Coherent and collective phenomena in quantum transport 8.513

- Lectures T, TR 1-2:30
- Homework handed out in class, collected two weeks later – except holidays and HW#1
- Term paper: choose topic by the end of October, submit before or in the last lecture
- Instructor: Leonid (aka Leo) Levitov, office 6C-345, email: levitov@mit.edu
- Course webpage: http://www.mit.edu/~levitov/8513
Quantum transport; Lecture I

• Localization vs. diffusion
• Anderson model, localization transition;
• Quantum-coherent effects in diffusive conductors: weak localization, negative magnetoresistance, Aharonov-Bohm effect ($2\Phi_0$ and $\Phi_0$)
• Transport as a scattering problem: conductance = transmission; Landauer formula
Absence of Diffusion in Certain Random Lattices

P. W. Anderson
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received October 10, 1957)

This paper presents a simple model for such processes as spin diffusion or conduction in the "impurity band." These processes involve transport in a lattice which is in some sense random, and in them diffusion is expected to take place via quantum jumps between localized sites. In this simple model the essential randomness is introduced by requiring the energy to vary randomly from site to site. It is shown that at low enough densities no diffusion at all can take place, and the criteria for transport to occur are given.
I was cited for work both in the field of magnetism and in that of disordered systems, and I would like to describe here one development in each field which was specifically mentioned in that citation. The two theories I will discuss differed sharply in some ways. The theory of local moments in metals was, in a sense, easy: it was the condensation into a simple mathematical model of ideas which were very much in the air at the time, and it had rapid and permanent acceptance because of its timeliness and its relative simplicity. What mathematical difficulty it contained has been almost fully cleared up within the past few years.

Localization was a different matter: very few believed it at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it.
Einstein Relation (1905)

$\sigma = e^2 D \nu$

$\nu = \frac{dn}{d \mu}$

Conductivity

Density of states

Diffusion Constant

No diffusion – no conductivity

Localized states – insulator

Extended states – metal

Metal – insulator transition
Correlations due to Localization in Quantum Eigenfunctions of Disordered Microwave Cavities

Prabakar Pradhan and S. Sridhar
Department of Physics, Northeastern University, Boston, Massachusetts 02115
(Received 28 February 2000)

\[ f = 3.04 \text{ GHz} \]

\[ f = 7.33 \text{ GHz} \]

Anderson Insulator  Anderson Metal
Fermi Pasta Ulam 1955

**Q:** Will a nonlinear system (system of interacting particles) completely isolated from the outside world evolve to a microcanonical distribution (reach equipartition).

Anderson 1958

**Q:** Will a density fluctuation (a wave packet) in a system of quantum particles in the presence of disorder dissolve in the diffusive way.
Localization of single-electron wave-functions:

\[
\left[-\frac{\nabla^2}{2m} + U(r) - \varepsilon_F \right] \psi_\alpha(r) = \xi_\alpha \psi_\alpha(r)
\]

\[\psi_\alpha(x)\]

\[\xi_{loc}\]

\[\psi_\alpha(x)\]

\[\xi_{loc}\]

\[\sigma \frac{L_x L_y}{L_z}; \text{ extended}\]

\[\alpha \exp\left(-\frac{L_z}{\xi_{loc}}\right); \text{ localized}\]

Disorder

Conductance

\[G = \frac{I}{V} \bigg|_{V \to 0}\]
Scattering centers, e.g., impurities

Models of disorder:
- Randomly located impurities
- White noise potential
- Lattice models
  - Anderson model
  - Lifshits model
Anderson Model

- \(-W < \varepsilon_i < W\) uniformly distributed

- Lattice - tight binding model
- Onsite energies \(\varepsilon_i\) - random
- Hopping matrix elements \(I_{ij}\)

\[
I_{ij} = \begin{cases} 
I & i \text{ and } j \text{ are nearest neighbors} \\
0 & \text{otherwise}
\end{cases}
\]

Anderson Transition

\[
\frac{I_c}{W} \approx \left(\frac{1}{2d}\right) \left(\frac{1}{\ln d}\right)
\]

- \(I < I_c\) Insulator
  - All eigenstates are localized
  - Localization length \(\xi\)

- \(I > I_c\) Metal
  - There appear states extended all over the whole system
Q:
Why arbitrary weak hopping is not sufficient for the existence of the diffusion

Einstein (1905): Marcovian (no memory) process → diffusion

Quantum mechanics is not marcovian
There is memory in quantum propagation!
Why?
Hamiltonian

\[ \hat{H} = \begin{pmatrix} \varepsilon_1 & I \\ I & \varepsilon_2 \end{pmatrix} \]

\[ \hat{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \]

\[ E_2 - E_1 = \sqrt{(\varepsilon_2 - \varepsilon_1)^2 + I^2} \]
\[ \hat{H} = \begin{pmatrix} \varepsilon_1 & I \\ I & \varepsilon_2 \end{pmatrix} \quad \text{diagonalize} \quad \hat{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \]

\[ E_2 - E_1 = \sqrt{(\varepsilon_2 - \varepsilon_1)^2 + I^2} \approx \frac{\varepsilon_2 - \varepsilon_1}{I} \quad \varepsilon_2 - \varepsilon_1 \gg I \]

\[ \varepsilon_2 - \varepsilon_1 \ll I \]

von Neumann & Wigner “noncrossing rule”
Level repulsion

What about the eigenfunctions?
\[ \hat{H} = \begin{pmatrix} \varepsilon_1 & I \\ I & \varepsilon_2 \end{pmatrix} \]

\[ E_2 - E_1 = \sqrt{(\varepsilon_2 - \varepsilon_1)^2 + I^2} \approx \frac{\varepsilon_2 - \varepsilon_1}{I} \quad \text{if} \quad \varepsilon_2 - \varepsilon_1 \gg I \]
\[ \quad \text{or} \quad \varepsilon_2 - \varepsilon_1 \ll I \]

What about the eigenfunctions?

\[ \phi_1 \varepsilon_1 ; \phi_2 \varepsilon_2 \leftarrow \psi_1, E_1 ; \psi_2, E_2 \]

\[ \varepsilon_2 - \varepsilon_1 \gg I \]

\[ \psi_{1,2} = \phi_{1,2} + O \left( \frac{I}{\varepsilon_2 - \varepsilon_1} \right) \phi_{2,1} \]

Off-resonance
Eigenfunctions are close to the original on-site wave functions

Resonance
In both eigenstates the probability is equally shared between the sites

\[ \psi_{1,2} \approx \phi_{1,2} \pm \phi_{2,1} \]
Anderson insulator
Few isolated resonances

Anderson metal
There are many resonances and they overlap
A selfconsistent theory of localization

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Received 12 January 1973

Abstract. A new basis has been found for the theory of localization of electrons in disordered systems. The method is based on a selfconsistent solution of the equation for the self energy in second order perturbation theory, whose solution may be purely real almost everywhere (localized states) or complex everywhere (nonlocalized states). The equations used are exact for a Bethe lattice. The selfconsistency condition gives a nonlinear integral equation in two variables for the probability distribution of the real and imaginary parts of the self energy. A simple approximation for the stability limit of localized states gives Anderson’s ‘upper limit approximation’. Exact solution of the stability problem in a special case gives results very close to Anderson’s best estimate. A general and simple formula for the stability limit is derived; this formula should be valid for smooth distribution of site energies away from the band edge. Results of Monte Carlo calculations of the selfconsistency problem are described which confirm and go beyond the analytical results. The relation of this theory to the old Anderson theory is examined, and it is concluded that the present theory is similar but better.
**Simplest example: Anderson Model Cayley tree:**

Parameters: \( I, W \) and branching number \( K \) (here \( K=2 \))

Crucial simplification: no loops

The probability amplitude to find the particle at a distance \( n \) is proportional to

\[
A(n) \propto I^n \prod_{j=1}^{n} \frac{1}{\varepsilon - \varepsilon_j} \approx I^n \left(\frac{K}{W}\right)^n
\]
The probability amplitude to find the particle at a distance \( n \) is proportional to

\[
A(n) \propto I^n \prod_{j=1}^{n} \frac{1}{\varepsilon - \varepsilon_j} \approx I^n \left( \frac{K}{W} \right)^n
\]

At each step among \( K \) site we can choose the one, which energy is the closest to \( \varepsilon \), i.e., \( |\varepsilon - \varepsilon_j| \approx W/K \)

**\( K > 1 \):** Competition between exponentially small amplitude of each path and exponentially large number of paths.

Conclusion: for \( I < I_c \), where \( I_c \approx W/K \) the system is an insulator, because \( A(n \to \infty) \to 0 \) In the opposite case – metal

More precisely \( I_c \approx W/(K \log K) \)
\[ A(n) \propto I^n \prod_{j=1}^{n} \frac{1}{\varepsilon - \varepsilon_j} \approx I^n \left( \frac{K}{W} \right)^n \]

Conclusion: for \( I < I_c \), where \( I_c \approx W/K \) the system is an insulator, because \( A(n \to \infty) \to 0 \). In the opposite case - metal

More precisely \( I_c \approx \frac{W}{(K \log K)} \)

\[ I > \frac{W}{K} \quad \text{Typically there is a resonance at every step} \]

\[ \frac{W}{(K \log K)} < I < \frac{W}{K} \]

\[ I > W \quad \text{Typically each pair of nearest neighbors is at resonance} \]

The particle can travel infinitely far through the resonances of sites, which are not nearest neighbors.
Quantum effects in diffusive transport
Weak localization

Phase Coherence Phenomena in Normal Conductors

How does disorder influence transport?

Classically, from Drude theory

![Formula: $\sigma = \frac{ne^2 \tau}{m}$]

$1/\tau$ scattering rate

Quantum mechanically? Naively...

(i) for $\ell \equiv v_F \tau \gg \lambda_F$, interference is unimportant & can add intensities $\sim$ Drude!

(ii) for $\ell \sim \lambda_F$ conductivity vanishes: metal-insulator transition

...However, mechanisms of quantum interference impact even on metallic phase

Feynman Trajectories

Transfer probability amplitude:

$$G(r, 0; t) = \langle r|e^{-iHt/\hbar}|0\rangle \theta(t)$$

Impurity average

i.e. over realisations of random impurity potential

$$\langle G(r, 0; t) \rangle_V = \left\langle \sum_i A_ie^{i\varphi_i} \right\rangle_V \sim e^{-t/2\tau}$$

i.e. random phase cancellation $\sim$ short-range correls.
Quantum diffusion

\[ G(r, 0; t) = \sum_i A_i e^{i\varphi_i} \]

\[
\begin{align*}
\langle P(r, t) \rangle_v & = \left\langle \sum_i A_i^2 \right\rangle_v^{\text{classical}} + \left\langle \sum_{i \neq j} A_i A_j \cos(\varphi_i - \varphi_j) \right\rangle_v^{\text{quantum}} \\
\langle |G(r, 0; t)|^2 \rangle_v & = \left\langle \sum_i A_i^2 \right\rangle_v^{\text{classical}} + \left\langle \sum_{i \neq j} A_i A_j \cos(\varphi_i - \varphi_j) \right\rangle_v^{\text{quantum}} \\
& \xrightarrow{\text{perturbation theory}} 0
\end{align*}
\]

\[ \partial_t P(r, t) - D \partial^2 P(r, t) = \delta(r) \delta(t) \]

& predicts classical Drude conductivity \( \sigma = e^2 \nu D \)

\[ |A_1 e^{i\varphi_1} + A_2 e^{i\varphi_2}|^2 = A_1^2 + A_2^2 + 2A_1 A_2 \cos(\varphi_1 - \varphi_2) \]

In \( T \)-invariant system, \( A_1 = A_2, \ \varphi_1 = \varphi_2 \)

i.e. \[ P_{\text{quantum}} = 2 \times P_{\text{classical}} \]

\[ \Rightarrow \text{tendency to localize} \]

\[ \Rightarrow \text{quantum correction to conductivity...} \]
Suppression of conductance

\[ \frac{\delta \sigma}{\sigma} = \frac{\delta P}{P} \sim - \int dP_{\text{return}} \sim -v_F\lambda_F^{d-1} \int_\tau^{L^2/D} \frac{dt}{(Dt)^{d/2}} \]

\rightarrow \text{singular correct}^{\text{NS}} \text{ in low dim.}

\[ \delta \sigma_{d=2} = -\frac{e^2}{\pi^2 \hbar} \ln \left( \frac{L}{\ell} \right) \]

...accumulation of WL correct\textsuperscript{NS}: scaling\textsuperscript{2} \rightarrow \text{Anderson localisation}

\textsuperscript{1}Gor'kov, Larkin & Khmel'nitskii '79
\textsuperscript{2}Abrahams, Anderson, Ramakrishnan & Liciardello '79
Long-range quantum coherence

- Quantum interference effects mediated by two long-ranged modes of density relaxation...

- ‘Diffuson’

$$\langle G^R(0, r; t) G^A(r, 0; t) \rangle_V = \frac{\text{e}^{\text{FT}}}{\text{Dq}^2 + i\omega}$$

- ‘Cooperon’

$$\langle G^R(0, r; t) \overline{G^A(0, r; t)} \rangle_V = \frac{\text{e}^{\text{FT}}}{\text{Dq}^2 + i\omega}$$

...together, diffusion modes form basic elements of diagrammatic perturbation theory

- Characteristic weak localization phenomena

- But magnetoresistance is not the only physical manifestation of quantum interference...

...effects recorded in fluctuations phenomena...
Scattering approach
Conductance from transmission

Heuristic discussion

Fermi energy left contact $\mu + eV$
Fermi energy right contact $\mu$
applied voltage $eV$
transmission probability $T$
reflection probability $R$

incident current

$$I_{in} = e v_F \Delta \rho$$

density

$$\Delta \rho = \left(\frac{d\rho}{dE}\right) eV$$

density of states

$$\frac{d\rho}{dE} = \left(\frac{d\rho}{dk}\right) \left(\frac{dk}{dE}\right) = \frac{1}{2\pi} \left(\frac{1}{\hbar v_F}\right)$$

$$I_{in} = \frac{(e/\hbar)eV}{\hbar} \text{ independent of material !!}$$

$$I = \frac{(e/\hbar)TeV}{\hbar} \Rightarrow$$

Landauer formula

$$G = \frac{dI}{dV} = \frac{e^2}{\hbar} T$$
Drift and diffusion

\[ j = \sigma E - eD dn/dx \]
\[ E = -dU/dx \]
\[ dn = \nu d\mu - e\nu dU \]

at constant \( \mu \)

\[ j = 0 = -\sigma dU/dx + e^2 D\nu (dU/dx) \]

\[ \Rightarrow \quad \sigma = e^2 D\nu \]

Electrochemical potential \( \mu - eU \)

Einstein relation

for space dependent \( \mu \)

\[ j = -e\nu D d\mu/dx \]
\[ j = e\nu D (\mu_L - \mu_R)/L \]
\[ j = (e^2 \nu D/L) V \]

\[ I = \frac{e^2}{h} TV \]
Scattering matrix

scattering state

\[ |\psi >_{inc} = e^{ikx} \]
\[ |\psi >_{ref} = r e^{-ikx} \]
\[ |\psi >_{tra} = t e^{ikx} \]

scattering matrix

\[
\begin{pmatrix}
  b_1 \\
  b_2
\end{pmatrix} =
\begin{pmatrix}
  r & t' \\
  t & r'
\end{pmatrix}
\begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix}
\]

current conservation \Rightarrow S is a unitray matrix

In the absence of a magnetic field S is an orthogonal matrix

\[ t' = t \]
Transfer matrix

\[
\begin{pmatrix}
\beta \\
\beta'
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\tilde{\beta} \\
\tilde{\beta}'
\end{pmatrix}
= 
\begin{pmatrix}
1/t^* & -r^*/t^* \\
-r/t & 1/t
\end{pmatrix}
\begin{pmatrix}
\beta \\
\beta'
\end{pmatrix}
\]

Transfer matrix is multiplicative  \implies arbitrary array of scatterers

One dimensional localization:

\[
\langle G \rangle = \frac{e^2}{\hbar} \exp(-L/\lambda)
\]

localization length \( \lambda \)

but \( \log G \) is normal distributed

characterize the sample through its distribution

\[
P(G) \ dG
\]

Discuss again later
Conductance from transmission

\[ G = \frac{dI}{dV} = \frac{e^2}{h} T \]

conductance quantum \[ \frac{e^2}{h} \]

dissipation and irreversibility

\[ W = I V = G V^2 \]

resistance quantum \[ \frac{h}{e^2} \approx 24 \text{ kOhm} \]
Conductance from transmission

\[ G = \frac{dI}{dV} = \frac{e^2}{h} T \]

conductance quantum

\[ \frac{e^2}{h} \]

dissipation and irreversibility

\[ W = I V = G V^2 \]

\[ R = \frac{dV}{dI} = \frac{h}{e^2} \frac{1}{T} \]

resistance quantum

\[ \frac{h}{e^2} \approx 24 \text{ kOhm} \]

Dissipation for elastic scattering?!
Conductance from transmission

\[ G = \frac{dI}{dV} = \frac{e^2}{h} T \]

conductance quantum \( \frac{e^2}{h} \)

\[ R = \frac{dV}{dI} = \frac{h}{e^2} \frac{1}{T} \]

resistance quantum \( \frac{h}{e^2} \approx 24 \text{ kOhm} \)

Dissipation for elastic scattering?! Energy is lost to the reservoirs.
General properties of S-matrix

Current conservation

Scattering matrix is a unitary matrix

\[
\begin{align*}
    s^\dagger s &= 1 \\
    r^* r + t^* t &= 1 \quad \Rightarrow \quad R + T = 1 \\
    t'^* r + r'^* t &= 0 \\
    r^* t' + t^* r' &= 0 \\
    t'^* t' + r'^* r' &= 1 \quad \Rightarrow \quad R' + T' = 1 \\
    s s^\dagger &= 1 \\
    \Rightarrow \quad R' + T = 1 \\
    \Rightarrow \quad R + T' = 1
\end{align*}
\]

\[
\begin{pmatrix}
    r \\
    t' \\
    t \\
    r'
\end{pmatrix}
\]
Magnetic field symmetry

\[
\begin{pmatrix}
  b_1 \\
  b_2
\end{pmatrix} = \begin{pmatrix}
  r & t' \\
  t & r'
\end{pmatrix} \begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix} \quad \begin{pmatrix}
  b_1 \\
  b_2
\end{pmatrix} = s(B) \begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix}
\]

Time reversal: Hamiltonian is invariant when all momenta and B field are reversed

\[
\begin{pmatrix}
  a_1^* \\
  a_2^*
\end{pmatrix} = s(-B) \begin{pmatrix}
  b_1^* \\
  b_2^*
\end{pmatrix} \Rightarrow \begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix} = s^*(-B) \begin{pmatrix}
  b_1 \\
  b_2
\end{pmatrix}
\]

\[
\Rightarrow s^*(-B)s(B) = 1 \Rightarrow s^\dagger(B) = s^*(-B) \Rightarrow
\]

\[s^T(B) = s(-B)\]

\[t'(B) = t(-B) \Rightarrow T'(B) = T(-B)\]

but \[T'(B) = T(B) \Rightarrow T(B) = T(-B)\]

\[G = \frac{dI}{dV} = \frac{e^2}{h} T\] is an even function of magnetic field
Aharonov-Bohm conductance oscillations

\[ \chi_1 = \int_{\text{upper}} dsA, \, \chi_2 = \int_{\text{lower}} dsA, \, \chi_1 - \chi_2 = 2\pi \Phi / \Phi_0, \]

\[ G(\Phi) = \frac{e^2}{h} T(\Phi) \]

\[ G(\Phi) = \sum_n G_n \cos(2\pi n \Phi / \Phi_0) \]

**Persistent current**
(periodic boundary conditions)

\[ \chi = \int_{\text{circle}} ds \ A = 2\pi \Phi / \Phi_0, \]

\[ F = \sum_n E_n(\Phi), \]

\[ I = -dF / d\Phi \]

\[ k = -(2\pi / L)(\Phi / \Phi_0), \]

\[ I = -dF / d\Phi = - \sum_n dE_n(\Phi) / d\Phi = - \sum_n (dE_n(k) / dk)(dk / d\Phi) \]

\[ I = (e / L) \sum_n v_n(k) \]
General properties of the S-matrix
Unitarity

Current conservation

Example 1: single channel, a 2x2 unitary matrix

Example 2: many channels, an NxN unitary matrix, eigenvalues of the form $S_j = \exp(2i\delta_j)$

$\delta_j$ scattering phases
Causality in EM and in QM

Cause-effect relation, linear response

\[ D(t) = \int_0^\infty \mathcal{K}(\tau) E(t-\tau) \, d\tau; \]

\[ \mathcal{E} = \int \mathcal{E}_\omega e^{-i\omega' t} \, d\omega, \quad \mathcal{D} = \int \mathcal{D}_\omega e^{-i\omega t} \, d\omega \]

\[ \mathcal{D}_\omega = \mathcal{E}_\omega \int_0^\infty \mathcal{K}(\tau) e^{i\omega \tau} \, d\tau, \]

\[ \mathcal{E}_\omega = \frac{\mathcal{D}_\omega}{\mathcal{E}_\omega} = \int_0^\infty \mathcal{K}(\tau) e^{i\omega \tau} \, d\tau. \]

Dielectric function \( \mathcal{E}(\omega) \) analytic in the upper half-plane

\[ \omega = \omega_0 + i\omega_1, \quad \omega_1 > 0, \]

b/c of exponentially decreasing \( e^{-\omega_1 \tau} \).

Out-state \( B = SA \)

In-state

\[ A(t) = 0 \text{ at } t < 0, \quad B(t) = 0 \text{ at } t < t_1, \quad t_1 > 0 \]

\[ A_\omega = \int_0^\infty A(t) e^{i\omega t} \, dt, \quad B_\omega = \int_{t_1}^\infty B(t) e^{i\omega t} \, dt. \]

\[ B_\omega = SA_\omega \]

S(\( \omega \)) could have singularities at the zeros of \( A(\omega) \), but this is impossible b/c S is a property of the scattering potential, independent of the in-state

As a function of energy, S-matrix is analytic in the upper complex half-plane.