partial \mathrm{A}/\partial t$$

Linear response theory: derive the Kubo formula

A system driven out of equilibrium, $H = H_0 + H'$, $H' = \sum_i O_i A_i(t)$,

$$\langle O_j(t)\rangle_{n.e.} = \langle O_j(t)\rangle + \int d\tau \chi_{ji}(t-\tau) A_i((\tau) + \ldots \tag{2}$$

Steps to derive the response function χ_{ji}: 1) Express χ_{ji} through the thermal equilibrium state in distant past $A_j(\tau) \to 0$ as $\tau \to -\infty$:

$\langle O_j(t)\rangle_{n.e.} = Z_0^{-1} \sum_\alpha e^{-\beta\epsilon_\alpha} \langle \alpha | U^\dagger(-\infty, t) O_j U(-\infty, t) | \alpha \rangle, \quad Z_0 = \mathrm{Tr} e^{-\beta H_0}$

2) Express the evolution operator as time-ordered power series

$U(t_0, t) = U_0(t - t_0) \times \mathrm{Texp}\left(-i \int_{t_0}^{t} dt' H_I'(t')\right)$. Here we are working in the "interaction representation" $H_I' = U_0^\dagger(t-t_0) H' U_0(t-t_0)$, $U_0(t-t_0) = \exp\left(-iH_0 t/\hbar\right)$. (the choice of the initial time t_0 is completely arbitrary)

3) Next, expand in H_I' as $U(t_0, t) = U_0(t-t_0)\left[1 - i\int_{t_0}^{t} dt' H_I'(t') + \ldots\right]$.

At 1st order in H_I' this gives (a result independent of the time t_0)

$$\chi_{ji}(t-t') = \Theta(t-t') \frac{i}{\hbar} \langle [O_j(t), O_i(t')] \rangle \tag{3}$$

The Heaviside function is a direct consequence of causality – that is, an applied field can impact the future dynamics but not the past dynamics.

Fourier representation of susceptibility (reminder)

Since the unperturbed Hamiltonian is time-independent it is clear that the linear response is diagonal in frequency. Namely, if the system is perturbed at a frequency ω, the linear response will be at frequency ω as well:

$$\langle O_j(\omega)\rangle = \sum_i \chi_{ji}(\omega)A_i(\omega)$$

where $\langle O_j(\omega)\rangle$, $\chi_{ji}(\omega)$ and $A_i(\omega)$ are the Fourier transforms of $\langle O_j(t)\rangle$, $\chi_{ji}(t)$ and $A_i(t)$:

$$A_i(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}A_i(t)dt, \quad \chi_{ji}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\chi_{ji}(t)dt$$

☺**:** Mathematically speaking, this is perfectly natural since under FT a convolution in Eq.(2) turns into a product.
☺**:** We will use both positive and negative frequencies!
☺**:** Since $f(\omega) = f^*(-\omega)$ for FT of a real-valued function, the real and imaginary parts of $\chi_{ji}(\omega) = \chi'_{ji}(\omega) + i\chi''_{ji}(\omega)$ are even and odd in ω, respectively.

The arrow of time and Fourier transform (reminder)

Because of causality, $\chi(\tau < 0) = 0$ in Eq.(2). The Fourier transform

$$\chi_{ij}(z) = \int_{-\infty}^{\infty} dt e^{izt} \chi_{ij}(t) = \int_{0}^{\infty} dt e^{izt} \chi_{ij}(t)$$

is therefore analytic in the upper half plane of complex frequency, $\mathrm{Im}\, z > 0$. This analyticity property is a nontrivial, but extremely useful mathematical consequence of the arrow of time.

Many constraints on the ω dependence, both the obvious ones and the surprising ones.

To illustrate the connection between causality and the analytic properties under Fourier transform consider $\chi(t) = \Theta(t) A e^{-\gamma t}$. This is a memory function with the memory loss rate $\gamma > 0$.

In this case we have $O_j(t) = \int_{-\infty}^{t} dt' A e^{-\gamma(t-t')} f_i(t')$. The Fourier transform

$$\chi(z) = \int_{0}^{\infty} dt A e^{izt - \gamma t} = \frac{A}{\gamma - iz}. \qquad (4)$$

This expression has a pole at $z = -i\gamma$ in the lower halfplane $\mathrm{Im} z < 0$, and is analytic at $\mathrm{Im} z > 0$.

Analytic functions? See excellent 18.04 notes, or a summary at the end

Sanity check: harmonic oscillator susceptibility (reminder)

Hamiltonian $H = \frac{p^2}{2m} + \frac{m\omega_0^2}{2}x^2 - exE(t)$. Find Kubo polarizability?
Dipole moment $d = (O_j) = ex$, the "force" E couples to $O_i = -d$.
Dynamic polarizabity, defined as $\langle d(t)\rangle = \int_{-\infty}^{t} \chi(t-t')E(t')dt'$, equals

$$\chi_{Kubo}(t-t') = -\frac{i}{\hbar}\langle G|[d(t), d(t')]|G\rangle$$

Quantum harmonic oscillator evolution is identical to the classical one.
Therefore $x(t) = x(t')\cos\omega_0(t-t') + \frac{p(t')}{m\omega_0}\sin\omega_0(t-t')$. Plugging it in the Kubo formula and combining with the equal-time commutators $[x(t'), x(t')] = 0$, $[x(t'), p(t')] = i\hbar$ gives a result (!!!) identical to the classical oscillator polarizability response

$$\chi_{Kubo}(t-t') = -\frac{ie^2}{\hbar} i\hbar \frac{1}{m\omega_0}\sin\omega_0(t-t') = \frac{e^2}{m\omega_0}\sin\omega_0(t-t')$$

Fourier transform (infinitesimal damping η added to control convergence)

$$\chi(\omega) = \int_0^\infty dt e^{i\omega t - \eta t}\chi(t) = \frac{e^2}{2im\omega_0}\left(\frac{1}{\eta - i(\omega+\omega_0)} - \frac{1}{\eta - i(\omega-\omega_0)}\right)$$

$$= \frac{e^2}{m(\omega_0^2 - (\omega + i\eta)^2)}, \quad \text{complex poles}: \omega_{1,2} = \pm\omega_0 - i\eta,\ \mathrm{Im}\,\omega_{1,2} < 0$$

The poles $\omega_{1,2}$ reside in the lower halfplane of complex ω. This agrees

Use the eigenstates of H_0, $\epsilon_\alpha|\alpha\rangle = H_0|\alpha\rangle$, and identity decomposition $1 = \sum_\alpha |\alpha\rangle\langle\alpha|$ to bring $\chi_{ji}(\omega) = \int dt e^{i\omega t}\frac{i}{\hbar}\langle[O_j(t), O_i(0)]\rangle$ to the form

$$\chi_{ji}(\omega) = \frac{i}{\hbar Z_0}\sum_{\alpha\beta} e^{-\beta\epsilon_\alpha}\langle\alpha|O_j|\beta\rangle\langle\beta|O_i|\alpha\rangle \int_0^\infty e^{i(\epsilon_\alpha-\epsilon_\beta)t}e^{i\omega t}e^{-\delta t}dt$$

$$-\frac{i}{\hbar Z_0}\sum_{\alpha\beta} e^{-\beta\epsilon_\beta}\langle\beta|O_j|\alpha\rangle\langle\alpha|O_i|\beta\rangle \int_0^\infty e^{i(\epsilon_\alpha-\epsilon_\beta)t}e^{i\omega t}e^{-\delta t}dt$$

$$= \frac{1}{Z_0}\sum_{\alpha\beta}\langle\beta|O_j|\alpha\rangle\langle\alpha|O_i|\beta\rangle \frac{e^{-\beta\epsilon_\beta} - e^{-\beta\epsilon_\alpha}}{\omega - (\epsilon_\beta - \epsilon_\alpha) + i\delta} \tag{5}$$

We swapped α and β in 2nd term, and added a factor $e^{-\delta t}$ to assure convergence.
This result is completely general (no approximations made!). We will use it later to derive the fluctuation-dissipation theorem and sum rules.

Eq.(5) is an explicit expression that would be useful if we knew the many-body eigenstates and the respective matrix elements. Usually we don't, so we will seek other ways to evaluate the response functions.

Since O_j are Hermitian operators, it follows that (check!)

$$\chi_{ji}(\omega) = -\chi_{ij}(-\omega) = -[\chi_{ji}(-\omega)]^* = [\chi_{ij}(\omega)]^*$$

is a Hermitian matrix. Decomposing into a sum of the real and imaginary parts

$$\chi_{ji}(\omega) = \chi'_{ji}(\omega) + i\chi''_{ji}(\omega)$$

and setting $j = i$ we see that $\chi''_{jj}(\omega)$ is real and an odd function of ω. Likewise, $\chi'_{jj}(\omega)$ is a real, even function of ω.
Other symmetry properties of χ_{ji} can be derived from symmetries of H. For instance, if H is time-reversal invariant, and if $f_i(t) \to \epsilon_i f_i(-t)$ under time-reversal, then it is easy to see that

$$\chi_{ji}(\omega) = -\epsilon_i\epsilon_j\chi_{ij}(-\omega) = \epsilon_i\epsilon_j\chi_{ji}(\omega)$$

The reason we need to include the "signature," ϵ_i, is that some operators that we are interested in, such as a position or an electric potential, are even under time-reversal, $\epsilon_i = 1$, while others, such as the current or the magnetic field, are odd, $\epsilon_i = -1$.

Identification of $\chi''_{ij}(\omega)$ with dissipation (reminder)

Consider the rate at which power is absorbed from a generic external field

$$P(t) = \frac{d\langle H\rangle}{dt} = \sum_j \frac{\partial\langle H\rangle}{\partial A_j}\dot{A}_j = \sum_j \langle O_j(t)\rangle_{n.e.}\dot{A}_j$$

$$= \int d\tau \chi_{ji}(\tau) A_i(t-\tau)\dot{A}_j(t) = \iint \frac{d\omega d\nu}{(2\pi)^2} e^{i(\omega-\nu)t}\chi_{ji}(\omega)A_i(\omega)i\nu A_j(-\nu)$$

Typically, we are not interested in the rapidly oscillating pieces of P but only in its time average. We thus integrate over t [to enforce approximate δ-function in frequency through $\int dt e^{i(\omega-\nu)t} = 2\pi\delta(\omega-\nu)$]:

$$\int dt P(t) = \int \frac{d\nu}{2\pi}\chi_{ji}(\nu)A_i(\nu)i\nu A_j(-\nu)$$

Since $A_j(t)$ is real, $A_j(-\omega) = A_j^*(\omega)$. Using $\chi_{ji}(-\nu) = \chi^*_{ji}(\nu)$ we have

$$\int dt P(t) = \int \frac{d\nu}{2\pi}\nu\chi''_{ji}(\nu)A_i(\nu)A_j^*(\nu)$$

Since dissipated power is always positive (2nd law of thermodynamics), it follows that $\nu\chi''_{ii}(\nu) \geq 0$. (Which agrees with the symmetry properties, see above)

This result checks with the harmonic oscillator response found above:

$\chi''(\omega) \sim \delta(\omega-\omega_0) - \delta(\omega+\omega_0))$ (odd in ω and positive for $\omega > 0$).

Equilibrium fluctuations are defined as a correlation function

$$S_{ij}(t) = \langle (O_i(t) - \langle O_i \rangle)\,(O_j(0) - \langle O_j \rangle) \rangle \qquad (6)$$

In solids, spatial and temporal correlations (of fluctuations) of particle density, magnetization, etc, are measured in the scattering experiments. Or, by noise measurements of current fluctuations in electric circuits, etc.

Relate fluctuations S to linear susceptibility χ?

Here we do it for the non-symmetrized correlator in Eq.(6), the quantity of interest for analyzing spatial and temporal correlations (scattering). Other quantities, such as current and voltage fluctuations, probed by noise measurements, are described by symmetrized correlators, discussed below.

Derivation of the Fluctuation-Dissipation Theorem

* Express S through microscopic states. It follows from the cyclic property of the trace that

$$S_{ij}(t) = \sum_{\alpha\gamma} e^{-\beta\epsilon_\alpha} \langle\alpha|\delta O_i(t)|\gamma\rangle\langle\gamma|\delta O_j(0)|\alpha\rangle = \sum_{\alpha\gamma} e^{-\beta\epsilon_\alpha + it(\epsilon_\alpha - \epsilon_\gamma)}$$

$$\times\langle\alpha|\delta O_i(0)|\gamma\rangle\langle\gamma|\delta O_j(0)|\alpha\rangle = [\alpha \leftrightarrow \gamma, i \leftrightarrow j] = S_{ji}(-t - i\beta).$$

* Detailed balance. Therefore, the Fourier transform $S(\omega) = \int_{-\infty}^{\infty} S(t)e^{i\omega t}dt$ obeys an interesting identity $S_{ij}(\omega) = S_{ji}(-\omega)e^{\beta\omega}$ known as the detailed balance relation.

* The key step. We can express $S_{ij}(\omega)$ through the many-body eigenstates of H_0 as

$$S_{ji}(\omega) = \int dt \tfrac{1}{Z_0} \textstyle\sum_{\alpha\beta} e^{-\beta\epsilon_\alpha} \langle\alpha|O_j|\beta\rangle\langle\beta|O_i|\alpha\rangle e^{i(\omega - \epsilon_\beta + \epsilon_\alpha)t}$$

$$= \frac{1}{Z_0}\sum_{\alpha\beta} e^{-\beta\epsilon_\alpha}\langle\alpha|O_j|\beta\rangle\langle\beta|O_i|\alpha\rangle 2\pi\delta(\omega - \epsilon_\beta + \epsilon_\alpha). \qquad (7)$$

Comparing Eqs. (7) and (5), we find an amazing fluctuation-dissipation relation

$$\chi''_{ji}(\omega) = S_{ji}(\omega)\frac{1}{2\hbar}(1 - e^{-\beta\hbar\omega})$$

Fluctuation-Dissipation Theorem (discussion)

A relation between two quantities that have quite different meaning:
* χ'' is the rate of dissipation of the nonequilibrium state after system is driven out of equilibrium by $A(t)$
* S describes fluctuations in pristine equilibrium state

The equivalence of χ'' and S permits us to predict a large host of non-equilibrium phenomena based exclusively on the knowledge of the equilibrium ensemble. Indeed, since we have identified $\chi''(\omega)$ with dissipation, we can think of it as being some measure of the "density of states" for excitations with energy $\hbar\omega$ (aka the spectral function).
In this way we can obtain an intuitive understanding of the equilibrium fluctuations of the system as related to the thermal occupation of a set of harmonic oscillator modes according to

$$S_{ij}(\omega) = 2\left\{\theta(\omega)\left[1+\bar{n}(\omega)\right] - \theta(-\omega)\bar{n}(|\omega|)\right\}\chi''_{ij}(\omega)$$

where $\bar{n}(\omega) = 1/(e^{\beta\omega}-1)$ is the Bose occupancy factor with chemical potential $\mu = 0$ describes "spontaneous" and "stimulated" processes.
The limit $\beta\omega \ll 1$ gives the classical version of the fluctuation-dissipation theorem,

$$S_{ij}(\omega) = \left[\frac{2k_B T}{\omega}\right]\chi''_{ij}(\omega).$$

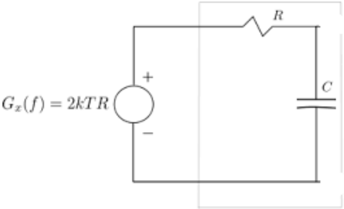
Fluctuation-Dissipation Theorem: two examples

The fluctuation-dissipation theorem says that when there is a process that dissipates energy, turning it into heat (e.g. friction), there is a reverse process related to thermal fluctuations.
One textbook example is the Brownian random-walk motion. A particle that is being kicked and dragged.
Langevin dynamics: $\mathrm{v} = \mu f(x) + \delta\mathrm{v}(t)$, where μ is mobility, $f(x) = -\nabla U(x)$ is external force, and velocity fluctuations $\delta\mathrm{v}(t)$ define diffusion constant $D = \int_0^\infty \frac{1}{3}\langle\delta\mathrm{v}(t)\delta\mathrm{v}(0)\rangle dt$.
Brownian motion converts heat energy into kinetic energy—the reverse of drag. Due to fluctuation-dissipation theorem, the mobility μ and diffusivity D are related by $D = k_B T\mu$.
In other words, the fluctuation of the particle at rest has the same origin as the dissipative frictional force one must do work against, if one tries to perturb the system in a particular direction [Einstein (1905)].

The relation $D = k_B T\mu$ is found by demanding that Boltzmann distribution $e^{-\beta U(x)}$ is a steady state of the Fokker-Planck equation $\partial_t p = D\nabla^2 p - \nabla(\mu \mathrm{f} p)$.

Fluctuation-Dissipation Theorem: two examples

Another example is the Johnson noise in an electrical resistance arising due to its inner thermal fluctuations.



The Kirchhoff-Langevin dynamics: $IR = V + \delta V(t)$, where V is external voltage (say, $V = -Q/C$ in the picture) and $\delta V(t)$ is Johnson noise intrinsic to the resistor.

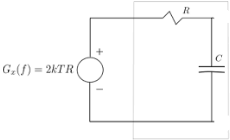
Noise spectral power $\langle \delta V(\omega) \delta V(-\omega) \rangle_{\hbar\omega \ll k_B T} = 2Rk_B T$ (Nyquist, 1928).

E.g. an RC circuit in thermal equilibrium, $\frac{1}{C} Q(t) = -R\dot{Q}(t) + \delta V(t)$.

Fluctuations δV are due to a small and rapidly-fluctuating current caused by the thermal fluctuations of the electrons and atoms in the resistor.

Johnson noise converts heat energy into electrical energy—the reverse of power dissipation by a resistor.

A direct derivation of Johnson noise (Nyquist thm)



Consider an RC circuit made of a capacitor C and resistor R in series with a Johnson noise source $\delta V(t)$: $\frac{Q}{C} + IR = \delta V(t)$.
In Fourier harmonics, this reads $Q_\omega \left(\frac{1}{C} + i\omega R\right) = \delta V_\omega$. The spectrum of charge fluctuations on the capacitor

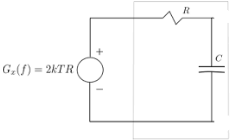
$$\langle Q_{-\omega} Q_\omega \rangle = \frac{\langle \delta V_{-\omega} \delta V_\omega \rangle}{\frac{1}{C^2} + \omega^2 R^2}$$

Demand that capacitor's thermal energy equals $\frac{1}{2} k_B T$:

$$E_c = \left\langle \frac{Q^2}{2C} \right\rangle = \int \frac{d\omega}{2\pi} \frac{\langle \delta V_{-\omega} \delta V_\omega \rangle}{2C(\frac{1}{C^2} + \omega^2 R^2)} = \frac{1}{4R} \langle \delta V_{-\omega} \delta V_\omega \rangle =? = \frac{1}{2} k_B T.$$

Which instantly gives $\langle V_{-\omega} V_\omega \rangle_{\hbar\omega \ll k_B T} = 2Rk_B T$. (Independent of C!)

Q: What about the HO kinetic energy? A: This is a dissipative HO with a thermal bath R.



"Canonical susceptibility" for a resistor $RI(t) = V(t)$?
Hamiltonian $H' = V(t)\Delta Q$, where $\Delta Q(t) = \int_{-\infty}^{t} I(t')dt'$ is the charge transfered through the resistor. Therefore, we want a relation of the form $\Delta Q_\omega = \chi(\omega)V_\omega$.
Comparing this to $R\Delta\dot{Q} = V$ gives $\Delta Q_\omega = \frac{1}{i\omega R}V_\omega$ and $\chi(\omega) = \frac{1}{i\omega R}$.
The FDT relation $S(\omega) = \hbar \coth\frac{\hbar\omega}{2T}\chi''(\omega)$ (this is the FDT statement for a symmetrized pair correlator S) gives charge and current fluctuations

$$\langle \Delta Q_{-\omega}\Delta Q_\omega\rangle = \hbar\coth\frac{\hbar\omega}{2T}\frac{1}{\omega R}, \quad \langle I_{-\omega}I_\omega\rangle = \hbar\omega\coth\frac{\hbar\omega}{2T}\frac{1}{R}$$

Noisy resistor is usually modeled as a noiseless resistor in series with the Johnson voltage noise source $\delta V_\omega = RI_\omega$ with the spectrum

$$\langle \delta V_{-\omega}\delta V_\omega\rangle = \hbar\omega\coth\frac{\hbar\omega}{2T}R = 2\hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right)R$$

Analogy with the Brownian random walks

Identify current with particle velocity, and capacitor charge — with particle displacement: $I \to v$, $-Q \to x$. Then $\frac{Q}{C} + IR = \delta V(t)$ turns into an equation for a Brownian particle moving due to thermal kicks and being dragged by an external force of a harmonic oscillator

$$v = \mu f(x) + \delta v, \quad \delta v = \frac{\delta V}{R}, \quad \mu = \frac{1}{R}, \quad f(x) = -\partial_x \frac{x^2}{2C} = -\frac{x}{C}$$

with the drag coefficient $\mu = \frac{1}{R}$.
This can be described by a diffusion equation for the probability distribution $p(x,t)$ of particle displacement (aka the Fokker-Planck equation): $\partial_t p(x,t) = D\partial_x^2 p(x,t) - \partial_x(\mu f(x) p(x,t))$. Derivation: $\partial_t p(x,t) = -\partial_x j$, $j = -D\partial_x p(x,t) + \mu f(x) p(x,t)$.
Now, demand that the equilibrium distribution $p(x) \sim e^{-\beta U(x)}$, $U(x) = \frac{x^2}{2C}$ describes the steady state. [Independent of $\mu = 1/R$!]
This predicts a relation between particle diffusivity and drag coefficient

$$D = k_B T \mu.$$

Combining it with the Einstein formula for particle diffusivity

$D = \int_0^\infty dt \langle \delta v(t) \delta v(0) \rangle = \frac{1}{2} \langle \delta v_{-\omega} \delta v_\omega \rangle$ gives the particle velocity noise spectrum $\langle \delta v_{-\omega} \delta v_\omega \rangle = 2\mu k_B T$. Going back to the electric quantities $\delta v = \delta I = \frac{1}{R}\delta V$, $\mu = \frac{1}{R}$ yields the Johnson noise spectrum $2Rk_B T$.

Einstein theory and Fluctuation-Dissipation Thm

Since the external force f couples to particle displacement, $\mathcal{H}' = -\mathrm{f}\mathrm{x}(t)$, the appropriate susceptibility is $\mathrm{x}_\omega = \chi(\omega)\mathrm{f}_\omega$, where we introduced Fourier harmonics $\mathrm{x}_\omega = \int dte^{i\omega t}\mathrm{x}(t)$, $\mathrm{f}_\omega = \int dte^{i\omega t}\mathrm{f}(t)$, etc. Comparing this to the equation of motion $\mathrm{v} = \mu\mathrm{f}$ gives

$$\chi(\omega) = \frac{i\mu}{\omega}.$$

The FDT relation (taken in the classical limit) is $S(\omega) = \frac{2k_BT}{\omega}\chi''(\omega)$, which predicts the displacement fluctuations spectral density

$$\langle \delta x_\omega \delta x_{-\omega} \rangle = \frac{2k_BT}{\omega^2}\mu.$$

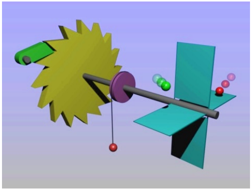
Multiplying both sides by ω and using the relation $\mathrm{v}_\omega = -i\omega\mathrm{x}_\omega$ gives velocity fluctuation spectrum

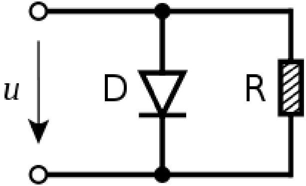
$$\langle \delta v_{x,\omega} \delta v_{x,-\omega} \rangle = 2k_BT\mu,$$

where $v_{x,\omega}$ are Fourier harmonics of the particle velocity x component, $v_{x,\omega} = \int dte^{i\omega t}v_x(t)$. Einstein relation then follows after expressing the diffusion constant through $\langle \delta v_{x,\omega} \delta v_{x,-\omega} \rangle$ in the limit of small ω.

Feynman's ratchet and pawl paradox

Can thermal bath do work?





Thermal noise can convert heat into mechanical work provided that the system is not in thermal equilibrium with the environment. Here temperatures of two susbsystems (ratchet and pawl) have to be imbalanced. No mechanical work can be produced if the ratchet and pawl temperatures are equal. A simplest heat engine, efficiency $\sim \Delta T$. The spinning direction is clockwise if $\Delta T > 0$ and counterclockwise if $\Delta T < 0$. This topic, in part because of the insightful discussion in Feynman lectures, has triggered a lot of theor and exper activity.

Symmetrized and non-symmetrized fluctuations

For symmetrized correlation function $\tilde{S}_{ij}(t) = \frac{1}{2}\langle O_i(t)O_j(0) + O_j(0)O_i(t)\rangle$ the Fluctuation-Dissipation theorem reads:

$$\tilde{S}_{ij}(\omega) = \frac{1}{2} i\hbar \left(\chi_{ji}^* - \chi_{ij}\right) \coth \frac{\hbar\omega}{2T}$$

For a single variable $O_i(t) = x(t)$ this gives

$$\langle x(\omega)x(-\omega)\rangle = \hbar\chi''(\omega) \coth \frac{\hbar\omega}{2T}.$$

The Johnson-Nyquist noise spectral function (symmetrized)

$$\langle \delta V(\omega)\delta V(-\omega)\rangle = \hbar\omega R \coth \frac{\hbar\omega}{2T}$$

at low frequency $\omega \to 0$ giving the textbook result $\langle \delta V^2\rangle = 2RT$

Both symmetrized and non-symmetrized fluctuations are measurable (yet by very different techniques). Which one is more 'natural', i.e. more easily measurable? It depends: e.g. scattering experiments access non-symmetrized fluctuations, whereas for Brownian motion or Johnson noise it is the symmetrized fluctuations that are being measured.

Johnson Noise Thermometry

JNT is a well established experimental technique that finds wide applications in temperature scale metrology and in the development of reliable thermometers for harsh environments.
Also, there've been much interest in the extensions of JNT and the Fluctuation-Dissipation Theorem to out-of-equilibrium systems. Here is one example from the literature.
Low-frequency current noise in a voltage-biased tunnel junction

$$S_I = \langle \delta I^2 \rangle = R^{-1} \left[T_n + \frac{eV}{2k_B} \coth\left(\frac{eV}{2k_B T} \right) \right]$$

can be used for high-precision temperature measurement [Spietz et al. Science 300, 1929 (2003)]

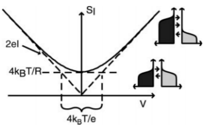


Fig. 1. Theoretical plot of current spectral density of a tunnel junction (Eq. 3) as a function of dc bias voltage. The diagonal dashed lines indicate the shot noise limit, and the horizontal dashed line indicates the Johnson noise limit. The voltage span of the intersection of these limits is $4k_BT/e$ and is indicated by vertical dashed lines. The bottom inset depicts the occupancies of the states in the electrodes in the equilibrium case, and the top inset depicts the out-of-equilibrium case where $eV \gg k_BT$.

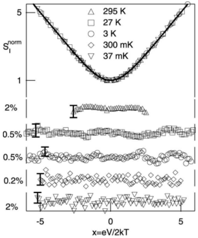


Fig. 3. Normalized junction noise plotted versus normalized voltage at various temperatures. Noise power is normalized to the zero bias (Johnson) noise, and bias voltage is scaled relative to temperature. In these units, the data follow the universal function xcoth(x), depicted by the solid line. The residuals have the indicated fractional standard deviations and are shown below. This plot shows that the "gas law" for the junction noise is obeyed over four decades in temperature, with a significant systematic effect at the room temperature. Error bars indicate stated approximate SD of residuals.

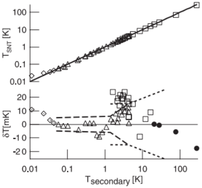


Fig. 4. Comparison of temperature as measured by the SNT (T_{SNT}) to temperature as measured by secondary thermometers ($T_{secondary}$). Temperature is displayed on logarithmic axes, and the solid line indicates the line $T_{SNT} = T_{second-}$

Anderson localization

A quantum mechanical analog of a random walk in a random environment. Anderson considered the tight binding approximation, in which the electrons can hop from atom to atom and are subject to an external random potential modeling the random environment. He gave some non-rigorous but convincing arguments that in this case such a system should loose all its conductivity properties for large enough disorder, that is, become an insulator. The electrons in such a system become trapped due to the external extensive disorder. This is in sharp contrast to the behavior in ideal crystals which are always conductors.

Today:

* Introduce and compare various models of localization
* The relation between localization (quantum random walks) and ohmic conductivity
* The mean-field picture (by Anderson, Thouless and others)
* Experimental observations. The minimum metallic conductivity
* Mobility edge

* The metal-insulator transition

Anderson localization overview

Models of disorder:
$\epsilon\psi(\mathrm{r}_i) = \epsilon_{i'}\psi(\mathrm{r}_i) + \sum_{|\mathrm{r}_{i'}-\mathrm{r}_i|=1} I\psi(\mathrm{r}_{i'})$, $-W < \epsilon_i < W$ random on-site energies (Anderson model on a d-dimensional lattice)
$\epsilon\psi(\mathrm{r}) = \left(\frac{p^2}{2m} + U(\mathrm{r})\right)\psi(\mathrm{r})$, $U(\mathrm{r}) = \sum_i u(\mathrm{r}-\mathrm{r}_i)$ the disorder potential (Lifshits model)
$\epsilon\psi(\mathrm{r}) = \left(\frac{p^2}{2m} + U(\mathrm{r})\right)\psi(\mathrm{r})$, $\langle U(\mathrm{r})U(\mathrm{r}')\rangle \sim \delta(\mathrm{r}-\mathrm{r}')$, $\langle U(\mathrm{r})\rangle = 0$ the white noise model

Microscopic picture:
The localized and extended (delocalized) states
The localized phase: absence of diffusion, dynamics nonergodic
The delocalized phase: normal diffusion/ergodicity; quantum-coherent effects and non-Markovian effects (long-time memory)

Striking manifestations in transport:
Zero-T conductance $G = \frac{I}{V}_{V\to 0} = \begin{cases} \sigma\frac{L_x L_y}{L_z} & \textit{extended} \\ \sim \exp(-L_z/\zeta) & \textit{localized} \end{cases}$
The transition between the two phases
The role of space dimensionality and decoherence (inelastic scattering)

In Anderson model, transition between localized and delocalized phases occurs at the critical value of hopping

$$I_c \sim \frac{W}{2d\log(2d)}$$

(Abou-Chakra, Anderson and Thouless, A selfconsistent theory of localization 1973)

PDF

Anderson localization in one dimension

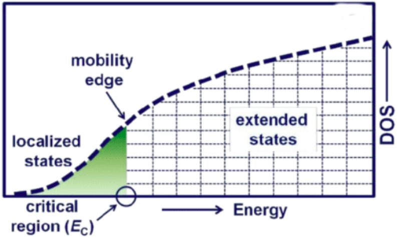
demo

The minimum metallic conductivity

Experimental observations:
Temperature dependence $d\rho/dT$ small and positive for a good metal (el-ph scattering)
but becomes large and negative when ρ exceeds values ranging around $80 - 180\mu\Omega cm$ (for instance, see: Mooij 1973).
Interpretation: an onset of the insulating behavior.
Quasiclassical picture: Drude conductivity $\sigma = \frac{ne^2\tau}{m}$ valid provided that the electron wavelength $\lambda_F = \frac{2\pi}{k_F}$ is much smaller than the mean free path $\ell = v_F\tau$
$k_F\ell \gg 1$ or $E_F\tau \gg 1$
Rewrite using $n = k_F^3/3\pi^2$ as $\sigma = \frac{e^2}{3\pi^2\hbar}k_F^2\ell$
Remembering that $\hbar/e^2 \approx 4.1k\Omega$ obtain the minimum conductivity
$\sigma\lambda_F \approx 5 \cdot 10^{-5}(k_F\ell)\Omega^{-1} \gg 5 \cdot 10^{-5}\Omega^{-1}$

Resistivity of a metal $\rho = \frac{1}{\sigma} \ll 200\mu\Omega \cdot \lambda_F$ $(\AA)$ (the Ioffe-Regel criterion)

Mobility edge in a disordered electron band



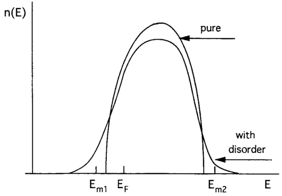
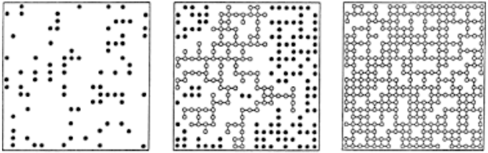


Figure 2.1 The density of states with and without disorder and the mobility edges in the former case (schematic). Note the smooth behavior near E_{mi}.
credit: Y Imry Introduction to mesoscopic physics

Electronic states in a disordered band. For each energy the states are either all localized or all extended (Mott theorem).
Sharp mobility edge in the spectrum separating localized and delocalized states. At $E < E_m$ the localization radius diverges as $E \to E_m$.
Different behavior for the Fermi level above and below the mobility edge:
metallic for $E_F > E_m$, resistivity $\rho(T)$ grows, takes a finite value at $T = 0$;
insulating for $E_F < E_m$: resistivity $\rho(T)$ decreases, becomes infinite at $T \to 0$.

Classical percolation in random resistor networks



a $p = 0.2$ b $p = 0.59$ c $p = 0.8$

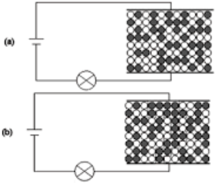


Figure 1. Pictorial representation of percolation. When a continuous chain from the top to the bottom is formed as in (b), there will be a percolating current and the light bulb (⊗) will turn on.

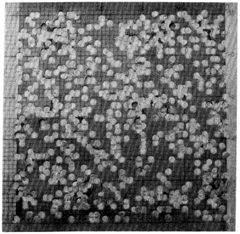


FIG. 1. Photograph of the sheet of conducting paper at the stage where the concentration of holes is 0.268.

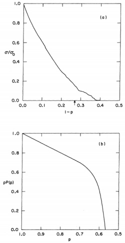


FIG. 2. (a) Graph of the conductivity as a function of the concentration of holes $(1-p)$. The bulk conductivity of the conducting paper is σ_0. The arrow shows the point at which the photograph of Fig. 1 was taken.

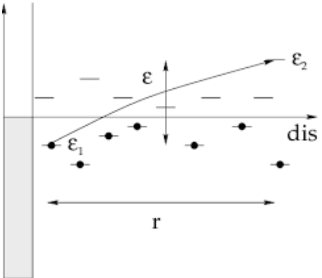
from: B.J. Last and D.J. Thouless, Percolation Theory and Electrical Conductivity, Phys.Rev.Lett. 27, 1719 (1971)

Thermally activated conduction in the localized regime, $E_F < E_m$

Conduction pathways:

1. Activation (phonon-assisted) above the mobiliy edge, $\sigma \sim e^{-\beta(E_m - E_F)}$
2. Hopping to a nearby localized state (phonon-assisted), percolation through random network of hopping-resistance links (Miller-Abrahams 1960). For localization radius ξ, the level spacing of states at $r < \xi$ that are directly accessible by hopping, $\Delta_\xi = (n_0 \xi^d)^{-1}$ with n_0 the density of states at E_F. This predicts $\sigma \sim e^{-\beta \Delta_\xi}$, which usually dominates over activation above the mobility edge

Experiment usually shows a much slower T dependence $\sigma \sim e^{-C(T_0/T)^\alpha}$, $\alpha < 1$. Origin: variable range hopping (Mott 1966, 1970)



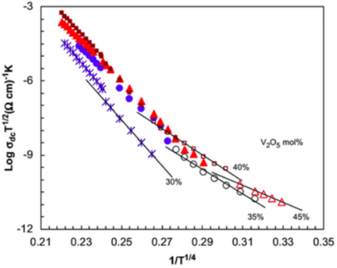


Fig. 11. Log $\sigma T^{1/2}$ vs. $1/T^{1/4}$ for $0.5[xAg_2O{-}(1-x)V_2O_5]{-}0.5TeO_2$ glasses. The solid lines are fit to Greaves' model.

Variable Range Hopping

Hopping to remote states at distances $L \gg \xi$?
Localized wavefunction overlap $|\langle L|0\rangle|^2 \sim e^{-2L/\xi}$
A larger number of states than at $r \sim \xi$, thus a smaller level spacing $\Delta_L = (n_0 L^d)^{-1}$, and a higher thermal activation rate $e^{-\beta\Delta_L}$
Putting everything together gives the VRH hopping rate $e^{-\beta\Delta_L - 2L/\xi} = e^{-(AL+B/L^d)}$

It pays to hop at $L \gg \xi$: optimal $L_M \sim \left(\frac{\beta\xi}{n_0}\right)^{1/(d+1)}$. These processes are relevant when $T < T_0 = \Delta_\xi$, predicting an insulating T dependence $d\sigma/dT > 0$:

$$\sigma_{VRH} \sim e^{-C(T_0/T)^\alpha}, \quad \alpha = \frac{1}{d+1} < 1$$

Values: $\alpha_{d=3} = 1/4$, $\alpha_{d=2} = 1/3$, $\alpha_{d=1} = 1/2$
More on the Miller-Abrahams network and Mott VRH can be found here.

The long-range Coulomb interactions, which are poorly screened in the insulating state, create an interesting correlated state with a Coulomb gap. This alters the α value, producing a universal dependence $\sigma \sim e^{-(T_0/T)^{1/2}}$ (Efros-Sklovskii theory)

Anderson localization in one dimension

demo

We're now consider quantum transport, at $T \approx 0$
(c.f. semi-classical Boltzmann transportation).

We consider now an external $\vec{E}$-field (and $\vec{B}$-field) summerized by an external $\vec{A}$-field. (i.e. take a Gauge where $U \equiv 0$)

Recall $\quad \vec{E} = \dot{\vec{A}} + \vec{\nabla}\Phi \quad ; \quad \vec{p} = \vec{p}_i + \frac{e}{c}\vec{A} \quad ;$

$$\mathcal{H} = H_0 + H_1 = H_0 + \left(-\frac{e}{c}\frac{1}{2m}(\vec{p}_i \cdot \vec{A} + \vec{A}\cdot\vec{p}_i) + \frac{e^2}{2mc^2}\vec{A}^2 \right)$$
$$= H_0 + \left(-\frac{1}{c}\vec{J}\cdot\vec{A} \right)$$

Note that in general, $\vec{J} = -\frac{e}{c}\sum_i \left(\vec{v}_i\,\delta(\vec{r}-\vec{r}_i) + \delta(\vec{r}-\vec{r}_i)\vec{v}_i \right)$

$$= -\frac{e}{2}\sum_i\left(\frac{\vec{p}_i}{m}\delta(\vec{r}-\vec{r}_i) + \delta(\vec{r}-\vec{r}_i)\frac{\vec{p}_i}{m}\right) \mapsto j_P \quad \text{(paramagnetic)}$$
$$-\frac{e^2}{mc^2}A(\vec{r})\sum_i \delta(\vec{r}-\vec{r}_i) \mapsto j_D \quad \text{(diamagnetic)}$$

So $\langle\vec{J}\rangle = \langle\vec{j}_P\rangle + \langle\vec{j}_D\rangle \quad ; \quad \langle \dot{j}_{P,\mu}(\vec{q})\rangle = -R_{\mu\nu}A_\nu(\vec{q})$

Kubo linear response theory: Drude conductivity

So $\langle \vec{j} \rangle = \langle \vec{j}_P \rangle + \langle \vec{j}_D \rangle$; $\langle j_{P,\mu}(\vec{q}) \rangle = -R_{\mu\nu} A_\nu(\vec{q})$

With $R_{\mu\nu}(\vec{q},t) = -i \langle 0 | [j_{P,\mu}(\vec{q},t), j_{P,\nu}(-\vec{q},0)] | 0 \rangle \, \theta(t-0)$

And $\langle j_D \rangle = \frac{e^2}{mc^2} \vec{A} \, n_0$ (to linear order)

So, $\langle j_\mu(\vec{q},\omega) \rangle = - K_{\mu\nu}(\vec{q},\omega) A_\nu(\vec{q},\omega)$

$$K_{\mu\nu} = R_{\mu\nu} + \frac{ne^2}{mc^2} \delta_{\mu\nu} .$$

Note that $\vec{E} = \dot{\vec{A}} = i\omega A(\vec{q},\omega)$

$$\Longrightarrow \qquad \sigma = \frac{J}{E} = \frac{1}{i\omega} K_{\mu\nu}$$

Kubo linear response theory: Drude conductivity

Recall that σ is complex, and it's real part corresponds to dissipation.

Now, inserting a complete set,

$$R_{j_\mu j_\mu} = i\sum_n |\langle 0|j_\mu|n\rangle|^2 \left\{ \frac{1}{\omega-(\varepsilon_n-\varepsilon_0)+i\eta} - \frac{1}{\omega+(\varepsilon_n-\varepsilon_0)+i\eta} \right\}$$

$$\Longrightarrow \quad \mathrm{Re}\{\sigma_{j_\mu j_\mu}(\vec{q},\omega)\} = \frac{\pi}{\omega}\sum_n |\langle 0|j_\mu(\vec{q})|n\rangle|^2 \{\delta(\omega-(\varepsilon_n-\varepsilon_0))\} \quad \text{for } \omega>0. \qquad (*)$$

So measuring σ gives information about excited state.

Also, we could have derived $(*)$ via Fermi golden rule. Suppose we shine light on the metal, it dissipate σE^2 energy, while emission rate is:

$$\frac{1}{\tau} = 2\pi A^2 \sum_n |\langle 0|j_x|n\rangle|^2 \delta(\omega-(E_n-E_0))$$

Equating, $\quad \frac{\hbar\omega}{\tau} \approx \sigma E^2$, and use $i\omega A = E \Rightarrow$ desired result.

For DC conductivity, we take $\vec{q} = 0$ and $\omega \to 0$

Now consider a disordered system (for ordered system, we know $\sigma \to +\infty$.)

WLOG assume homogenity:

$$\sigma'(\vec{q},\omega) = \frac{1}{\omega}\int d(\vec{r}-\vec{r}\,')\int dt\; e^{-i\omega t}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}\,\theta(t)\;\underbrace{\overline{\langle 0|\,[\,j_{P,\mu}(\vec{r},t)\,,\, j_{P,\mu}(\vec{r}\,',0)]\,|0\rangle}^{\text{disorder average}}}_{=F(\vec{r}-\vec{r}\,')}$$

$= F(\vec{r}-\vec{r}\,')$, and has translation symmetry

[While for EACH config. in average, the translation symmetry is destroyed].

$$= \frac{1}{\omega}\underset{\text{volume}}{\frac{1}{\Omega}}\int d\vec{r}\, d\vec{r}\,' \int dt\; e^{-i\omega t}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}\;\overline{\langle 0|\,[\,j_{P,\mu}(\vec{r},t)\,,\, j_{P,\mu}(\vec{r}\,',0)]\,|0\rangle}\;\theta(t)$$

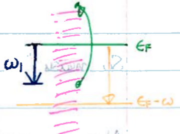
Taking $\vec{q} \to 0$, rearranging:

$$\sigma'(\vec{q},\omega) = \frac{\pi}{\omega}\frac{1}{\Omega}\sum_n \overline{\langle 0|\int d\vec{r}\, j_{\vec{q},\mu}(\vec{r})|n\rangle\langle n|\int d\vec{r}'\, j_{\vec{q},\mu}(\vec{r}')|0\rangle}\ \delta(\omega-(E_n-E_0))$$

Now, $\underbrace{H = H_0 + V(r)}_{\text{single particle Hamiltonian}}$, where $V(r)$ is random, in single particle approximation.

We may label states by label α, $H|\alpha\rangle = E_\alpha|\alpha\rangle$ ← single particle state.

Then, $|n\rangle = |\underset{\text{particle}}{\beta}\,\underset{\text{hole}}{\bar{\alpha}}\rangle$ with $\varepsilon_\beta > \varepsilon_F$, $\varepsilon_\alpha < \varepsilon_F$



(Note that $j \propto c^\dagger_{\vec{r}} c_{\vec{r}}$ is single particle operator)

converting from many-body matrix element to single-particle matrix element (easy since we're in free e^- model)

$$\Rightarrow \int dr \langle n|j_\mu(\vec{r})|0\rangle = \int d\vec{r}\, \frac{e}{m}\int d\vec{r}'\, \left(\phi^*_\beta(\vec{r}')\, \nabla_{\vec{r}}\, \delta(\vec{r}-\vec{r}')\, \phi_\alpha(\vec{r}')\right)$$

$$= \frac{e}{m}\int \phi^*_\beta(\vec{r}')\, \vec{\nabla}_{\vec{r}'}\, \phi_\alpha(\vec{r}')\, d\vec{r}'$$

$$= \frac{e}{m}\langle\beta|\vec{\nabla}|\alpha\rangle$$

limit determined by f_α, f_β

$$\Rightarrow \sigma'_{\mu\mu} = \frac{e^2}{\omega}\frac{1}{\Omega}\int_{-\omega}^{0} d\omega_1 \sum_\alpha \delta(\omega_1-E_\alpha)\sum_\beta \delta(\omega-E_\beta+\omega_1)\ \overline{|\langle\beta|\frac{\nabla_\mu}{m}|\alpha\rangle|}$$

$$= \frac{e}{m}\langle\beta|\vec\nabla|\alpha\rangle$$

limit determined by f_α, f_β

$$\Rightarrow \sigma_{\mu\mu}' = \frac{e^2}{\omega}\frac{1}{\Omega}\int_{-\omega}^{0} d\omega_1 \sum_\alpha \delta(\omega_1 - E_\alpha)\sum_\beta \delta(\omega - E_\beta + \omega_1)\,\left|\langle\beta|\frac{\nabla_\mu}{m}|\alpha\rangle\right|$$

$$\left(\because \sigma_{\mu\mu}' = \frac{e^2}{\omega}\frac{1}{\Omega}\sum_{\alpha,\beta}\left|\langle\beta|\frac{\nabla_\mu}{m}|\alpha\rangle\right|^2 \delta(\omega - (E_\beta - E_\alpha))\, f(E_\alpha)\,(1 - f(E_\beta))\right)$$

where we've take $\epsilon_F = 0$

[$\sum_{\alpha,\beta}\delta(\ldots)\delta(\ldots)$ depends on eigenvalue distribution, $|\langle\beta|\nabla|\alpha\rangle|^2$ depends on eigenvector so make sense to separate.]

In approximation,

$$\sigma_{\mu\mu}' = \frac{e^2}{\omega}\frac{1}{\Omega}\int_{-\omega}^{0} d\omega_1 \underbrace{\overline{\sum_\alpha \delta(\omega_1 - E_\alpha)}}_{N(\omega)}\ \underbrace{\overline{\sum_\beta \delta(\omega - E_\beta + \omega_1)}}_{N(\omega-\omega_1)}\ \overline{\left|\langle\beta|\frac{\nabla_\mu}{m}|\alpha\rangle\right|^2}$$

pick some typical $|\beta\rangle, |\alpha\rangle$ and compute.

By randomness, $N(\omega) \approx N(\omega-\omega_1) \approx N(\epsilon_F) = N(0)$.

Note also that we're in $N\to\infty$ limit first, before taking $\omega\to 0$

$\overline{\sum_\alpha \delta(\omega - E_\alpha)\sum_\beta \delta(\omega - E_\beta + \omega_1)} \approx \overline{\sum_\alpha \delta_\alpha}\cdot\overline{\sum_\beta \delta_\beta}$ since the level distribution is random at the coarse grained scale.

Combining, $\sigma_{\mu\mu} = \frac{e^2\pi[N(0)]^2}{\Omega}\overline{|\langle\beta|\frac{\nabla_\mu}{m}|\alpha\rangle|^2} = \frac{e^2\pi(N(0))^2}{\Omega}\overline{V^2}$

In the $\underbrace{\text{weak disorder limit}}$ (i.e. $k_F\ell \gg 1$), the wavefunctions are locally plane wave

ℓ mean-free path (our phenomenological parameter)

$\Longrightarrow$ $\phi_\alpha(\vec r) = e^{i\vec k\cdot\vec r + \phi_0}$ in scale $|\vec r| < \ell$. where $|\vec k| \approx k_F$; $k_F\ell \ll 1$.

And $\vec k$ and ϕ_0 are slow varying functions in $\vec r$.

Divide the volume into boxes of dimension $\ell\times\ell\times\ell$. Assume $\phi_\alpha(\vec r) \approx e^{i\vec k\cdot\vec r+\phi_0}$ inside each box.

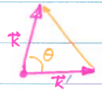
Then, $V_{\alpha\beta} = \langle\beta|\frac{\nabla}{m}|\alpha\rangle = \sum_{i=1}^{\Omega/\ell^3}\delta_i$, where $\delta_i = \int_{\ell^3}\psi^*_{\vec k'}\frac{1}{m}\nabla\psi_{\vec k}\, d^3\vec r$

Kubo linear response theory: Drude conductivity

Then, $V_{\alpha\beta} = \langle \beta | \frac{\vec{\nabla}}{m} | \alpha \rangle = \sum_{i=1}^{\Omega/\ell^3} \delta_i$, where $\delta_i = \int_{\ell^3} \psi^*_{\vec{k}'} \frac{1}{m} \vec{\nabla} \psi_{\vec{k}} \, d^3\vec{r}$

Now, since there is an overall random phase, all cross terms cancels,

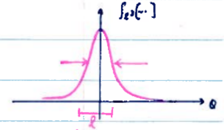
$$\overline{V^2} = \frac{\Omega}{\ell^3} \overline{|\delta|^2}$$



Next, $\delta_i \approx e^{i\phi_i} \left(\int_{\nu} \frac{k}{m} \frac{e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}}{\Omega} d^3\vec{r} \right)$. where $|\vec{k}-\vec{k}'| \approx 2k_F \sin\left(\frac{\theta}{2}\right)$

Since contributions come only from situation where $\vec{k}-\vec{k}'$ is small, $|\vec{k}-\vec{k}'| \approx 2k_F\theta$

$$\longrightarrow \quad \delta_i \approx \begin{cases} \frac{1}{m}\frac{k_F \nu}{\Omega} e^{i\phi_i} & \text{if } (k_F\theta)\ell < 1 \\ 0 & \text{otherwise} \end{cases}$$



$$\longrightarrow \quad \overline{V^2} = \left(\frac{\Omega}{\nu}\right)\left(\frac{k_F \nu}{m\Omega}\right)^2 \cdot \underbrace{\int_0^{1/k_F\ell}\int_0^{2\pi} \frac{\sin\theta \, d\phi \, d\theta}{4\pi}}_{\text{impurity average (fraction of boxes with non-zero integral)}} \approx \frac{\pi\ell}{3m^2\Omega}.$$

Therefore, $\sigma = \frac{2e^2\pi^2}{3m^2}\left(\frac{N(0)}{\Omega}\right)^2 \ell$ For free fermion, $\frac{N(0)}{\Omega} = \frac{mk_F}{2\hbar^2\pi^2}$

$$\Longrightarrow \quad \sigma = \frac{e^2 k_F^2 \ell}{6\pi^2\hbar}$$

And $\sigma_{\text{Boltzmann}} = \frac{ne^2\tau}{m} = \frac{e^2 k_F^2 \ell}{3\pi^2\hbar}$ (agree)

$\tau = \frac{\ell}{m}$, $n = \frac{k_F^3}{3\pi^2}$

Recall that $\frac{e^2}{\hbar}$ appears in quantum Hall effect and is the quantum unit of conductance. And $\sigma = \left(\frac{e^2}{\hbar}\right)\left(\frac{k_F^2 \ell}{6\pi}\right)$

Also, $\frac{h}{e^2} = \frac{2\pi\hbar}{e^2} = 25.8\,(k\Omega)$

And as it turns out... $\sigma = \frac{e^2}{\pi\hbar}(k_F \ell)$ in 2D

(Since $\frac{N(0)}{\Omega} \propto m$)

The minimum metallic conductivity is found by setting $k_F\ell \approx 1$
Obtain $\sigma_{3D}^{min} = \frac{e^2}{3\hbar}\lambda_F$ and $\sigma_{2D}^{min} = \frac{e^2}{\pi\hbar}$

This agrees with the estimates based on the Ioffe-Regel criterion

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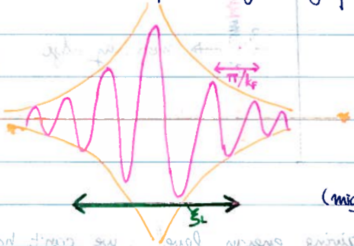
Kubo linear response theory: localized phase

We've seen that when $k_F \ell \gg 1$, then we have metal.

Next we want to consider $k_F \ell \ll 1$.

We expect the wavefunction to have exponentially decaying envelop near scatterer.



(might have $\xi_L > \ell$).

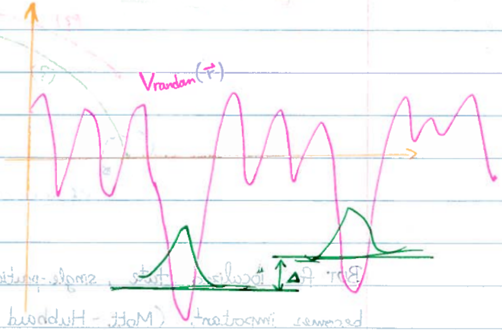
From Kubo formula, $\sigma = \frac{1}{\omega} \sum_{\alpha,\beta} |\langle\alpha|j|\beta\rangle|^2 \, \delta(\omega - (E_\alpha - E_\beta)) f_\alpha (1 - f_\beta)$

with localization, $\langle\alpha|j|\beta\rangle \propto \langle\alpha|v|\beta\rangle = \langle\alpha|[H, x]|\beta\rangle$

$\Longrightarrow \quad \sigma = \omega \sum_{\alpha,\beta} |\langle\alpha|x|\beta\rangle|^2 \, \delta(\omega - (E_\alpha - E_\beta)) \underbrace{f_\alpha (1 - f_\beta)}_{\text{phase space } \sim \omega} \longrightarrow 0$ as $\omega \to 0$

Kubo linear response theory: localized phase

In the random potential picture:



Locally, the probability of finding two states in resonance is

$$P_r \propto \frac{1}{N(E)\cdot L^d}$$

While the tunneling probability is

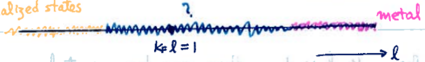
$$P_t \propto e^{-\xi/L}$$

Thus, far away, there is no overlap between states localized in a trough.

$\Longrightarrow$ localization is common (for sufficient low energy).

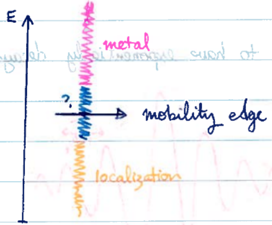
Remark: Although wavefunction has qualitative difference, density of states look more-or-less the same.

Kubo linear response theory: localized phase



(Anderson)

Alternatively, think in terms of energy: (Mott)



(At a given energy, states are either all localized or all extended.
For if not, extended state and localized state can mix.)

Now, at a giving energy level, we can't have both metallic state and localized state. Otherwise they will mix.

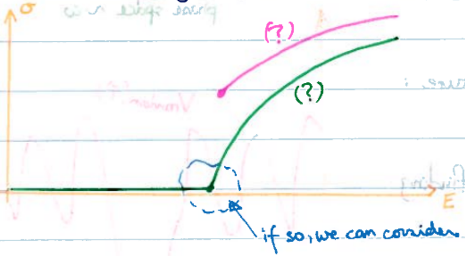
$\Longrightarrow$ Mobility edge is sharp.

Kubo linear response theory: localized phase

Now, at a giving energy level, we can't have both metallic state and localized state. Otherwise they will mix.

$\Longrightarrow$ Mobility edge is sharp.

But the transition may take several forms



Relate conductivity and diffusivity for disordered electrons?

This can be done in a very general way using the fluctuation-dissipation theorem

Recall Einstein relation for a Brownian random walker: $\mu = TD$

In a similar vein, here we will need the Einstein relation for a conductor at $T = 0$:

$$\sigma = e^2 N_0 D, \quad N_0 = \frac{dn}{d\mu}$$

It is an exact relation between two observables (no approximation made)

Proof: write electric current as a sum of the ohmic and diffusive parts,

$$\mathrm{j} = \sigma \mathrm{E} - eD\nabla n$$

and demand that it vanishes in a steady state in the presence of a static potental: $\mathrm{E} = -\nabla\delta\phi(r)$, $n(r) = n_0 + \frac{dn}{d\mu}e\delta\phi(r)$.

Scaling theory. Dimensionless conductance

Define dimensionless conductance $g = \frac{G}{2e^2/h} = \pi \frac{G}{e^2/\hbar}$.
Express the conductance of a box of size L in terms of the diffusion time and level spacing Δ:

$$G = \sigma L^{d-2} = 2e^2 \frac{dn}{d\mu} D L^{d-2} = 2\frac{e^2}{\hbar}\frac{\hbar D}{L^2}\frac{1}{\Delta}, \quad \Delta = \frac{1}{L^d dn/d\mu}$$

where the factor of 2 is spin degeneracy, and Δ is the single-particle level spacing near E_F.
So for free fermions $G = 2\frac{e^2}{\hbar}\frac{\hbar}{\tau_{\rm T}}\frac{1}{\Delta}$, where we introduced the Thouless transport time defined as $\frac{1}{\tau_{\rm T}} = \frac{D}{L^2}$, the inverse time for a random walker to diffuse through legth scale L. Or, think of $\tau_{\rm T}$ as a time to escape from a box of dimension L.

Therefore, we find a fundamental relation $g = 2\pi \frac{E_{\rm T}}{\Delta}$, where we defined the Thouless energy $E_{\rm T} = \hbar/\tau_{\rm T}$.

Compare this picture to our discussion of resonances in the localized phase

$$H = \begin{pmatrix} \epsilon_1 & V \\ V & \epsilon_2 \end{pmatrix}, \quad E_\pm = \frac{\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4V^2}}{2}$$

Resonances ("delocalized states") occur for detuning less than hopping, $\epsilon_1 - \epsilon_2 \lesssim V$.

Now, in dimensionless conductance $g = 2\pi \frac{E_T}{\Delta}$ identify the Thouless energy $E_T = \hbar/\tau$ with V, and the level spacing Δ with $\epsilon_1 - \epsilon_2$.

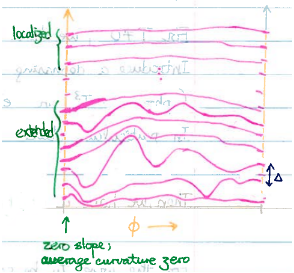
Then the Thouless criterion — localization at $g < 1$, delocalization at $g > 1$ — can be viewed as nothing but a "block form" of the pair resonance condition $\epsilon_1 - \epsilon_2 \lesssim V$.

Thouless criterion for Anderson localization

How do we find $E_T = \hbar/\tau$?

Sensitivity to boundary conditions: Thouless energy and time

Demo



Thouless energy and transport time: $\frac{\hbar}{\tau_{\mathrm{T}}} \sim \frac{\partial^2 E_i}{\partial \phi^2}$, $E_{\mathrm{T}} = \frac{\hbar}{\tau_{\mathrm{T}}}$

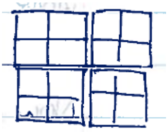
$$\sqrt{\overline{\left(\frac{\partial^2 E_i}{\partial \phi^2}\right)^2}} = \hbar \frac{\pi D}{L^2} = \pi E_{\mathrm{T}}$$

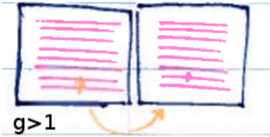
This is a generalization of the result from scattering theory for a time delay for the scattering of a wave packet, $\Delta t \sim \hbar d\delta(E)/dE$.

Dimensionless conductance. Block picture:

for $g \ll 1$:

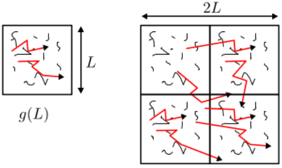
(local can still be identified with individual box)



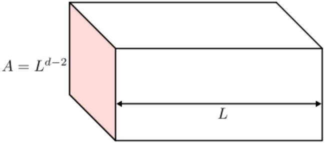


recall classical scaling: $G = \sigma A/L$, $g(L) = g_0 L^{d-2}$, $g_0 \sim k_F^{d-1}\ell$.

Expect $d = 2$ to be the critical dimension.



$g(L)$ $g(L)$



Generalize the classical scaling $g(L) = g_0 L^{d-2}$ to the quantum-coherent transport problem?

Wanted: a scaling theory for $g(L)$. An RG flow

$$\frac{\partial \log g(L)}{\partial \log L} = \beta(g)$$

with β a function of g only (assume universality).

Motivated by QFT in high-energy physics and the scaling theory of phase transitions.

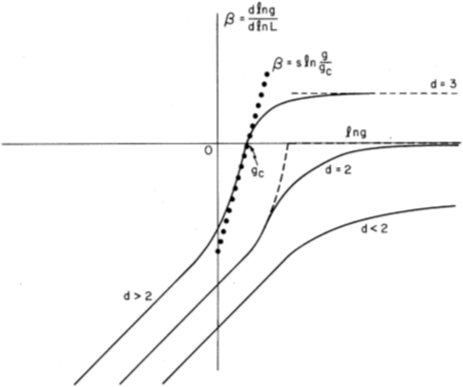
Peturbation theory in weak disorder $\frac{1}{g} \sim \frac{1}{k_F \ell} \ll 1$:

$$\beta(g) = d - 2 - \frac{C}{g} + O(g^{-2})$$

Scaling theory of localization

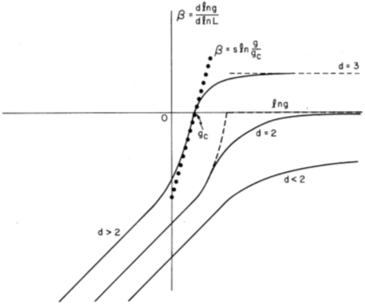
Abrahams, Anderson, Licciardello, Ramakrishnan, PRL 42 673 (1979):

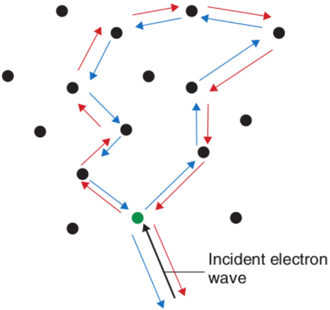
Anderson transition as an RG fix point: A critical point for $d > 2$; insulator $d < 2$; subtle $d = 2$



The minimum metallic conductance value $g_{d=3} \sim 1$

Metallic phase: phase-coherent transport





$\beta(g) = d - 2 - c/g$ with $c > 0$ for scalar potential disorder (weak localization), $c < 0$ for spin-orbit scattering (weak antilocalization). Macroscopic phase-coherent behavior at weak disorder. Memory effects due to electron wave interference. At large lengthscales these effects are sensitive to ultralow magnetic fields. Negative magnetoresistance (B field suppressing the interference, "undoing" localization) and $d\rho/dT < 0$

Anderson transition in a 1D quasiperiodic potential

Harper equation, duality and Anderson transition in one dimension

In a tight-binding problem with a quasiperiodic potential,

$$\epsilon\psi_n = 2t' \cos(2\pi\omega n + \theta)\psi_n + t\psi_{n-1} + t\psi_{n+1}$$

the eigenstates can be either localized or delocalized depending on the ratio of t and t'. There is an Anderson transition when $t = t'$.
To understand the origin of this behavior, we define a duality transformation connecting the real and reciprocal space as follows.

- Consider Fourier-transformed wavefunction, $\psi_n = \int_{-\pi}^{\pi} \psi(p) e^{ipn} \frac{dp}{2\pi}$ and rewrite Schroedinger equation for ψ_p.
- The shift $n \to n \pm 1$ translates into multiplication by a phase factor $\psi(p) \to e^{\pm ip}\psi(p)$; conversely, the Fourier transform of $2\cos(2\pi\omega n + \theta)\psi_n$ is $e^{i\theta}\psi(p + 2\pi\omega) + e^{-i\theta}\psi(p - 2\pi\omega)$. Therefore
$$\epsilon\psi(p) = 2t\cos(p)\psi(p) + t'\psi(p + 2\pi\omega) + t'\psi(p - 2\pi\omega)$$
where without loss of generality we set $\theta = 0$.
- After rescaling, $p = 2\pi\omega\tilde{p}$ this gives a dual problem with $t \rightleftharpoons t'$
$$\epsilon\psi(\tilde{p}) = 2t\cos(2\pi\omega\tilde{p})\psi(\tilde{p}) + t'\psi(\tilde{p} + 1) + t'\psi(\tilde{p} - 1).$$
- From the above, we conjecture that states are localized when $t' > t$ and extended when $t' < t$.
- Confirm these conclusions by solving the problem numerically by using direct diagonalization of the Hamiltonian for a finite system.