Random Dimer Model: Escape from Localization

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Abstract

The Anderson localization is introduced as well as the scaling theory of localization. These predict the absence of the metallic state in 1 and 2 dimensions. In such a theoretical background, the random dimmer model is shown to be novel due to its ability to escape from localization. This model is also shown to be applicable to describe the insulator-metal transition in a wide range of conducting polymer, such as polyaniline.

1 Introduction

Most of the Modern devices are build upon the property of a small particle: electron. The electrons in devices have two basic types of states, moving around the device or staying in a certain point or region. This makes the metal-insulator transition(MIT) an important issue in condensed matter physics. Experimentally, to characterize the difference of these two states, we can measure the DC conductivity $\sigma(0)$. For metallic state, we have $\sigma(0) \neq 0$, for insulator state, $\sigma(0) = 0$. Theoretically, we view the metal as a extended state which means that the charge carriers can move around from one side of the sample to the other side. While we call the insulator state localized state which means the charge carrier can only move inside a small region of a sample and cannot move from one side to the other side.

There are mainly three kind of insulators, so called the band insulator, Mott insulator and Anderson insulator. Also there respectively have three kind of MIT. These different insulating state arise from different mechanisms. For band insulator, due to the periodic lattice potential, the energy of the electrons form different energy bands between which there exist band gaps. The electrons cannot move freely in the fully filled band due to the Pauli exclusive principle. For Mott insulator, the strong Coulomb interaction make the moving of the electron (or other boson such as Cooper pairs) cast a large energy, so called the Mott gap. This energetic unfavorable motion is forbidden if the gap is much large the kinetic energy of the charge carrier, which is the insulating state. For the Anderson insulator, the insulating state is mainly from the incoherence scattering from the random static potential, which makes a destructive interference of the propagating wave, thus make the forward motion of charge carrier impossible. My essay mainly focus on the Anderson insulator state, or Anderson localization and the defiant of Anderson localization, one of which is the random dimer model.

This essay is organized as following, in section (II) the Anderson localization is introduced based on a 1 dimensional site-disordered model. In section (III) The scaling theory of localization is shown to predict the absence of metal phase in 1 or 2 dimension disordered system. After all this theoretical background introduction, the random dimer model is presented in section (IV). In section (V), a possible experimental system showing the behavior of random dimer model is introduced.

2 Anderson localization: A site-disordered model based on perturbation theory

In 1958,Anderson give rise the first localization model[2],so-called the site-disordered model. The model is shown as the figure(1) The electron (or spin) on the site n has energy E_n. The energy is has a random distribution $P(E)$ which has a width W (2nd order moment). The hoping matrix element is $V_{jk}(r_{jk})$, which transfer a electron on one site to the other (we assume it is not a random variable here).

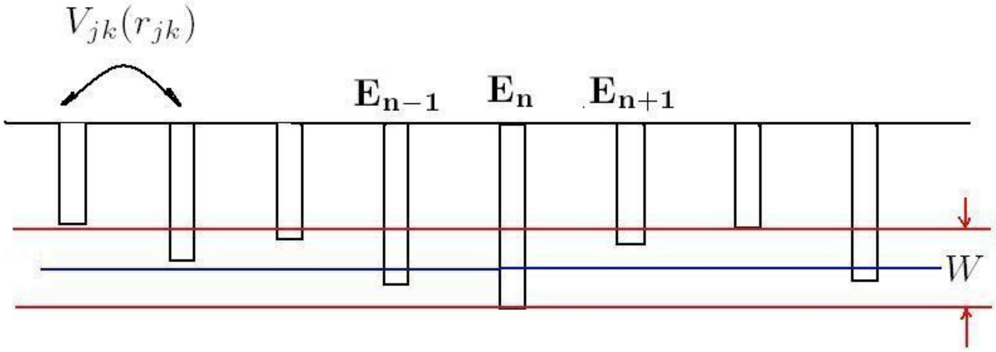

Figure 1: The site-disordered model

The Hamiltonian is,

$$H = \sum_n E_n c_n^+ c_n + \sum_{m,n} V_{m,n} c_m^+ c_n + c.c. \tag{1}$$

where $c_n^\pm$ is the creating and anihilating operators of electron on site n. The Hamiltonian consists of on site potential energy and the hoping term. Here, we only consider the motion of a single electron on this chain. If we set the wavefunction as,

$$\Phi(t) = \sum_n a_n(t) c_n^+ \left|\texttt{vacuum}\right\rangle \tag{2}$$

We will get the equation of motion as,

$$i\frac{da_j}{dt} = E_j a_j + \sum_{k \neq j} V_{jk} a_k \tag{3}$$

After a Laplace transformation $f_j(s) = \int_0^\infty e^{-st} a_j(t) dt$ and setting the initial condition as $a_0(0) = 1$,$a_{j\neq 0}(0) = 0$, we have the following equation of motion,

$$\begin{aligned} i[sf_j(s) - a_j(0)] &= E_j f_j + \sum_{k\neq j} V_{jk} f_k(s) \\ f_j(s) &= \frac{i\delta_{0j}}{is - E_j} + \sum_{k\neq j} \frac{1}{is - E_j} V_{jk} f_k(s) \end{aligned} \tag{4}$$

This equation can be solved by iteration, which reads,

$$f_0(s) = \frac{1}{s + iE_0 - iV_c(0)} = \frac{1}{s + Im[V_c(0)] + i(E_0 - ReV_c(0))} \tag{5}$$

$$V_c(0) \equiv \sum_k \frac{V_{0k}^2}{is - E_k} + \sum_{k,i} \frac{V_{0k}V_{kl}V_{l0}}{(is - E_k)(is - E_l)} + \cdots \tag{6}$$

For simplify, we can assume $V_{k\neq j\pm 1} = 0$ and $V_{j\pm 1,j} = V$, that is the on-site disorder tight-binding model.

To tell whether the system is in a localized state (insulating state) or extended state (metallic state), we need a quantity. The most natural way is the conductivity (or conductance which will be used on next section). But since we are solving the wavefunction, a quantity directly related to the wavefunction will be more convenience. This quantity is so-call `return probability`. It is defined as the probability to find the electron on the initial original site 0. If we can find the electron on the original site with a probability one, that means it is a localized state, i.e. the system is a insulator. If this probability is zero, which means the electron has gone away, thus we have a extended state or metallic state. We have two limit cases, one is $W = 0$ which means the on site potential is fixed constant. We know this situation correspond to the Bloch wave which is a extended state. Another limit case is $V = 0$ which means no hoping from site to site, that is the localized state. This two cases can be characterized by a quantity $\frac{W}{V}$ of which is 0 and ∞ respectively. And between these two limit cases, we should have a transition which is the so called Anderson transition at a critical value $(\frac{W}{V})_c$.

The return probability is determined by $|a(t \to \infty)|^2$ thus by $f_0(s)$. And the property of $f_0(s)$ is determined by the crucial quantity $V_c(0)$. You can see from equation(5), the physical meaning is that a state with a perturbation energy $(E_0 - ReV_c(0))$ will decay at a rate of $e^{-Im[V_c(0)]t}$. Thus,if $Im[V_c(0)] \neq 0$, the life time for this state is $1/Im[V_c(0)]$, which means that it will die out and cannot go back to the original site. That is the extended state. On the other hand, if $Im[V_c(0)] = 0$, this state doesn't decay. Then the electron always have enough time to can go back to its original site although it has a finite amplitude $a_0(t \to \infty)$ smaller than one due to spread to the neighbor site. It is the localized state.

In his paper, Anderson used the perturbation theory order by order and discuss the convergence of the series. Because the energy E_j is a random variable, the calculation becomes more complicated, the result is the quantity of $V_c(s)$ with probability distribution. The conclusion is just as what we have said, there is a region in which $Im[V_c(0)] \to 0$ as $Re[s] \to 0$ with a probability one. That is the localized state.

3 Scaling theory of localization

In the above section,we have introduced a simplified on-site disorder model based on perturbation theory. This model give rise the conclusion that disorder can induced localized state. In this section, we will use a more powerful tools, renormalization group to get some more general knowledge about the localization. That is the so called scaling theory of localization[4].

This theory based on one character quantity, dimensionless conductance (NOT conductivity), defined as,

$$g(L) = \frac{2\hbar}{e^2} G(L) \tag{7}$$

Where L is the system size. Our purpose is to see how the dimensionless conductance varies with the system size L. If $L \to \infty$, $g(L)$ divergent, then we have extended state. On the contrary, if $g(L)$ monotonically tend to zero, then it is localized state. The behavior of the conductance $g(L)$ is determined by a function $\beta(g(L)) = \frac{d\ln(g(L))}{d\ln(L)}$ as we always define in renormalization group theory. If β is positive, we have divergent $g(L)$ as $L \to \infty$, thus extended state. If β is negative, we have zero $g(L)$ thus the localized state.

The basic idea is assuming that $\beta(g(L))$ is a monotonic increasing function (The first assumption). Then for the large and small $g(L)$, the author argue the asympotitics of $\beta(g(L))$ from general physical consideration.

For large $g(L)$, the macroscopic transport theory work well. The conductance depends on the following variables,

$$\frac{2\hbar}{e^2} G(L) = \frac{\Delta E(L)}{dE(L)/dN} \tag{8}$$

$\Delta E(L)$ is the geometric mean of flucutuation in energy level (not exactly but accuarate enough here), $dE(L)/dN$ is the mean spacing of the energy levels. Supposing that we have a constant density of charge carrior n_e, $dE(L)/dN = (n_e L^d)^{-1}$. $\Delta E = \frac{\hbar}{\tau}$ where τ is the mean free time. If assuming that the pure system (without disorder) can be described by the Fermi liquid theory (The second assumption), $\tau = (\frac{L}{2})^2/D_0$ where D_0 is the diffusion constant. So the dimensionless conductance behavior as,

$$G(L) = \frac{g(L)}{2\hbar/e^2} = \sigma L^{d-2} \tag{9}$$

so that,

$$lim_{g\to\infty} \beta_d(g) = d - 2 \tag{10}$$

For small $g(L)$, exponential localization is expected, so,

$$g = g_a e^{-\alpha L} \tag{11}$$

Hence,

$$\lim_{g\to 0} \beta_d(g) = -\alpha = \ln[g/g_a(d)] \tag{12}$$

Combining the above the asymptotic behavior, we have,

$$\frac{dg}{d\ln L} = g(d - 2 - \alpha/g) \tag{13}$$

$$\frac{d\ln g}{d\ln L} = (d - 2 + ...) \tag{14}$$

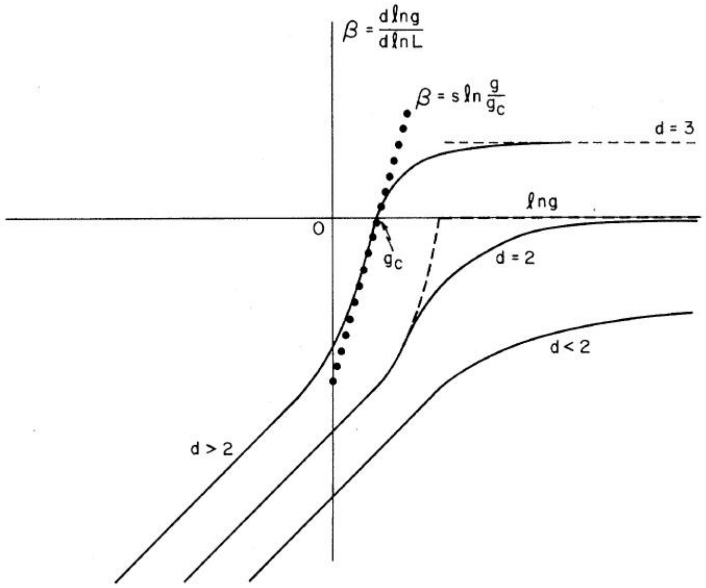

Figure 2: Plot of $\beta(g)$ vs $\ln g$ for $d > 2$, $d = 2$, $d < 2$. From [4]

A schematic curve for $d \ln g/d \ln L$ vs $\ln g$ is shown in figure(2). We can see for $d \leq 2$, we always have negative $\beta(g)$, so the conductance $g(L)$ will always decay to zero. This implies the absence of metallic state in $d \leq 2$ dimensions.

For $d > 3$ dimension, there exist a critical value g_c such that $\beta(g_c) = 0$. By linearizing the $\beta(g)$ function around g_c, another result from scaling theory is that near the critical point on the extended state side (more specifically, the mobility edge), the conductivity is,

$$\sigma = A \frac{e^2}{\hbar} \frac{g_c}{L_0^{d-2}} |\epsilon|^{(d-2)/s} \tag{15}$$

where A L_0 are constant, g_c is the critical point of g and $|\epsilon|$ is the distance to the mobility edge. $s = 1/\nu$ and ν is the exponent of the localization length. The exponent $(d-2)\nu$ is the conductivity exponent which can be measured from experiments.

4 Escape from localization: random dimer model

In the above section a strong conclusion is draw that for $d \leq 2$, the metallic state behavior is absence and the conductivity behavior as a power law on the mobility sides. This agrees with some experimental result such as conductivity exponent results. But it is also contradict to some experiments which show the existence of metallic state in $d \leq 2$ in disordered system. So physicist need to explain why.

According the Anderson localization theory based on perturbation theory, the localization appear only at some circumstance such a fitable value of W/V,or density. If you get out of these parameter region, we can escape from localization. But the point is for the scaling theory, there always is absence of metallic state no matter the parameter values. So we need a circumstance for the scaling theory to fail. As we have mention, the scaling theory based on two assumptions, one is that $\beta(g)$ is a monotonically increasing function. The second one is for pure system, it can be described by a `Fermi liquid`[1]. So we can have a possible way to escape from localization. That is the pure system is in the superconductivity state. Although the electron will be localized by disorder, if they form Cooper pairs, they can escaper from localization. But in this section, we focus on another possibility to escape from the localization, that is the quantum dimmer model.

For the on site disorder model of Anderson, one always assume that the site energy or the matrix elements are statistically independent. That is E_n is statistically independent to $E_{n\pm1}$ and other site energy. But in a real system, the site energy and matrix elements are always statistically dependent. We consider a modified on-site disorder tight-binding model. For simplify, the site energy are assumed to have only two value E_a and E_b with probability q and $1-q$. The equation of motion becomes,

$$i\frac{da_n}{dt} = E_n a_n + V\left(a_{n+1} + a_{n-1}\right) \tag{16}$$

The initial condition is set to $a_m(0) = \delta_{m,0}$ and choosing the most disorder case $q = \frac{1}{2}$. And from the site amplitude $a_n(t)$, the mean square displacement can be calculated to see whether it is a extended state or a localized state.

$$\bar{m^2} = \sum_m |a_m(t)|^2 \tag{17}$$

For different $(E_a - E_b)/V$, the $\frac{\bar{m^2}}{(Vt)^{3/2}}$ versus t are shown in figure(3)

We can see for $\frac{(E_a-E_b)}{V} < 2$, the mean square displacement divergent with time, thus the extended state. $\frac{(E_a-E_b)}{V} \geq 2$, the mean square displacement is decay to zero, thus the localized state.

To understand this, let us have look at the scattering process first. Assuming the random dimer is on the site $0, 1$ and assuming the following site amplitude,

$$a_n = \begin{cases} e^{ikn} + Re^{-ikn} & (n \leq -1) \\ Te^{ikn} & (n \geq 1) \end{cases}$$

$$a_0 = 1 + R = T\left(E_- e^{-ik} + V\right)/V \tag{18}$$

$$E_- = E_a - E_b \tag{19}$$

Then the refection probability is,

$$|R|^2 = \frac{(W + \cos k)^2}{(W + \cos k)^2 + \sin^2 k} \texttt{ where } W \equiv \frac{E_-}{2V} \tag{20}$$

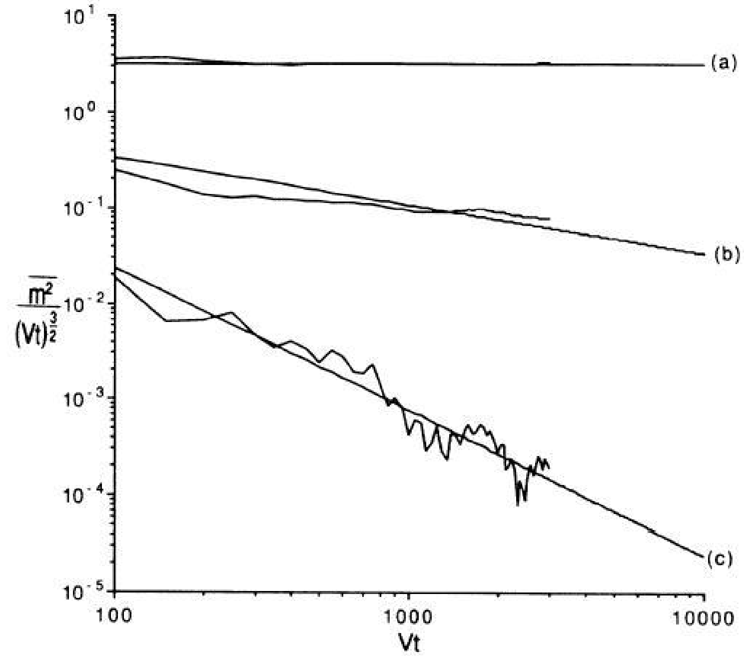

Figure 3: The mean square displacement divided by $(Vt)^{3/2}$ for different disorder (a) $\frac{(E_a-E_b)}{V}=1$ (`superdiffusion`) (b) $\frac{(E_a-E_b)}{V}=2$ (`diffusion`) (c) $\frac{(E_a-E_b)}{V}=3$ (`localized`) From[5]

We can see if $W = -\cos k$, $R = 0$ which mean a perfect transmitted electronic state at $k_o = \cos^{-1} W$. This is possible when $W \in [-1, 1]$. In fact, it is a kind of resonance effect that the refection from the second site of the dimer is completely out of phase with one from the first site.

From this scattering process, we can see at $k_o = \cos^{-1} W$ electron can propagate through any dimer with a perfect transmission. Now we need to consider the disordered chain case. The transport across the chain can be described by the product of transfer matrixes,

$$T_a^{n_1} T_b^{2n_2} T_a^{n_3} T_b^{2n_4} \cdots \tag{21}$$

And the tranfer matrix is defined as,

$$\left(\begin{array}{c} a_{n+1} \\ a_n \end{array} \right) = \left[\begin{array}{cc} \frac{E-E_n}{V} & -1 \\ 1 & 0 \end{array} \right] \left(\begin{array}{c} a_n \\ a_{n-1} \end{array} \right) \tag{22}$$

The transmition through the dimer T_b is,

$$T_b = \left[\begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right] \quad T_b^2 = (-1) \left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right] \tag{23}$$

So the phase change through a dimer is $-2k + \pi$. So the phase of different site are[1],

$$e^{-i2k}, e^{ik}, 1, -e^{-ik}, -1, e^{ik}, 1, e^{2ik}, \ldots \tag{24}$$

It is still Bloch wave that can propagate through the whole chain.

Here the situation is different from Anderson's model. In Anderson's model,if W is less than a certain critical value W_c ($W_c < 1$), we always have extended state. That is independent of the wave vector. In the random dimer model, $W \leq 1$ is not enough to give rise a extended state. To have a extended state, we should have a certain resonance wave vector. So we can have a region $[W_c, 1]$ in which state should be localized predicted by the Anderson localization theory, but in fact it could be extended state due to resonance. That is the main result of random dimer model.

5 Numerical Experiment: Polyaniline as a Random Dimer Model

The above model seems theoretical beautiful. But is it just a idealized model of theory, or a real model based on real world? In this section, a suitable material which will be shown to have the behavior of quantum-dimer model,the Plyaniline, is introduced.

Based on the scaling theory of localization, in 1 dimension disordered system, there is not metallic state. But in some experiments, physicist do find the

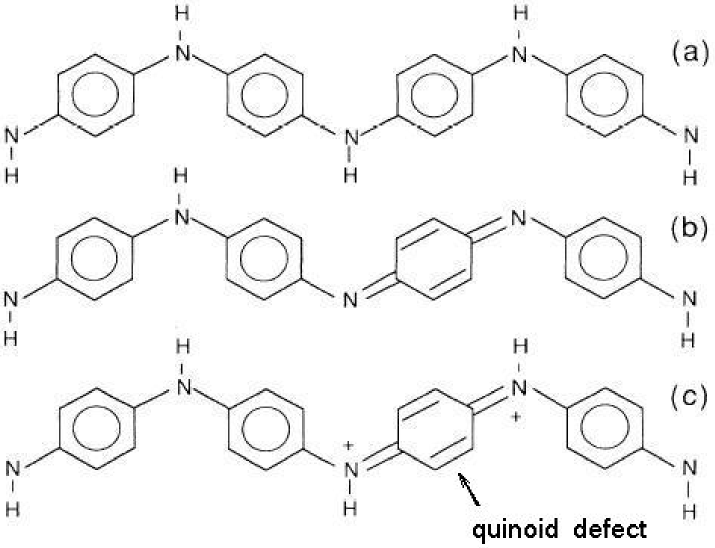

Figure 4: Parent forms of polyaniline: (a) leucomeraldine, (b) emeraldine ,`((a) & (b) are unprotonated)` (c) `protonated` emeraldine. From [6]

insulator-metal transition in the disordered conducting polymer. A example is the Polyaniline.

The Polyaniline are linear chain constructed by connection of three parent forms which are shown on the figure(4),

The quinoid defect in the emeraldine can be viewed as a dimmer (shown in figure(4,5)). The polyaniline can be map to random dimer model in the following way, see figure(5),

The different between the reduced model with the original one is that there are two transfer matrix elements on this model. Just following the calculation of the random dimer model, the reflection probability is,

$$|R|^2 = \frac{(V_1^2 - V_0^2 - W^2 - 2V_0 W \cos k)^2}{(V_1^2 - V_0^2 - W^2 - 2V_0 W \cos k)^2 + (2V_0 V_1 \sin k)^2} \tag{25}$$

In the real system, using the resonance energy for benzene which is ≈ 2.5`eV` as unit of energy β, and just noticing that $E(\beta)$ could be viewed as $\hbar^2 k^2/2m$, the numerical results are shown in figure(5),

For both protonated and unprotonated quinoid,the reflection coefficient is zero between -0.32β and -0.29β. This means that at this region, the electron are completely unscattered by the quinoide defect thus, behavior as a metallic state. This result agree with the numerical calculation which shows that at a protonated level of 50% (most disordered case), at the range of -0.21 to -0.35β, this kind of polymer exhibits its maximum conductivity (more metallic state).

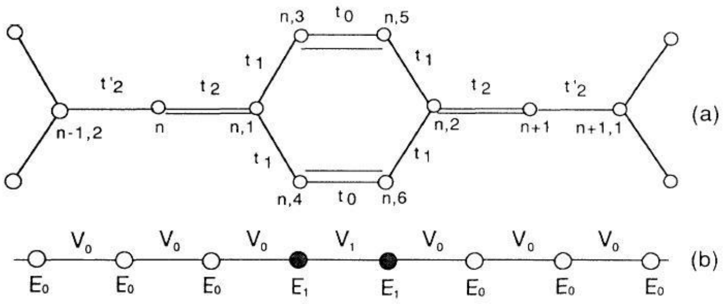

Figure 5: (a) A typical quinoid defect in emeraldine. n `(nitrogen atoms)` t_i `(transfer matrix elements)` (b) The random-dimer model of meraldine. V_i `(effective transfer matrix elements)` E_i `(on site energy)` From[6]

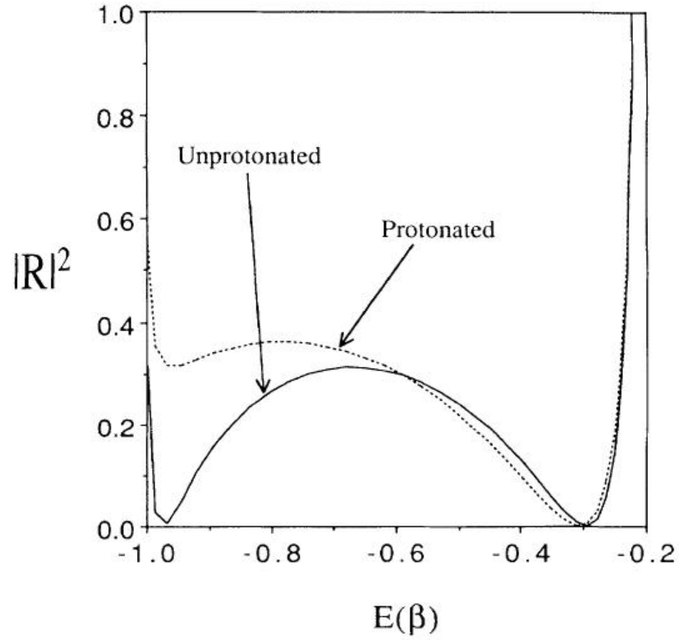

Figure 6: Reflection coefficient through a protenated and unprotonated quinoid defect

6 conclusion

This term essay have reviewed some important results on Anderson localization ,scaling theory of localization and the defiant of localization, especially on random dimer model. Application of the random dimmer model to the real polymer conductor are also introduced . This model are shown to be applicable to the insulator-metal transition in the conducting polymers.

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