Self-avoiding random walks and the two-dimensional localization theorem

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We have addressed one of the most important and basic results in disordered systems, namely the complete localization of noninteracting electrons in two dimensions even at infinitesimal disorder. We present a proof of this assertion by combining some finer aspects of the behavior of self-avoiding random walks with Anderson's original approach to localization where a renormalized perturbation expansion of self-energy, whose terms have the self-avoiding random-walk character, was analyzed.

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Anderson's demonstration that an electron can be spatially localized in a medium of random potential[1] has had far reaching impact on a number of areas of physics. One result that significantly guided the development of the subject, not only in respect to electrons, but also in respect to localization in disparate circumstances such as that of light and other classical waves,[2] is that all states in two dimensions ought to be localized no matter how weak the disorder is.[3,4] Interestingly this result, in spite of being widely applied to rather general situations like a theorem, lacks a proof.

The sensitivity of localization to the dimensionality of the medium was realized soon after its discovery by Mott and others.[5] In one dimension there is Borland's theorem[5] that states that infinitesimal disorder can cause all eigenstates of a noninteracting electron to be localized. It took nearly two decades to realize that the situation in two dimensions could be similar to that in one dimension. However, a substantive formal demonstration of complete localization in two dimensions has eluded us all along.

The two-dimensional localization came in focus when the quantum Hall effect was discovered in two dimensions because extended states were required to carry the Hall current. Soon it was found that the magnetic field could delocalize at least those electrons in two dimensions that were *weakly* localized.[6] As this source of delocalization was found in two dimensions the question whether *all* the rest of the electrons were indeed localized in the Anderson's sense[1] was apparently not probed further. Another situation where the need to scrutinize the two-dimensional localization theorem was felt rather urgently arose when some recent experiments showed a distinct metal-insulator transition in two-dimensional electron systems, albeit as a function of the electron concentration in very dilute electron systems.[7] Studies[8] do indicate that the newly found metal-insulator transition is due to very different conditions than those that were responsible for the previous result[4] that showed absence of the metal-insulator transition in two dimensions. However, notwithstanding the mechanism of the recent result, a convincing way of showing that it has a different origin than the previous result[4] is to show that the previous result can be *proven* to be well founded and correct within the conditions in which it was predicted and observed.

We take this approach and scrutinize Anderson's original theory of localization rather than the scaling theory[4] because of the following dichotomy. Anderson's original tight-binding approach,[1] which was expected to favor localization, did not show the absence of a metallic phase in two dimensions, whereas the scaling theory did, although at the outset it appeared to favor delocalization. Anderson considered an electron as initially localized on a site and then turned on the nearest-neighbor interaction to allow it to diffuse away, whereas the scaling theory treated the electron as a plane wave which was perturbed by disorder. So it should be interesting to take a close look at Anderson's original approach and examine where two-dimensionality plays a special role. We will outline essentials of Anderson's approach, highlight the role of self-avoiding random walks, and invoke their statistics to address the problem at hand.

The renormalized perturbation theory

Anderson[1] studied the diffusion of a noninteracting electron in a lattice whose site energies are random and sufficiently local, overlapping only with those on the nearest-neighbor sites. Whether the electron would be spatially localized or diffuse indefinitely was shown to depend on the convergence or otherwise of the following renormalized perturbation series (RPS) for self-energy S_i on site i:

$$S_i(Z) = \sum_{j\neq i}\left[V_{ij}g_j^iV_{ji} + \left(\sum_{k\neq i,j} V_{ij}g_j^iV_{jk}g_k^{i,j}V_{ki} + \cdots\right)\cdots\right]. \tag{1}$$

Here $g_n^{i,j,\ldots,n-1}=(Z-e_n-S_n^{i,j,\ldots,n-1})^{-1}$ is the Green function; e_n is the site energy on site n, which varies randomly from one site to another; V_{nm} is the transfer integral between the nearest-neighbor sites n and m and takes a fixed nonrandom value, say V; Z is the complex energy $E\pm is$. The RPS converges and is defined term by term if the electron is spatially localized and is unable to diffuse away to infinity.[1] Note that the terms in the RPS have the character of self-avoiding random walks (SAWs) since the superscripts denote the sites excluded once they are traversed in the course of a random walk (i.e., a site is replaced by an infinite potential after the walker steps out of it).

The structure of the RPS is quite involved—not only does it extend to infinity, but each denominator expands into a hierarchy of infinite continued fractions. Each level of the

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continued fractions is an infinite series in which each term sends down infinite continued fractions. This is evident in the following expanded version of Eq. (1):

$$S_i(Z) = \sum_{j\neq i} \frac{V_{ij}}{Z - e_j - \sum_{k\neq i,j} \frac{V_{jk}}{Z - e_k - \cdots}[V_{kj} + \sum_{l\neq i,j,k}, \ldots]} \times \left\{ V_{ji} + \sum_{k\neq i,j} \left[\frac{V_{jk}}{\cdots}[V_{ki} + \cdots] \right] \cdots \right\}. \quad (2)$$

While each term of the RPS represents a closed self-avoiding ring originating and terminating on a particular site (such as $i\to j\to i$, $i\to j\to k\to i$, etc.), a continued fraction represents an open SAW diverging away from a site in a self-avoiding ring without ever returning to it. The latter walks proceed along a hierarchy of rings joined to each other (for an illustration see Ref. 9).

In spite of its complicated structure the RPS has simple convergence properties[1,10,11] as summarized below.

(1) If the RPS for S_i converges then it implies that (a) each term in it is well defined; (b) all the self-energies that appear in the denominators of Eq. (1), i.e., S_j^i, $S_k^{i,j}$, ..., necessarily converge. For if, say, one of these did not converge, then it would not be defined term by term and since the terms appearing in it also appear in the RPSs of other S's (including the S_i), all the RPSs would cease to be defined term by term; (c) all the S's, i.e., S_j^i, $S_k^{i,j}$, ..., must be nonzero. If, say, S_j^i is zero, then it will have to be due to the divergence of $S_k^{i,j}$, in which case the latter will not be defined term by term and in turn, as argued above, all the S's will cease to be precisely defined.

(2) The RPS for S_i can diverge (and cease to be defined) if one of the denominators, say $(Z-e_n-S_n^{i,j,\ldots,n-1})$, vanishes. But such a pole acquired by S_i will be of no consequence, since it will coincide with a zero of the Green function, $g_i(Z)=(Z-e_i-S_i)^{-1}$, which lies outside the energy spectrum.

(3) However, the complex singularities like branch cuts will be of interest. Note that the branch cut of S_i coincides with that of the Green function g_i and therefore represents the spectrum of extended states. Also, the branch cuts of all the S's–S_i, S_j^i, $S_k^{i,j}$,... coincide with each other over the same range of the real Z axis. (In fact this is another way of saying that if there is a range of energy over which the RPS of S_i is not defined, then the RPSs of all the S's will not be defined in the same energy range.)

It is apparent that the extended states will exist in a disordered system, i.e., S_i will have a branch cut, only if the continued fractions in its RPS extend to infinity and they do not converge. This will be possible only if there are SAWs in the system that grow indefinitely. It is in this connection that the dimensionality of the lattice underlying the system plays the central role. The growth of the SAWs as they appear in the RPS is crucially different in two dimensions than in the higher dimensions and this, we will show, is responsible for the special status of localization in two dimensions.

To address the question of complete localization in two dimensions we should first explore if both the RPS of S_i and all the continued fractions emanating from it extend to infinity for all the energies in the spectrum, and if they do, then study their convergence. Their infinite extent would imply that all the S's in the denominators of the S_i RPS, namely S_j^i, $S_k^{i,j}$, ..., are finite and nonzero. If the RPS and the continued fractions were of finite extent, then the RPS would converge trivially. So we should know the conditions under which the SAWs could grow indefinitely in the two dimensions.

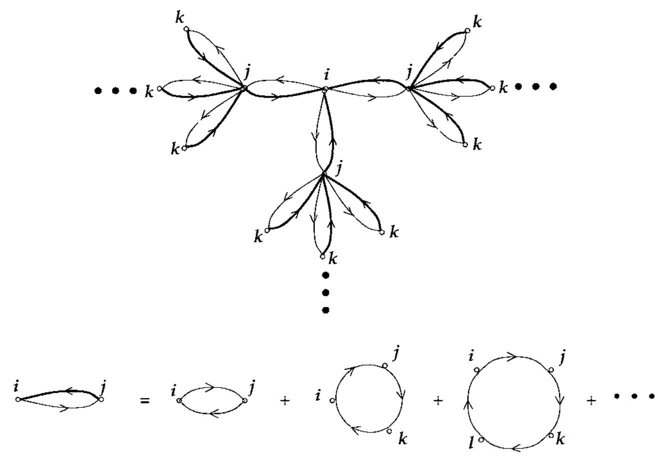

FIG. 1. Schematic representation of the RPS of Eqs. (1) and (2) as a cactus for a square lattice. The SAW rings that make a typical lobe shown are explained in the text.

It is important to realize at the outset that the higher terms in the RPS's of $S_i, S_j^i, S_k^{i,j}$, ..., etc. appear with rapidly decreasing probability because as the number of steps n increases the probabilities for a SAW to (i) cross itself before returning to the origin, or (ii) end up in a cage[12] at one stage or another, build up rapidly. In fact, the probability of *initial ring closure* (i.e., of a SAW terminating at its origin) decreases as $n^{-\theta}$ with θ=11/6 in two dimensions and 23/12 in three dimensions.[13] So the higher terms in the RPS contribute with the weights vanishing as $n^{-\theta}$, and the RPS can be treated as effectively finite. Thus, we ought to only check if the continued fractions in the RPS can be of infinite extent in spite of the above, and if so, whether they would converge.

To visualize the hierarchical arrangement of the RPS terms, which form self-avoiding rings and open SAWs, we represent the RPS of S_i as a cactus, shown in Fig. 1. All the possible SAW rings that originate and terminate at a particular site are represented by a lobe. A lobe is characterized by two sites, the origin and its nearest neighbor to which the walker takes the *first* step, e.g., the lobe attached to the site j represents *all* those SAW rings that originate and terminate at j and necessarily pass through the nearest-neighbor site k. To distinguish between the stepping-out and stepping-in portions of the SAWs, the latter is shown by thicker lines. Note that the set of lobes joined to a site, say i, represents the full RPS and the sets of lobes attached to them represent the RPSs with the site i excluded. The open SAWs that grow along the continued fractions are formed as the walker leaves a lobe after taking the first step and hops on to an adjoining one, and moves on like this.

If we follow the SAWs in a real lattice and map them on to the SAWs in the cactus of Fig. 1, we will realize that the number of SAWs in the cactus is in fact far too large for the

SAWs that can be actually performed in the lattice,[9,14] but the latter form a subset of the former. The situations outlined above require many of lobes in the cactus to be cut off. If, by stepping on a site, the walker is led into a cage, or it tries to cross its path by stepping on a site a second time, then the lobes attached to such sites would become unapproachable and consequently cannot contribute to the RPS. Such lobes and the whole hierarchies of lobes underneath them would become redundant and would have to be cut off. Thus, the cactus of our interest would be a highly trimmed one and would include only those SAWs that can grow *indefinitely* in the given lattice. These SAWs contribute to the denominators of the RPS. Consequently, a rather sparse set of continued fractions in the RPS is of infinite extent and therefore relevant if the extended states have to exist.

An *unrestricted* SAW is certain (with probability 1) to be trapped well before diverging to infinity in a lattice of any dimensionality.[15] In these SAWs the probability of taking a step is $1/q_0$, where q_0=(lattice coordination number 1). However, these SAWs are not the ones that appear in the RPS of S_i. Since in the RPS a traversed site is replaced by an infinite potential, and it becomes inaccessible to the walker when it comes near it, the "one step probability" for the SAWs is 1/(number of unoccupied sites). These SAWs are referred to in the literature as *growing* SAWs (or GSAWs).[16] The short-range memory of these SAWs makes them behave very differently in two dimensions than in three dimensions. We will see in the following that while the probability that a GSAW can grow *indefinitely* approaches 1 in three dimensions as the number of steps n diverges, in two dimensions it approaches *zero* as approximately $n^{-0.64}$. Our strategy is to make it as convenient as possible for a GSAW to grow indefinitely and then study its growth behavior. If in spite of this it shows a tendency to return to a traversed site with probability 1, then we should conclude that a continued fraction in the RPS must terminate at one stage or another as $n \to \infty$.

Indefinitely growing SAWs (IGSAWs)

A GSAW can get terminated if it steps into a cage.[12] By constraining it from entering into a cage we can isolate the SAWs that grow indefinitely (the IGSAWs) from those that get terminated in the cages and get the upper bounds on the probability for a GSAW to grow indefinitely (and therefore for the existence of the infinite continued fractions in the RPS) in two dimensions and three dimensions. We will call this the "smartness condition" because such a walker can sense and avoid going in the direction that leads into a cage. The latter is achieved by setting the probability to step in the direction of the cage to *zero*. In the present context this would mean that in two dimensions, the smartness condition will have to be applied with probability approaching 1 as $n \to \infty$ for a GSAW to grow indefinitely, whereas in three dimensions this probability approaches 0 as $n \to \infty$. The arguments are as follows.

Recall the number of SAWs of n steps is given as

$$Z^{SAW} \propto n^{\gamma-1} q_{eff}^n, \tag{3}$$

where q_{eff} is the effective connectivity of the SAWs (or the number of unoccupied sites) and $\gamma=43/32$ for two-dimensional SAWs as well as GSAWs since they belong to the same universality class.[16] For the number of IGSAWs we make the following ansatz:

$$Z^{IGSAW} \propto n^{\gamma'-1} q'^n, \tag{4}$$

where q' is the effective connectivity of the IGSAWs; $1 < q' \leqslant q_{eff}$. To determine γ' and q' we use the data in the Table 2 of Kremer and Lyklema.[17] By eliminating q' in Eq. (4) we can write γ' for an n-step IGSAW as

$$\gamma'(n) = 1 + \frac{\ln\left(\frac{\zeta(n+1)}{\zeta(n-1)}\right) - \ln\left(\frac{\zeta(n)}{\zeta(n-2)}\right)}{\ln \frac{(n+1)(n-2)}{(n-1)n}}. \tag{5}$$

For brevity we have used ζ for Z^{IGSAW}. Table I lists $\gamma'(n)$ for up to $n=21$. Taking the odd-even fluctuations into account, we get

$$0.695 \leqslant \gamma' \leqslant 0.720. \tag{6}$$

To estimate q', we plotted the ratio of the successive terms in the second column of Table 2 of Ref. 17 as a function of $1/n$ and found that $q'=q_{eff}$=2.638 for the square lattice, which is very close to the best estimate, 2.638 16 of Ref. 18, as expected. We can safely assume that in general, $q'=q_{eff}$ for two dimensions. Thus, we will have

$$Z^{IGSAW}/Z^{SAW} \sim n^{\gamma'-\gamma} \simeq n^{-0.64}. \tag{7}$$

This is a crucial result, as it shows that the fraction of existing SAWs of length n that are able to grow indefinitely in two dimensions approaches *zero* as $n \to \infty$. That is, the infinite continued fractions in the RPS for two dimensions contribute with vanishing weights. The reason for this is the drastic decrease in the value of the exponent γ as we isolate the IGSAWs from the SAWs. This is due to the long-range correlation in two dimensions between the *tip* of a walk (which is the leading point of a walk that moves forward) and the *bead* (which is a traversed point that compels the tip to make the decision to keep away from it) and is responsible for the walker to return to the traversed sites no matter how far away it has gone from them. It therefore increases the frequency of the need for the application of the smartness condition in two dimensions as n increases to force a walk to grow. However, in spite of this, eventually, in the limit of $n \to \infty$, the probability that a SAW can grow indefinitely goes to zero due to the result in Eq. (7).

While in two dimensions a closed loop automatically defines a trap or a cage, the situation in three dimensions is

TABLE I. The IGSAW exponent γ' of Eq. (4) as a function of number of steps n.

$\gamma'(n)$	n
0.7258877	21
0.6920597	20
0.7328707	19
0.6911360	18

much different. In order to define a cage in three dimensions, a closed "basket" has to be present, which does not allow the walk to leak out. A cage the walker can be trapped in, has to be a part of the hull of a connected three-dimensional cluster. The simplest version, which requires the smallest number of steps, is a hole with a surface made of Hamiltonian walks (a completely surface covering SAW in two dimensions).[19] For such cages, however, q_{eff}(Ham. walk) $<$ q_{eff}(SAW, two dimensions) $<$ q_{eff}(SAW, three dimensions).[20] The probability that a region of size L^3 (say) forms a cage goes to zero at least as $[q_{eff}$(Ham. walk in $D-1$ dimensions)/q_{eff}(SAW in D dimensions)$]^{L^2}$. Thus the probability of forming a large cage in three dimensions, in contrast to two dimensions, converges rapidly to 0. So, in three dimensions a cage can always be avoided with the help of the smartness condition and a SAW can grow indefinitely without ever returning to its origin. This would also imply that γ' should be the same as γ in three dimensions.

In conclusion, we have investigated one of the most fundamental questions in condensed matter physics and its allied areas: why should an infinitesimal disorder in potential cause all states of an electron to be localized in two dimensions? We find that the answer was embedded in Anderson's original paper[1] on electron localization. The clues lay in the fact that the number of SAWs contributing to the RPS of the self-energy is far too small than what Anderson considered. Besides, and more importantly, in two dimensions these SAWs have the intrinsic tendency to rapidly return to their origin in spite of the severe constraints we can put to facilitate their growth. This accounts for the convergence of the RPS under all circumstances relevant to the noninteracting electrons in a tight-binding Hamiltonian. The result is applicable to all the situations that can be mapped on to the framework of the electronic problem.

It is also important to note that new insights into the localization in three dimensions can be gained if q' is computed for the IGSAWs in different three-dimensional lattices. This will enable the exact calculation of a number of localization properties using the formalisms developed in Refs. 21 and 22.

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