Anderson Localization Explained simply
MIT Grad Student Seminar
October 4th, 2013

Consider the Anderson model: (electron on a lattice)

$$\boxed{\mathcal{H} = \sum_i \varepsilon_i c_i^+ c_i - t \sum_{\langle ij \rangle} c_i^+ c_j + c_j^+ c_i}$$

where $\{c_i^+, c_j\} = \delta_{ij}$, $\{c_i, c_j\} = \{c_i^+, c_j^+\} = 0$

and ε_i are on site energies that are distributed according to a probability distribution with width W

e.g. $P(\varepsilon) = \frac{1}{W} \Theta(\frac{1}{4}W^2 - \varepsilon^2)$

or $P(\varepsilon) = \frac{1}{W\sqrt{2\pi}} e^{-\varepsilon^2/2W^2}$

c_i^+ creates an electron at site i with atomic orbital wavefunction $\varphi(\vec{r} - \vec{r}_i)$

Limit 1 : $\{\varepsilon_i\} = 0$; $\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^+ c_j + c_j^+ c_i$

This can be diagonalized : $c_i \equiv \sum_k e^{i\vec{k}\cdot\vec{r}_i} c_k$, $c_i^+ = \sum_k e^{-i\vec{k}\cdot\vec{r}_i} c_k^+$

$$\Longrightarrow \quad \mathcal{H} = + \sum_k \epsilon_k c_k^+ c_k \quad \text{where } \epsilon_k = -2t \sum_\delta \cos(\vec{k}\cdot\vec{\delta})$$

1d chain : $\epsilon_k = -2t \cos ka$ ($a \equiv$ lattice spacing)
2d square lattice: $\epsilon_k = -2t(\cos k_x a + \cos k_y a)$
3d cubic lattice: $\epsilon_k = -2t(\cos k_x a + \cos k_y a + \cos k_z a)$

Notice that, even though we have not set restrictions on $\vec{k}$ by boundary conditions, energy states are periodic in k. Inequivalent energy states are labeled by $k \in [-\pi/a, \pi/a]$ in the 1st BZ

Also notice for a d-dimensional cubic lattice

$$|\epsilon| \leq 2td \Rightarrow \text{bandwidth } \boxed{B \equiv \epsilon_{max} - \epsilon_{min} = 4td}$$

Aside density of states

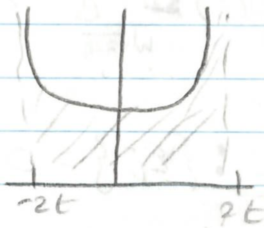
$$D(\epsilon) = \frac{1}{(2\pi)^d} \int_{-\pi/a}^{\pi/a} \prod d k_i \, \delta(\epsilon + 2t \sum_i \cos k_i a) \equiv \sum_k \delta(\epsilon - \epsilon_k)$$

using $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-iyx)$

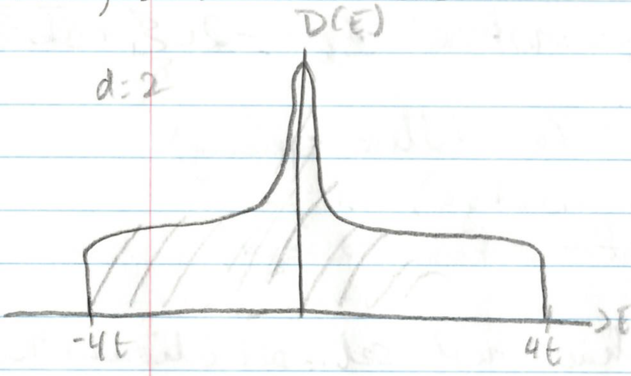
& $I_0(x) = \frac{1}{\pi} \int_0^{\pi} \exp(x \cos y \, dy)$ & $I_0(-ix) = J_0(x)$

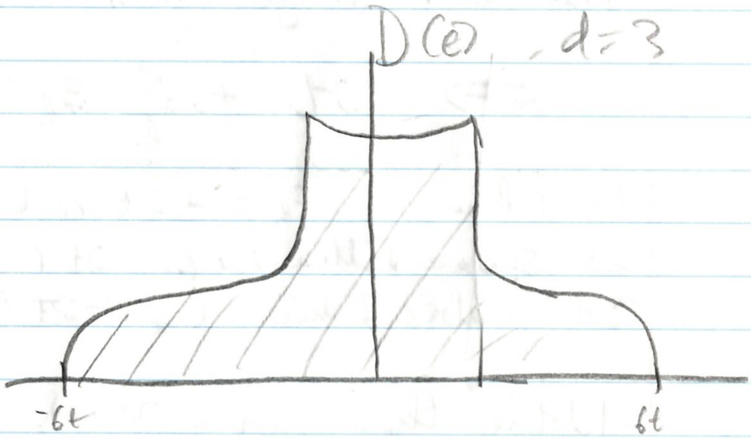
Find $$\boxed{D(\epsilon) = \frac{1}{a^d \pi} \int_0^{\infty} dy \cos(y\epsilon) J_0^d(2ty)}$$

$d=1$ $D(\epsilon) = \frac{1}{\pi a} \frac{1}{\sqrt{4t^2 - \epsilon^2}}$



$d = 2, 3$: numerics





These momentum eigenstates are <u>delocalized</u>

1d Intuitive example : initial wavepacket $\psi_0 \sim e^{-x^2}$
free particle

Then solving Schrodinger's eq: $\psi(\tau, x) \sim \frac{\exp(-x^2/1+2i\tau)}{\sqrt{1+2i\tau}}$

and $\langle |x| \rangle \sim \tau$ for large τ, the packet diffuses away.

Limit 2 $t = 0$ $\{\varepsilon_i\} \neq 0$

$\mathcal{H} = \sum_i \varepsilon_i c_i^\dagger c_i \Rightarrow$ this is already diagonal in the lattice index

Eigenstates are atomic orbital states at site i with energy ε_i. These are <u>localized</u>

Note if ε_i are all the same, then superpositions of states localized on many sites are now eigenstates, and we no longer have localization.

Important that we have a spread of ε_i sampled from a distribution of width W.

<u>Have shown so far</u>: $W = 0, t \neq 0$ States delocalize
$W \neq 0, t = 0$ States localize

<u>What about $W \neq 0, t \neq 0$?</u> Can we say anything?

Consider $|\psi\rangle = \sum_i a_i |0 \ldots i = 1, 0 \ldots\rangle$ Then:

$$H|\Psi\rangle = \sum_i E a_i|i\rangle = \sum_i \varepsilon_i a_i|i\rangle - t\sum_{\langle ij\rangle} a_j|i\rangle$$

So we have a matrix equation for the a_i

$$E a_i = \varepsilon_i a_i - t\sum_{j=i+\delta} a_j \qquad \delta$$

If $a_i \equiv a_i(\tau)$ $\quad i\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \Rightarrow \boxed{i\dot{a}_i = \varepsilon_i a_i - t\sum_{j=i+\delta} a_j}$ (*)

Now say $\quad a_m(\tau=0) = 1 \quad \& \quad a_{i\neq m}(\tau=0) = 0$

We want to solve $a_m(\tau\to\infty)$.

If: $\quad a_m(\tau\to\infty) = 0 \longrightarrow$ delocalized

$\quad\quad a_m(\tau\to\infty) \neq 0 \longrightarrow$ localized

<u>How did Anderson approach the problem?</u>

Consider Laplace transforming (*) $\quad \tilde{a}_i(E) = \int_0^\infty e^{iE\tau} a_i(\tau)\,dt$

where E has a positive imaginary part for convergence

$$\therefore\ [E\tilde{a}_i - i a_i(0)] = \varepsilon_i \tilde{a}_i - t\sum_{j=i+\delta} \tilde{a}_j$$

$$\boxed{\tilde{a}_i = \frac{i\delta_{mi}}{E-\varepsilon_i} + \sum_j \frac{T_{ij}}{E-\varepsilon_i}\tilde{a}_j}$$

where $T_{ij} = -t$ for ij spaced on lattice site apart.

Strategy, solve iteratively:

$$\tilde{a}_{j\neq m} = \frac{1}{E-\varepsilon_j} T_{jm}\,\tilde{a}_m(E) + \sum_k \frac{1}{E-\varepsilon_j} T_{jk} \frac{1}{E-\varepsilon_k} T_{km}\,\tilde{a}_m(E) + \dots$$

And also

$$\tilde{a}_m = \frac{i}{E-\varepsilon_m} + \sum_k \frac{1}{E-\varepsilon_m} T_{mk} \overbrace{\left(\frac{T_{km}}{E-\varepsilon_k} + \sum_l \frac{T_{kl}}{E-\varepsilon_k} \frac{T_{lm}}{E-\varepsilon_l} + \dots \right)}^{\text{Write as } (\delta e + i\gamma - EK) \text{ for small imaginary part of } E} \tilde{a}_m$$

<u>We are really interested only in $\tilde{a}_m(E)$</u>

Can solve $\boxed{\tilde{a}_m(E) = \dfrac{i}{E(1+K) - (\varepsilon_m + \delta e) - i\gamma}}$ energy correction

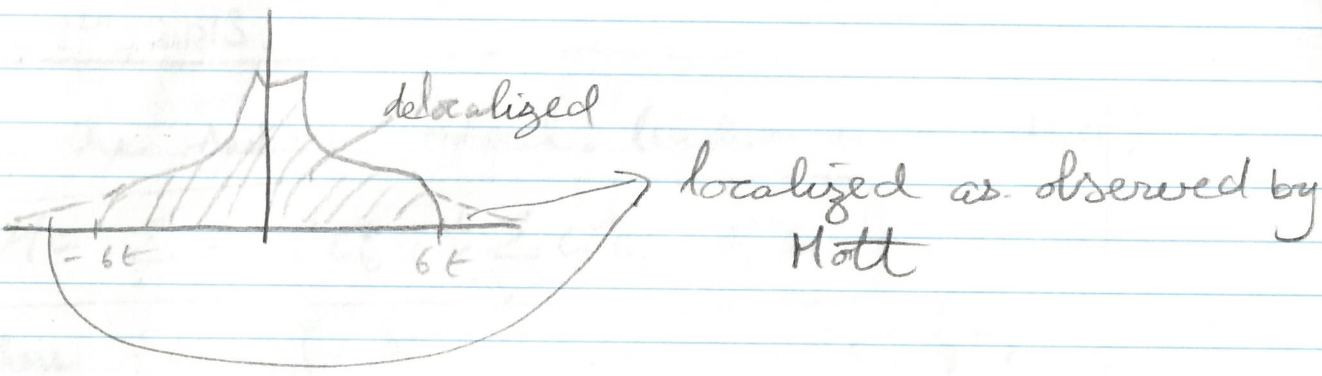
If $\gamma \neq 0$, the state decays $\tau \to \infty$ and there is no localization
if $\gamma = 0$, the state does not decay $a_m(\tau \to \infty) \neq 0$
<u>localization</u>!

From above, it is clear that γ depends on $\varepsilon_i, \varepsilon_j \dots$
which are sampled from a probability distribution $p(\varepsilon)$
with width W.

$\to$ Statements about γ must be made <u>on average</u>

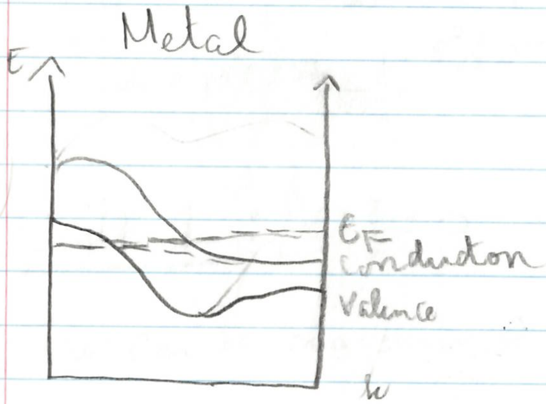
$\to$ In the above argument we are perturbing the localized Hamiltonian in t, this makes sense because states are localized when $t=0$ and we want to see if they remain localized for $t \neq 0$

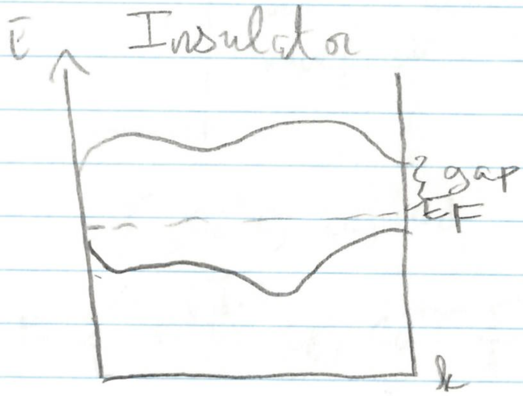
What happens if $W \sim B$? density of states looks like



<u>What does this escplain?</u>

This explains disorder induced metal → insulator transitions





The lack of a gap between valence & conduction band means states are extended.

If there is a gap, states are localized.

<u>Caveats</u> In 1 & 2d localization happens as long as $W > 0$.

This happens because of multiple scattering.