Waves in non crystalline structures

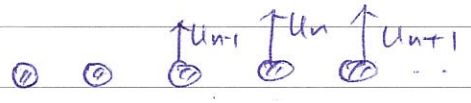
Real materials are not in perfect crystal structures. It's therefore important to understand how electrons / waves behave differently from the Bloch states

Even in the perfect periodic structures, it is still possible to have non-Bloch states.

These are known as evanescent modes.
We shall start from evanescent modes and go into other non-Bloch states.

Evanescent modes

We shall take 1D elastic waves as an example.



$$M\frac{d^2u_n}{dt^2} = K(u_{n+1} + u_{n-1} - 2u_n)$$

We have shown that the travelling waves

$$u_n \propto Re\left[e^{ik(na) - i\omega t}\right]$$

are the solutions provided that

$$-M\omega^2 = K(e^{ika} + e^{-ika} - 2)$$

This results in

$$\omega^2 = \frac{4K}{M} \sin^2 \frac{ka}{2}$$

$$\therefore \omega = 2\sqrt{\frac{K}{M}} \left| \sin \frac{ka}{2} \right| \leq 2\sqrt{\frac{K}{M}}$$

A natural question is why $\omega > 2\sqrt{\frac{K}{M}}$ can't exist ?

What about if one forces the elastic string to oscillate at $\omega > 2\sqrt{\frac{K}{M}}$?

What will happen ?

The reason why $\omega \leq 2\sqrt{\frac{K}{M}}$ is based on the assumption k = real.

To go beyond $2\sqrt{\frac{K}{M}}$, k must be complex and it is still a solution.

Suppose $k = K + i\beta$, we have

$$\sin ka/2 = \sin \frac{Ka}{2} \cos i\frac{\beta a}{2} + \cos \frac{Ka}{2} \sin i\beta a/2$$

$$= \sin \frac{Ka}{2} \cosh \beta a/2 + i \cos \frac{Ka}{2} \sinh \beta a/2$$

$$\therefore \omega = 2\sqrt{\frac{K}{M}} \sin \frac{ka}{2} = 2\sqrt{\frac{K}{M}} \left(\sin \frac{Ka}{2} \cosh \frac{\beta a}{2} + i \cos \frac{Ka}{2} \sinh \frac{\beta a}{2} \right)$$

$\therefore \omega = \text{real}$

$\therefore \cos\frac{ka}{2} \underbrace{\sinh\frac{\beta a}{2}}_{\neq 0} = 0$

$\therefore \cos\frac{ka}{2} = 0 \Rightarrow \sin\frac{ka}{2} = 1 \qquad k = \frac{\pi}{a}$

For $k_{max} = K = \pi/a$.

Hence $\omega = 2\sqrt{\frac{K}{M}}\cosh\frac{\beta a}{2} > 2\sqrt{\frac{K}{M}} = \omega_c$

$\therefore$ For $\omega > \omega_c$, $k = \frac{\pi}{a} + i\beta$

$\omega < \omega_c$, k = real, $\beta = 0$

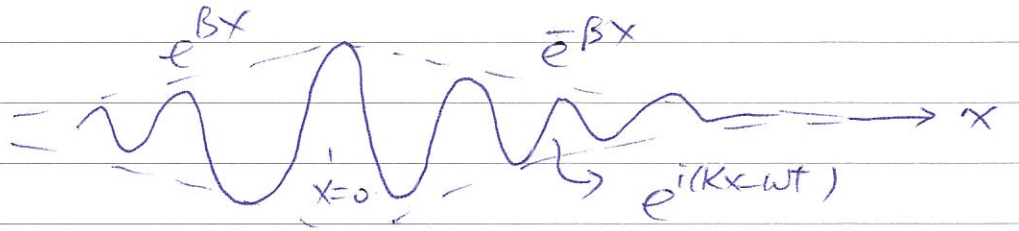
$u(x) = Re\left[e^{ikx - i\omega t}\right]$

$= Re\left[e^{-i\omega t} e^{iKx}\right] e^{-\beta x}$

$\beta > 0$ decays

$\beta < 0$ increasy exponentially x

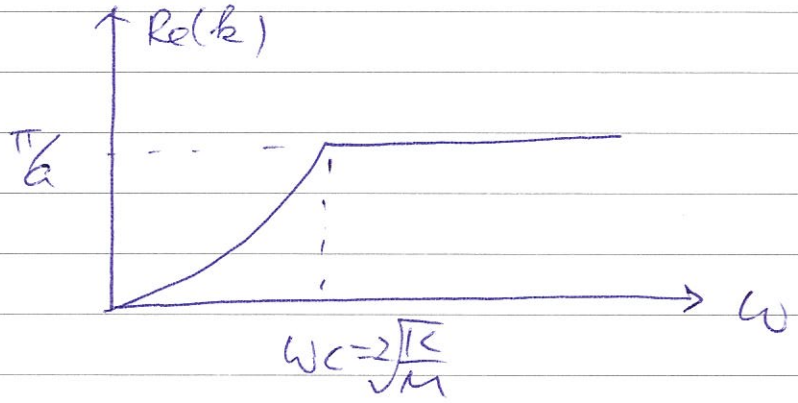
$\therefore$ If we force $x=0$ of a string to oscillate at $\omega > \omega_c$, one gets

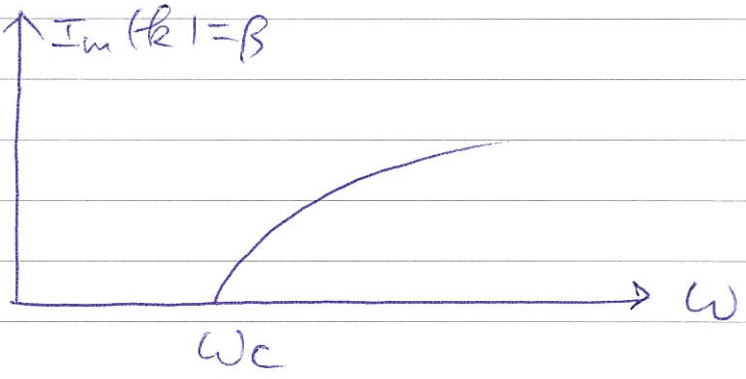


There are evanescent modes and they do not

exist without forcing / breaking translational invariance!

Dispersions of these modes are





Surface / edge states

The evanescent modes can be stablized by breaking translational invariance.

In this case, they become surface states, edge states, or defect / impurity states.

The simplest case is the surface state.

In general, the real surface is rather complex, involving rearrangements of atomic configuration.

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Here we shall simply the discussion by assuming an ideal surface.

Metal surface

In this case, electronic states are delocalized. Two parameters are important to characterize the metalic surface: work function and surface energy

Work function: ΔE between the electron at vacuum level (the) & at the Fermi surface

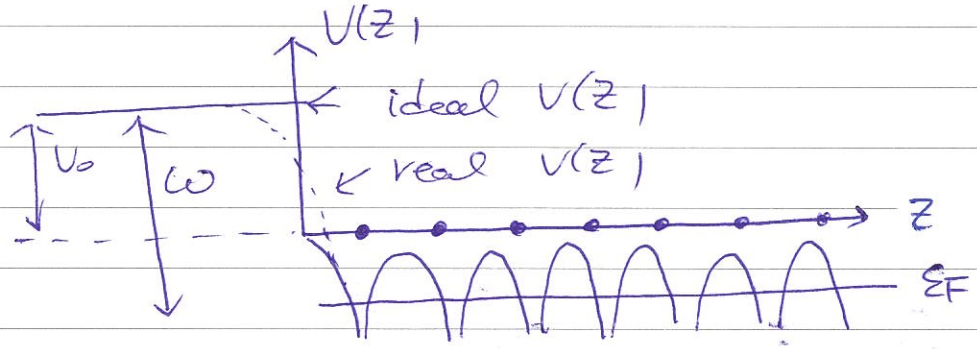


Fig. 12.1

$$W = V(-\infty) - V(0) - \varepsilon_F \simeq V_0 - \varepsilon_F$$

W determines thermionic & field emissions.

$J = AT^2 e^{-W/k_BT}$ (Richardson-Dushman eq.)

Surface energy: energy required to create a unit surface area

= Δ electronic energy for a metal when all bonds across a planar surface are truncated!

In the nearly free electron model, one has

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dz^2} + U(z)\right]\psi(z) = \mathcal{E}\,\psi(z)$$

$$U(z) = U_0 \qquad z<0$$

$$= \sum_{n=1}^{\infty} U(z+na) \qquad z>0$$

as shown in the above figure. (Fig 12.1)

$$\psi(z) = \begin{cases} A\, e^{\frac{1}{\hbar}\sqrt{2m(U_0-\mathcal{E})}\, z} & z<0 \\ B\,u_k e^{ikz} + C\,u_{-k} e^{-ikz} & z>0 \end{cases}$$

for $\mathcal{E} < U_0$, u_k is the Bloch function.

Roughly, we have

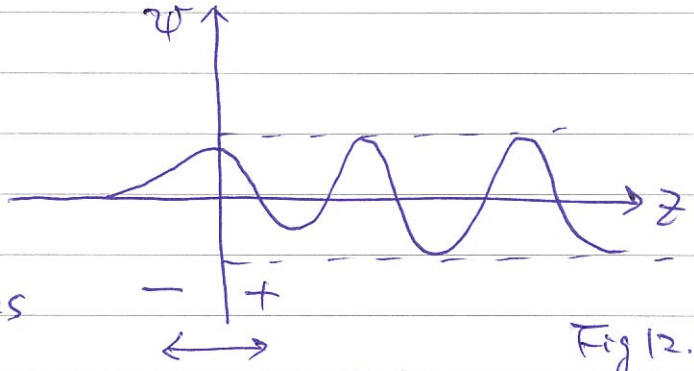


Fig 12.2

dipolar bilayer.

The dipolar field is the cause for the step (U_0) as shown in Fig. 12.1.

In approaching $z=-\infty$, the potential is in fact not flat and can be described by the image potential, $V \sim \frac{1}{z}$.

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Friedel oscillation near surface

The confinement potential in a metal changes the wave function of electrons from the Bloch wave to a mixture of $+k$ & $-k$.

In the nearly-free approximation, one has

$$\psi_k(z) = \sqrt{\frac{2}{L}} \sin kz \quad , \quad k = \frac{n\pi}{L}, \quad n = 1, 2, \cdots$$

which is quite different from the plane wave $\frac{1}{\sqrt{L}} e^{ikz}$, $k = \frac{2n\pi}{L}$, $n = 0, \pm 1, \pm 2 \cdots$

The total density can be found

$$\rho(z) = \sum_{n=1}^{N} \psi_n^*(z) \psi_n(z)$$

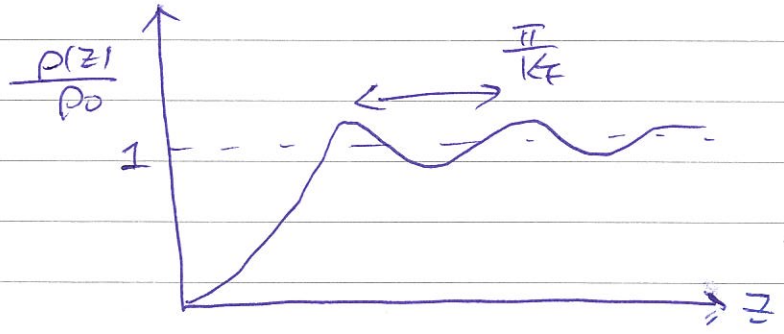
$$= \frac{2}{L} \sum_{n=1}^{N} \sin^2 \frac{n\pi z}{L} = \frac{N+\frac{1}{2}}{L} - \frac{\sin\left[\frac{2\pi(N+\frac{1}{2})z}{L}\right]}{2L \sin \pi z/L}$$

In the limit of $L \to \infty$, while $\rho_0 = N/L$ is fixed, (one spin) one finds

$$\rho(z) = \rho_0 - \frac{\sin 2\pi\rho_0 z}{2\pi z}$$

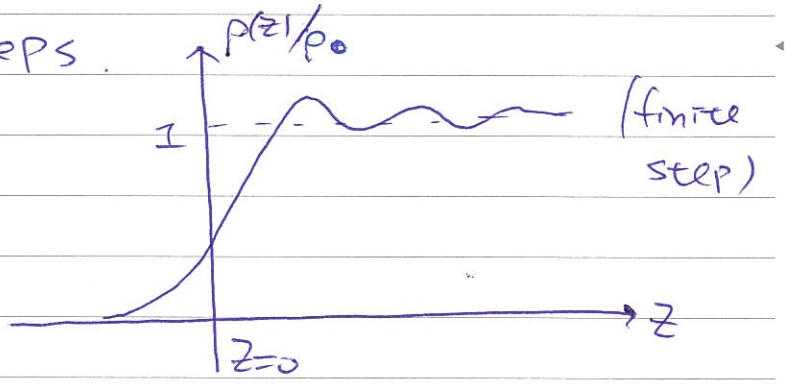
$\because \Delta k = \pi/L$, $\frac{k_F}{\pi/L} = N$ $\therefore$ $\pi\rho_0 = k_F$

$$\therefore \rho(z) = \rho_0 - \rho_0 \frac{\sin 2k_F z}{2k_F z}$$



The oscillation has a period $\sim \lambda_F$, which is know as the Friedel oscillation.

The above analysis is overly simplified. However, this type of oscillation persists to finite potential steps.



Semiconductor surface states.

For the surface of a semiconductor, localized states can be stablized within the gap of the semiconductor. These are known as surface states.

To illustrate the existence of surface states, we shall consider K near π/a of a one dimensional lattice in the nearly-free electron approximation.

We have $\psi_K(z) = C_K e^{iKz} + C_{K-G} e^{i(K-G)z}$ $\quad z = \frac{z\pi}{a}$ --- (2)

for $z \gg 0$

$$\begin{pmatrix} \varepsilon_K^0 - \varepsilon & U_G \\ U_G^* & \varepsilon_{K-G}^0 - \varepsilon \end{pmatrix} \begin{pmatrix} C_K \\ C_{K-G} \end{pmatrix} = 0 \qquad \varepsilon_K^0 = \frac{\hbar^2 K^2}{2m}$$

As we have solved before, we have

$$\varepsilon_\pm = \frac{1}{2}(\varepsilon_K^0 + \varepsilon_{K-G}^0) \pm \sqrt{\left(\frac{\varepsilon_K^0 - \varepsilon_{K-G}^0}{2}\right)^2 + |U_G|^2}$$

Near π/a, $K = \pi/a + q$

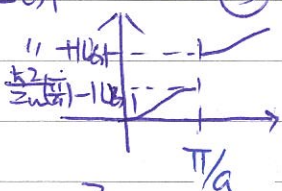
$$\frac{1}{2}(\varepsilon_K^0 + \varepsilon_{K-2\pi/a}^0) = \frac{1}{2}\left[\frac{\hbar^2}{2m}\left[(\pi/a + q)^2 + (\pi/a - q)^2\right]\right]$$

$$= \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + \frac{\hbar^2}{2m} q^2$$

$$\frac{1}{2}(\varepsilon_K^0 - \varepsilon_{K-2\pi/a}^0) = \frac{1}{2} \times \frac{\hbar^2}{2m} \times 2\frac{\pi}{a} q \times 2$$

$$= \frac{\hbar^2 \pi}{ma} q$$

$$\therefore \varepsilon_\pm = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + \frac{\hbar^2 q^2}{2m} \pm \sqrt{\left(\frac{\hbar^2 \pi}{ma}\right)^2 q^2 + |U_G|^2} \quad \text{--- (3)}$$



$$\therefore C_{K-G} = \frac{\varepsilon - \varepsilon_K^0}{U_G} C_K$$

$$C_{K-G}^\pm = \frac{\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + \frac{\hbar^2 q^2}{2m} \pm \sqrt{\quad} - \frac{\hbar^2}{2m}\left(\frac{\pi}{a} + q\right)^2}{U_G} C_K$$

$$= \frac{-\frac{\hbar^2\pi}{ma}q \pm \sqrt{\left(\frac{\hbar^2\pi}{ma}q\right)^2 + |U_G|^2}}{U_G} C_K$$

$$\therefore \psi_\pm(z) = A\left[e^{i\frac{\pi z}{a}} + \frac{|U_G|}{U_G}(-\gamma \pm \sqrt{1+\gamma^2})\, e^{-i\frac{\pi z}{a}}\right] e^{iqz} \quad \text{--- (4)}$$

$\uparrow$
$\psi_K(z)$ for $z >> 0$

A = some constant

$$\gamma = \frac{\hbar^2\pi q}{ma|U_G|}$$

To satisfy $\psi(z \to -\infty) = 0$, one forms the linear combination of $\psi_K(z)$ & $\psi_{-K}(z)$

resulting wave function are shown in Fig 12.2.

Similar

As in the case of 1D elastic waves, One can form surface states by setting

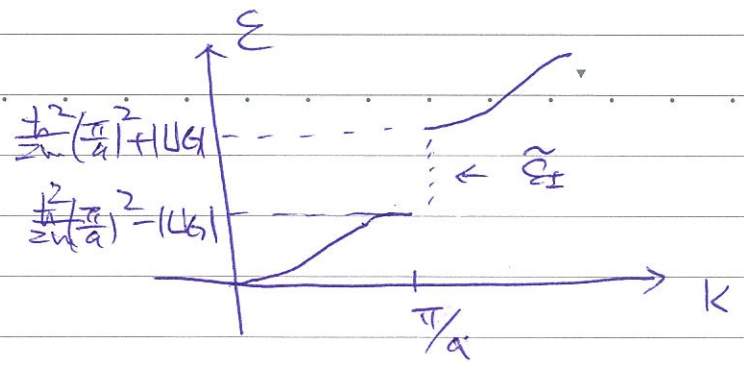
$$q = iK$$

In this case, eq. (3)

$$\Rightarrow \tilde{\varepsilon}_\pm = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{a}\right)^2 - K^2\right] \pm |U_G|\sqrt{1 - \left(\frac{\hbar^2\pi K}{ma|U_G|}\right)^2}$$

$$\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 - |U_G| < \tilde{\varepsilon}_\pm < \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 + |U_G|$$

$\therefore \tilde{\varepsilon}_\pm$ falls within the gap



$$C^{\pm}_{k-G} = \frac{-\frac{i\hbar^2\pi k}{ma} \pm \sqrt{|U_G|^2 - (\frac{\hbar^2\pi k}{ma})^2}}{U_G} C_k$$

$|\text{numerator}| = |U_G| \quad \therefore \text{numerator} = e^{\pm i\delta} |U_G|$

$$\tan\delta = \frac{\frac{-\pi k\hbar^2}{ma}}{\sqrt{|U_G|^2 - (\frac{\hbar^2\pi k}{ma})^2}}$$

$$\therefore C^{\pm}_{k-G} = e^{\pm i\delta} \cdot \frac{|U_G|}{U_G}$$

$$\psi(z) = A\left[e^{i\frac{\pi z}{a}} + \frac{|U_G|}{U_G} e^{-i\frac{\pi}{a}z \pm i\delta} \right] e^{-kz}$$

which decays away from $z=0$ into $z>0$.

Note that for $z<0$, one has to set

$q = -ik$ so that $C^{\pm}_{k-G} = e^{\mp i\delta} \frac{|U_G|}{U_G}$.

$$\psi(z) = A\left[e^{i\frac{\pi z}{a}} + \frac{|U_G|}{U_G} e^{-i\frac{\pi z}{a}} e^{\mp i\delta} \right] e^{kz}$$

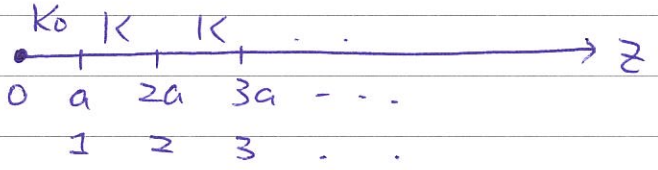
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Surface vibrations

As we indicated, $\omega > 2\sqrt{\frac{K}{M}}$: elastic waves may be stablized near the surface. This can be more formally solved.

Consider a semi-infinit chain as shown in below



The elastic constant between the 1st two atoms is different and is K_0.

$$\therefore \quad M\ddot{u}_0 = -K_0(u_0 - u_1) \qquad \text{(F)} - 1$$

$$M\ddot{u}_1 = -K_0(u_1 - u_0) - K(u_1 - u_2) \qquad \text{(F)} - 2$$

$$M\ddot{u}_n = -K(u_n - u_{n-1}) - K(u_n - u_{n+1}) \quad n \geq 2 \qquad \text{(F)} - 3$$

Clearly, only u_0 is different, so we seek the solution

$$u_0 = A_0 e^{-i\omega t}$$

$$u_n = A\, e^{ik(na) - i\omega t} \quad n \geq 1$$

for surface waves.

Substituting u_n into eq. (F)-3, one obtains the bulk dispersion relation

$$\omega^2 = \frac{4K}{M} \sin^2 \frac{ka}{2} \qquad \text{---} (6)$$

Here k is not specified yet. As in the case of infinite chain, one needs to consider the boundary condition.

to fix k. This is done by examing eqs. ⑤-1 & ⑤-2, we find

$$-M\omega^2 A_0 = -K_0(A_0 - e^{ika}A)$$

$$-M\omega^2 A = -K_0(A - A_0 e^{-ika}) - K(A - A e^{ika})$$

By using eq. ⑥, $M\omega^2 = 2K\frac{1+\cos ka}{2}$, the above equations reduce to

$$[K_0 - 2K(1-\cos ka)]A_0 - K_0 e^{ika} A = 0$$

$$-K_0 e^{-ika} A_0 + [K_0 - K(1-e^{-ika})]A = 0$$

∴ To get nonvanishing A_0 & A, one finds that the determinant $= 0$

$$\therefore \quad [K_0 - 2K(1+\cos ka)][K_0 - K(1+e^{-ika})] = K_0^2$$

$$\therefore \quad -2K_0(1-\cos ka) - K_0(1+e^{-ika}) + 2K(1+\cos ka)(1-e^{-ika}) = 0$$

Clearly, $e^{ika} = 1$ is a solution which, however, is a rigid translation of the chain.

Replacing $\cos ka$ by $\frac{1}{2}(e^{ika} + e^{-ika})$, we find

$1+\cos ka = \frac{1}{2}(1-e^{ika})(1-e^{-ika})$. Hence

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$\cdots (1-e^{ika})\left[(k_0-k)e^{ika}+2k-2k_0-ke^{-ika}\right]=0 \cdots$

$$\therefore e^{ika} = 1 \pm \sqrt{1+\frac{k}{k_0-k}} \equiv 1 \pm \sqrt{1+\frac{1}{\varepsilon}}$$

$\because k, k_0 > 0, \quad \therefore \varepsilon \equiv \frac{k_0-k}{k} > -1$ One has two possibilities

(i) $k_0 < k, \quad -1 < \varepsilon < 0, \quad 1+\frac{1}{\varepsilon} < 0$

$$\therefore e^{ika} = 1 \pm i\sqrt{-1-\frac{1}{\varepsilon}}$$

Clearly, this is not possible for localized surface modes since if k = complex $\equiv k_2 + i\beta$, one has $e^{ika}e^{-\beta a} = 1 \pm i\sqrt{1-1/\varepsilon}$

$$e^{-\beta a} = |1 \pm i\sqrt{1-1/\varepsilon}| > 1$$

which is not decaying for e^{ika}!

$\therefore$ This is not possible.

(ii) $k_0 > k, \quad \varepsilon > 0, \quad \therefore |e^{ika}| = |1+\sqrt{1+1/\varepsilon}| > 1$

$\therefore$ it's not decaying too! (k = purely imaginary)

$\therefore$ Only $e^{ika} = 1-\sqrt{1+1/\varepsilon}$ is a possible solution for decaying solution.

In this case, $\therefore 1-\sqrt{1+1/\varepsilon} < 0, \quad \therefore k = \pi a + i\beta$

$$e^{-\beta} = \sqrt{1+1/\varepsilon} - 1, \quad \beta = -\ln(\sqrt{1+1/\varepsilon} - 1)$$

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$$= -\ln \frac{1+\xi^{-1}}{1+\sqrt{1+1/\xi}} = -\ln \frac{1}{\xi+\sqrt{\xi^2+\xi}}$$

$$= \ln\left(\xi+\sqrt{\xi^2+\xi}\right) > 0 \quad \text{if it's decaying.}$$

$$\therefore \xi+\sqrt{\xi^2+\xi} > 1$$

$$\therefore \xi > 1/3 \quad , \quad \frac{K_0}{K} > \frac{4}{3}$$

Hence for $K_0/K > 4/3$, one has a localized edge mode with

$$\omega_s^2 = \frac{2K}{M}(1+\cos ka)$$

$$= \frac{2K}{M}(1+\cosh\beta) \quad \text{above the bulk} \quad \omega = 2\sqrt{\frac{K}{M}}\left|\sin\frac{ka}{2}\right|$$

The solution $u_n = A(1)^n e^{-n\beta}$ for $n \geq 1$.

Point-like defects/impurities

Point-like impurities or defects are the most (often) encountered objects that break the translational invariance of crystals.

Ideally, one introduces a potential $U(\vec{r}-\vec{r}_0)$ to simulate a single impurity (Compensated impurities) at $\vec{r}_0$.

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Usually, there is charge imbalance at the impurity site. so that $U(r-r_0)$ is long-ranged. $\left(\frac{1}{|r-r_0|}\right)$ However, due to the presence of other electrons, as we shall see, these charge imbalance will be compensated so that $U(r-r_0)$ becomes short-ranged. In the extreme case, $U(r-r_0) \propto \delta(r-r_0)$ is highly localized at r_0.

The scattering of an electron off from $U(r)$ can be best described by the Green's function.

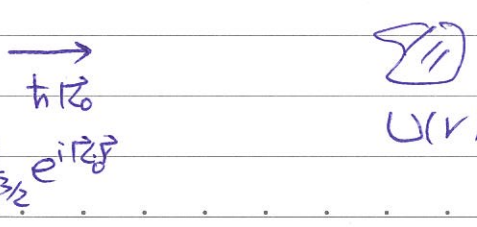
Method of Green function for single electron

For a given scattering potential $U(r)$, the Schrödinger equation for the electron is

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right]\psi(r) = E\psi(r) \quad \cdots (6)$$

To consider the elastic scattering, we shall assume that the electron comes in at $\vec{r}=-\infty$ with momentum $\hbar\vec{k}_0$ so that

$$E = \frac{\hbar^2 k_0^2}{2m} = \frac{\hbar^2 k^2}{2m}$$



Eq. (6) can be cast in a general form...

$$(H_0 + U)|\psi\rangle = E|\psi\rangle$$

Hence $$(E - H_0)|\psi\rangle = U|\psi\rangle \quad \text{--- (7)}$$

We may try to write

$$|\psi\rangle = |\phi\rangle + \frac{U}{E+H_0}|\psi\rangle \quad \text{--- (8)}$$

with $|\phi\rangle$ satisfies $(E - H_0)|\phi\rangle = 0$ --- (9)

i.e. $\frac{-\hbar^2}{2m}\nabla^2\phi = E\phi = \frac{\hbar^2 k_0^2}{2m}\phi$

$\phi(r)$ can be fixed by the boundary condition at $r \to -\infty$, $\phi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k_0}\cdot\vec{r}}$

(or $\frac{1}{\sqrt{V}} e^{i\vec{k_0}\cdot\vec{r}}$)

The correct way to solve eq. (7) is to invert $E - H_0$ correctly as follows

$$|\psi^{\pm}\rangle = |\phi\rangle + \frac{1}{E + H_0 \pm i\varepsilon} U|\psi^{\pm}\rangle, \quad \varepsilon \to 0^+ \quad \text{--- (10)}$$

(the Lippmann-Schwinger equation)

$\pm i\varepsilon$ are needed to avoid divergence.

In real space, Eq (10) takes the following form

$$\psi^{\pm}(r) = \phi(r) + \int dr' \, G_0^{\pm}(r - r') \, U(r') \, \psi^{\pm}(r') \quad \text{--- (11)}$$

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Here $G_0^{\pm}(r, r') \equiv \langle r | \frac{1}{E - H_0 \pm i\varepsilon} | r' \rangle$

$= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \frac{1}{E - \frac{\hbar^2 k^2}{2m} \pm i\varepsilon}$ satisfies

$$(E - H_0)\, G_0(r, r') = \delta(r - r') \quad ---(12)$$

$$(E - H_0)\, G_0(r, r') = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \frac{E - \frac{\hbar^2 k^2}{2m}}{E - \frac{\hbar^2 k^2}{2m}}$$

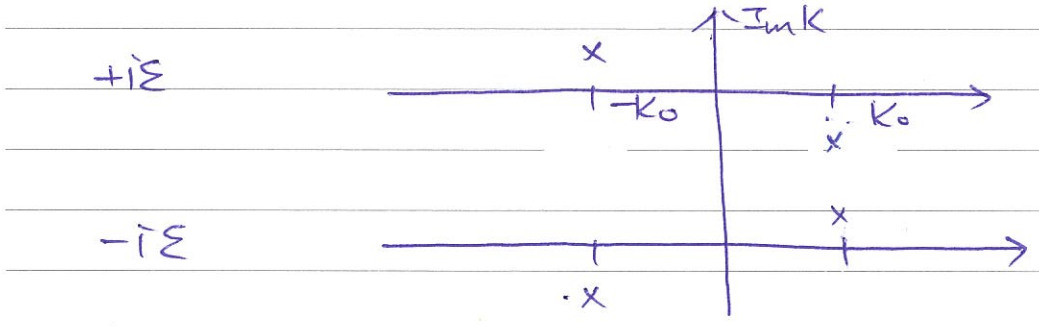
$$= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} = \delta(r - r') \;)$$

G_0 is known as the Green's function.

$\pm i\varepsilon$ shift poles in k off from real axis so that the integral is meaningful:

$$\frac{1}{E - \frac{\hbar^2 k^2}{2m} \pm i\varepsilon} \to -\frac{2m}{\hbar^2} \frac{1}{k^2 - k_0^2 \mp i\varepsilon} \qquad \frac{2m}{\hbar^2}\varepsilon \to \varepsilon.$$

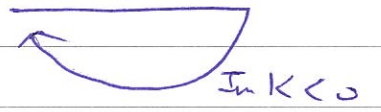
poles: $k^2 = k_0^2 \pm i\varepsilon = \begin{cases} (k_0 + i\varepsilon)^2 \text{ or } (-k_0 - i\varepsilon)^2 \\ (k_0 - i\varepsilon)^2 \text{ or } (-k_0 + i\varepsilon)^2 \end{cases}$



$\therefore e^{ik|r-r'|} \to 0$ only when $\mathrm{Im}\, k > 0$

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∴ It's clear that for $+i\varepsilon$, one has to choose the contour



∴ pole at K_0 contributes, one gets

$$G_0^+(r,r') = -\frac{2m}{\hbar^2}\frac{e^{ik_0|r-r'|}}{4\pi|r-r'|} \quad \text{---(13)}$$

for $-i\varepsilon$, $G_0^-(r,r') = -\frac{2m}{\hbar^2}\frac{e^{-ik_0|r-r'|}}{4\pi|r-r'|}$ --(14)

Combined with $e^{-i\omega t}$; it's clear that G^+ describes waves propagate outward, while G^- describes waves " inward.

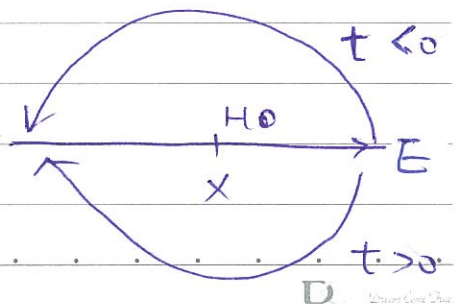
In general, G^+ is known as retarded Green's function (G_R), while G^- is known as the advanced Green's function (G_A).

$$G^{R/A} = \frac{1}{E - H_0 \pm i0^+}$$

In the time domain, it's clear that $G^R(t)=0$ if $t<0$

$$G^R(t) = \int_{-\infty}^{\infty} dE\, e^{-\frac{iEt}{\hbar}} G^R$$

$$= e^{-\frac{i\hat{H}_0 t}{\hbar}}\theta(t)$$



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Hence $\langle \vec{r}|\hat{G}^{R(+)}|\vec{r}'\rangle$

$= \langle \vec{r}| e^{\frac{i}{\hbar}\hat{H}_0 t}|\vec{r}'\rangle\,\theta(+t)$

is the time-evolution from $\vec{r}'$ to $\vec{r}$ for $t>0$.

On the other hand, $G^{A(+)} = e^{-\frac{i}{\hbar}\hat{H}_0 t}\theta(-t)$,

$\therefore$ $G^{A(+)}$ propagates backwards in time.

In the following, unless specified, we shall use G to refer G^R.

T-matrix & S-matrix

It's often define a T-matrix by

$$U|\varphi^+\rangle \equiv T|\Phi\rangle$$

$$\therefore \underbrace{U|\varphi^+\rangle}_{T|\Phi\rangle} = U|\Phi\rangle + U\frac{1}{E-H_0+i\varepsilon}T|\Phi\rangle$$

$$T = U + U\frac{1}{E-H_0+i\varepsilon}T \quad \cdots (11)$$

Since Eq. (11) takes the following form

$$\varphi(\vec{r}) = \Phi(r) - \frac{2m}{\hbar^2}\int d^3\vec{r}'\,\frac{e^{ik_0|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|}U(\vec{r}')\varphi(\vec{r}')$$

For $r \gg r'$, $\frac{1}{|\vec{r}-\vec{r}'|} \sim \frac{1}{r}$

but $|\vec{r}-\vec{r}'| = r\sqrt{1-2\frac{\vec{r}\cdot\vec{r}'}{r^2}+\left(\frac{r'}{r}\right)^2} \simeq r-\vec{r}\cdot\vec{r}'$

$$e^{ik_0|\vec{r}-\vec{r}'|} \approx e^{ik_0 r} e^{-i\vec{k}\cdot\vec{r}'}$$

$$\therefore \psi(\vec{r}) = \phi(\vec{r}) - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ik_0 r}}{r}\int d^3r'\, e^{-i\vec{k}'\cdot\vec{r}'} U(\vec{r}')\psi(\vec{r}')$$

$$= \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}_0\cdot\vec{r}} + \frac{e^{ikr}}{r} f(\vec{k},\vec{k}_0)\right]$$

$T|k_0\rangle = T|\phi\rangle$

where $f(\vec{k},\vec{k}_0) = \frac{-1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3 \int d^3r' \frac{e^{-i\vec{k}\cdot\vec{r}'}}{(2\pi)^{3/2}} U(\vec{r}')\langle\vec{r}'|\psi\rangle$

$= \langle\vec{k}'|T|k_0\rangle$

is the scattering amplitude that gives the differential cross section $\sigma(\theta,\phi) = |f(\vec{k},\vec{k}_0)|^2$

The S-matrix is defined by

$$\langle\phi_f|S|\phi_i\rangle = \lim_{\substack{t\to\infty \\ t\to-\infty}} \langle f|\hat{U}(t',t)|i\rangle \Rightarrow \text{shift } t\to 0,\ t'\to\infty$$

$e^{\frac{-iH}{\hbar}t} \to e^{-\epsilon t}$

In the ω-space, $\frac{1}{i\hbar}\int_0^\infty dt\, e^{i\omega t} U(t)$

$$= \frac{1}{\hbar\omega - H + i\varepsilon}$$

$$\therefore S(E) = \frac{1}{E - H_0 + i\varepsilon + U}$$

$$= \frac{1}{E-H_0+i\varepsilon} + \frac{1}{E-H_0+i\varepsilon}U\frac{1}{E-H_0+i\varepsilon} + \frac{1}{E-H_0+i\varepsilon}U\frac{1}{E-H_0+i\varepsilon}U\frac{1}{E-H_0+i\varepsilon}$$

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$$\frac{1}{E-H_0+i\varepsilon} + \cdots$$

$$= \frac{1}{E-H_0+i\varepsilon} + \frac{1}{E-H_0+i\varepsilon}\hat{T}\frac{1}{E-\hat{H}_0+i\varepsilon}$$

$\therefore$ S describes the transition (total) in the scattering (amplitude)

while T describes the scattering (into other state) amplitude.

Shielding effect of a charged center

Using the Green's function, we can calculate the charge distribution near a static impurity charge embedded in a metal.

To find the total effects due to U, one needs to find T in eq. (15).

If U is not strong, T can be found perturbatively as

$$T = U + U\frac{1}{E-H_0+i\varepsilon}U + U\frac{1}{E-H_0+i\varepsilon}U\frac{1}{E-H_0+i\varepsilon}U + \cdots$$

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In the leading order approximation, $T \simeq U$, this is known as the Born approximation. One has

$$\psi_{\vec{k}_0}(\vec{r}) = \frac{1}{\sqrt{V}}\left[e^{i\vec{k}_0\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\int d\vec{r}\,' \frac{e^{ik_0|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} U(\vec{r}\,') e^{i\vec{k}_0\cdot\vec{r}\,'}\right]$$

$$\therefore \rho(r) = \sum_{k_0<k_F} \psi^*_{k_0}(r)\,\psi_{k_0}(r)$$

$$= \frac{1}{V}\left\{ \sum_{k_0<k_F} - \sum_{(\vec{k}_0<k_F} \frac{m}{2\pi\hbar^2}\int d\vec{r}\,' U(\vec{r}\,') \right.$$

$$\times\left[\frac{e^{ik_0|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} e^{i\vec{k}_0(\vec{r}\,'-\vec{r})} + \frac{e^{-ik_0|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} e^{-i\vec{k}_0\cdot(\vec{r}\,'-\vec{r})}\right]$$

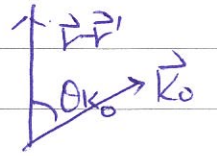
$$\left. + O(U^2)\right\}$$

$$= \rho_0 - \frac{2m}{(2\pi)^4\hbar^2}\int d\vec{r}\,' U(\vec{r}\,') \int_{k_0<k_F} d^3\vec{k}_0 \left[\frac{e^{ik_0|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} e^{i\vec{k}_0\cdot(\vec{r}\,'-\vec{r})}\right.$$

$\uparrow$ $\frac{N}{V}$

$$\left. + \frac{e^{-ik_0|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} e^{-i\vec{k}_0\cdot(\vec{r}\,'-\vec{r})}\right]$$

$$\int d\Omega_{\vec{k}_0}\, e^{i\vec{k}_0\cdot(\vec{r}-\vec{r}\,')} = \int \sin\theta_{k_0}\, d\theta_{k_0}\, 2\pi\, e^{ik_0|\vec{r}-\vec{r}\,'|\cos\theta_{k_0}}$$



$$= 2\pi \frac{1}{ik_0|\vec{r}-\vec{r}\,'|}\left(e^{ik_0|\vec{r}-\vec{r}\,'|} - e^{-ik_0|\vec{r}-\vec{r}\,'|}\right)$$

$$= 4\pi \frac{\sin k_0|\vec{r}-\vec{r}\,'|}{k_0|\vec{r}-\vec{r}\,'|}$$

Similarly, $\int d\Omega_{k_0}\, e^{-i\vec{k}_0(\vec{r}-\vec{r}\,')} = \frac{4\pi \sin k_0|\vec{r}-\vec{r}\,'|}{k_0|\vec{r}-\vec{r}\,'|}$ too!

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$$\rho = \rho_0 - \frac{2m}{(2\pi)^4 \hbar^2} \int d\vec{r}\,' U(\vec{r}\,') \int_0^{k_F} dk\, 4\pi k^2 \frac{\sin k|r-r'|}{k|r-r'|} \times \frac{2\cos k|r-r'|}{|\vec{r}-\vec{r}\,'|}$$

After integrating over k, we get

$$\rho(r) - \rho_0 = -\frac{m k_F^2}{2\pi^3 \hbar^2} \int d\vec{r}\,' U(r') \frac{j_1(2k_F|r-r'|)}{|\vec{r}-\vec{r}\,'|^2} \quad \cdots (16)$$

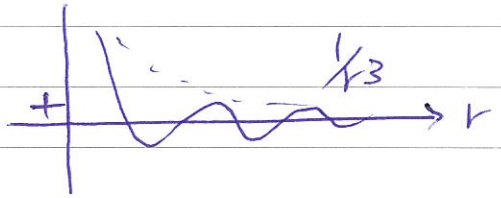
where $j_1(x) = \frac{\sin x - x\cos x}{x^2}$ is the 1st order spherical Bessel function.

For $U = U_0 \delta(r)$, Eq. (16) implies

$$\rho(r) - \rho_0 \sim \frac{j_1(2k_F r)}{r^2} \sim \frac{\sin 2k_F r - 2k_F r \cos 2k_F r}{r^4}$$

$$\sim \frac{2\cos 2k_F r}{r^3}$$

which shows the Friedel oscillation of electron density.



The accumulated electrons try to screen the charge. One can derive the screened potential by using the Poisson eq.

To find localized modes, (by using the Green's func.) we first ...

notice that

$$\hat{G}^R(E) = \frac{1}{E - \hat{H} + i\varepsilon} = \left(\sum_n |E_n\rangle\langle E_n|\right)\frac{1}{E-\hat{H}}$$

$$= \sum_n \frac{|E_n\rangle\langle E_n|}{E - E_n + i\varepsilon} \quad \cdots (19)$$

Hence, all energy eigenvalues will appear as poles of $\hat{G}(E)$.

For E near a particular E_n,

$$\frac{1}{E - E_n + i\varepsilon} = P\frac{1}{E-E_n} - i\pi\delta(E-E_n)$$

↑ Cauchy principal value

$$\therefore \hat{G}^R(E) \simeq |E_n\rangle\langle E_n| \left\{ P\frac{1}{E-E_n} - i\pi\delta(E-E_n) \right\}$$

Furthermore, one has

$$-\frac{1}{\pi} \mathrm{Im} \langle \vec{r}|\hat{G}^R(E)|\vec{r}\rangle = \sum_n \delta(E-E_n)|\langle \vec{r}|E_n\rangle|^2$$

$$\equiv \text{local density of states} \quad \cdots (19)$$

i.e. $\frac{-1}{\pi}\mathrm{Im}\, G^R(\vec{r},\vec{r},E)$ measure density of states ...

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$$\nabla^2 U = -4\pi(\rho - \rho_0)$$

$$= \frac{2me^2 k_F^2}{\pi \hbar^2} \int d\vec{r}\,' \, U(r') \frac{j_1(2k_F|r-r'|)}{|r-r'|^2}$$

The self-consistent solution is found to be $U(r) \sim \frac{\cos 2k_F r}{r^3}$ which also shows the Friedel oscillations, which can be checked by the Knight shifts measuring in NMR-type expt.

Localized modes near a single impurity

To understand the scattering of an electron off from a single impurity, we shall consider the simplest model – the tight-binding model to illustrate the possibility of localized modes.

In this case, the impurity is compensated so that one can set $U = U_0 \delta_{\vec{r},0}$

The Hamiltonian is

$$\hat{H} = \sum_{\langle \vec{r},\vec{r}' \rangle} t|\vec{r}\rangle\langle\vec{r}'| + t|\vec{r}'\rangle\langle\vec{r}| + U_0|0\rangle\langle 0| \quad \leftarrow (1.1)$$

weighted by the probability $|\langle \vec{r}|E_n\rangle|^2$ at $\vec{r}$.

Since $\sum_{\vec{r}} |\langle \vec{r}|E_n\rangle|^2 = \sum_{\vec{r}} \langle E_n|\vec{r}\rangle\langle \vec{r}|E_n\rangle = \langle E_n|E_n\rangle$

$= 1$,

one gets $\sum_{\vec{r}} \frac{1}{\pi} \mathrm{Im}\, G^R(\vec{r},\vec{r},E) = \sum_n \delta(E-E_n)$

$= D(E)$ (density of state, global)

$\dots$ (20)

Single impurity

To find localized modes of $\hat{H}$ defined in eq. (17), we set $\hat{H}_0 = \sum_{\langle \vec{r},\vec{r}'\rangle} t\,|\vec{r}\rangle\langle \vec{r}'| + t\,|\vec{r}'\rangle\langle \vec{r}|$

$\hat{H}_I = U_0 |0\rangle\langle 0|$

$\therefore \hat{G}^R = \frac{1}{E-\hat{H}_0+i\varepsilon-\hat{H}_I} = \left[(E-\hat{H}_0+i\varepsilon)\left(1-\underbrace{\frac{1}{E-\hat{H}_0+i\varepsilon}}_{G_0}\hat{H}_I\right)\right]^{-1}$

$= (1-\hat{G}_0\hat{H}_I)^{-1}\underbrace{\frac{1}{E-\hat{H}_0+i\varepsilon}}_{G_0}$

$= (1+\hat{G}_0\hat{H}_I + \hat{G}_0\hat{H}_I\hat{G}_0\hat{H}_I + \hat{G}_0\hat{H}_I\hat{G}_0\hat{H}_I\hat{G}_0\hat{H}_I\cdots)\,G_0$

$= G_0 + G_0\hat{H}_I G_0 + G_0\hat{H}_I G_0\hat{H}_I G_0 + G_0\hat{H}_I G_0\hat{H}_I G_0\hat{H}_I G_0 + \cdots$

$= G_0 + G_0\hat{H}_I G = G_0 + G_0 T G_0$

For $\hat{H}_I = U_0 |0\rangle\langle 0|$, the above equation reduces to

$$\hat{G}^R = \hat{G}_0 + \hat{G}_0|0\rangle U_0\langle 0|\hat{G}_0 + \hat{G}_0|0\rangle U_0\langle 0|\hat{G}_0|0\rangle U_0\langle 0|\hat{G}_0 + \cdots$$

$$= \hat{G}_0 + \frac{\hat{G}_0|0\rangle U_0\langle 0|\hat{G}_0}{1 - U_0\langle 0|\hat{G}_0|0\rangle}$$

Hence, there are new poles defined by

$$1 = U_0 \, \mathrm{Re}\langle 0|\hat{G}_0|0\rangle \quad \cdots (21)$$

i.e. $$\frac{1}{U_0} = \mathrm{Re}\,\hat{G}_0(0,0,E)$$

There are many solutions to eq. (21) denoted by E_n.

$$\therefore 0 = 1 - U_0 \, \mathrm{Re}\langle 0|\hat{G}_0(E)|0\rangle = -U_0 \cdot \langle 0|\hat{G}_0'(E_n)|0\rangle (E - E_n) + \cdots$$

$$\hat{G}_0'(E) = \frac{d\hat{G}_0}{dE}$$

$$\therefore \hat{G}^R \simeq \hat{G}_0(E) - \frac{\hat{G}_0(E_n)|0\rangle\langle 0|\hat{G}_0(E_n)}{U_0 \, \mathrm{Re}\langle 0|\hat{G}_0'(E_n)|0\rangle} \frac{1}{E - E_n}$$

$$\sum_n \frac{|E_n\rangle\langle E_n|}{E - E_n}$$

$$\therefore |E_n\rangle \simeq \frac{\hat{G}_0(E_n)|0\rangle}{\sqrt{-\mathrm{Re}\langle 0|\hat{G}_0'(E_n)|0\rangle}} \quad \cdots (22)$$

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$\psi_n(r) = \langle r | E_n \rangle$

$$= \frac{1}{\sqrt{\mathrm{Re}\langle 0|\tilde{G}_0'(E_n)|0\rangle}} \sum_m \frac{\phi_m^{0*}(r)\,\phi_m^0(0)}{E_n - E_m^0 + i\varepsilon} \quad \cdots (23)$$

If E_n falls outside bands formed by $\{E_m^0\}$, $\psi_n(r)$ will decay as $r \to \infty$ and is a localized state.

Impurities in 1D

In 1D, the eigenvalue of $H_0 = -2t\cos k \equiv \varepsilon_0(k)$.

For finite systems, $k = k_1, k_2, \ldots$, $\varepsilon_0(k)$ can be ordered as $-2t \le \varepsilon_1^0 < \varepsilon_2^0 < \cdots < \varepsilon_N^0 \le 2t$

$$\langle 0|G_0|0\rangle = \sum_{n=1}^{N} \frac{|\phi_n^0(0)|^2}{E - \varepsilon_n^0 + i\varepsilon} \quad \therefore \mathrm{Re}\,G_0 = \sum_{n=1}^{N} P\frac{1}{E - \varepsilon_n^0}|\phi_n^0(0)|^2$$

which is $+\infty$ for $E \simeq \varepsilon_n^{0+}$ and $-\infty$ for $E \simeq \varepsilon_n^{0-}$.

There for, $\mathrm{Re}\,G_0(0,0,E)$ roughly looks like

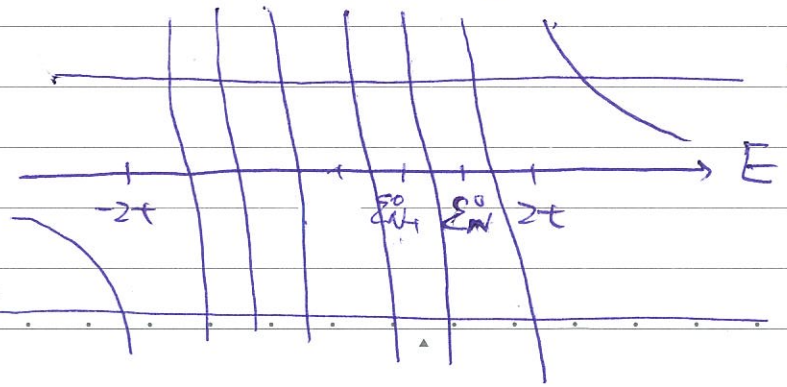


Fig 12.3

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Hence eq. (21) implies that there exists ...

a interaction of $1/U_0$ with $\mathrm{Re}\, G_0$ at $E > 2t$ for $U_0 > 0$, at $E < -2t$ for $U_0 < 0$

These are localized modes.

The above analysis is for finite systems and seems to be applicable to $d = 2$ & $d = 3$, but this is not correct in the limit of infinite systems in which degeneracies of E play important role.

To find localized modes, one needs to evaluate $\mathrm{Re}\, G_0(0, 0, E)$.

For 1D, we have

$$\langle x|G_0|x'\rangle = \sum_k \frac{\langle x|k\rangle\langle k|x'\rangle}{E - \varepsilon_0(k) + i\varepsilon}$$

$$\langle x|k\rangle = \frac{1}{\sqrt{N}} e^{ikx}$$

N = # of lattice

$$= \frac{1}{N}\sum_k \frac{e^{ik(x-x')}}{E - \varepsilon_0(k) + i\varepsilon}$$

$k \to ka$

$$= \int_0^{2\pi} \frac{dk}{2\pi} \frac{e^{ik(n-n')}}{E - 2t\cos k + i\varepsilon}$$

$x, x' = na, na'$

It's convenient to set $z = e^{ik}$, $dk = \frac{dz}{iz}$

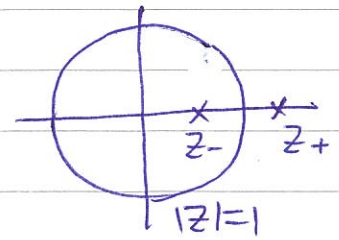
$$\langle x|G_0|x'\rangle = \oint \frac{dz}{2\pi i} \frac{z^{n-n'}}{z[E - t(z+z^{-1})] + i\varepsilon z}$$

$$= \oint \frac{dz}{2\pi i} \frac{z^{n-n'}}{Ez - tz^2 - t + i\varepsilon z}$$

The integrand has poles at

$$z_\pm = \frac{1}{2t}\left[E + i\varepsilon \pm \sqrt{(E+i\varepsilon)^2 - 4t^2}\right]$$

$\varepsilon \to 0^+$, $z_+ z_- = 1$, $|z_-| < 1$, $|z_+| > 1$ for $E^2 > 4t^2$, $E > 0$



the integration gives

$$\langle x|G_0|x'\rangle = \frac{E}{|E|} \frac{1}{\sqrt{E^2 - 4t^2}} \left[\frac{E}{2t} - \frac{E}{|E|}\sqrt{\left(\frac{E}{2t}\right)^2 - 1}\right]^{n-n'} \cdots (24)$$

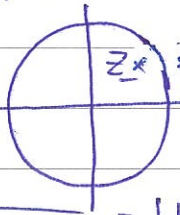
For $E^2 < 4t^2$, $\sqrt{E^2 - 4t^2} = \sqrt{4t^2 - E^2}\, i$

$$\left|\frac{1}{2t}\left(E \pm \sqrt{4t^2 - E^2}\, i\right)\right| = 1$$

$\pm i\varepsilon$ shifts $\sqrt{(E+i\varepsilon)^2 - 4t^2} = \sqrt{E^2 - 4t^2 + 2i\varepsilon E} = \sqrt{(4t^2 - E^2)}\, e^{i(\pi - \varepsilon E)}$

$$= \sqrt{4t^2 - E^2}\, i\, e^{i\varepsilon E} \approx \sqrt{4t^2 - E^2}\, i\,(1 - i\varepsilon E)$$

$\therefore |z_+| = 1^+$, $|z_-| = 1^-$ (for $E > 0$)



one gets

$$\langle x|G_0|x'\rangle = \frac{i}{\sqrt{4t^2 - E^2}} \left[\frac{E}{2t} + \frac{1}{i}\sqrt{1 - \left(\frac{E}{2t}\right)^2}\right]^{|n-n'|} \cdots (25)$$

∴ For $E^2 > 4t^2$, one gets

$$\langle 0|G_0|0\rangle = \frac{\pm 1}{\sqrt{E^2-4t^2}}$$

Eq. (21) implies that the energies of localized modes

$$E_{loc} = \pm\sqrt{4t^2+U_0^2} \qquad (U_0>0\ +,\ U_0<0\ -)$$

Furthermore,

$$\langle X=na|G^0(E_{loc})|0\rangle$$

$$= \frac{1}{U_0}\left[\frac{E_{loc}}{2t} \pm \sqrt{\left(\frac{E_{loc}}{2t}\right)^2-1}\right]^{|n|}$$

$$= \frac{1}{U_0}\left[\pm\right]^n\left[\frac{\sqrt{4t^2+U_0^2}}{2t} - \frac{|U_0|}{2t}\right]^{|n|}$$

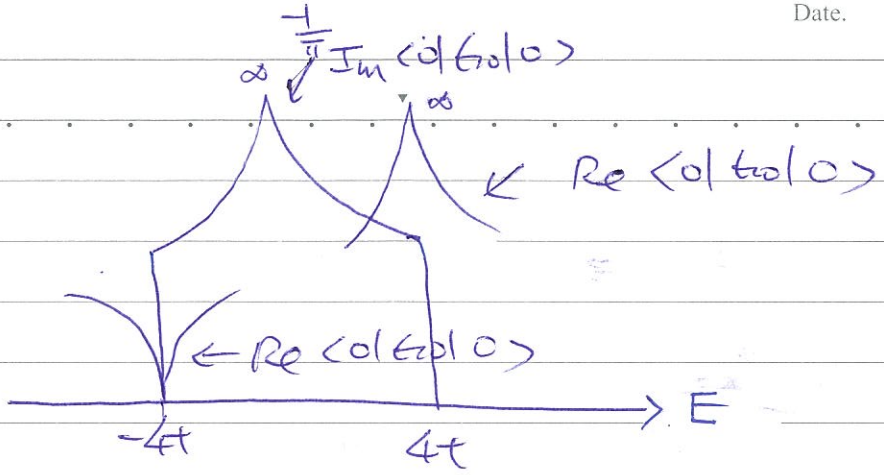
$$= \frac{(\pm 1)^n}{U_0}\left[\underbrace{\sqrt{1+\left(\frac{U_0}{2t}\right)^2} - \frac{|U_0|}{2t}}_{<1}\right]^{|n|} \Rightarrow \text{decays.}$$

Single impurity in 2D & 3D

$$\langle 0|G_0(E)|0\rangle$$

$$= \frac{1}{(2\pi)^2}\int_0^{2\pi} dk_x \int_0^{2\pi} dk_y \frac{1}{E-2t(\cos k_x+\cos k_y)+i\varepsilon} \quad \text{for 2D}$$

The imaginary part & real part are (~ density of states) sketched as follows



Near the band edge $(-4t)$, $\bar{E} = \delta E - 4t$

$$\langle 0|\hat{G}_0|0\rangle = \frac{1}{(2\pi)^2}\int d^2k \frac{1}{\delta E - 4t - 2t(\cos k_x + \cos k_y)}$$

$$\sim \frac{1}{2\pi}\int k\,dk \frac{1}{\delta E - tk^2}$$

↑ expand around (π, π)

$$\sim \frac{\ln(-\delta E/t)}{4\pi t}$$

$$\therefore \frac{1}{U_0} \sim \frac{\ln(-\delta E_{loc}/t)}{4\pi t}$$

For $U_0 = -|U_0| < 0$

$$\delta E_{loc} \cong -t\, e^{-4\pi t/|U_0|}$$

$$E_{loc} \cong -4t - t\, e^{-4\pi t/|U_0|}$$

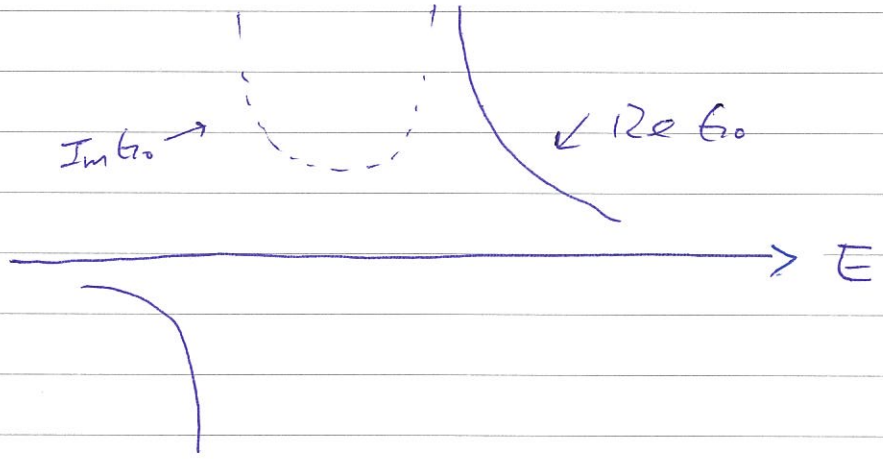
∴ The bounding energy $\delta E_{loc} \to 0^-$ as $|U_0| \to 0$

but no matter how weak the attraction potential $U_0 = -|U_0|$ is, there is always a bound state! (This feature reflects in the Cooper pairs in 2D, and many other problems in 2D.)

3D

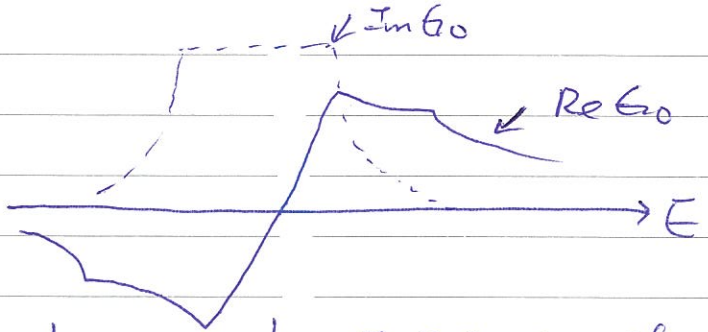
As we have seen, localized impurity states always exist in 1D & 2D.

The basic reason is due to the divergence of $Re\langle o|G_o|o\rangle$ at band edge. For instance, for 1D tight binding model, one has



Hence there is always a local state for a single impurity.

At 3D, however, both Im G_o & Re G_o are finite:



Therefore, U_o has to be strong enough to yield localized bound states! (for non compensated impurity).

Impurity vibration modes

Similar localized modes exist for phonons when (local mass (or spring constant) / α) is different.

Suppose that the bulk phonons is (Hamiltonian of)

$$H = \sum_i \frac{\vec{P}_i^{\,2}}{2M} + \frac{1}{2} \sum_{\substack{ij \\ \alpha\beta}} u_\alpha(r_i)\, \Phi_{\alpha\beta}(r_i - r_j)\, u_\beta(r_j)$$

(we reserve $D_{\alpha\beta}$ for the Green's function of phonons)

The eq. of motion is

$$M \frac{d^2 u_\alpha(\vec{r}_i)}{dt} = - \sum_{j\beta} \Phi_{\alpha\beta}(\vec{r}_i - \vec{r}_j)\, u_\beta(\vec{r}_j)$$

For a given frequency ω, one gets

$$\omega^2 u_\alpha - \frac{1}{M} \sum_{j\beta} \Phi_{\alpha\beta}(\vec{r}_i - \vec{r}_j)\, u_\beta = 0 \quad \cdots \quad (26)$$

If the atom at $r=0$ has different mass M_0 (isotope)

Eq. (26) becomes

$$\omega^2 \vec{u}(\vec{r}) - \frac{1}{M} \sum_{r'} \overleftrightarrow{\Phi}(\vec{r} - \vec{r}') \cdot \vec{u}(\vec{r}') + \frac{\delta M}{M} \omega^2 u_0\, \delta_{\vec{r},0} = 0$$

with $\delta M = M_0 - M$ . . . . . (27)

Clearly, $\frac{\delta M}{M}\omega^2 u_0 \delta_{\vec{r},0}$ plays the role ... as $U_0 \delta_{\vec{r},0}$ for the electronic problem.

Formally, we can rewrite eq. (27) as

$$[K(\omega^2) + \delta K(\omega^2)]\, u = 0 \qquad \text{--- (28)}$$

with $K(\omega) = \omega^2 \mathbb{I} - \frac{1}{M}\overleftrightarrow{\Phi} \leftrightarrow E - H_0$

$$\delta K(\omega^2) = \frac{\delta M}{M}\omega^2 \quad \delta_{\vec{r},0} \leftrightarrow -U_0 \delta_{\vec{r},0}$$

This is similar to the Schrödinger eq., we get

$$\vec{u}^{\pm} = \vec{u}^0 + \frac{1}{\omega^2 \mathbb{I} - \frac{1}{M}\overleftrightarrow{\Phi} \pm i\varepsilon}(-\delta K)\,\vec{u}^{\pm}$$

Here $\overleftrightarrow{D}^{\pm} = \frac{1}{\omega^2 - \frac{1}{M}\overleftrightarrow{\Phi} \pm i\varepsilon}$ are classical retarded / advanced Phonon Green's functions. and $\vec{u}^0$ is the solution to $(\omega^2 \mathbb{I} - \frac{1}{M}\overleftrightarrow{\Phi})\cdot \vec{u}_0 = 0$

In the k-space, one has $\vec{u}_0 = \vec{u}_k e^{i\vec{k}\cdot\vec{r}}$

$$K(\omega^2)\, u \to (\omega^2 - \omega_k^2)\, u_k \qquad \vec{u}_{k}^{+} = (\vec{u}_k)^*$$

$$\therefore \overleftrightarrow{D}^{\pm}(\vec{r}-\vec{r}') = \frac{1}{N}\sum_k \frac{\vec{u}_k \vec{u}_k^{+}}{\omega^2 - \omega_k^2 \pm i\varepsilon} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \qquad \varepsilon \to 0^+$$

is a 3×3 matrix!

(Note that this is quite different from the real quantum Green's function for phonons, $D^+ = \frac{2\omega_k}{\omega^2 - \omega_k^2 + i\varepsilon}$, we shall come back to it later.)

Similar to the electronic problem, the condition (eq (21)) for localized vibration mode is

$$\Pi' = -D(0,0,\omega^2)\,\delta K(\omega^2)$$

$$\therefore \quad \frac{1}{N}\sum_K \frac{U_K U_K^*}{\omega_K^2 - \omega^2}\frac{\delta M}{M}\omega^2 = \Pi \quad \cdots (29)$$

This is a 3×3 matrix condition. More precisely, one has

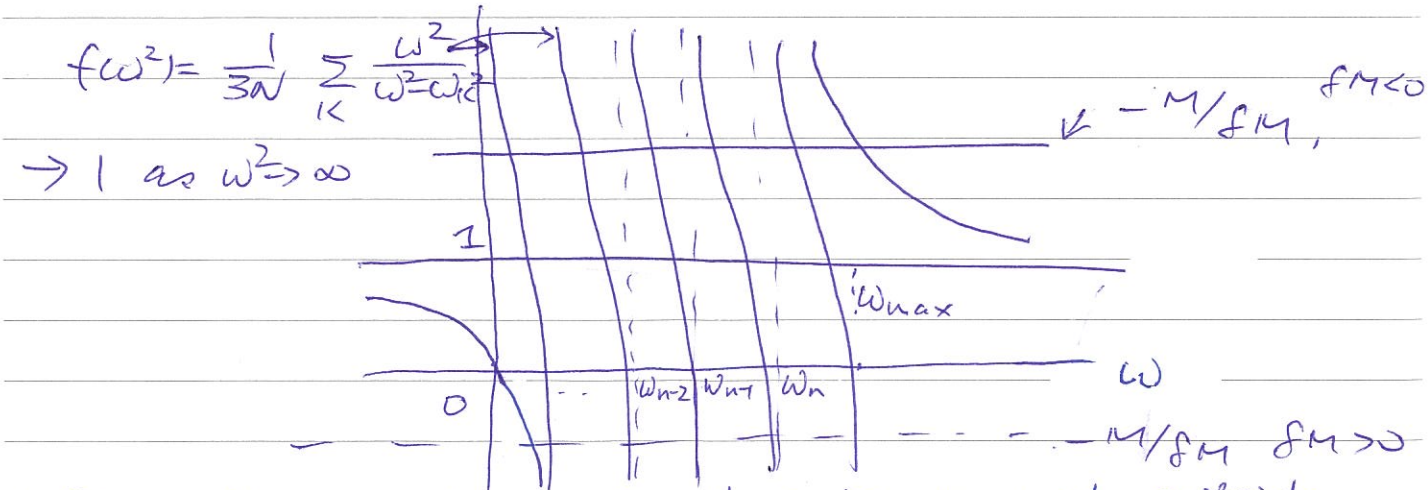
$$\frac{\delta M}{NM}\sum_K U_{K\alpha} U_{K\beta}^* \frac{\omega^2}{\omega_K^2 - \omega^2} = \delta_{\alpha\beta} \quad \cdots (30)$$

For a defect in a cubic crystal,

$$U_{K\alpha} U_{K\beta}^* = \tfrac{1}{3}\delta_{\alpha\beta}$$

(30) becomes $$\frac{\delta M}{3NM}\sum_K \frac{\omega^2}{\omega_K^2 - \omega^2} = 1$$

Graphically, this is similar to Fig 12.3:



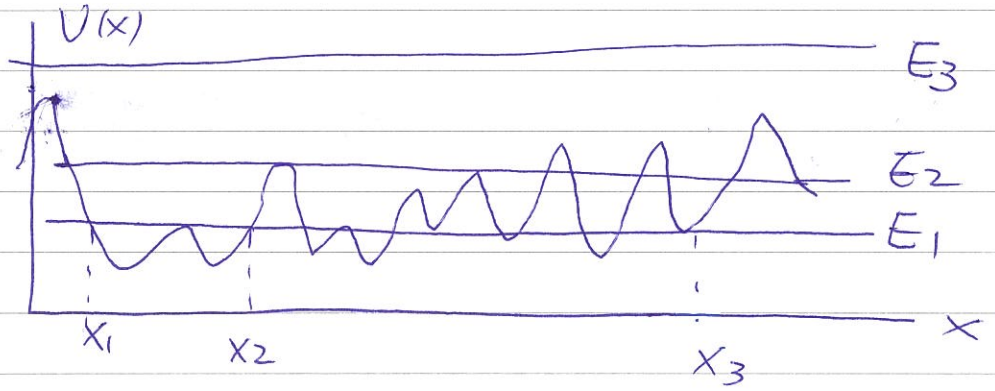
$\therefore \delta M > 0$ (heavier impurity), there is no mode outside the band, hence there is no localized mode.

Only lighter impurity ($-M < \delta M < 0$) supports a localized mode!

Localization

We have treated the problem of a single impurity and see that there exist (may) one localized mode.

What happens when we have many impurities, or finite density of impurities $\frac{N_I}{V} \equiv n_I$?
Does the system just posses N_I localized states?
Naively, for many impurities, the potential $V(x)$ of the system as shown in below



For $E = E_1$, the wavefunction is localized between x_1 & x_3. This is understandable because outside (x_1, x_3), $V > E_1$, $\psi \sim e^{\frac{-1}{\hbar}\sqrt{2m(E-V)}}$.

Similarly, for $E = E_2$, ψ is also localized.

What about $E = E_3$?

The intuition would say that ψ is extended. In 1958, however, Anderson pointed that for lower dimensions, all ψ are localized.

The mechanism is no longer based on energy consideration. Instead, it's due to the wave nature: interference would confine the particle and leads to localization of the wave. In fact, Anderson pointed out that all waves are localized for lower dimenson and strong enough random potential. So that the system is an insulator. The transition to all localized states is a metal–insulator transition. As we shall see, current understanding is for $d \leq 2$, the system is insulator for any disorder
$d > 2$ localization for strong enough disorder.

Localization in 1D

Anderson's original model grew out of a series of electron spin resonance experiments by Feher & collaborators on donor impurities (such as P & As) in Si. Feher & collaborators found that the electron spin on each P nucleus retained its characteristic frequency

on a timescale from seconds to minutes (i.e. life time). This is quite different from that predicted by the simple golden rule calculation in which impurities would interact with other impurities and lead to $0.1-10^{-6}$ sec. It indicated the spin diffusion is absent among ^{31}P impurity spins.

To capture the essence of quantum diffusion in the presence of disorders, Anderson proposed the tight-binding model

$$H = \sum_n \varepsilon_n C_n^+ C_n + V \sum_{n,m} C_n^+ C_m \quad \cdots (39)$$

where ε_n is a random number, uniformly distributed over $(\frac{-W}{2}, \frac{W}{2})$, i.e., the probability density, $P(\varepsilon_n) = \frac{1}{W}\,\theta(\frac{W}{2}-\varepsilon_n)\,\theta(\varepsilon_n+W/2)$

The Anderson model is effectively a 1D model. Clearly, it describes localization-delocalization transition as $V=0$, when none of sites are connected, all states are localized; when $W=0$, the system is described by a 1D band and all states are delocalized.

It turns out that in 1D, all states are localized once $W \neq 0$, in this case, one can find explicit expression for the characteristic length over which wave functions decay. (localization length)

(Definitions)

Criteria for localization

(i) To see if a particle is localized, a natural quantity to consider is the probability that the particle returns to its original position at $t \to \infty$.

Let $C_n(t)$ be the probability amplitude that an electron is on site n at time t,

We shall be interested in $\lim_{t\to\infty} |C_n(t)|^2$.

Using the Anderson model, eq. (30), we find

$$i\dot{C}_n(t) = \varepsilon_n C_n + \sum_m V_{nm} C_m \quad \cdots (31)$$

where we generalized V to V_{nm}, hopping amplitude between n & m sites.

After Fourier transformation, eq (31) becomes

$$C_n(E) = \frac{C_n(t=0)}{E-\varepsilon_n} + \sum_{m\neq n} \frac{V_{nm} C_m(t)}{E-\varepsilon_m} \quad \cdots (32)$$

Here $C_n(E) = \int_{-\infty}^{\infty} e^{iEt/\hbar} C_n(t)\, dt$ .....

& $C_n(t) = \int \frac{dE}{2\pi} e^{-iEt/\hbar} C_n(E)$

and the behavior $t \to \infty$ is related to the behavior of $C_n(E)$ at $E \to 0$.

At $t=0$, $C_n(t=0) = \delta_{n,0}$, then eq (32) can be solved by iteration, one gets

$$C_0(E) = \frac{1}{E-\varepsilon_0} + \sum_{m\neq 0} \frac{V_{0m} V_{m0}}{(E-\varepsilon_0)(E-\varepsilon_m)}$$

$$+ \sum_{\substack{\ell, m\neq 0 \\ m\neq \ell}} \frac{V_{0m} V_{m\ell} V_{\ell 0}}{(E-\varepsilon_m)(E-\varepsilon_\ell)(E-\varepsilon_0)} + \cdots \quad (33)$$

∴ The nth term in the probability amplitude is a self-avoiding random of n steps that starts and ends at the origin.

Since it's clear that each term contains $\frac{1}{E-\varepsilon_0}$, one can sum the series by defining

$$C_0(E) = \frac{1}{E - \varepsilon_0 - S_0(E)}$$

with $S_0(E) = \sum_{m\neq 0} \frac{V_{0m} V_{m0}}{E-\varepsilon_m} + \cdots$

In general, the recurring probability amplitude ...

for nth site is

$$G_n(E) = \frac{1}{E - \varepsilon_n - S_n(E)} \quad \cdots (34)$$

Since $G_n(t) = \int \frac{dE}{2\pi} e^{-iEt/\hbar} G_n(E)$, it is clear that if $\mathrm{Im} S_n(E)$ for E lies on real axis ($\neq 0$), $\int dE$ will pick up a decay term: $e^{-t/\tau}$ with $\tau = 1/\mathrm{Im} S_n(\varepsilon_n')$. ε_n' is shifted pole satisfying: $\varepsilon_n' - \varepsilon_n - \mathrm{Re}\, S_n(\varepsilon_n') = 0$

In other words, the state with ε_n' has a finite lifetime, the returning probability $|G_n(t)|^2 \to 0$ as $t \to \infty$!

Hence $S_n(E)$ is the crucial quantity to determine whether E is localized or not.

$\mathrm{Im} S_n(E = \text{Real}) \neq 0 \Rightarrow$ localized $\cdots (35)$

$S_n(E)$ is known as site self-energy

However, $S_n(E)$ themself depends on n and are random variables too! Therefore, the signature of the absence of extended states is the vanishing of the probability distribution of the site self-energy for all energies along the Real E axis $\cdots (36)$

The returning probability amplitude $G_n(E)$ in eq. (36) can be also more convenient derived using the Green's function in below.

(ii) Green's function & returning probability amplitude

Since $G = (E-H)^{-1}$, one has

$$(E-H)\,G = \mathbb{I}$$

That is $$(E - H_0)\,G = \mathbb{I} + VG$$

where $H_0 = \sum_n \varepsilon_n c_n^+ c_n$, $V = \sum_{n,m} V_{nm} c_n^+ c_m$

In terms of matrix elements, one finds

$$(E-\varepsilon_n)\,G_{nm}(E) = \delta_{nm} + \sum_{\ell \neq n} V_{n\ell}\, G_{\ell m}(E)$$

$$\therefore G_{nn}(E) = \frac{1}{E-\varepsilon_n} + \sum_{\ell \neq n} \frac{V_{n\ell}\, G_{\ell n}}{E-\varepsilon_n}$$

$$= \frac{1}{E-\varepsilon_n} + \sum_{\ell \neq n} \frac{V_{n\ell}\, V_{\ell n}}{(E-\varepsilon_n)(E-\varepsilon_\ell)} + \cdots$$

$$n \neq \ell \quad G_{n\ell}(E) = \frac{1}{E-\varepsilon_n} \sum_{m \neq n} V_{nm}\, G_{m\ell}(E)$$

Which is the same as eq. (33).

Therefore, $$G_{nn}(E) = \frac{1}{E - \varepsilon_n - \Sigma_n(E)}$$

In other words, the returning amplitude is ....

Simply $G(r,r,E)$ and the signature for absence of extended states is

$$\mathrm{Im}\, G(r,r,E) = 0 \quad \text{on real } E \text{ axis} \quad \text{--- (37)}$$

Exact results in 1D using spreading out amplitude

Once the state is localized, one expects the state is peaked somewhere in the lattice and decays as $e^{-m/\lambda}$, where m is the distance from the peak. Here λ is the localization length. Suppose the peak is at $x=0$,

$$\therefore \langle m|G^R(E)|0\rangle = \sum_n \frac{\langle m|E_n\rangle\langle E_n|0\rangle}{E - E_n + i\eta}$$

$$= \int dE'\, D(E') \frac{\langle m|E'\rangle\langle E'|0\rangle}{E - E' + i\eta} \qquad D(E') = \text{DOS}$$

$$\approx D(E)\, i\pi \langle m|E\rangle \sim e^{-m/\lambda} e^{i\phi}$$

$\phi =$ phase of matrix element

Hence one defines λ by

$$\lambda^{-1}(E) \equiv \lim_{m\to\infty} \frac{-1}{2m} \ln \overline{|\langle 0|\hat{G}(E)|m\rangle|^2} \quad \text{--- (38)}$$

where $\overline{\cdots}$ indicates the average over random on site energies ε_n!

If we can show that for <u>all E, $\lambda(E)$ is finite, then all states are localized</u>!

According to eq. (38), to find λ, one needs to calculate $\langle 0|\hat{G}(E)|m\rangle$.

We shall consider only the nearest neighbour hopping:

$$V\sum_{nm} c_n^+ c_m \rightarrow t\sum_n c_n^+ c_{n+1} + c_{n+1}^+ c_n \quad \cdots (39)$$

Let $\langle n|\hat{G}_0|m\rangle = \frac{\delta_{nm}}{E-\varepsilon_n}$, one has

the first nonzero term $\langle 0|\hat{G}|m\rangle$

is $\langle 0|\hat{G}_0|0\rangle t\langle 1|\hat{G}_0|1\rangle t\langle 2|\hat{G}_0|2\rangle t \cdots t\langle m|\hat{G}_0|m\rangle$

higher-order terms then involve back and forth walks between 0 & m.

Clearly, if we denote

G^ℓ = Green's function in which the electron is forbidden to visit site ℓ $\cdots$ (40)

$$F(g,E) = {}^{t}/_{g^2} \int dg'\, P(E - {}^{t}/_{g} - tg')\, F(g', E)$$

... (45)

Eq. (45) is the integral equation that $F(g,E)$ obeys. Once $F(g,E)$ is found, eq (42) implies

$$\lambda^{-1}(E) = -\int dg\, F(g,E) \ln|g| \quad \text{... (46)}$$

so that $\lambda(E)$ is found.

In the limit of <u>small w/t</u>, we have $P(E) = \delta(E)$ and it's suffice to consider $E \Rightarrow 0$

$\therefore$ Eq. (45) implies $F(g,0) \equiv f(g)$

$$f(g) = {}^{t}/_{g^2} \int dg'\, \delta(\underbrace{E}_{\parallel 0} - {}^{t}/_{g} - tg')\, f(g')$$

$$= \frac{1}{g^2} f(-1/g) \quad \text{- - - (47)}$$

The solution to eq. (47) is

$$f(g) = \frac{0.2646}{\sqrt{1+g^4}} \quad \left(\int_{-\infty}^{\infty} dg\, f(g) = 1\right) \quad \text{... (48)}$$

This is independent of w/t. Substituting eq. (48)

From eq. (44), one can deduce the probability (density) for $t\vec{G}^{\ell}$ $(\equiv g)$: $F(g, E)$

$$F(g,E) = \int \prod_n P(E_n)\, dE_n\, \delta(g - \langle \ell+1 | t\vec{G}^{\ell} | \ell+1 \rangle$$

By translational invariance, it's suffice to consider $g = t\vec{G}^{0}$ so that

$$F(g,E) = \int \prod_n P(E_n)\, dE_n\, \delta(g - \langle 1 | t\vec{G}^{0}(E) | 1 \rangle)$$

$$= \int \prod_n P(E_n) dE_n\, \delta\left(g - \frac{t}{E - E_1 - t^2\langle 2|\vec{G}'|2\rangle}\right)$$

↑ eq. (44)

$\therefore E_1$ can be integrated out

$$\int dE_1\, P(E_1)\, \delta\left(g - \frac{t}{E - E_1 - t^2\langle 2|\vec{G}'|2\rangle}\right)$$

$$= \int dE_1\, P(E_1)\, \delta\left(\frac{g(E - E_1 - t^2\langle 2|\vec{G}'|2\rangle) - t}{E - E_1 - t^2\langle 2|\vec{G}'|2\rangle}\right)$$

$$= \int dE_1\, (E - E_1 - t^2\langle 2|\vec{G}'|2\rangle)\, P(E_1)\, \delta\left(g(E - E_1 - t^2\langle 2|\vec{G}'|2\rangle) - t\right)$$

$$= \frac{t}{g} \cdot \frac{1}{g}\, P\left(E - t/g - t^2\langle 2|\vec{G}'|2\rangle\right)$$

$$\therefore F(g,E) = \frac{t}{g^2} \int \prod_{n\neq 1} P(E_n) dE_n\, P\left(E - t/g - t^2\langle 2|\vec{G}'|2\rangle\right)$$

$$= t/g^2 \int \prod_n P(E_n) dE_n \int dg'\, P\left(E - t/g - tg'\right) \delta\left(g' - t\langle 2|\vec{G}'|2\rangle\right)$$

$\int P(E_1) dE_1 = 1$

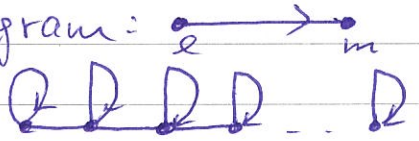
Then

$$\langle \ell | \hat{G} | m \rangle = \langle \ell | \hat{G} | \ell \rangle t \langle \ell+1 | \hat{G}^{\ell} | m \rangle \quad \text{---} (41)$$

A straightforward generalization of (41) is

$$\langle \ell | \hat{G} | m \rangle = \langle \ell | \hat{G} | \ell \rangle + \langle \ell+1 | \hat{G}^{\ell} | \ell+1 \rangle + \langle \ell+2 | \hat{G}^{\ell+1} | \ell+2 \rangle$$

$$\cdots + t \langle m | G^{m-1} | m \rangle =$$

Diagram: $\ell \rightarrow m$ = 

After averaging over ε_n, one expects

$$\overline{\langle \ell+1 | \hat{G}^{\ell} | \ell+1 \rangle} = \overline{\langle \ell+2 | \hat{G}^{\ell+1} | \ell+2 \rangle} =$$

$$\cdots = \overline{\langle m | G^{m-1} | m \rangle} \quad \text{(site independent!)}$$

Therefore, eq. (38) becomes

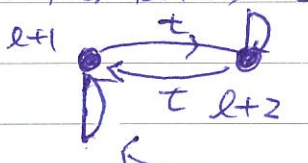
$$\lambda^{-1} = - \overline{\ln | \langle \ell+1 | + t \hat{G}^{\ell} | \ell+1 \rangle |} \quad \text{---} (42)$$

Now, according to the perturbation theory,

$$\langle \ell+1 | \hat{G}^{\ell} | \ell+1 \rangle = \langle \ell+1 | G^{0} | \ell+1 \rangle$$

$\uparrow$ zeroth order of t $\quad \bullet_{\ell+1}$

$$+ \langle \ell+1 | G^{0} | \ell+1 \rangle t \langle \ell+2 | \hat{G}^{\ell+1} | \ell+2 \rangle t \langle \ell+1 | \hat{G}^{\ell} | \ell+1 \rangle$$



$$\text{---} (43)$$

Solving eq. (43), we obtain $\langle \ell+1 | \hat{G}^{\ell} | \ell+1 \rangle = \dfrac{1}{\epsilon - \varepsilon_n - t^2 \langle \ell+2 | \hat{G}^{\ell+1} | \ell+2 \rangle}$

$$\text{---} (44)$$

into eq. (4), one finds, to first iteration, ...

$$f(g) = \frac{t}{g^2} \int dg'\, P(-t/g - tg')\, \frac{c}{\sqrt{1+g'^4}} \qquad c = 0.2696.$$

$$P(\epsilon) = \frac{1}{W} \quad \text{for} \quad -\frac{W}{2} \le \epsilon \le W/2$$

From $f(g)$, one deduces (HW. I)

$$\lambda^{-1} = -\int_{-\infty}^{\infty} dg\, f(g) \ln|g|$$

$$= 0.1142\, \frac{W^2}{t^2} \quad \therefore \quad \lambda = \text{finite as long as } W \neq 0 !$$

That is, states are localized.

(iii) Inverse participation number

Another way to characterize whether a state is localized or not is to consider the second moment of the probability density (due to Wegner 1980)

$$P^{-1} = \sum_r |\psi(r)|^4$$

Here ψ is normalized: $\sum_r |\psi(r)|^2 = 1$

Examples: ① plane waves $\psi(r) = \frac{1}{\sqrt{V}} e^{ikr}$

$\therefore |\psi|^4 = \frac{1}{V^2}$, $P^{-1} = \frac{1}{V^2} \times V = \frac{1}{V}$, $\therefore P = V = L^d$.

② $\psi_{i=0} = 1, \quad \psi_{i\neq 0} = 0$

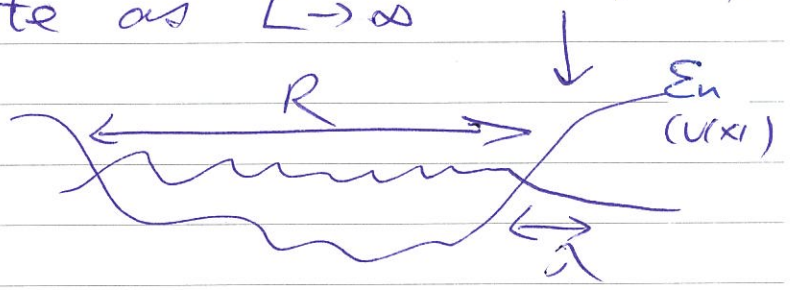
$|\psi(r)|^4 = \delta_{r,0} \quad \therefore \sum_r |\psi(r)|^4 = 1$

$P = 1$

in general, for localized states,

$P \sim R^d$ $\quad R$ = average diameter of the state $\pm \xi$ (localization length)

$\therefore$ P remains finite as $L \to \infty$



③ Critical State

$P \sim L^{d^*}$ with $d^* \neq d$ being some fractal dimension.

Such a state is also extended but not the same as plane waves.

(iii) Average P^{-1} : If we sum over states and average, we get

$$\overline{P^{-1}} = \frac{1}{N(E)} \sum_{n,r} \overline{|\psi_n(r)|^4 \delta(E - E_n)}$$

$N(E)$ = # of states near $E = \sum_n \delta(E - E_n)$

$$= \frac{1}{N(E)} \sum_{n,r} \overline{\langle r|E_n\rangle^2 \delta^2(E-E_n) (\langle E_n|r\rangle)^2 \frac{1}{\delta(E-E_n)}}$$

$$= \frac{1}{N(E)} \sum_r \overline{\langle r|\delta(E-H)|r\rangle^2 \left[\frac{1}{\delta(E-H)}\right]}$$

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Here $\delta(E-H) = -\frac{1}{\pi} \mathrm{Im} \frac{1}{E-H+i\delta} = \frac{1}{\pi} \frac{\delta}{(E-H)^2+\delta^2}$

and $\left[\frac{1}{\delta(E-H)}\right] = \frac{1}{\pi}\frac{1}{\delta}$ at $E=H$

$\therefore \overline{P^{-1}} = \frac{\pi V}{N(E)} \lim_{\delta\to 0} \delta A(0,E,\delta) = \frac{\pi}{\rho(E)} \lim_{\delta\to 0} \delta A(0,E,\delta)$

where $A(0,E,\delta) = \overline{\left(-\frac{1}{\pi}\mathrm{Im}\langle r| \frac{1}{E-H+i\delta} |r\rangle\right)^2}$

$\simeq$ average return probability with a time interval δ^{-1}

$\therefore \overline{P^{-1}}$ corresponds to the probability that a particle will return to the same site after ∞ time interval.

(iv) Transfer matrix and Lyapunov exponents.

For 1D and quasi-1D systems, localization length can be also calculated from the limiting behavior of products of random matrices.

Consider a tight-binding 1D model,

$$H = \sum_n \varepsilon_n c_n^+ c_n + t \sum_n c_n^+ c_{n+1} + h.c.$$

The eigenstate ψ_n satisfies

$$t(\psi_{n-1} + \psi_{n+1}) + \varepsilon_n \psi_n = E\psi_n$$

$$\therefore \quad (\varepsilon_n - E)\psi_n + t(\psi_{n+1} + \psi_{n-1}) = 0$$

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{E-\varepsilon_n}{t} & -1 \\ 1 & 0 \end{pmatrix}}_{T_n} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}$$

$T_n \equiv$ transfer matrix

$\therefore$ Starting from $\begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}$, one has

$$\begin{pmatrix} \psi_{L+1} \\ \psi_L \end{pmatrix} = \underbrace{T_L T_{L-1} \cdots T_1}_{\Theta_L} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \quad -- (4)$$

Define

$$\Gamma \equiv \lim_{L\to\infty} (\Theta_L \Theta_L^+)^{1/2L}$$

The eigenvalues of Γ can be put in the form e^{γ_i}. $\gamma_i \equiv$ Lyapunov exponents of Θ_L.

The smallest of γ_i determines the slowest possible exponential increase of state for $L\to\infty$

$\therefore$ The smallest γ_i can be identified as the inverse of longest λ.

It can be shown (HW.2) that the conductance of the system is

$$G = \frac{e^2}{h} Tr \frac{2}{QQ^+ + (QQ^+)^{-1} + 2}$$

Using γ_i, one has

$$G = \frac{e^2}{h} \sum_{j=1}^{N} \frac{2}{\cosh^2 \gamma_j - 1} \qquad N = 2 \text{ in this case}$$

Localization and conductance : metal–insulator transition

The localization of wavefunction can be also manifestated in the measurement of conductance. As we have seen in the discussion of Lyapunov exponents, the conductance is found once all exponents are known.

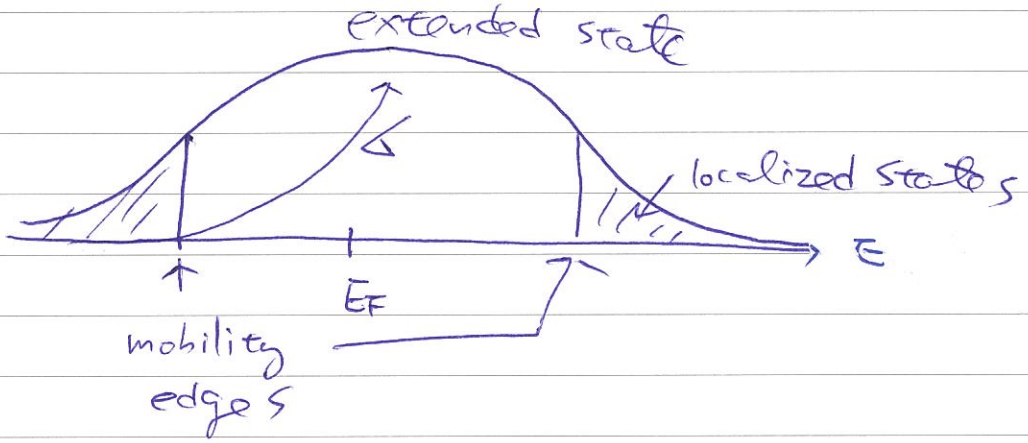
What is the behavior of the conductance when the strength of impurities increases?

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Mobility edge

After Anderson's proposal of localization, the relevance of localization to transport properties was discussed by Mott (1964). Mott proposed the concept of mobility edge which separates the localized states from the extended states as shown in below



If E_F falls in the range of extended states, the conductivity σ is large, otherwise, $\sigma = 0$ for $T = 0$. Therefore, there will be a metal-insulator transition as one tunes the Fermi energy!

Is the transition continuous or discontinuous? This transition is quite different from the

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Usual phase transitions that we have talked about. The usual phase transitions exhibit anomalies in thermodynamic measurements such as specific heat & magnetization. Here the density of state is smooth and there is no anomalies in specific heat. The anomaly shows up in the transport measurements, which as we shall see, are <u>non-equilibrium properties</u> of the system.

Mott proposed that σ jumps discontinuously from some σ_{min} to zero, based on the appealing of Drude conductivity: $\sigma = \frac{ne^2\tau}{m}$

$\therefore \begin{cases} n \sim a^{-d} \\ a = \text{lattice constant} \\ \ell = v_F \tau, \end{cases}$ $\quad v_F = \frac{\hbar k_F}{m} \simeq \frac{1}{m}\frac{\hbar}{a}$

$\therefore \sigma \sim \frac{e^2 a^{-d} \ell}{\hbar/a} \sim \frac{e^2}{\hbar}\frac{a^{2-d}}{\pi}\frac{\ell}{a}$

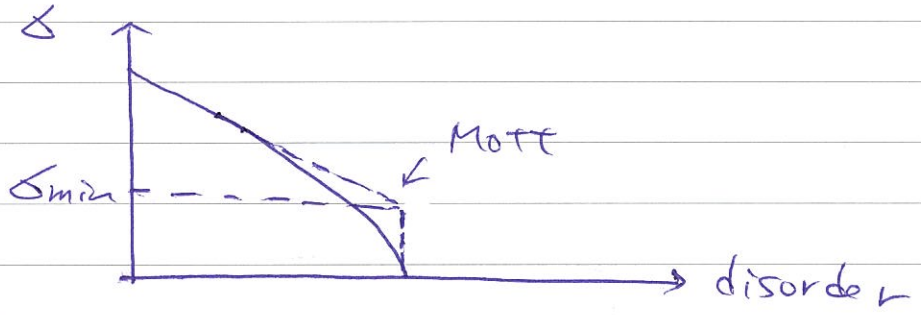
Since ℓ can not be smaller than a,

$\sigma \gtrsim \sigma_{min} = \frac{e^2}{\hbar}\frac{a^{2-d}}{\pi}$, there is a min σ.

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This turns out to be incorrect. The transition is continuous as shown in below.



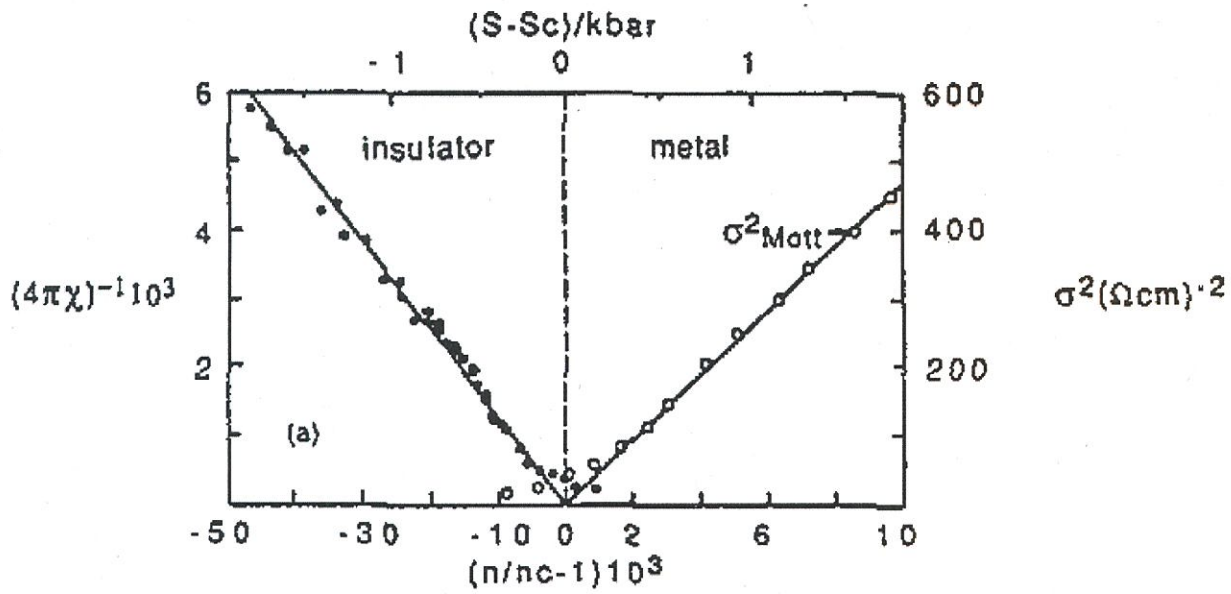
(expt. see over)

Variable range hopping

The insulator, usually termed Anderson insulator, is insulating only at T=0.

At finite T, an electron can move by thermally activated hopping. Every time an electron moves from one localized state to another state which has overlap with the first state. Since in general, two localized states do not have the same energy, the electron must exchange energy with a phonon each time it moves. The hopping is limited by phonon frequency.

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Metal-Insulator transition in uncompensated Si:P, P= dopant atoms

M.A. Paalanen & G.A. Thomas, Helv. Phys. Acta 56, 27, 1983

$$\sigma \sim \omega_{phonon}\, e^{-2\alpha r - \frac{\Delta\varepsilon}{k_B T}}$$

r = distance between localized centers

$\alpha \triangleq$ localized length ~ const

$\Delta\varepsilon$ = energy difference

Both r & $\Delta\varepsilon$ fluctuate. but for σ, we replace r & $\Delta\varepsilon$ by their averages.

Let $g(\epsilon)$ be DOS per volume, $g(\epsilon) r^d$ is then # of states available within distance r. $\therefore \Delta\varepsilon \sim \frac{A}{g(\epsilon) r^d}$ A being some constant.

$$\therefore \sigma \sim e^{-2\alpha r - \frac{A}{g(\epsilon) k_B T r^d}}$$

Minimizing $2\alpha r + \frac{A}{g(\epsilon) k_B T r^d}$ would lead to largest possible σ:

$$\frac{d}{dr}\left[2\alpha r + \frac{A}{g(\epsilon) k_B T r^d}\right] = 0$$

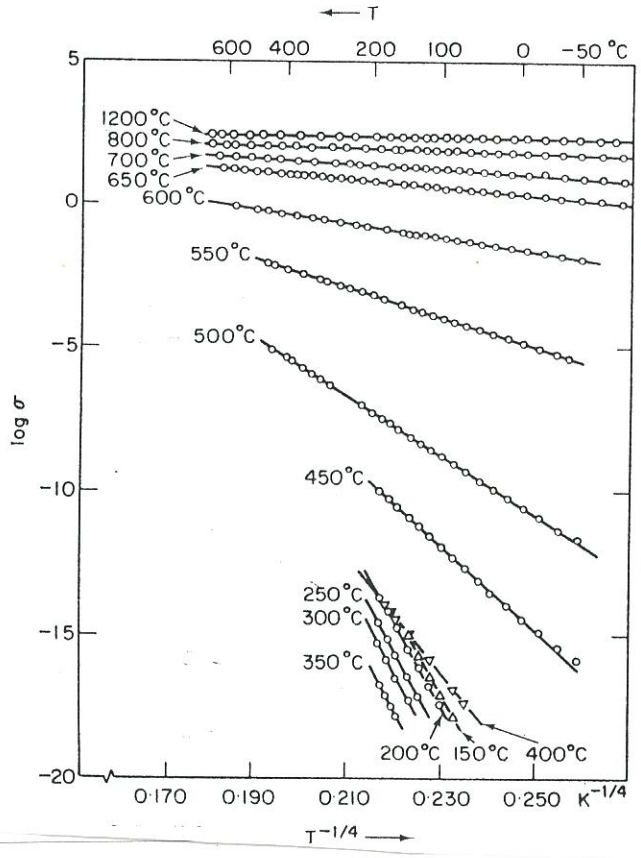
$$\therefore r^{d+1} \sim \frac{A}{\alpha g(\epsilon) k_B T}, \quad r \sim \frac{1}{T^{\frac{1}{d+1}}}.$$

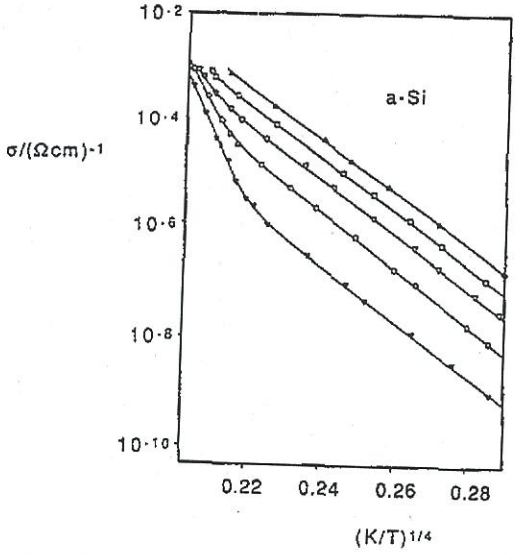
$\therefore$ The leading behavior of $\sigma \sim e^{-\left(\frac{T_0}{T}\right)^{\frac{1}{d+1}}}$

At $d=3$, $\sigma \sim e^{-\left(\frac{T_0}{T}\right)^{\frac{1}{4}}}$ (Mott.) ... (46)

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This behavior was proposed by Mott and was observed in many samples such as doped & compensated $Si_{1-x}P_x$, VO_x, $La_{1-x}Sr_xVO_3$ & pyrolytic carbon annealed as different T. See Below (Bücker 1993)





W. Beyer, 1974
Ph.D. Thesis
Universität
Marburg.

Level spacing statistics

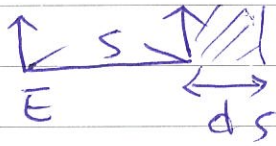
Another signature of metal-insulator due to impurities is the statistics of level spacings.

$$P(S) = \sum_i \delta\left(S - \frac{E_{i+1} - E_i}{\Delta}\right).$$

For localized states, each state occupied different localization and hence is independent. The spectrum is uncorrelated.

$P(S)\,dS$ = [probability for there is no energy level in $(E, E+S)$]

× [under the condition that there is no energy level in $(E, E+S)$ but there is an energy level in $(E+S, E+S+dS)$]



$= r(S)\cdot dS$

$$= \int_S^\infty P(x)\,dx$$

(level spacing $> S$)

$$\therefore P(S) = r(S) \int_S^\infty P(x)\,dx$$

If the spectrum is uncorrelated, $r(S) = \text{const} \equiv r_0$

$$\therefore P(S) = r_0 \int_S^\infty P(x)\,dS$$

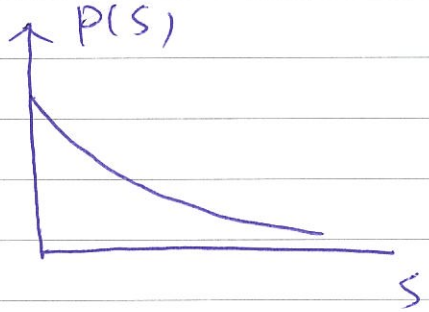
$$\frac{dP(S)}{dS} = -\gamma_0 P(S)$$

$$\therefore P(S) = P_0 e^{-\gamma_0 S}$$

$$\because \int_0^\infty P(S)\,dS = 1 \quad \therefore \quad P_0 = \gamma_0$$

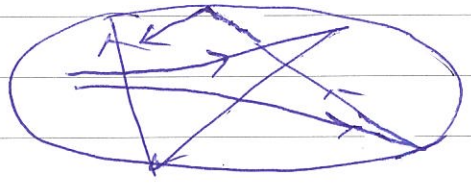
$$\langle S \rangle = \int_0^\infty S\,P(S)\,dS = \frac{1}{\gamma_0}$$

$$\therefore P(S) = \frac{1}{\langle S \rangle} e^{-S/\langle S \rangle}$$



This is the Poisson distribution.

On the other hand, for extended states, disorders tends to make the system chaotically: slightly different initial conditions lead to divergence of classical paths



accordiy to Bohr-Sommerfeld quantization $\oint p \cdot dr = nh$ their energies tend to repel.

The simplest form to account for repulsion of levels is $r(S) = \alpha S$

$$\therefore P(S) = \alpha S \int_S^\infty P(x)\,dx$$

$$\frac{dP(S)}{dS} = \alpha \int_S^\infty P(x)\,dx + \alpha S(-P(S)) = \frac{P(S)}{S} - \alpha S P(S)$$

$$\therefore P(s) = As\, e^{-\alpha s^2/2}$$

Normalization : $\int_0^\infty ds\, P(s) = 1$

$$\therefore A = \alpha \quad , \quad P(s) = \alpha s\, e^{-\alpha s^2/2}$$

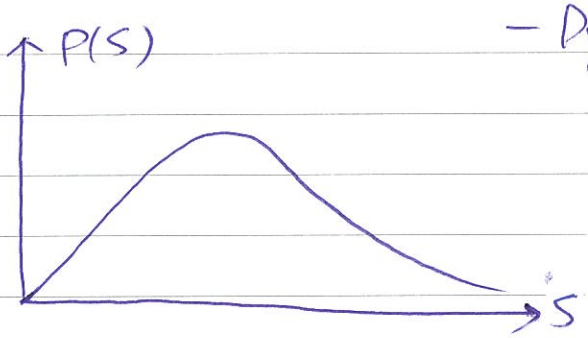
$$\langle s \rangle = \int_0^\infty s\, p(s)\, ds = \alpha \int_0^\infty s^2 e^{-\alpha s^2/2} ds$$

$$= \alpha \left(-\frac{d}{d\beta}\right) \int_0^\infty e^{-\beta s^2} ds \,\Big|_{\beta = \alpha/2}$$

$$= \sqrt{\frac{\pi}{2\alpha}}$$

$$\therefore P(s) = \frac{\pi s}{2\langle s \rangle^2}\, e^{-\frac{\pi s^2}{4\langle s \rangle^2}}$$

This is the Wigner - Dyson distribution.



Classical chaotic systems, when quantized, should exhibit the Wigner - Dyson distribution. This is known as the Bohigas - Giannoni - Schmit conjecture.

Integrable classical motions, when quantized, exhit the Poisson statistics. This is known as the Eutzwiller - Berry - Tabor conjecture.

From the above discussion, the metal-insulator (Anderson) transition is a divided line between Insulator $\longleftrightarrow$ Poisson statistics

Strong disorder $\swarrow$ Disorder metal $\longleftrightarrow$ Wigner-Dyson statistics

$\nwarrow$ Weak disorder

Note that in general, the Wigner-Dyson statistics may not be the standard one. For most general level repulsions, $P(s) \sim s^{\beta} e^{-\alpha s^{\beta+1}}$.

At the transition, the system is critical.

(i) $P(s) \sim s^{\beta}$ $s \ll 1$

$P(s) \sim e^{-As}$ $s > 1$

(ii) ψ_E is multifractals

$$\int |\psi_E|^{2q} d^d r \sim L^{-D_q(q-1)}$$

(iii) $\overline{\rho(E)\rho(E')}$ ... scale invariance.

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The scaling theory of localization

The most powerful theory of localization is a scaling theory developed by Abraham, Andersan, Licciardello, & Ramakrishnan (PRL, 42, 673, 1979) in 1979. The idea is that since the metal-insulator transition is continuous, one expects scaling phenomenon should be exhibited close to the transition.

The question is then: how scaling would be exhibited?

In the usual critical phenomena, the order parameter ψ is so-called a scaling field so that $\langle \psi(r)\psi(r')\rangle \sim \frac{1}{|r-r'|^{d-2+\eta}}$

η = anomalous dimension. L-(47)

The point is that if one counts the dimension of ψ in the Ginzburg-Landau Hamiltonian, one finds $[\psi] = \frac{d-2}{2}$ and hence η is anomalous.

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Mathematically, the reason why η appears in eq. (47) is that there is a prefactor a^η as a coefficient in eq. (47) with a = lattice constant.

In general, there may be more scaling fields (such as $\psi^2 \to$ specific heat)

However, in the Anderson transition, Abraham et al. assume that there is one scaling parameter.

This is the key assumption:

the dimensionless conductance

$$g(L) = \frac{2\pi\hbar}{e^2} G(L) \quad \cdots \quad (48)$$

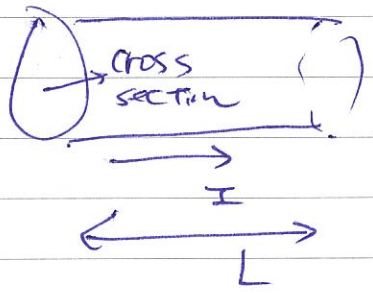
is a universal function of the sample size L^d.

Here $G(L)$ is the conductance.

Simple dimensional analysis tells us.

$$G(L) = \sigma L^{d-2} \quad \cdots \quad (49)$$

$\because J = \sigma E$ $\quad I = J \cdot$ cross section



$= \sigma \cdot E \cdot$ cross section

$= \sigma \frac{EL}{L} L^{d-1}$

$\equiv G V$

$\therefore G = \sigma \cdot L^{d-2}$

$$\frac{G(L)}{G(L')} = \left(\frac{L}{L'}\right)^{d-2}$$

The key assumption of one scaling parameter can be motivated by considering changes of energy eigenstates made by changing sizes of the system $L_1 \to L_2$.

When the system size changes, energy levels will be shifted resulted in ΔE. Also the energy level spacing S will be changed too, ΔS.

Therefore, the crucial dimensionless quantity changed is $\Delta E / \Delta S$.

For localized states, their energies are not sensitive to the boundary.

$\therefore \Delta E_{\text{localized}} \simeq 0$

Only extended states are sensitive to the boundary condition and ΔE is often calculated by finding the energy difference of periodic & antiperiodic boundary conditions.

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The mean spacing between energy levels ...

is $\Delta\varepsilon = \frac{1}{n L^d}$

$\therefore \Delta E = \hbar/\tau_D$, τ_D = typical time scale with transport (extended states) from the center to the edge

(ΔE = Thouless energy scale) $\equiv E_T$

$\tau = \frac{(L/2)^2}{D_0}$ D_0 = diffusion constant

Einstein relation $\sigma = 2e^2 n \cdot D_0$ $D = \frac{\tau v^2}{d}$

$n = D_0 E$

$\therefore \Delta E = 2\hbar\sigma / e^2 n L^2$

$\therefore \frac{\Delta E}{\Delta\varepsilon} = \frac{2\hbar}{e^2}\sigma L^{d-2} = \frac{2\hbar}{e^2} G(L) = g(L)$

(dimensionless Thouless conductance)

Consistent with the previous assumption.

Given one scaling parameter, one can address how $g(L)$ changes eventually as $L \to \infty$

This is examined by defining

$$\frac{d \ln g(L)}{d L} = \beta \quad \cdots \quad (10)$$

where $\beta = \beta(g)$ is referred as the beta function. The central physics of localization is contained in $\beta(g)$, which is a universal function of g, depending only on dimensions d.

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If $L \to \infty$, $\beta(g) > 0$, $g(L)$ must diverge.
This is the signature of extended states.
On the other hand, $\beta(g) < 0$, $g(L) \to 0$.
∴ all of states are localized!

In the extreme case (weak disorder limit),
one has the Ohmic law : $G = \sigma L^{d-2}$

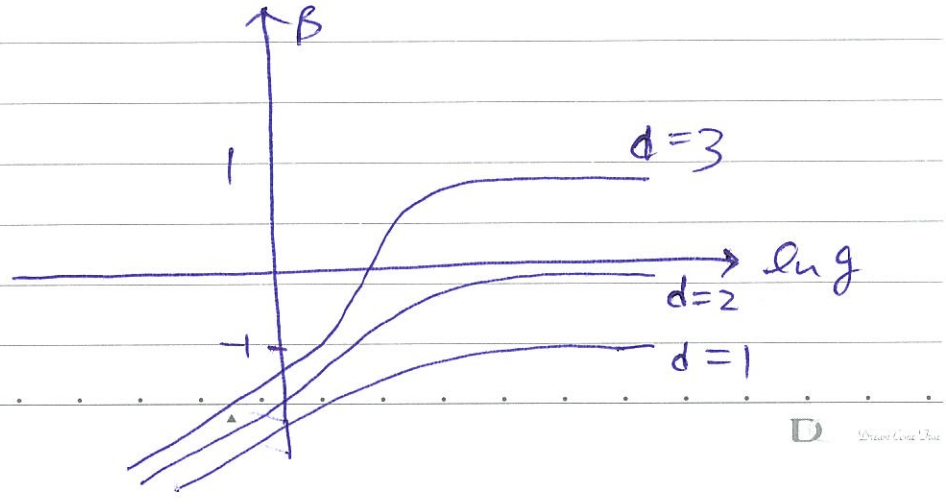
$\therefore \beta(g) = d-2$. $(g >> 1,\ E_T >> \Delta S)$

In the limit of strong disorder, the
localization length $\xi << L$, $G \sim e^{-L/\xi}$

$$\beta(g) = -L/\xi = \ln g \qquad (g << 1,\ E_T << \Delta S)$$

To gain insight (further), Abraham et al. made
the 2nd key assumpt : $\beta(g)$ is monotonic.

This enables one to connect $\ln g$ to $d-2$
as follows



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It's clear from this figure that for $d=1,2$, all states are localized

For $d=3$, $\beta(g)$ crosses $\ln g$ axis and approaches 1 asymptotically.

The transition from $\beta(g)<0$ to $\beta(g)>0$ is continuous and hence there is no minimum metallic conductivity.

The above assumption receives confirmation from the perturbative calculation which is valid in weak-disorder limit: $\beta(g) = d-2-\frac{A_d}{g}$ $A_d>0$ constant

Nonetheless, there is no rigorous mathematical proof for all strength disorders, even though the one-parameter scaling theory provides an important phenomenology of localization.

Assuming its correctness, near $\beta(g)=0$ at $g=g_c$ $(d=3)$, we can approximate

$$\beta(g) = \frac{g-g_c}{\nu g_c} \equiv \frac{\delta g}{\nu}$$

ν = a positive # determined by the slope.

$$\therefore \frac{d\ln g}{d\ln L} = \frac{1}{g}\frac{\delta g}{d\ln L} \sim \frac{1}{g_c}\frac{\delta g}{d\ln L}$$

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$$\therefore \frac{1}{g_c}\frac{dg-g_c}{d\ln L} \sim \frac{g-g_c}{\nu g_c}$$

$$\frac{d\ln g-g_c}{d\ln L} \simeq \frac{1}{\nu}$$

$$\ln\frac{g-g_c}{g_0-g_c} = \ln\left(\frac{L}{L_0}\right)^{\frac{1}{\nu}}$$

$$\left(\frac{L}{L_0}\right) = \left(\frac{g-g_c}{g_0-g_c}\right)^{\nu} \quad \cdots (1)$$

L_0, g_0 are some constants

In the localized regime, $g_0 < g_c$.

If we define $\xi = L_0\left(\frac{g_c}{g_0-g_c}\right)^{\nu} \equiv L_0|\epsilon|^{-\nu}$

$$g = g_c\left(1-\left(\frac{L}{\xi}\right)^{\frac{1}{\nu}}\right)$$ decreases as $L\uparrow$

The length scale ξ diverges at g_c. Since the localization length also diverges at g_c, one identifies $\xi = \lambda$ (localization length) and ν being the exponent. Similar to the exponent for the correlation length.

Eq. (1) is valid for $\xi \gg L$. For large L, one expects Ohm's law is applicable.

$$\therefore g \sim \left(\frac{L}{\xi}\right)^{d-2} \sim \xi^{2-d} \sim |\epsilon|^{(d-2)\nu} \equiv |\epsilon|^{s}$$

with $s = (d-2)\nu$ $\quad \cdots (2)$

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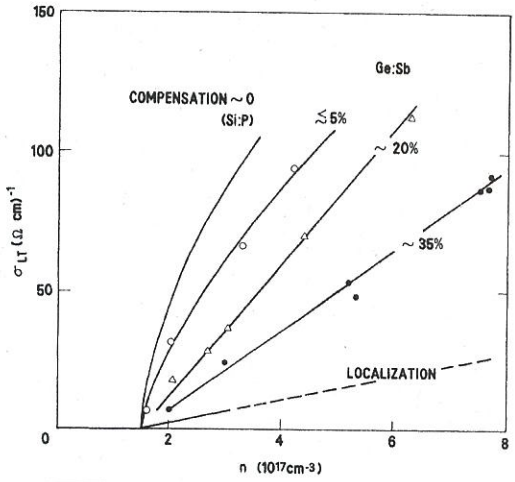
Hence the conductivity vanishes continuously with the power s.

It can be shown if $\beta(g) = d-2 - \frac{A_d}{g}$ $A_d > 0$,

$s=1$ (Hw. 3)

Experimentally, this can be checked and s appears to vary between 1/2 and 1:

G. A. Thomas et. al, Phy. Rev. B 25, 4288 (1982)



Low T → Conductivity

One sees that s evolves from $s=1/2$ in the uncompensated semiconductor, Si:P, toward $s=1$ as the compensation is increased in Ge:Sb ($s=0.55$ at 0%, $s=0.7 \pm 0.2$ at ~5%, $s \approx 1$ at 20%, and $s \approx 1$ for 35% compensation)

Note that the random potential is due to the charged P-ions. In Si:P, each P gives up an electron, In the compensated Ge:Sb, equal amounts of Sb & B are added so that # of scatters exceeds # of charge carriers

in the compensated samples. Hence, disorder plays a larger role in the compensated samples & causes the improved agreement with scaling theory. In the uncompensated materials, spin-orbit & e-e interactions are in action, reducing S to 1/2.

Weak localization and quantum interference

In the weak disorder limit, one can treat the random potential perturbatively. As we shall see, $\beta(g) = d - 2 - \frac{A_d}{g}$ with $A_d > 0$.

At $d=2$, $\beta(g) = -\frac{A_d}{g}$, $\frac{d\ln g}{d\ln L} = -\frac{A_d}{g}$

$$\| $$

$$\frac{1}{g}\frac{dg}{d\ln L}$$

$\therefore g = g_0 - A_d \ln L/L_0$ with L_0 being some macroscopic length scale. This is valid only for $L < L_0$ and $g \uparrow$ as $L \to L_0$ & then goes to strong disorder regime. Hence the logarithmic variation of conductance represents a precursor to the localization and is often termed as weak localization (localization is manifested as $g \uparrow 0$ but not really localized.)

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At finite temperatures, electrons can diffuse around. The mean free path $\sim \sqrt{D\tau}$

τ = scattering time D = diffusion const.

$\therefore$ One expects $L \sim \sqrt{D\tau}$ and $\tau \sim T^{-P}$

$P \sim 1$

$\therefore \delta g \sim A_d \frac{D}{2} \ln T/T_0$

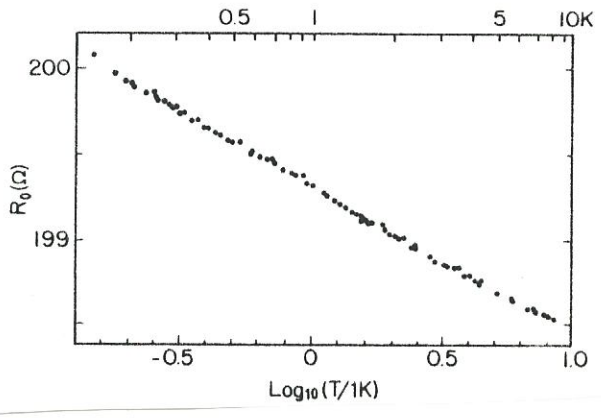
In other words, the deviation from the Drude formula should be

$$\Delta\sigma \propto \ln T/T_0 \quad \text{---} (52)$$

i.e. as $T \downarrow 0$, $\sigma \downarrow$, $(R \uparrow)$ logarithmically.

This logarithmic variation is well exhibited in the data on copper film. See below

S. Kobayashi et. al.
J. Phys. Soc. Jpn. 49, 1635, 1980



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Disorder and quantum interference

The limit of weak disorder was realized to be important for understanding the localization problem in fo's after the work by Abrahams et al. By summing a certain class of diagrams in perturbation theory (maximally crossed diagrams), the above log correction to δ can be deduced for $d = 2$.

Since $T \to 0$, $\Delta\delta \propto \ln T/T_0 \to -\infty$, eventually one reaches the regime where total δ vanishes. Hence all states are localized at $T=0$ for $d=1,2$. Even though this was an analysis for weak disorders, it is believed that all states are also localized in the strong disorder limit.

One of the important points as we shall see in this developement is that these diagrams

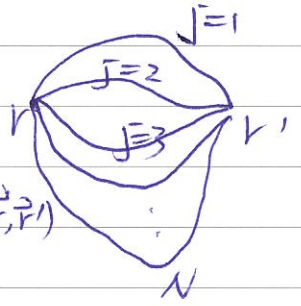
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Can be interpreted as quantum interference ... processes that give rise to an enhanced backscattering.

Quantum interference and classical propagation

Wave propagation and classical propagation are different. Their difference can be best illustrated by considering the probability of going from $\vec{r}$ to $\vec{r}'$: $P(r, r')$



Classically: the probability is a summation of probability $P_j(\vec{r}, \vec{r}')$ for each possible path

$$P(\vec{r}, \vec{r}') = \sum_{j=1}^{N} \overline{P_j(\vec{r}, \vec{r}')} \quad (13)$$

($\overline{\cdots}$ is the average over disorders)

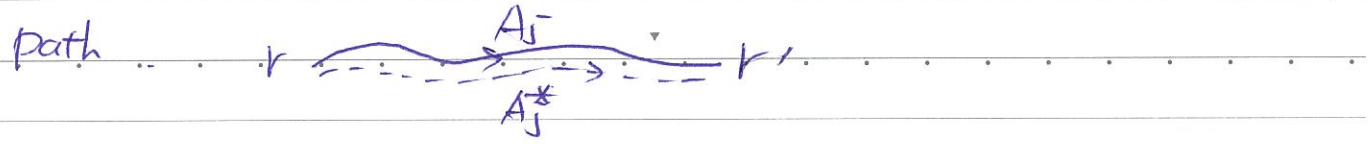
Quantum diffusion, however, is different. The fundamental quantity is the amplitude $G_j(\vec{r}, \vec{r}')$ for path j

and

$$P(\vec{r}, \vec{r}') = \left| \sum_j G_j(\vec{r}, \vec{r}') \right|^2 = \sum_{i,j} G_i^*(r, r') G_j(r, r') \quad (14)$$

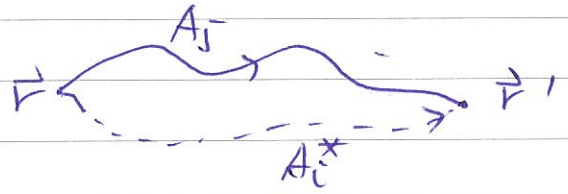
Therefore, one needs to assign two amplitudes ... (complex conjugate to each other) for each ...

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Clearly, classical probability only accounts for terms with $i=j$ in eq. (14) shown in the above figure.

The most general terms, shown in below, would exhibit quantum interference.



Phase coherence, Aharonov-Bohm effects & universal fluctuations

To be able to see the interference effect, waves have to be coherent.

The characteristic length scale that the electron is coherent is called phase-coherent length l_ϕ. l_ϕ is different from the mean free path λ, which is the characteristic length that the momentum of the electron changes.

For elastic scatterings, since the energy of

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The electron is not charge, $e^{\frac{-iEt}{\hbar}}$ is not changed. Therefore, the electron is coherent.

Only when the scattering is inelastic and occurs with a given probability, the electron will become incoherent : $e^{\frac{-i}{\hbar}\Delta E_1 t}$ $e^{\frac{-i}{\hbar}\Delta E_2 t}$ ....

↑ ↗

randomly occurring ...

In solids, such inelastic scatterings happen with the participation of phonons.

Mesoscopic systems λ_ϕ is usually larger than λ. (~100 μm for very good semiconductors)

It's clear that one can have different regimes

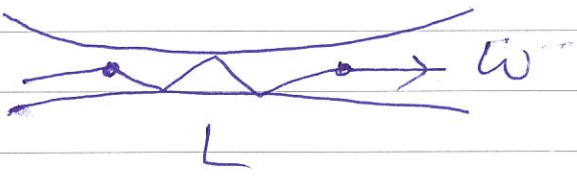
Classical

$\lambda_\phi << W, L$



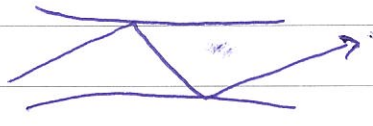
Diffusive

$\lambda < W, L < \lambda_\phi$



Ballistic

$W, L < \lambda$

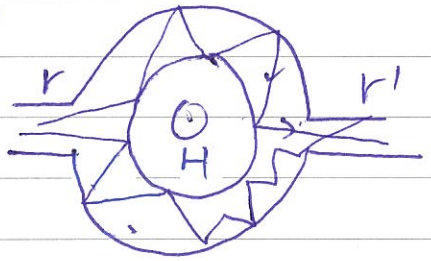


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The system when $L < \lambda_\Phi$ is called a mesoscopic systems. In these systems, electrons keep their phase coherent when they are transported. Hence it is possible to observe quantum interference.

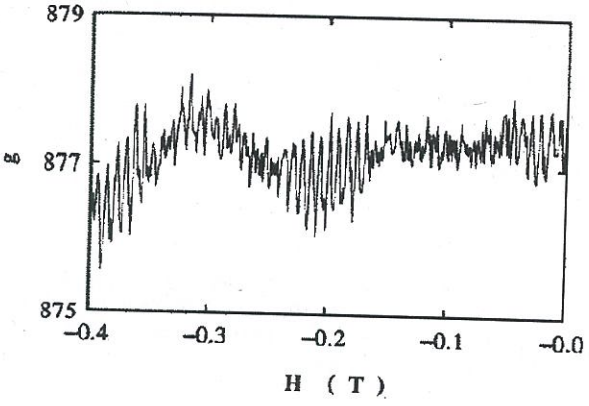
Aharanov-Bohm effect

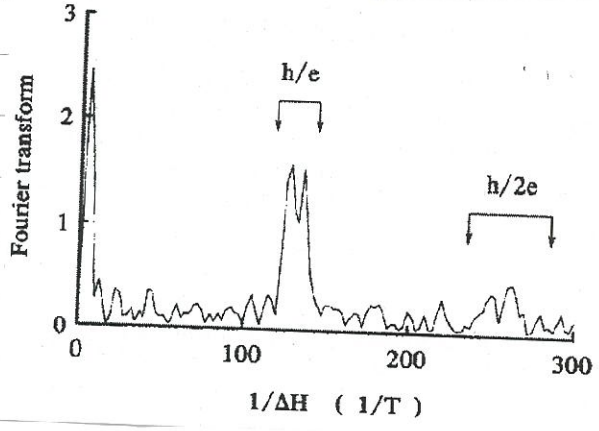
A classical experiment to show the effect of interference is the Aharanov-Bohm effect. Here a ring of size $< \lambda_\Phi$ is made with magnetic field H penetrating inside the ring.



Typical measurements of g show oscillations

After Fourier transformation, one finds





see S. Washburn, in Mesoscopic Phenomena in Solids. eds. Altshuler, Lee & Webb, Elsevier (1991)

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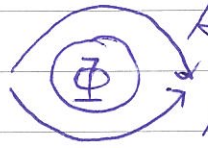
How do we understand these periods & oscillations?

Eq. (14) can be rewritten as

$$P(\vec{r},\vec{r}') = \sum_i A_i^2 + 2\sum_{i\neq j} A_i A_j \cos(\phi_i - \phi_j) \quad \cdots (15)$$

when we have set $G_i(\vec{r},\vec{r}') = A_i e^{i\phi_i}$.

In the Ahanorov-Bohm expt, the presence of a hole distinguishes two paths as follows



with $A_i \sim A_j$, $\phi_i \sim \phi_j$

In the presence of magnetic fields, however,

$$\phi_j - \phi_i = \frac{e}{\hbar}\int_j \vec{A}\cdot d\vec{e} - \frac{e}{\hbar}\int_i \vec{A}\cdot d\vec{e}$$

$$= \frac{e}{\hbar}\oint \vec{A}\cdot d\vec{e} = \frac{e}{\hbar} \times \int \vec{B}\cdot da = \frac{e\Phi}{\hbar}$$

with Φ being the flux enclosed by the ring.

Hence eq. (15) becomes

$$P(\vec{r},\vec{r}') \sim 2A^2 + 2A^2\cos\frac{e\Phi}{\hbar}$$

$$= 2A^2 + 2A^2\cos\left[2\pi\frac{e\Phi}{h}\right]$$

This results in oscillations with period $\Phi = \frac{h}{e} = \Phi_0$

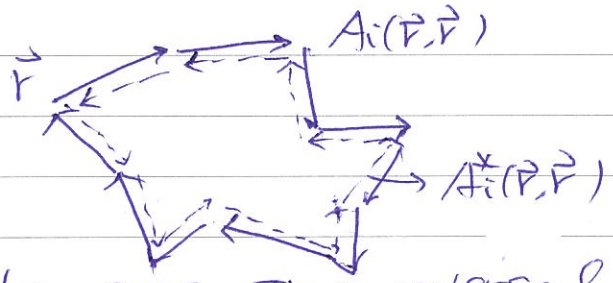
and this is the standard Ahanorov-Bohm effect.

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How to account for the period of h/e?

The h/e oscillation turns out to be the mechanism for same for weak localization.

To see it, as we indicated, if the returning probability is finite, the particle will be localized. To find the returning probability, we note that for waves, there are two ways to return to the original location for each given path configuration:



The two paths are time reversal to each other.

In the absence of magnetic field, eq. (11) implies that $\phi_i = \phi_j$

$$P(\vec{r},\vec{r}) = 2A_i^2 + 2A_i^2 = 4A_i^2$$

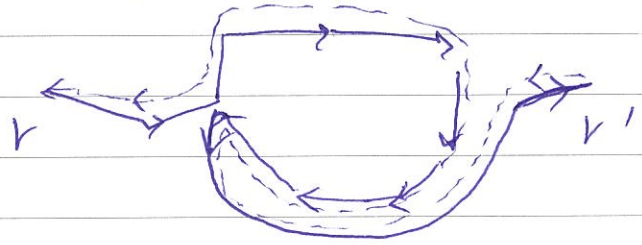
Hence it is 2 times of the classical probability

Hence, the 2nd term (which is the original for interference) enhances the returning probability! and this is the interference mechanic for localization.

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In the presence of magnetic field, A_i & A_i^* are no longer the same and hence the returning probability may not be enhanced. (for weak H, the enhancement is always weakened!)
In the case of Ahanorov-Bohm effect,
the corresponding two paths are



The phase difference is $\frac{e}{\hbar}\left[\oint - \oint\right]\vec{A}\cdot d\vec{s}$

$$= \frac{2e}{\hbar} \times \Phi$$

$$\therefore P(r,r') \sim 2A^2 + 2A^2 \cos\frac{2e}{\hbar}\Phi$$

$$= 2A^2\left[1 + \cos 2\pi \frac{e}{h}\Phi\right]$$

This results in oscillations with period

$$\Phi = \frac{h}{2e}.$$

Universal conductance fluctuations & speckles

When the system size $L \gg \lambda_\phi$, the system can be considered as a collection of $N = \left(\frac{L}{\lambda_\phi}\right)^d$ subsystems which are statistically independent (because they are not coherent!).

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A physical quantity defined in each subsystem ... will then take on N random values.

The value of the whole system is then the summation over these N random values and exhibit <u>self-averaging</u>, i.e.,

= <u>the ensemble average of the quantity</u>

.. <u>For $L \gg \lambda_\phi$</u>, one expects for <u>weak disorders</u>

$$\frac{\sqrt{\overline{(\delta G)^2}}}{\bar{G}} \simeq \frac{1}{\sqrt{N}} \simeq \left(\frac{\lambda_\phi}{L}\right)^{d/2} \quad \cdots (56)$$

where $\delta G = G - \bar{G}$. $\bar{G} = \bar{G}_{ce} = \sigma L^{d-2}$

$\therefore \overline{(\delta G)^2} \propto L^{d-4}$

$\therefore$ For $d \leq 3$, $\overline{\delta G^2} \to 0$ as $L \to \infty$, the system is said to be self-averaging (no fluctuation)

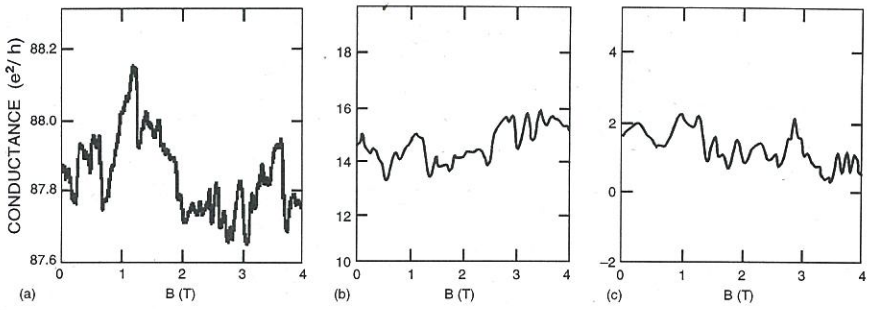
In contrast, <u>for $L < \lambda_\phi$</u>, the electron is phase coherent. (mesoscopic regime)

Experimentally, it's found $\sqrt{\overline{\delta G^2}} \simeq$ constant $\cdot \frac{e^2}{h}$

The fluctuation is independent of <u>size of the system</u> and the <u>amount of disorders</u>, depending only on the geometry of the system. For a given realization of disorders, the dependence of

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fluctuations on external parameters (such as magnetic fields or Fermi energy) are reproducible and be around e^2/h. We term it as universal conductance fluctuations. The followings are some experimental examples:



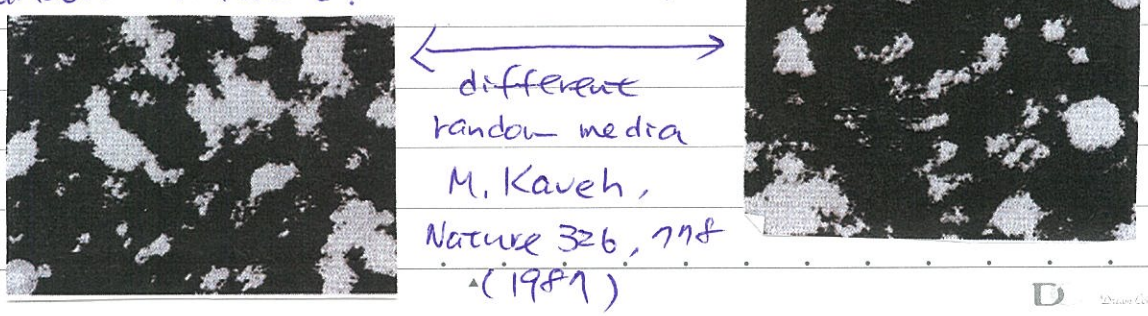
↑ Gold ring of diameter 0.8 mm

Si-MOSFET

numerical simulation of Anderson model

P.A. Lee, A.D. Stone, & H. Fukuyama
PR B 35, 1039 (1987)

Similar phenomenon was also observed in scattering of coherent light from an inhomogeneous medium with refractive index fluctuating in space on a scale comparable to the wavelength of the light. This results in the speckle pattern, representing the fingerprint of the random obstacle. (see below.)



different random media

M. Kaveh, Nature 326, 778 (1987)

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Correction of conductivity due to interference

As indicated, the time reversal invariance implies that the electron's returning probability is enhanced. Hence one expects that there will be correction of σ due to interference.

Eq. (5-2) is a hand-waving result for $d=2$.

To derive $\delta\sigma$, one needs to calculate σ via the perturbation theory (weak disorder).

Starting from the full Green's function

$$\hat{G} = (\hat{G}_0^{-1} - V)^{-1} \qquad \hat{G}_0 = (E - \hat{H}_0)^{-1}, \quad \hat{H} = H_0 + U(r)$$

where if the impurity is a Gaussian ensemble, the average over disorders is

$$\overline{U(r)} = 0 \qquad \overline{U(r)\,U(r')} = B(r-r') \quad \cdots (5\text{-}7)$$

For white noises, $\overline{V(r)V(r')} = B\delta(r-r') \quad \cdots (5\text{-}8)$

If we consider microscopic nature of disorders, we have

$$U(r) = \sum_{j=1}^{N_I} v(r - r_j)$$

where v is the potential due to the impurity.

This is the Edwards model (Philos. Mag. 3, 1020, 1958).

In this model, if the volume of the sample is V, then the probability density is simply

$$\prod_{j=1}^{N_I} \frac{d\vec{r}_j}{V} \quad \cdots \quad (59)$$

In general, one needs not only $\bar{V}$ and $\overline{V(r_1)V(r')}$ but also $\overline{V(r_1)V(r_2)\cdots V(r_n)}$. For this purpose, one forms the generating functional

$$\Phi[g] \equiv \overline{e^{\int d\vec{r}\, g(\vec{r})V(\vec{r})}} \quad \cdots \quad (60)$$

Obviously, $$\left.\frac{\delta^2\Phi[g]}{\delta g(r)\delta g(r')}\right|_{g=0} = \overline{V(r)V(r')} \quad \cdots \quad (61)$$

$$\left.\frac{\delta^n\Phi[g]}{\delta g(r_1)\delta g(r_2)\cdots\delta g(r_n)}\right|_{g=0} = \overline{V(r_1)V(r_2)\cdots V(r_n)} \quad \cdots \quad (62)$$

that's why it is termed as generating functional.

Substituting $V(r) = \sum_{j=1}^{N_I} v(r-r_j)$ into eq. (60), we find

$$\Phi[g] = \int \prod_{j=1}^{N_I} \frac{dr_j}{V} e^{\underbrace{\int d\vec{r}\, v(\vec{r}-\vec{r}_j)g(\vec{r})}_{F(\vec{r}_j)}}$$

$$= \left[\int \frac{dr}{V} e^{F(\vec{r})}\right]^{N_I}$$

We shall let $V\to\infty$ and keep $\frac{N_I}{V} = n_I$ fixed.

$$\therefore \Phi[g] = \left[1 + \frac{n_I}{N_I}\int d\vec{r}\; e^{F(r)} - 1\right]^{N_I}$$

$$\to e^{n_I \int d\vec{r}\,(e^{F(r)}-1)} \quad \cdots (63)$$

Therefore, the cumulant expansion of Φ is

$$\ln \Phi[g] = \sum_{K=1}^{\infty} \frac{n_I}{K!}\int d\vec{r}\,[F(\vec{r})]^K \quad \cdots (64)$$

$$F(\vec{r}) = \int d\vec{r}\,' g(\vec{r}\,') v(\vec{r}-\vec{r}\,')$$

Using eqs. (61) & (62), one finds

$$\overline{V(r)} = n_I \int dr'\, v(r'-r)\left[\frac{\delta F}{\delta g(r)}\right]$$

$$\overline{V(r)V(r')} = n_I \int dr''\, v(r''-r)\, v(r''-r')$$

$$\overline{V(r_1)V(r_2)\cdots V(r_n)}$$

$$= n_I \int d\vec{r}\; v(r-r_1)v(r-r_2)\cdots v(r-r_n)$$

Hence it is no longer Gaussian.

In the weak disorder limit, $n_I \to 0$ & $v \to 0$,

$$\overline{V(r)} = n_I v_{q=0} = 0$$

$$\overline{V(r)V(r')} = B(r-r') = n_I \int d\vec{r}\,'' v(r''-r)\, v(r''-r')$$

$$B(q) = n_I \tilde{v}^2(q) \quad \cdots (65)$$

are two dominating terms. One recovers the Gaussian model.

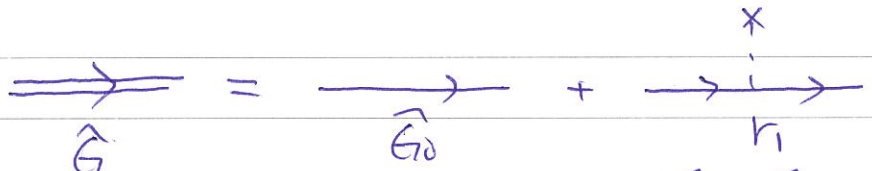
If $v(r) = v_0 f(r)$, $B(r-r') = n_I v_0^2 f(r-r')$ is a white noise -- (66)

Multiple scattering expansion

One can expand $\hat{G} = (\hat{G}_0^{-1} - V)^{-1}$

into $\hat{G} = \hat{G}_0 + \hat{G}_0 V \hat{G}_0 + \hat{G}_0 V \hat{G}_0 V \hat{G}_0 + \cdots$ (67)

Graphically, one has the representation



$\hat{G}$ $\quad$ $\hat{G}_0$ $\quad$ $\hat{G}_0 V \hat{G}_0$

$G(r,r')$ $\quad$ $G_0(r,r')$ $\quad$ $\int dr_1 G_0(r,r_1) V(r_1) G_0(r_1,r')$



$\hat{G}_0 V \hat{G}_0 V \hat{G}_0$

$= \int dr_1 \int dr_2 \, G_0(r,r_1) V(r_1) G_0(r_1,r_2) V(r_2) G_0(r_2,r')$

The graphs are called Feynman diagrams which help us to bookkeep perturbation terms.

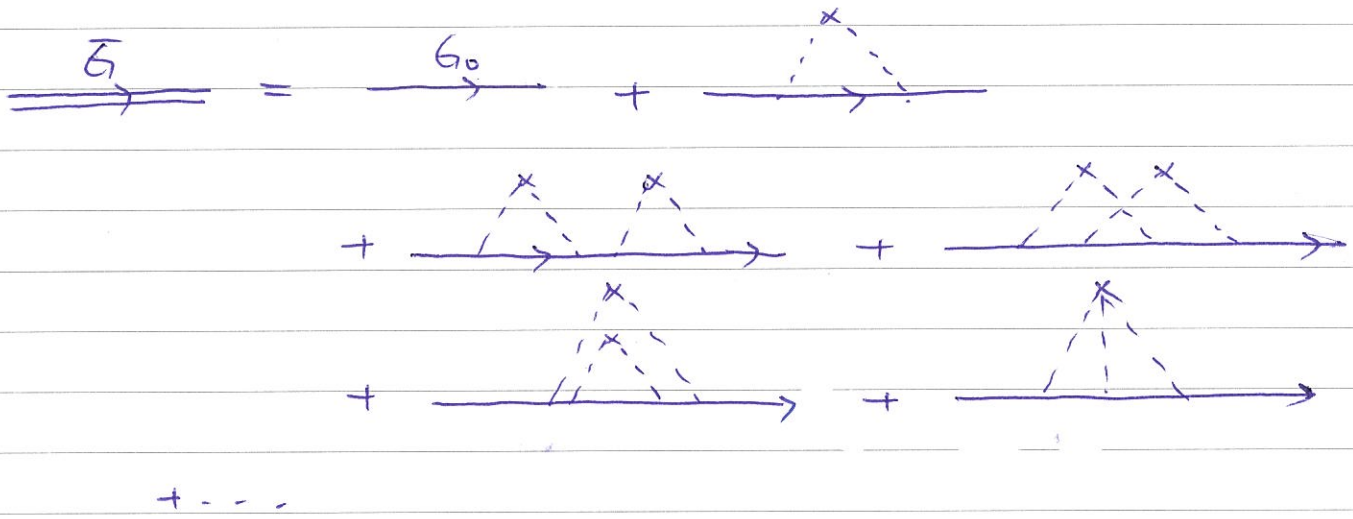
To go back mathematical expressions, one needs the Feynman rules which in this case are


$= G_0(r,r')$



$= \int dr_1 \, V(r_1)$

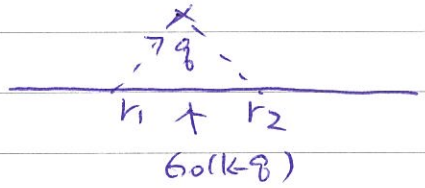
Upon averaging over disorders, one gets . . . .



+ . . .

The averaging joins two crosses due to $\overline{U(r)U(r')}$

$= B(r-r') \neq 0$

For instance, 

$$= \int dr_1 \int dr_2 \, G_0(r, r_1) \, G_0(r_1, r_2) \, G_0(r_2, r') \, B(r_1, r_2)$$

(68)

Apparently, there are two types of diagrams:

one-particle reducible (OPR): cutting a solid line will separate the diagram into two diagrams.

one-particle irreducible: can't be separated into two diagrams by cutting one solid line.

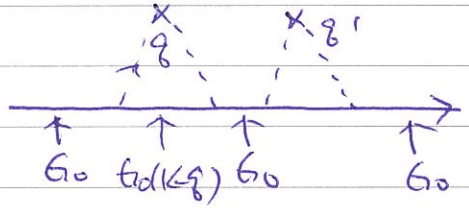
In the k space, the term of eq. (68) becomes

$$\frac{1}{V} \sum_q B_0(q) \, G_0(k) \, G_0(k-q) \, G_0(k) = G_0^{(k)} \left[\frac{1}{V} \sum_q B(q) \, G_0(k-q) \right] G_0(k)$$

The impurity takes a momentum & away . . . . . .

This is the result for a typical OPI diagram.

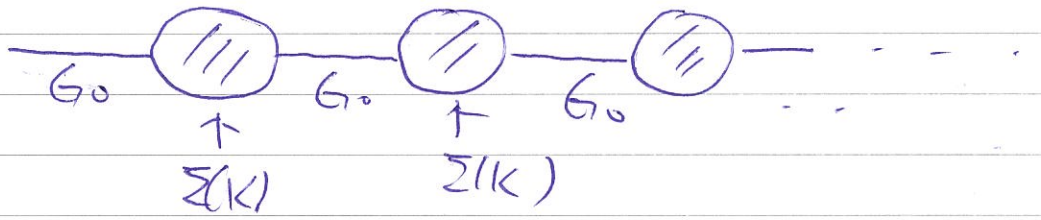
For reducible diagrams, for instance, the

diagram 

$$= \frac{1}{V^2} \sum_{q} \sum_{q'} G_0(k)\, B(q)\, G_0(k-q)\, G_0(k)\, B(q')\, G_0(k-q')\, G_0(k)$$

$$= G_0 \left[\frac{1}{V} \sum_{q} B(q)\, G_0(k-q)\, G_0(k) \right]^2$$

In general, for reducible diagrams, one has



$$= G_0 (\Sigma(k)\, G_0)^n \quad \text{where } \Sigma \text{ is irreducible.}$$

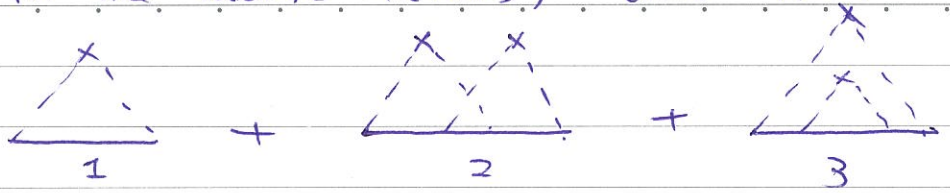
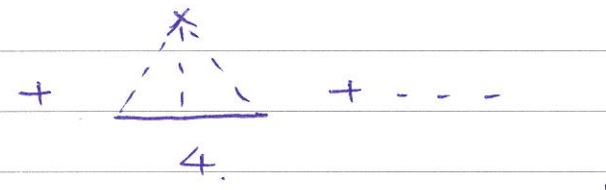
$$\therefore \bar{G}(k,E) = G_0(k,E) + G_0(k,E) \sum_{n=1}^{\infty} [\Sigma(k,E)\, G_0(k,E)]^n$$

$$= G_0(k,E) + G_0(k,E)\, \Sigma(k,E)\, \bar{G}(k,E)$$

$$\bar{G}(k,E) = \frac{G_0(k,E)}{1 - G_0(k,E)\,\Sigma(k,E)} = \frac{1}{E - \varepsilon(k) - \Sigma(k,E)}$$

$\Sigma(k,E)$ is similar to $S_n(E)$ in the analysis of the Anderson model and is termed as self-energy.

Clearly, in the lowest terms, one has

$\Sigma =$  + 

$$G^{A,R}(K,E) = \frac{1}{E \pm i\epsilon - \varepsilon(k) - \Sigma^{R,A}(k, E \pm i\varepsilon)}$$

For the lowest order, one has

$$\Sigma^{(1)} = \frac{1}{V} \sum_q B(k-q)\, G_0(q)$$

The real part of $\Sigma^{(1)}$ shifts the pole $\varepsilon(k)$, so only the imaginary part is important.

$$\mathrm{Im}\,\Sigma^{(1)}(K,E) = -\frac{\pi}{V} \sum_q B(k-q)\, \delta(E-\varepsilon(q))$$

$$= -\pi \int \frac{d^3\vec{q}}{(2\pi)^3} B(|\vec{k}-\vec{q}|)\, \delta(E-\varepsilon(q))$$

$\because \varepsilon(q) = \frac{\hbar^2 q^2}{2m}$ $\quad \int d^3\vec{q} = \int q^2\, dq\, dp\, d\Omega_q$, $q = \sqrt{\frac{2mE}{\hbar^2}}$

$$\therefore \mathrm{Im}\,\Sigma^{(1)} = -\pi \left(\frac{2mE}{\hbar^2}\right)^2 \frac{1}{(2\pi)^3} \underbrace{\int d\Omega_q}_{4\pi} \underbrace{\int \frac{d\Omega_q}{4\pi} B(k, \hat{k}-\hat{q})}_{\text{III}}$$

$\rho_0(E)$

$\langle B(k, \hat{k}-\hat{q}) \rangle$ average over angle of $\hat{q}$

$$= -\pi \rho_0(E) \langle B(k, \hat{k}-\hat{q}) \rangle_{\hat{q}}$$

Im Σ defines a characteristic timescale τ_e called elastic collision time.

$$\frac{\hbar}{2\tau_e} \equiv -\,\mathrm{Im}\,\Sigma^R(k,\varepsilon) \quad \cdots \quad (69)$$

In the lowest order, one gets

$$\frac{\hbar}{2\tau_e} = \pi \rho_0 \gamma_e$$

with $\gamma_e = \langle B(k-q)\rangle_{\hat{q}}$

Note that for white noises, $B(k-q) = \delta(k-q) \times n_I V_0^2$

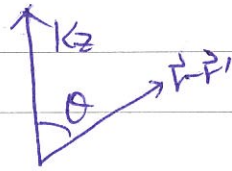
$$\therefore \quad \mathrm{Im}\,\Sigma^{(1)} = -\pi \rho_0(E)\cdot n_I V_0^2$$

$$\therefore \quad \frac{\hbar}{2\tau_e} = \pi \rho_0 n_I V_0^2 \quad \cdots \quad (69)-1$$

In the elastic scattering experiment, the energy of the incident wave E is conserved. If we set $E = \frac{\hbar^2 k_0^2}{2m}$,

$$G^R = \frac{1}{E - \frac{\hbar^2 k^2}{2m} + i\varepsilon + \frac{i\hbar}{2\tau_e}} = \frac{2m}{\hbar^2}\,\frac{1}{k_0^2 - k^2 + i0^+ + \frac{m}{\hbar\tau_e} i}$$

$$G^R(\vec{r}-\vec{r}') = \frac{2m}{\hbar^2}\int \frac{d^3k}{(2\pi)^3}\,\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{k_0^2 - k^2 + i\varepsilon + i\frac{m}{\hbar\tau_e}}$$



$$e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} = e^{ik|r-r'|\cos\theta}$$

$$\int \sin\theta\, d\theta\, d\phi\; e^{ik|r-r'|\cos\theta} = \frac{2\pi}{ik}\left(\frac{e^{ik|r-r'|} - e^{-ik|r-r'|}}{|r-r'|}\right)$$

One finds

$$G^R(r-r') = \frac{1}{4\pi i}\frac{2m}{\hbar^2}\frac{1}{|\vec{r}-\vec{r}'|}\int_{-\infty}^{\infty} z\,dz\,\frac{e^{iz|r-r'|} - e^{-iz|r-r'|}}{z^2 - k^2 + i\varepsilon + i\frac{m}{\hbar^2 z\ell_e}}$$

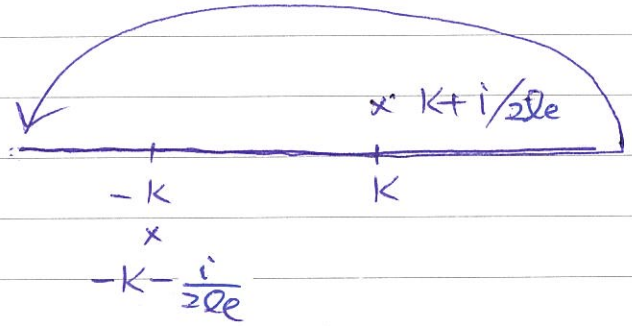
poles are at $z = \pm\sqrt{k^2 - i\varepsilon - i\frac{m}{\hbar^2 z\ell_e}}$ $\quad \varepsilon \to 0^+$

$$= \pm k\left(1 - i\frac{m}{k\hbar^2 z\ell_e}\right)^{\frac{1}{2}}$$

$$\simeq \pm k\left(1 + \frac{im}{2k\hbar^2 z\ell_e}\right) \quad \text{assuming } \frac{k\hbar^2 z\ell_e}{m} >> 1$$

It's convenient to define $\ell_e = \frac{k\hbar z\ell_e}{m} = v\tau_e$

In the limit $k\ell_e >> 1$ (long wave length limit), one gets, $z \cong \pm k\left(1 + \frac{i}{2k\ell_e}\right)$



Choose the contour ↶, One finds

$$\int_{-\infty}^{\infty} z\,dz\,(\cdots)$$

$$= \frac{2\pi i}{2k}\,k\,e^{ik|r-r'|}\,e^{-\frac{|r-r'|}{2\ell_e}}$$

$$\therefore G^R(r-r', E) = -\frac{2m}{\hbar^2}\frac{e^{ik|r-r'|}}{4\pi|r-r'|}\,e^{-\frac{|r-r'|}{2\ell_e}} = G_0^R(r-r')\,e^{-\frac{|r-r'|}{2\ell_e}} \quad \text{--- (10)}$$

Therefore, ℓ_e is identified as elastic mean free path.
($E = \hbar^2k^2/2m$)

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Two-particle Green's function

From the definition, it is clear that the conditional probability density of going from $\vec{r}'$ to $\vec{r}$ is $P(\vec{r},\vec{r}';t) = |\langle \vec{r}| e^{-\frac{i}{\hbar}Ht} |\vec{r}'\rangle \theta(t)|^2$.

$\because \int dt\, e^{\frac{i}{\hbar}Et} e^{-\frac{i}{\hbar}Ht} = \frac{\hbar/i}{E-H} = \hbar/i\, \hat{G}(E)$

$\therefore P(\vec{r},\vec{r}',t) = \hbar^2 |G^R(\vec{r},\vec{r}';t)|^2 = \hbar^2 G^R(\vec{r},\vec{r}';t) G^{R*}(\vec{r},\vec{r}';t)$

L-(71)

Note that $\int P(\vec{r},\vec{r}';t)\, d\vec{r}' = 1$ is correctly normalized ---(72)

Now, $\because G^R(\vec{r},\vec{r}';t) = \int d\omega\, e^{-i\omega t} \frac{-2m}{\hbar^2} \frac{e^{ik|\vec{r}-\vec{r}'|} - \frac{|\vec{r}-\vec{r}'|}{2\ell_e}}{4\pi|\vec{r}-\vec{r}'|}$

$G^A(\vec{r},\vec{r}';t) = \int d\omega\, e^{-i\omega t} \frac{-2m}{\hbar^2} \frac{e^{-ik|\vec{r}-\vec{r}'|} - \frac{|\vec{r}-\vec{r}'|}{2\ell_e}}{4\pi|\vec{r}-\vec{r}'|}$

$G^{R*}(\vec{r},\vec{r}';t) = \int d\omega\, e^{i\omega t} \frac{-2m}{\hbar^2} \frac{e^{-ik|\vec{r}-\vec{r}'|} - \frac{|\vec{r}-\vec{r}'|}{2\ell_e}}{4\pi|\vec{r}-\vec{r}'|}$

Here in G^R $e^{-i\omega t}$ is actually $e^{i\omega(t'-t)}$, in G^A $e^{i\omega t}$ is $e^{-i\omega(t'-t)}$

$\therefore G^{R*}(\vec{r}t;\vec{r}'t') = G^A(\vec{r}'t';\vec{r}t)$, $G^{R*}(\vec{r},\vec{r}',t) = G^A(\vec{r}'t,\vec{r})$

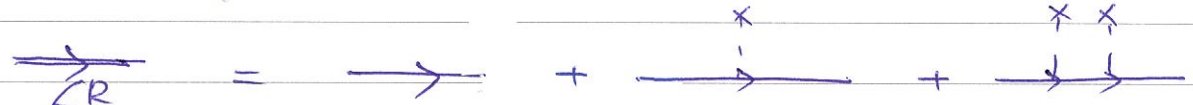
$\therefore P(\vec{r},\vec{r}',t) = \hbar^2\, G^R(\vec{r},\vec{r}';t)\, G^A(\vec{r}'t,\vec{r})$ is proportional to the average of two-particle Green's function.

In fact, as we shall see in the linear response theory, the conductivity can be described by the so-called Kubo formula which also involves two-particle Green's function

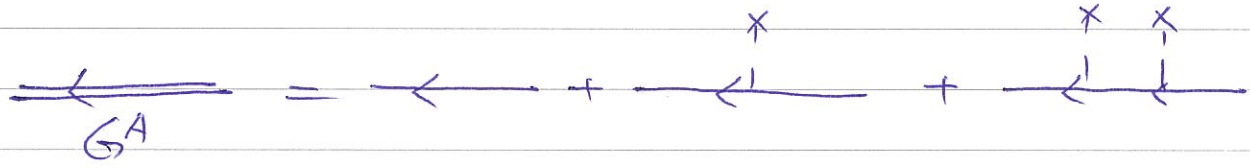
$$\sigma_{dc} = \frac{2e^2}{h} \lim_{\varepsilon\to 0^+} 4\varepsilon^2 \lim_{q\to 0} \Omega_q^2 \sum_{kk'} G^R(k,k+q) G^A(k',k+q)$$

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Diagramatically, as we have shown, before the average

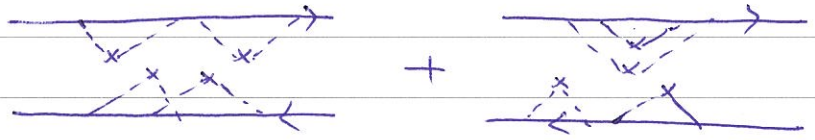


$G^A = \frac{1}{E - \varepsilon(k) - i0^-}$ is propagating in the opposite direction, just as a hole which propagates in opposite direction to the electron.



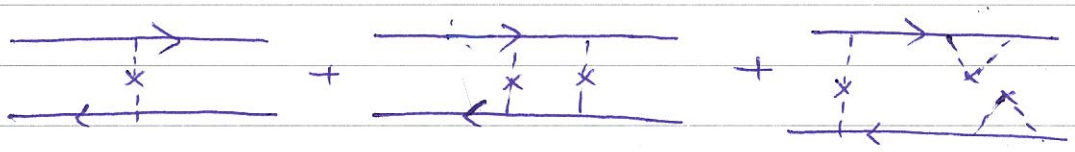
Clearly, when we take the average, there are three possibilities:

(i)



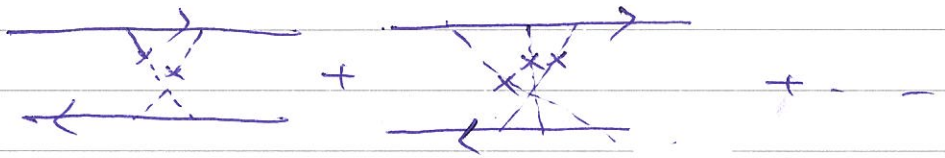
$= \overline{G^R} \cdot \overline{G^A}$

(ii)



two-particle reducible

(iii)



two-particle irreducible

The collisionless approximation : Drude-Boltzman approximation

In the first approximation, there is no crossing between G^R and G^A.

$$P(\vec{r},\vec{r}',t) = \frac{1}{\hbar^2}\overline{G^R(r,r',+)}\;\overline{G^A(r',+,r)} \equiv P_0(\vec{r},\vec{r}',+)$$

$$P_0(\vec{r},\vec{r}',+) = \frac{1}{\hbar^2}\int dt\; e^{-i\omega t}\int\frac{d\omega_1}{2\pi}\;\overline{G^R(r,r',\omega_1)}\;e^{+i\omega_1 t}$$
$$\int\frac{d\omega_2}{2\pi}\;\overline{G^A(r',r,\omega_2)}\;e^{-i\omega_2 t}$$

$$\int dt = 2\pi\,\delta(\omega_2+\omega-\omega_1)$$

$$\therefore \frac{1}{\hbar^2}P_0(\vec{r},\vec{r}',t) = \iint\frac{d\omega_1 d\omega_2}{2\pi}\,\delta(\omega_2+\omega-\omega_1)\;\overline{G^R(r,r',\omega_1)}\;\overline{G^A(r',r,\omega_2)}$$

$$= \int\frac{d\Omega}{2\pi}\;\overline{G^R(r,r',\Omega)}\;\overline{G^A(r',r,\Omega-\omega)}$$

or more symmetric

$$= \int\frac{d\Omega}{2\pi}\;\overline{G^R(r,r',\Omega+\omega/2)}\;\overline{G^A(r',r,\Omega-\omega/2)}$$

Similarly, $\overline{G^R(r,r')}\;\overline{G^A(r',r)}$

$$= \int\frac{d^dk_1}{(2\pi)^d}\,e^{i\vec{k}_1\cdot(\vec{r}-\vec{r}')}\,\overline{G^R(k_1,\Omega)}\int\frac{d^dk_2}{(2\pi)^d}\,e^{i\vec{k}_2\cdot(\vec{r}'-\vec{r})}\,\overline{G^A(k_2,\Omega-\omega)}$$

$$= \int\frac{d^dq}{(2\pi)^d}\int\frac{d^dk}{(2\pi)^d}\,e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\;\overline{G^R(k,\Omega)}\;\overline{G^A(k-q,\Omega-\omega)}$$

(k ↕ k_1; q ↑ k_1-k_2)

$$\therefore \frac{1}{\hbar^2}P_0(q,\omega) = \int\frac{d\Omega}{2\pi}\int\frac{d^dk}{(2\pi)^d}\;\overline{G^R(k,\Omega)}\;\overline{G^A(k-q,\Omega-\omega)} \quad --(13)$$

Now, $G^R(k,E) = \dfrac{1}{E-\varepsilon_k+i\varepsilon+\frac{i\hbar}{2\tau_e}}$ $\quad\because \hbar\Omega = E$

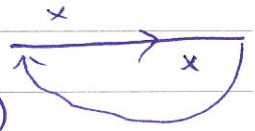
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$$\therefore \quad G^R(k,\Omega) = \frac{\hbar^{-1}}{\Omega - \xi_k + i\eta + \frac{i}{2\tau_e}} \qquad \xi_k \equiv \varepsilon_k/\hbar$$
$$\eta = \varepsilon/\hbar \to 0^+$$

$$\therefore \int \frac{d\Omega}{2\pi} \overline{G^R(k,\Omega)}\ \overline{G^A(k-q,\omega-\Omega)}$$

$$= \frac{1}{\hbar^2}\int \frac{d\Omega}{2\pi} \frac{1}{(\Omega - \xi_k + i\eta + \frac{i}{2\tau_e})(\Omega - \omega - \xi_{k-q} - i\eta - \frac{i}{2\tau_e})}$$



$$= \frac{1}{\hbar^2}\frac{(-2\pi i)}{2\pi} \frac{1}{\xi_k - \omega - \xi_{k-q} - i/2\tau_e} \qquad (\eta \to 0)$$

$$\xi_{k-q} - \xi_k = -\vec{q}\cdot\vec{v}$$

$$= \frac{1}{\hbar^2} \frac{1}{1/2\tau_e - i\omega + i\vec{v}\cdot\vec{q}}$$

$$= \frac{\frac{1}{\hbar^2}\cdot 2\tau_e}{1 - i\omega 2\tau_e + i\vec{v}\cdot\vec{q}\,2\tau_e}$$

$$\therefore P_0(q,\omega) = \int \frac{d^dk}{(2\pi)^d} \frac{2\tau_e}{1 - i\omega 2\tau_e + i\vec{v}\cdot\vec{q}\,2\tau_e} \qquad \cdots (74)$$

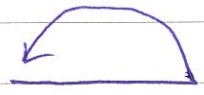
Now. $\int P_0(\vec{r},\vec{r}',\omega)\, d\vec{r}' = \int P_0(\vec{r}-\vec{r}',\omega)\, d\vec{r}'$

$$= \int P_0(\vec{R},\omega)\, d\vec{R} = P_0(q=0,\omega)$$

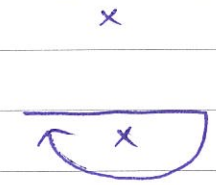
$$= \int \frac{d^dk}{(2\pi)^d} \frac{2\tau_e}{1 - i\omega 2\tau_e} = \frac{2\tau_e}{1 - i\omega 2\tau_e}$$

(volume of B.Z. $= (2\pi)^d$ a is absorbed)

$$\therefore \int P_0(\vec{r},\vec{r}',t)\, d\vec{r}' = \int \frac{d\omega}{2\pi} e^{-i\omega t} \frac{i}{\omega + i/2\tau_e}$$

$t<0$ 

$= 0$

$t>0$ 

$= \frac{(-2\pi i)\, i}{2\pi} \cdot e^{-t/2\tau_e} = e^{-t/2\tau_e}$

$$\therefore \int P_0(\vec{r},\vec{r}',t)\, d\vec{r}' = e^{-t/2\tau_e}\theta(t)$$

Note that the relaxation approximation $G^R = \frac{1}{E - \xi_k + i\Sigma + \frac{i\hbar}{2\tau_e}}$

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does maintain normalization (eq. (72)) correctly.

To restore correct normalization, one multiply does not need to P_0 by any correction.

$\therefore$ We have $\int P_0(\vec{r},\vec{r}',t)\,d\vec{r}' = \theta(t)\, e^{-t/\tau_e}$ -- (75)

Eq. (75) is exactly the same as predicted by the Drude model:

probability occurs during dt

$$= \frac{dt}{\tau_e}$$

Hence starting from $t=0$, if the probability for there is no collision before t is $P(t)$, then

$$P(t+\Delta t) = P(t)\left(1 - \frac{\Delta t}{\tau_e}\right)$$

$$\therefore \frac{dP}{dt} = -\frac{1}{\tau_e} P(t), \quad P(t) = e^{-t/\tau_e}$$

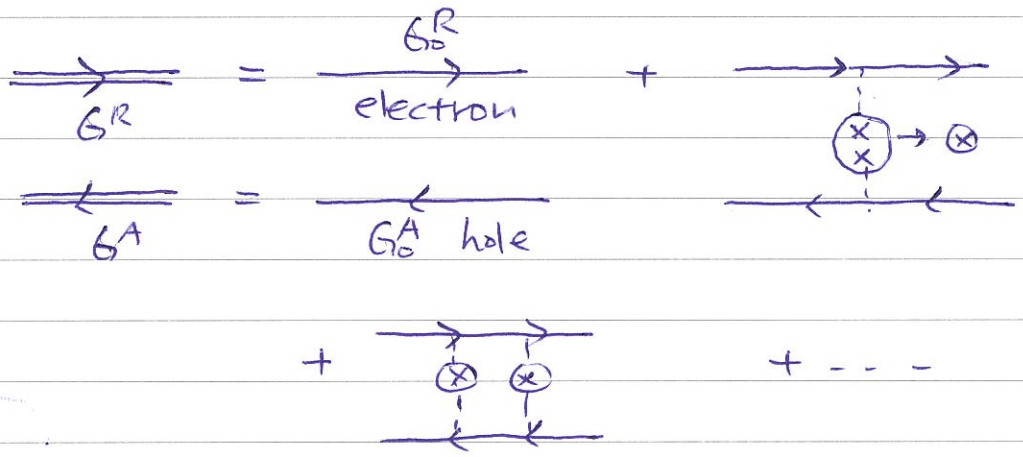
which coincides with eq. (75) exactly.

It can be shown directly by using the Kubo formula that the no-collision approximation leads to the Drude formula for σ.

Therefore, the no-collision approximation is the Drude-Boltzman approximation.

Diffuson

The simplest approximation that has the meaning of the probability is to connect



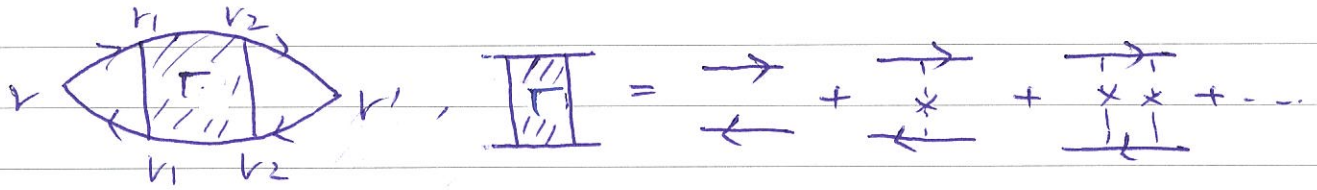
i.e. $G^R(r-r') = \cdots + \sum_{r_1 r_2} G_0^R(r-r_1)\,U(r_1)\,G_0^R(r_1-r_2)\,U(r_2)\,G_0^R(r_2-r_3)\,U(r_3)\cdots$

$G_0^{R*} = G^A(r', r) = \cdots + \sum_{r_1 r_2} G_0^{R*}(r-r_1)\,U(r_1)\,G_0^{R*}(r_1-r_2)\,U(r_2)\,G_0^{R*}(r_2-r_3)\,U(r_3)\cdots$

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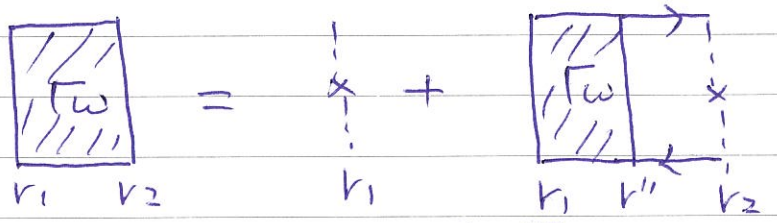
The associated two-particle Green's function is called Diffuson with diagrams



If the Fourier transformation over t is performed, one has $\Gamma \to \Gamma_\omega$ (eq. (13))

$$P_D(r,r',\omega) = \hbar^2 \int \frac{d\Omega}{2\pi} \int dr_1 \int dr_2 \; \overline{G^R(r,r_1,\Omega)\, G^A(r_1,r,\Omega-\omega)} \times \overline{G^R(r_2,r',\Omega)\, G^A(r',r_2,\Omega-\omega)}\, \Gamma_\omega(r_1,r_2)$$

and $\Gamma_\omega(r_1,r_2)$ satisfies L-(16)



$$\Gamma_\omega(r_1,r_2) = n_I v_0^2 \delta(r_1-r_2) + \underbrace{n_I v_0^2}_{\hbar/2\pi\tau^2} \int dr'' \, \Gamma_\omega(r_1,r'')\, \overline{G^R(r'',r_2,\Omega)} \times \overline{G^A(r_2,r'',\Omega-\omega)} \quad \text{-- (17)}$$

is called diffusion propagator!

It's more convenient to work in the K-space.

First, we have generally

$$P(\vec{r},\vec{r}',\omega) = \frac{1}{\hbar^2} \int \frac{d\Omega}{2\pi} \; \overline{G^R(r,r',\Omega)\, G^A(r',r,\omega-\Omega)} \quad \text{L-(18)}$$

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Here unlike the derivation of eq. (73), $G^R(r,r')$ & $G^A(r',r)$ are not translation before the average is taken.

But note that $P(r,r',\omega) = P(r-r',\omega)$

$$= \int P(q,\omega) \frac{d^d q}{(2\pi)^d} e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}$$

To go into the k-space, one first writes

$$G^R(r,r') = \int_{k_1}\int_{k_2} e^{i\vec{k}_1\cdot\vec{r} + i\vec{k}_2\cdot\vec{r}'} G^R(k_1,k_2,\Omega)$$

$$G^A(r',r) = \int_{k_1'}\int_{k_2'} e^{-i\vec{k}_1'\cdot\vec{r}' - i\vec{k}_2'\cdot\vec{r}} G^A(k_1',k_2',\Omega-\omega)$$

$r < k_1, k_2'$; $k_1', k_2' > r'$

$\therefore \vec{k}_1 - \vec{k}_2' = \vec{q}$, $\vec{k}_2 - \vec{k}_1' = -\vec{q}$

(associated with $\vec{r}$) (associated with $\vec{r}'$)

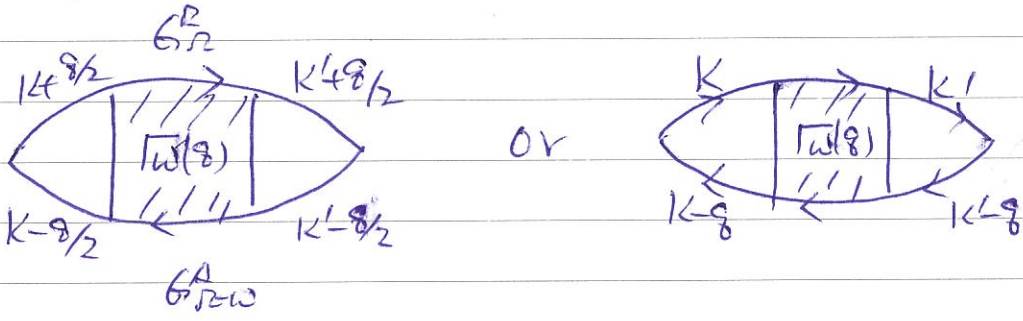
$$\therefore \int_\Omega \overline{G^R(r,r',\Omega)\, G^A(r',r,\omega-\Omega)}$$

$$= \int_q e^{i\vec{q}\cdot(\vec{r}-\vec{r}')} \int_\Omega \overline{G^R(k+\tfrac{q}{2}, k'-\tfrac{q}{2}, \Omega)\, G^A(k'+\tfrac{q}{2}, k-\tfrac{q}{2}, \Omega-\omega)}$$

k_1 k_2 k_1' k_2'

$$\therefore P(q,\omega) = \hbar^2 \int \frac{d\Omega}{2\pi} \overline{G^R(k+q/2, k'-q/2, \Omega)\, G^A(k'+q/2, k-q/2, \Omega-\omega)}$$

Graphically, one has



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Similarly, the Fourier transformation of eq. (76) is (From eq. (77), $\Gamma_\omega = \Gamma_\omega(r_1 - r_2)$)

$$P_D(r, r', \omega)$$

$$= \hbar^2 \int \frac{d\Omega}{2\pi} \int_{K_1} \int_{K_2} \int_{K_3} \int_{K_4} \int_{K_5} \overline{G^R(K_1, \Omega)}\ \overline{G^A(K_2, \Omega-\omega)}$$

$$\overline{G^R(K_3, \Omega)}\ \overline{G^A(K_4, \Omega-\omega)}\ \Gamma_\omega(K_5)$$

$$\int dr_1 \int dr_2\ e^{iK_1(r-r_1)}\ e^{iK_2(r_1-r)}\ e^{iK_3(r_2-r')}\ e^{iK_4(r'-r_2)}$$

$$\times\ e^{iK_5(r_1-r_2)}$$

$$\int dr_1 \int dr_2 = (2\pi)^2 \delta(K_1 - K_2 + K_5)\, \delta(K_4 - K_3 - K_5)$$

$$e^{i(K_1-K_2)r}\ e^{i(K_4-K_3)r'}$$

Clearly, set $K_5 = -q$.

$$P_D(\vec{r}, \vec{r}', \omega) = \hbar^2 \int_q e^{i\vec{q}\cdot(r-r')} \int_\Omega \int_K \overline{G^R(K, \Omega)}\ \overline{G^A(K-q, \Omega-\omega)}$$

$$\times \int_{K'} \overline{G^R(K', \Omega)}\ \overline{G^A(K'-q, \Omega-\omega)}\ \Gamma_\omega(q)$$

Eq. (77)

$$\Rightarrow \Gamma_\omega(q) = n_I v_0^2 + n_I v_0^2\, \Gamma_\omega(q) \int_K \overline{G^R(q, \Omega)}\ \overline{G^A(K-q, \Omega-\omega)}$$

$$\therefore \Gamma_\omega(q) = \frac{1}{(n_I v_0^2)^{-1} - \int_K \overline{G^R(q, \Omega)}\ \overline{G^A(K-q, \Omega-\omega)}} \quad \cdots (79)$$

is the diffusion propagator and is determined by.

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the bubble : $\Sigma_D(q,\omega) = \int_K \overline{G^R(q,\Omega)\ G^A(K-q, \Omega-\omega)}$

or more symmetrically

$$\Sigma_D(q,\omega) = \int_K \overline{G^R(K+q/2, \Omega+\omega/2)\ G^A(K-q/2, \Omega-\omega/2)}$$

$$= \int_K \frac{1}{E\Omega + E/2 - \varepsilon_{K+q/2} + i\Sigma + \frac{i\hbar}{2\tau_e}} \frac{1}{E\Omega - E/2 - \varepsilon_{K-q/2} - i\Sigma - \frac{i\hbar}{2\tau_e}}$$

with $E\Omega = \hbar\Omega$, $E = \hbar\omega$.

$$\therefore \Sigma_D(0,0) = \int_K \frac{1}{E\Omega - \varepsilon_K + i\hbar/2\tau_e} \frac{1}{E\Omega - \varepsilon_K - i\hbar/2\tau_e}$$

$\int_K \sim \rho_0(E_F) \int d\varepsilon$

$$\therefore \Sigma_D(0,0) \sim \rho_0(\varepsilon_F) \int d\varepsilon \frac{1}{E\Omega - \varepsilon + i\hbar/2\tau_e} \frac{1}{E\Omega - \varepsilon - i\hbar/2\tau_e}$$

$$= \rho_0(\varepsilon_F) \frac{2\pi i}{i\hbar/\tau_e}$$

Using eq. (6P)-1, we get

$$\Sigma_D(0,0) = (n_I v_0^2)^{-1}$$

Hence the denominator of $\Gamma_\omega(q)$, when expanded in $q \to 0$ & $\omega \to 0$, has no constant term.

For finite $\vec{q}$, ω, we have

$$\Sigma_D(q,\omega) = \rho_0(\varepsilon_F) \underset{\text{over } \hat{q}}{\langle} \int d\varepsilon \frac{1}{E\Omega + E/2 - \varepsilon - \frac{q}{2}\vec{v} + i\hbar/2\tau_e} \frac{1}{E\Omega - E/2 - \varepsilon + \frac{q}{2}\vec{v} - i\hbar/2\tau_e}$$

$$= \rho_0(\varepsilon_F) \left\langle \frac{2\pi i}{E - \hbar\vec{v}\cdot\vec{q} + i\hbar/2\tau_e} \right\rangle_{\hat{q}}$$

$$= \rho_0(\varepsilon_F) \frac{2\pi\tau_e}{\hbar} \left\langle \frac{1}{1 - i\frac{E\tau_e}{\hbar} + i\,\vec{v}\cdot\vec{q}\,\tau_e} \right\rangle_{\hat{q}}$$

$$= (n_I v_0^2)^{-1} \left[1 + \frac{iE\tau_e}{\hbar} - i\cdot\tau_e\underbrace{\langle\vec{v}\cdot\vec{q}\rangle}_{0} - \underbrace{\tau_e^2 \langle(\vec{v}\cdot\vec{q})^2\rangle}_{\left(\frac{\tau_e}{\hbar}\right)^2 \frac{v_F^2}{d} q^2} + \cdots \right]$$

∴ The diffuson propagator is

$$T_\omega(q) = \frac{n_I v_0^2/\tau_e}{i\omega - Dq^2} \qquad \text{---- (80)}$$

with $D = \tau_e v_F^2/d$ being the classical diffusion constant.

Diffusion of energy (or other quantities)

$$J_u = \langle c\cos\theta\, u(x_0 - \ell\cos\theta) \rangle$$

$$= \int_0^\pi c\cos\theta\, u(x_0 - \ell\cos\theta) \frac{2\pi d\theta}{4\pi} \sin\theta$$

$$= \frac{1}{2}\int_{-1}^{1} y\,dy\, c\, \underbrace{u(x_0 - \ell y)}_{u(x_0) - \ell y \frac{du}{dx}}$$

$$= -c\ell \frac{du}{dx} \frac{1}{2}\int_{-1}^{1} y^2 dy$$

$$= \underbrace{\frac{1}{3} c\ell}_{D} \frac{du}{dx} \qquad D = \frac{1}{3}c\ell = \frac{1}{3}c^2\tau, \quad c = v_F,\ d = 3$$

Eq. (f2) implies that the diffuson propagator is simply the classical diffusion. After appropriately normalized, one has

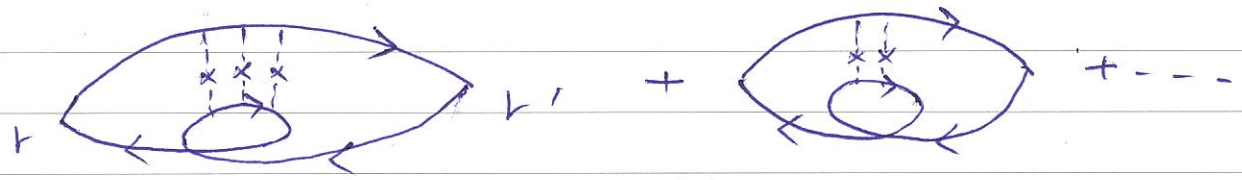
$$P(r,r',+)\big|_{\text{Diffusion}} \equiv \Pi_D(r-r';+)$$

$$= \frac{1}{(2\pi Dt)^{d/2}} e^{-\frac{|r-r'|^2}{2Dt}} \quad \cdots (f1)$$

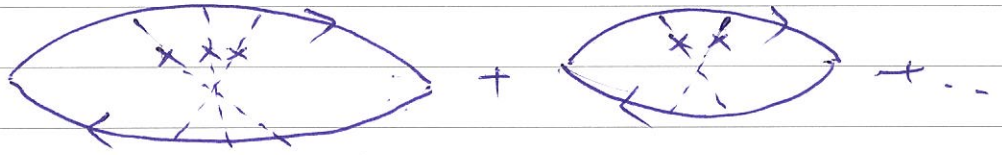
$$\left(\int dr' P(r,r';+) = 1\right)$$

Cooperon

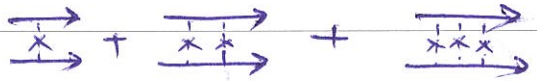
The ladder diagrams are those contributions with low phase mismatch. Another possible configaration to form ladder is the Cooperon shown in below



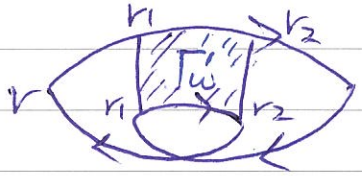
or can be drawn as



Hence these diagrams are maximally crossed. The ladders involved are



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is the Cooperon contribution

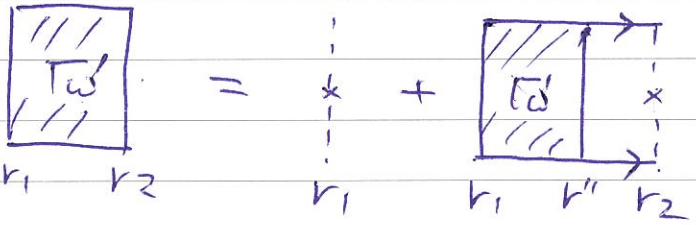
with $\chi_c(r,r';\omega) = \hbar^2 \int \frac{d\Omega}{2\pi} \int dr_1 \int dr_2 \; \overline{G^R(r,r_1,\Omega)} \overline{G^R(r_2,r',\Omega)}$

$\times \overline{G^A(r_2,r,\Omega-\omega)} \; \overline{G^A(r',r_1,\Omega-\omega)} \; \Gamma_\omega'(r_1,r_2)$

— (82)

with

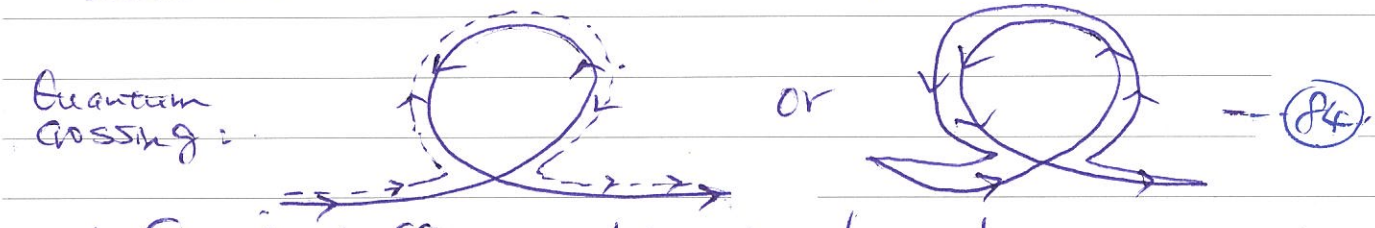
$$\Gamma_\omega'(r_1,r_2) = n_I U_0^2 \delta(r_1-r_2) + n_I U_0^2 \int \Gamma_\omega'(r_1,r'') \overline{G^R(r'',r_2,\Omega)} \times \overline{G^A(r'',r_2,\Omega-\omega)} \, dr''$$



— (83)

being the Cooperon propagator.

It's clear that the Cooperon describes propagation of two Green's functions through the same scattering path but in reversed direction as shaw below (old graphical representation



— (84)

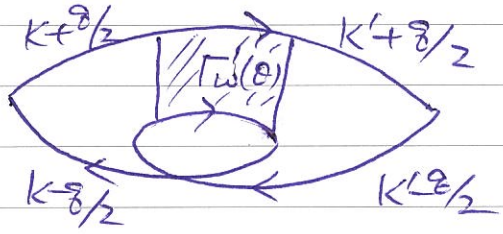
while the diffusion has no loop!

Hence there is no classical analogy of the Cooperon. It's purely due to quantum mechanics: amplitudes is the fundamental object: a_j & a_j^* can propagate in different directions!

The name Cooperon derives from the strong analogy to Cooper pair propagation in the theory of superconductivity.

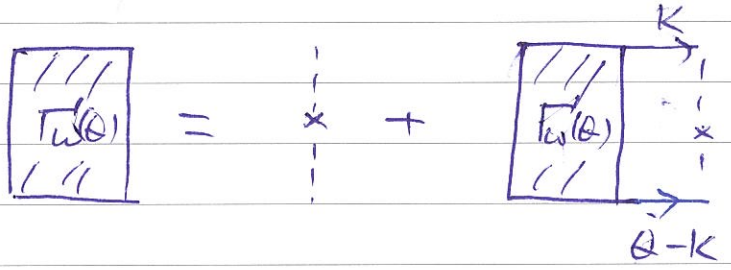
In the K-space, we have

$$\chi_c(q,\omega) =$$



$Q = K + K'$ (C.M. momentum)

with the Cooperon propagator being given by



$$\chi_c(q,\omega) = \hbar^2 \int_\Omega \int_{KK'} \overline{G^R(q,\Omega)}\ \overline{G^A(K-q,\Omega-\omega)}$$

$$\times\ \overline{G^R(q,\Omega)}\ \overline{G^A(K'-q,\Omega-\omega)}\ \Gamma_\omega(K+K')$$

$$\Gamma_\omega(Q) = n_I v_0^2 + n_I v_0^2 \int_K \Gamma_\omega(Q)\ \overline{G^R(K,\Omega)}\ \overline{G^A(Q-K,\Omega-\omega)}$$

$$\therefore \Gamma\omega'(\Theta) = \frac{1}{(n_I \nu_0^2)^{-1} \int_K \overline{G^R(K,\Omega)}\, \overline{G^A(\Theta-K,\Omega+\omega)}} \quad \text{--- (85)}$$

which has the same structure as that of the diffuson.

$$\therefore \Gamma\omega'(\Theta) = \frac{n_I \nu_0^2/2e}{i\omega - D\Theta^2} \quad \text{--- (86)}$$

↳ is also diffusion-like

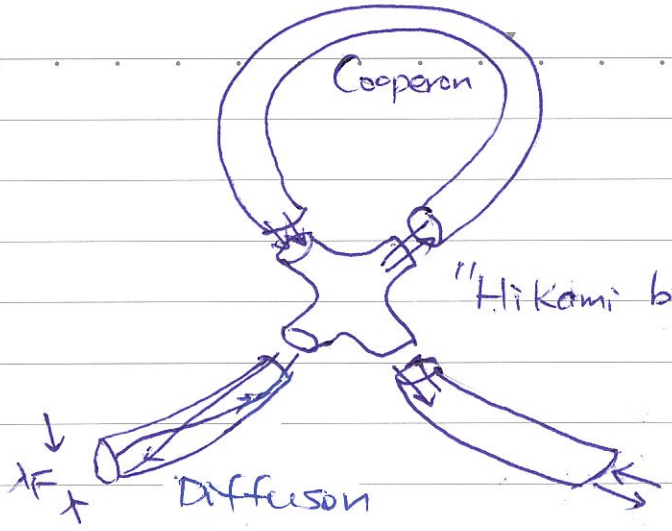
Hence the difference between the Cooperon & the diffusion is the quantum crossing. ↓ $\Pi_c(r-r';t)$

Weak localization

From the two building blocks Π_D of Π_C, one can evaluate the transfer probability.

As indicated, the quantum correction is due to the diagram shown in eq. (84).

Such paths are not unique because nearby paths (similar to the path integral) contribute equally. Roughly, paths with this distance λ_F are roughly the same phase. Hence lines in eq. (84) are replaced by tubes of cross section λ_F^{d-1} as follows:



The crossing area is called Hikami box and must occur near a scattering center

∴ The size of crossing area $\sim \lambda_F^{d-1} l_e$
(l_e = mean free path)

The above path provides a quantum correction to the diffusion constant D and a correction to the conductivity σ (both σ & $D \propto \tau_e$, $\therefore \frac{\delta\sigma}{\sigma} = \frac{\delta D}{D}$).

Estimate of δD is obtained by accounting for the returning probability ($\frac{1}{(Dt)^{d/2}}$, term of eq. (81)) at any point along the trajectory from $t > \tau_e$ (diffusion is valid) until the Thouless time τ_D (reach the boundary)

$$\frac{\delta D}{D} = \frac{\delta P}{P} \cong -\int_{\tau}^{\tau_D} \frac{\lambda_F^{d-1} \cdot \tau_F dt}{(Dt)^{d/2}} \times \text{returning probability} \quad \text{(tube volume)} \quad \text{--- (87)}$$

Here $\tau_D = L^2/D$

$$\therefore \frac{\delta D}{D} \cong -\nu_F \lambda_F^{d+1} D^{-d/2} \frac{1}{1-d/2} t^{1-d/2} \Big|_{\tau}^{\tau_D}$$

$$= -\frac{2}{2-d} \lambda_F^{d+1} D^{-d/2} \left[\tau_D^{\frac{2-d}{2}} - \tau^{\frac{2-d}{2}}\right]$$

$$\lambda_F^{d+1} D^{-d/2} \tau_D^{2-d/2} = \lambda_F^{d+1} D^{-d/2} L^{2-d} D^{\frac{d}{2}-1}$$

$$= \frac{\lambda_F^{d+1}}{D} L^{2-d}$$

$$\lambda_F^{d+1} D^{-d/2} \tau^{2-d/2} = \frac{\lambda_F^{d+1}}{D} \ell^{2-d}$$

$$\uparrow$$

$$\tau = \ell/\nu_F = \frac{\ell^2}{\tau \nu_F^2} = \frac{\ell^2}{D}$$

$$\therefore \frac{\delta\sigma}{\sigma} = \frac{\delta D}{D} \simeq -\frac{\lambda_F^{d+1}}{D} \frac{2}{2-d} \left(L^{2-d} - \ell^{2-d}\right)$$

$$d \to 2^+ \quad \frac{1}{2-d}\left(L^{2-d} - \ell^{2-d}\right) \to \ln L/\ell$$

$$\therefore \frac{\delta\sigma}{\sigma} = -\frac{\lambda_F^2}{D} \ln L/\ell$$ Consistant with the exact diagrammatic calculation

$$\delta\sigma = -\frac{e^2}{\pi^2 \hbar} \ln L/\ell \quad \text{---} (88)$$

(L.P. Gor'kov, et. al., JETP 30, 328. 1970)

& confirm the scaling analysis (see p. 12-72)

One can also use $\Gamma w'(\theta)$ to calculate the returning probability

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$$\frac{\delta D}{D} \sim -\int_{1/L}^{1/\ell} \frac{d\mathbf{Q}}{(2\pi)^d} \cdot \frac{n_z v_0^2/2e}{D Q^2}$$

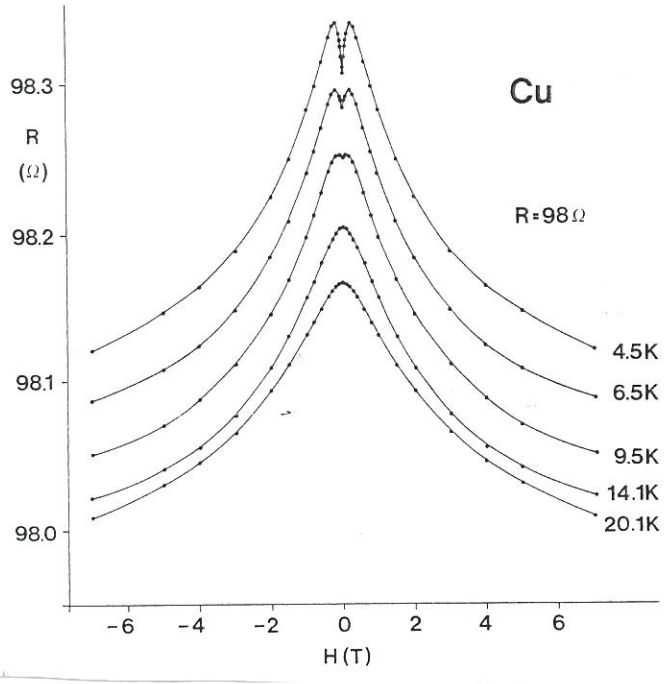
at $d=2$ $\quad \sim -\frac{n_z v_0^2/2e}{D} \ln L/\ell$

$$\therefore \delta\sigma \sim -A \ln L/\ell$$

Effect of weak magnetic field

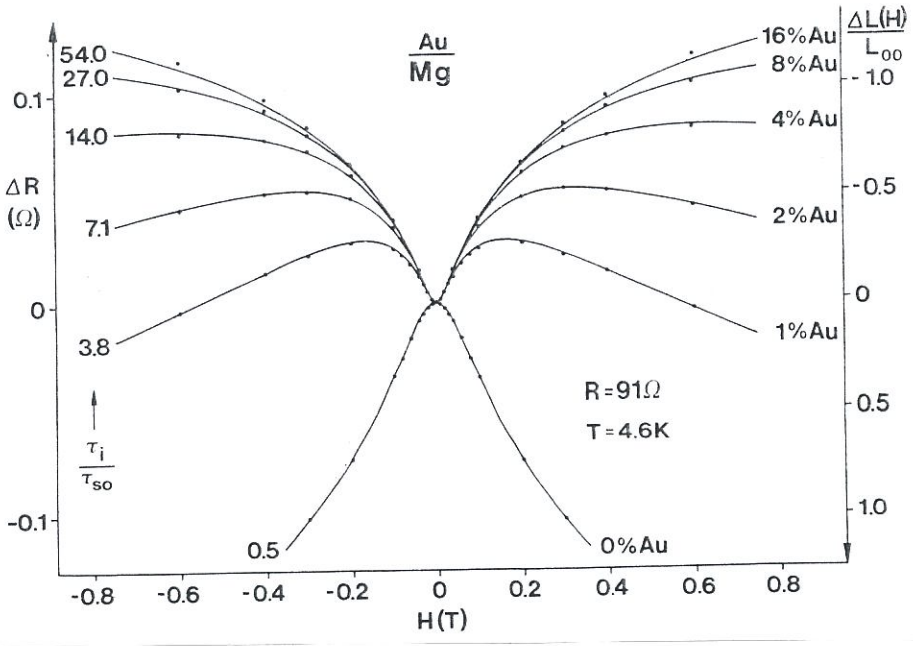
In the presence of weak magnetic field, time reversal paths are no longer equivalent and hence returning probability is reduced. $\delta\sigma \uparrow$, i.e, resistivity decreases. This is an important signature of weak localization.

(Note that $\vec{Q} \to \vec{Q} - \frac{2e}{c}\vec{A}$ in the weak field)



Cu-film (magneto-resistance) $d = 80A^\circ$
$\ell \sim 10A^\circ$ (mean free path) G. Bergman, Phys. Rep. 107, 1, 1984

Normal clean materials' magnetoresistance in this regime is featureless



Magnetoresistance of thin Mg films. When there is no coverage of Au atoms, it shows weak localization phenomenon. When there are Au atoms, spin-orbital effects become important.

Weak localization at finite T

At finite temperatures, electrons can interact with phonons so that phase coherence may get lost. Let τ_ϕ be the phase coherent time ($l_\phi = v_F \tau_\phi$), eq. (85) becomes

$$\frac{\delta\sigma}{\sigma} = -v_F \lambda_F^{d-1} \int_{\tau}^{\tau_\phi} \frac{dt}{(Dt)^{d/2}} \quad \cdots (86)$$

or $\frac{\delta D}{D} \sim \int \frac{d^d q}{(2\pi)^d} \frac{\hbar^2 v_F^2 / 2e}{D[\tau_\phi^{-2} + q^2]}$

$d=1$ $\frac{\delta\sigma}{\sigma} = -v_F \frac{2}{\sqrt{D}} (\sqrt{\tau_\phi} - \sqrt{\tau})$ $\because \tau_\phi \gg \tau$

$\simeq -\frac{2 v_F \sqrt{\tau}}{\sqrt{D}} \sqrt{\frac{\tau_\phi}{\tau}}$

$d=2$ $\frac{\delta\sigma}{\sigma} = -\frac{v_F \lambda_T}{D} \ln \tau_\phi/\tau$

$d=3$ $\frac{\delta\sigma}{\sigma} = -\frac{2 v_F \lambda_T^2}{D^{3/2}} \left(\frac{1}{\sqrt{\tau}} - \frac{1}{\sqrt{\tau_\phi}}\right)$

Clearly, for $d=1, 2$, as $T \downarrow$, quantum interference correction (due to τ_ϕ) decreases σ!

($\because \tau_\phi \gg \tau$)

In particular, at $d=2$, the dependence is logarithmic.

At $d=3$, however, lowering T, eventually, quantum interference correction is not important!

τ_ϕ is determined by phonon scattering or e-e interactions.

As we have seen in the last semister, τ_ϕ usually is proportional to inverse of power of T. (depending on scattering also $N_{phonon} \sim T^3$ in

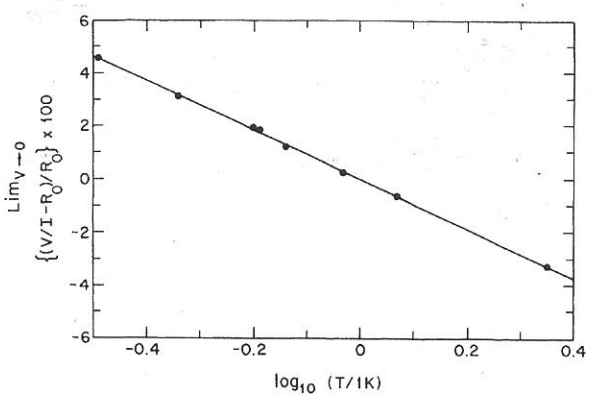
law T)

$\therefore \tau_\phi \sim T^{-\eta}$

Hence, $\frac{\delta G}{G_0} \propto \begin{cases} -T^{-\eta/2} & d=1 \\ -\ln \frac{T_0}{T} & d=2 \\ \text{const independent of } T & d=3 \text{ (very low T)} \\ \sim T^{\eta/2} \text{ (due to } \tau_\phi) & \end{cases}$

$\therefore$ For $d \leq 2$, δG diverges as $T \to 0$.

Since δG can't be negative, eventually, it means that weak perturbation theory breaks down and signifies an onset of the strong localization regime. The logarithmic T dependance is verified in expt. see below.



weakly disordered thin films of Palladium

G. J. Dolan & D. D. Osheroff
Phys. Rev. Lett 43, 721 (1979)

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Exceptions

Even though the scaling argument indicates that electrons are localized at $d=2$, the (key) assumption is: The Fermi-liquid theory completely describes the clean system. (We shall discuss the Fermi-liquid theory, essentially, it is similar to the Fermi gas system.)

In reality, this is not necessarily correct. There are exceptions.

Insulator - Superconductor transition

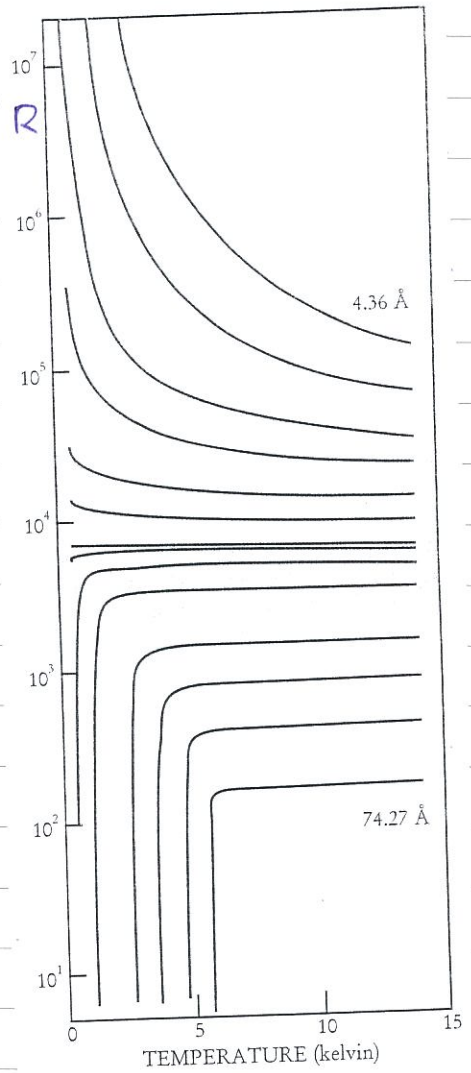
The superconducting state is not the Fermi-liquid. Therefore, it can be an exception.

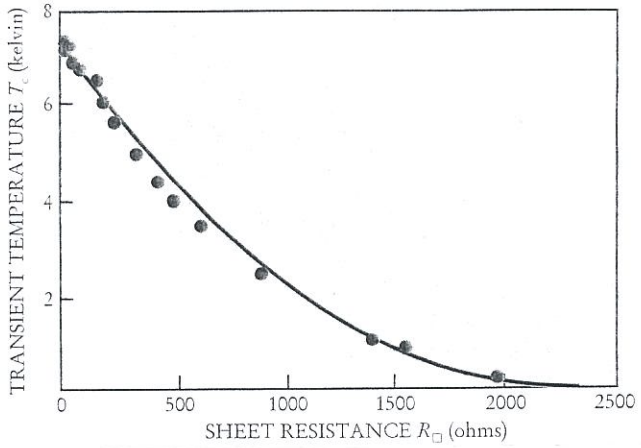
In the presence of disorders, Cooper pairs can be destroyed. In 3D, the broken pairs simply become two electrons and eventually the system goes back to disordered metal. In 2D, there is no metallic state, hence, when superconductivity is destroyed, it goes into the state of an insulator, causing the Insulator - Superconductor transition.

This has been observed in thin films either by

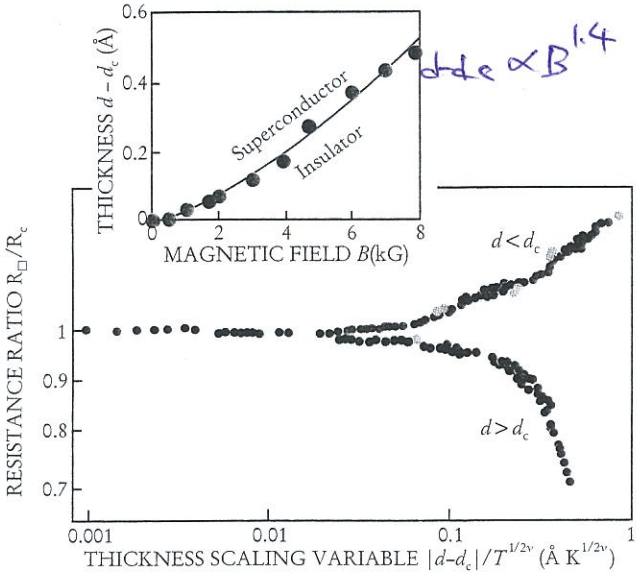
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Changing the thickness of the film or the magnetic field (which are essentially controling the strength of disorders.) A.M. Goldman & N. Markovic Physics Today Nov. V51, 31-44 (1998)





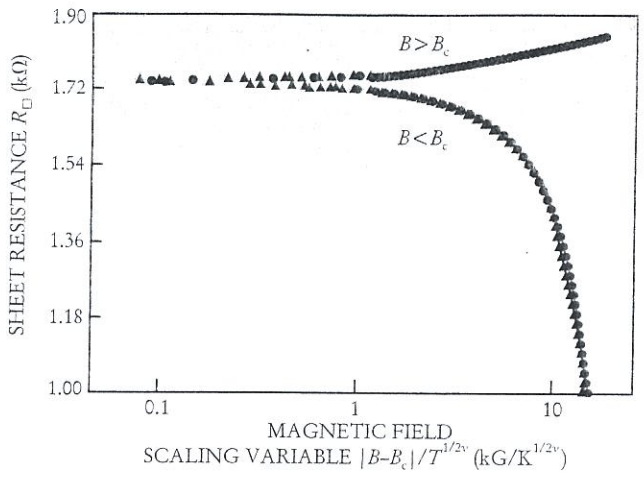
← Temperature dependence of sheet resistance for various thickness of bismuth film
$R_c \simeq 6450 \; (= h/4e^2)$



Scaling behavior:
$R > R_c$ & $R < R_c$ curves can be collapsed into two universal curves
Here $2\nu = 1.4 \pm 0.1$
d_c = critical thickness

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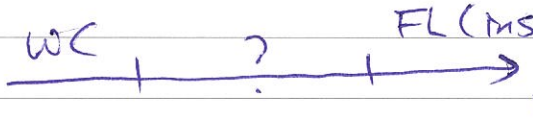
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Scaling analysis of temperature & magnetic field dependence shows that $B>B_c$ & $B<B_c$ curves can be collapsed into two universal curves. Here $B_c = 4.19$ KG. $z\nu = 1.36$.

Metalic state driven by Coulomb interaction

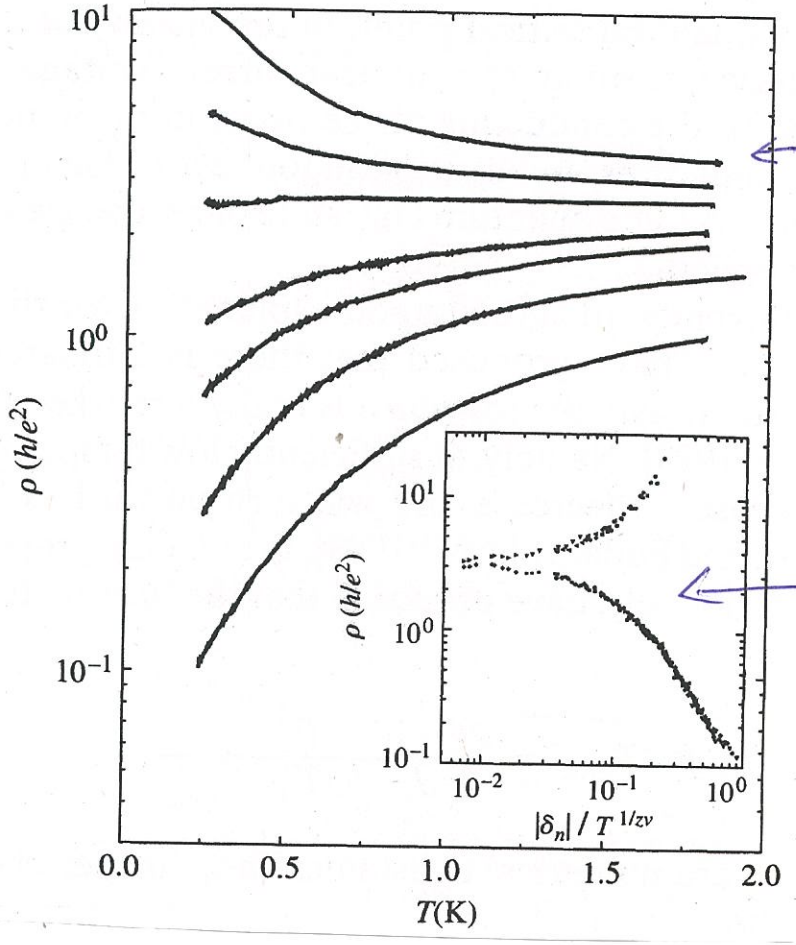
So far, we have neglected the Coulomb interaction. Naively, the Coulomb interaction tends to repel electrons and thus may enhance delocalization. However, the effective strength of the Coulomb interaction depends on the inter-particle distance. Hence, it will depend on the density of electrons. We have not addressed the issue of Coulomb interaction and come back to it later. But essentially, for low density, the electrons form so-called Wigner crystals; while for high densities, screening becomes important, the system is insulator. In between, it is yet unknown.



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(metal-insulator transition) 12-17.

Experimetally, quantum phase-transition like behavior is observed in 2D electrons (Si metal-oxide or GaAs -semiconductor-field-effect transistor, MOSFET). (First observed by S.V. Kravchenko et. al, PRL 77, 4938, 1996)



$n = 0.86 \times 10^{11}$ per cm^2
0.88
0.90
0.93
0.95
0.99
1.10

collapse of data

$\delta_n = \frac{n - n_c}{n_c}$

$z = 0.8$

$\nu = 1.5$

Key features : (i) exist n_c

(ii) on the conducting side

$\rho \sim \rho_1 + \rho_0(T)$ $\rho_0(T) \sim e^{T_0/T}$

(iii) Critical scaling

(iv) non-linear I V curve

(v) conducting phase suppressed by B

Currently, there is no consensus whether this is a true transition as T does not really go to zero. It is thus an open question. (Reading report.)

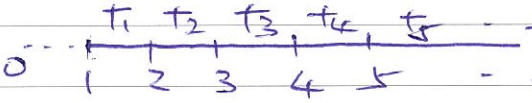
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Extended states in random hopping model

It is known that if the randomness is due to hopping, there may exis delocalized states even in 1D.

(see S. Alexander et. al, Rev. Mod. Phys. 53, 175, 1981; B.L. Huang, S.T. Wu & C.Y. Mou, PRB 70, 205440 f, 2004)

For example, consider a 1D random hopping model near a wall.



$t_{i-1}\psi_{i-1} + t_i\psi_{i+1} = E\psi_i$

$\because \psi_0 = 0$. $\therefore$ There exists a solution at $E=0$ such that $\psi_0 = \psi_2 = \psi_4 = \cdots = 0$

and for odd sites $t_{i-1}\psi_{i-1} + t_i\psi_{i+1} = E\cdot 0 = 0$

for even sites $t_{i-1}\underset{0}{\psi_{i-1}} + t_i\underset{0}{\psi_{i+1}} = E\psi_{odd}$

$\therefore E=0$

$\therefore \psi_{i+1} = -\frac{t_{i-1}}{t_i}\psi_{i-1}$ $\therefore \psi_3 = -\frac{t_1}{t_2}\psi_1$

$\psi_5 = -\frac{t_3}{t_4}\psi_3 = \frac{t_1 t_3}{t_2 t_4}\psi_1$

$\therefore |\psi_{2N+1}| = \frac{t_1}{t_2}\frac{t_3}{t_4}\frac{t_5}{t_6}\cdots\frac{t_{2N-1}}{t_{2N}}$ $\because t_i$ is random

$\therefore X_i \equiv \left|\frac{t_{2i-1}}{t_i}\right|$ is also random.

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Clearly,

$$\ln|\psi_{2N+1}| = \sum_{i=1}^{N} \ln x_i = \text{sum of random \#s}$$

$$\ln|\psi_{2N+1}| - \ln|\psi_{2N-1}| = \ln x_N = \text{random}$$

$\therefore \ln|\psi|$ performs random walking on the lattice

$\therefore$ Random walkers have high probability of going to ∞, $\therefore |\psi|$ is not localized.

Indeed, $\because \overline{(\ln|\psi_0^{2N+1}|)^2} = \sqrt{N}\,\sigma$

σ = standard deviation of $\ln x$

$\therefore |\psi_0^{2N+1}| \sim e^{-\sigma\sqrt{N}}$ which is semi-localized

(not $e^{-r/\xi}$ localized as) and is a resonant state.