Brief explanation and summary of Anderson localization in three dimensional systems

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In this paper, we briefly explain and summarize the central concepts of the well-known original work about Anderson localization[1]. We first describe the disordered model and how to see the localization in detailed math. Then we briefly summarize the reasoning Anderson used to give a generic condition for the absence of the transport in a three dimensional system, without describing the probability analysis in detail. In the end we will come to the conclusion of the condition for Anderson localization in three dimensions, which is the ratio of the disorder energy bandwidth and the interaction strength being larger than a critical value.

Anderson localization refers to the statement that, for a disordered system, transport will not happen for some conditions. In three dimensions, there exists a critical disorder bandwidth such that if the random disorder is stronger than the critical value, transport will not be able to happen and the system will become insulating. In dimensions $d \leq 2$, localization will always happen for arbitrary weak disorder, demonstrated by a scaling theory[2]. This is a significant finding providing insights into how transport properties in real materials can be affected by defects or impurity. In this paper, we briefly explain and summarize the derivations Anderson used to determine the condition for the absence of the transport in a three dimensional system.

The disordered model can be described by the Hamiltonian,

$$H = \sum_l E_j C_j^\dagger C_j + \sum_{j,k} V_{jk} C_j^\dagger C_k, \tag{1}$$

where E_j is the energy for a spin on site j. It is a random variable distributed with a probability distribution $P(E)dE$ within a bandwidth W. V_{jk} is the interaction term that may be or may not be a random variable with a probability distribution. C_j and $C_j^\dagger$ are the Fermion operators at site j. We know the time evolution of C_j,

$$i\frac{\partial}{\partial t}C_j = [C_j, H] \tag{2}$$

$$\{C_j, C_k^\dagger\} = \delta_{jk}. \tag{3}$$

The technique is that we initially place a single spin on site n at time $t = 0$, and study the probability of finding it at site n at a later time t. For temperature $T = 0$, the probability amplitude $a_j(t)$ of finding a particle on site j at time t is defined as,

$$a_j(t) = \theta(t)\langle 0|C_j(t)C_n^\dagger(0)|0\rangle. \tag{4}$$

The time evolution of $a_j(t)$ thus satisfies

$$i\tfrac{\partial}{\partial t}a_j(t) \tag{5}$$

$$= \delta(t)i\langle 0|C_j(t)C_n^\dagger(0)|0\rangle + \theta(t)\langle 0|[C_j, H](t)C_n^\dagger(0)|0\rangle \tag{6}$$

$$= \delta(t)ia_j(t=0) + \theta(t)E_j a_j(t) + \theta(t)\textstyle\sum_{k\neq j} V_{jk}a_k(t) \tag{7}$$

For convenience for the following derivation, we want $a_j(t)$ to be a differentiable function. So we only consider $a_j(t)$ in Eq 4 at $t \geq 0$ and redefine the behavior of $a_j(t = 0^-)$ as following.

$$a_j(t) = \langle 0|C_j(t)C_n^\dagger(0)|0\rangle. \tag{8}$$

$$i\frac{\partial}{\partial t}a_j(t) = E_j a_j(t) + \sum_{k\neq j} V_{jk}a_k(t). \tag{9}$$

And the initial condition is described by

$$a_n(t=0) = 1 \tag{10}$$

$$a_{j\neq n}(t=0) = 0. \tag{11}$$

Our goal is to obtain $\langle a_j(t=\infty)\rangle$. We first perform the Laplace transform of $a_j(t)$,

$$f_j(s) = \int_0^{+\infty} e^{-st}a_j(t)dt, \tag{12}$$

where s is an arbitrary complex number with positive or zero real part. From the final value theorem, $\lim_{s\to 0^+} sf(s) = \lim_{t\to+\infty} f(t)$, so we can investigate the behavior of $a_j(t = +\infty)$. From Eq. 9, we have

$$(is - E_j)f_j(s) = ia_j(t=0) + \sum_{k\neq n} V_{jk}f_k(s) \tag{13}$$

Here we have used that if $a_j(t)$ is a differentiable function, Laplace transform of $\frac{\partial}{\partial t}a_j(t)$ is $\int_0^{+\infty} e^{-st}\frac{\partial}{\partial t}a_j(t)dt = sf_j(t) - a_j(t = 0^+)$. So,

$$f_j(s) = \frac{i\delta_{jn}}{(is - E_j)} + \sum_{k\neq n}\frac{1}{(is - E_j)}V_{jk}f_k(s). \tag{14}$$

For $j \neq n$, $f_j(s)$ can be expressed in terms of $f_n(s)$ as

$$f_j(s) = \frac{1}{is-E_j} V_{jn} f_n(s) \quad (15)$$
$$+ \sum_k \frac{1}{is-E_j} V_{jk} \frac{1}{is-E_k} V_{kn} f_n(is) + \dots . \quad (16)$$

And for site n,

$$f_n(s) = \frac{i}{is-E_n} + \sum_k \frac{1}{is-E_n} V_{nk} (\frac{V_{kn}}{is-E_k} \quad (17)$$
$$+ \sum_l \frac{1}{is-E_k} V_{kl} \frac{1}{is-E_l} V_{ln} + \dots) f_n(s). \quad (18)$$

Then we can define $V_c(n)$ as

$$V_c(n) \equiv \sum_k \frac{(V_{nk})^2}{is-E_k} + \sum_{k,l} \frac{V_{nk}V_{kl}V_{ln}}{(is-E_k)(is-E_l)} + \dots . \quad (19)$$

And $f_n(s)$ can be expressed as

$$(1 - \frac{1}{is-E_n} V_c(n)) f_n(s) = \frac{i}{is-E_n} \quad (20)$$
$$f_n(s) = \frac{1}{s + iV_c(n) + iE_n} \quad (21)$$

At the limit of $s \to 0$, the leading order of $V_c(n)$ can be written as

$$\lim_{s\to 0} \sum_k \frac{(V_{nk})^2}{is-E_k} \quad (22)$$
$$= \lim_{s\to 0} \sum_k (V_{nk})^2 (\frac{-E_k}{s^2+E_k^2} - \frac{is}{s^2+E_k^2}) \quad (23)$$

The first term $-\Delta E^{(2)} \equiv \lim_{s\to 0} \sum_k (V_{nk})^2 \frac{-E_k}{s^2+E_k^2} = -\sum_k \frac{(V_{nk})^2}{E_k}$ is the second-order perturbation of the energy at site n. The second term

$$\lim_{s\to 0} \sum_k (V_{nk})^2 \frac{-is}{s^2+E_k^2} \quad (24)$$
$$= -i\pi \sum_k (V_{nk})^2 \delta(E_k) - is \sum_{k, E_k \neq 0} \frac{(V_{nk})^2}{E_k^2} \quad (25)$$

Here we have used that $\delta(x) = \frac{1}{\pi} \lim_{\epsilon\to 0} \frac{\epsilon}{x^2+\epsilon^2}$. We define the first term $-i\pi \sum_k (V_{0k})^2 \delta(E_k) \equiv -\frac{i}{\tau}$ and the second term $is \sum_{k, E_k \neq 0} \frac{(V_{nk})^2}{E_k^2} \equiv -isK$. Obviously if the first term is non-zero, the second term is indeterminate. If τ is finite and only the leading order of Eq. 19 is taken into account, Eq. 17 becomes

$$f_n(s) = \frac{i}{is-E_n} + \frac{(-\Delta E^{(2)} - \frac{i}{\tau} - isK)}{is-E_n} f_n(s). \quad (26)$$

The solution for f_n is

$$f_n(s) = \frac{1}{s(1+K) + (1/\tau) + i(E_n - \Delta E^{(2)})}. \quad (27)$$

If τ is finite, the contribution from K is neglectable. Thus,

$$f_n(s) = \frac{1}{s + (1/\tau) + i(E_n - \Delta E^{(2)})}, \quad (28)$$

So $a_n(t) = e^{-t/\tau - i(E_n - \Delta E^{(2)})t}$, since

$$\int_0^{+\infty} e^{-st} a_n(t) dt = \int_0^{+\infty} dt e^{-st - t/\tau - i(E_n - \Delta E^{(2)})t} \quad (29)$$
$$= \frac{1}{s + (1/\tau) + i(E_n - \Delta E^{(2)})}. \quad (30)$$

From the expression of $a_n(t)$, we know it represents a state of perturbed energy $E_n - \sum_k \frac{(V_{nk})^2}{E_k}$ decaying at the rate $\sim e^{-t/\tau}$ after a long enough time. In the case τ is infinite,

$$f_n(s) = \frac{1}{s(1+K) + i(E_n - \Delta E^{(2)})}, \quad (31)$$

and

$$a_n(t) = \frac{1}{1+K} e^{-i\frac{E_n - \Delta E^{(2)}}{1+K} t}. \quad (32)$$

The $a_n(t)$ does not satisfy $a_n(t=0) = 1$, because from Eq.24 to Eq.25, we take the limit of s to 0 to analyze $a(t)$ at the limit of t to $+\infty$. So in this case, $a_n(t \to +\infty)$ is reduced from 1 to $1/(1+K)$ rather than decaying to 0 at $t = +\infty$, which means the transport can not really happen. So whether the absence of transfer happens is determined by the convergence of $\mathrm{Im}(V_c(n))$ as $s \to 0$ in Eq. 21. Actually to the leading order, it is already shown in Eq. 23 that,

$$\mathrm{Im}(V_c(n)) = -s \sum_k \frac{|V_{nk}|^2}{s^2 + E_k^2} \sim -s \sum_{j\neq n} \frac{|f_j(s)|^2}{|f_n(s)|^2}. \quad (33)$$

So this also indicates that finite $\mathrm{Im}(V_c(n))/s$ at the limit of $s = 0^+$ means no real transport.

To determine the condition of $V_c(n)$ to be convergent, Anderson introduced a probability distribution for terms in

$$V_c(n) = \sum T_L \quad (34)$$
$$= \sum_{j,k,l\dots \neq n} V_{nj} \frac{1}{is-E_j} V_{jk} \frac{1}{is-E_k} V_{kl} \frac{1}{is-E_l} \dots V_{mn}. \quad (35)$$

The terms here in the expansion should also include repeated indices by definition. However, we can eliminate all of them by including in the energy denominator for atom k the perturbed energy $V_c(k)$. Specifically, if we want the term

$$V_{03} \frac{1}{e_3} V_{32} \frac{1}{e_2} V_{21} \frac{1}{e_1} V_{10}, \quad (36)$$

we can include the effect from the closed paths with repeated indices in $e_j = is - E_j - V_c(j)$ (Fig. 1). For example for this specific path in expression 36, $e_2 = is - E_2 - \sum_{j,k,l\neq 0,1} V_{2j} \frac{1}{e_j} V_{jl} \frac{1}{e_l} \dots \frac{1}{e^k} V_{k2}$. Also here, the indices in this series can not be repeated and can not include 0 or 1 which appear before e_2 in the expression 36. So,

$$\frac{1}{e_2} \simeq \frac{1}{is-E_2} (1 + \sum_{j,k,l\neq 0,1} V_{2j} \frac{1}{e_j} V_{jl} \frac{1}{e_l} \dots \frac{1}{e^k} V_{k2} \frac{1}{is-E_2}) \quad (37)$$

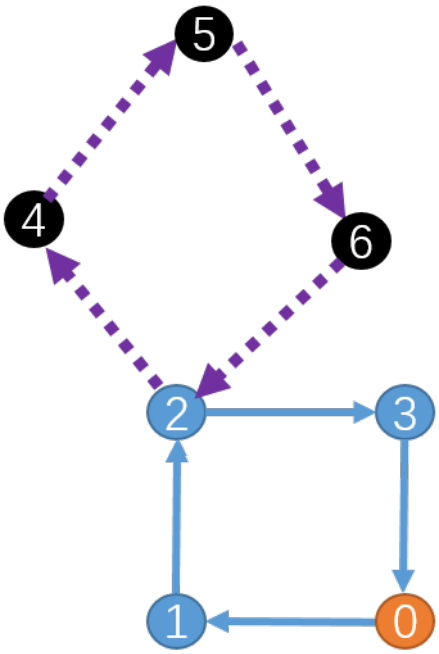

FIG. 1: Diagram for the expression of $V_c(n=0)$ in Eq.36. The blue solid path indicates the term in Eq.36. The purple dashed path indicates one of the paths whose effect is included in the denominator of site 2, e_2.

Inserting Eq. 37 to expression 36, we can see it includes the effect from all the repeated indices.

Some unimportant simplification is made as following. The probability distribution of E_j within the bandwith W is

$$P(E) = 1/W \quad \text{for} \quad -\frac{1}{2}W < E < \frac{1}{2}W \tag{38}$$

$$P(E) = 0 \quad \text{for} \quad |E| > \frac{1}{2}W, \tag{39}$$

Defining average number of terms of length L between T_L and $T_L + dT_L$ as $n(T_L)dT_L$, they come up with $n(T)$ of the following general form considering different cases:

$$n(T)dT = [F(\kappa, W/V)]^L \frac{dT}{T^2}\mathcal{L}(T) \tag{40}$$

where $\mathcal{L}(T)$ is a slowly varying function relative to T. For the following discussion, we assume V_{jk} is finite only when j and k are nearest neighbour and it is a constant $V_{jk} = V$ for all sites. Using the percolation theory, we can define

$$\Sigma = \sum_{n=1}^{\kappa^L} (\pm T_n), \tag{41}$$

where κ is the connectivity in percolation theory so the number of nonrepeating paths of length L leading from any given atom is $\sim \kappa^L$, considering the lattice only with near-neighbor connections. So Σ is the sum of the terms with path of length L. Thus the probability distribution for Σ is

$$P(\Sigma)d\Sigma \sim F^L(\kappa, W/V)\frac{d\Sigma}{\Sigma}\mathcal{L}(\Sigma). \tag{42}$$

We can define $(W/V)_0$ to satisfy

$$F^L(\kappa, (W/V)_0)\mathcal{L}(1) = 1. \tag{43}$$

From some probability analysis, the paper[1] concludes that if (W/V) is slightly larger than $(W/V)_0$, the most probable value of Σ is small of order e^{-L}. And the probability of $\Sigma = 1$ is also of order e^{-L}. For the limit of $L \to +\infty$, the value of Σ is less than $\sim e^{-L}$ with a probability $\sim 1 - e^{-L}$. But the number of $\Sigma' s$ only increases as L. So the series of Eq. 19 can almost always converge if $(W/V) > (W/V)_0$, which is the condition for Anderson localization to happen in a three dimensional system. The paper[1] also gave a typical estimation $(W/V)_0 = 26$ for $K = 4.5$ for the simple cubic lattice. Contrary to three dimensional systems where strong enough disorder is needed for electrons to be localized, in dimensions $d \leq 2$, it is proved in a scaling theory[2] that localization always happens for arbitrary weak disorder.

[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958), URL https://link.aps.org/doi/10.1103/PhysRev.109.1492.

[2] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979), URL https://link.aps.org/doi/10.1103/PhysRevLett.42.673.