Weak Disorder in a Two Dimensional Lattice

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1 Introduction

In 1958, P. W. Anderson showed that for particles in a lattice with strong disorder, the wavefunctions do not diffuse through the system in the way that is expected from Bloch waves. Instead, they are located in a single region, with an exponential amplitude falloff as you travel further from the center of the wavefunction. This property of the wavefunction became known as localization.

The existence of localized states, versus extended states, is important because of its application to the behavior of electrons in solids. The localization of electrons within a solid is inversely correlated to the conductivity of that solid. Conductors, which approach finite conductivity as you go to lower and lower temperatures, have extended electron states. Insulators, whose conductivity goes to zero as temperature goes to zero, have localized states. Because of the significance of the concept of localization through disorder, for his work in on the subject, Anderson eventually earned the Nobel Prize.

However, practically, we are interested in cases where the disorder of the solid is not necessarily strong. For example, a doped semiconductor can be thought of as a weakly disordered lattice. Though, when considering weak disorder, the behavior of electrons within the lattice is less clear. For a one dimensional lattice, any amount of disorder results in localization. But, for a two dimensional lattice there isn't consensus on the behavior of the electrons. There have been attempts to show that any amount of disorder in two dimensions result in localized states. However, we have found 2D objects which appear to be conductors.

Thus, we investigate weak disorder in the two dimensional case. We would like to know what kind of disorder is required to produce localization.

2 Anderson Model

The model we use to investigate disorder is the same as the one Anderson used in his 1958 paper. We consider a single electron and a square lattice, where the electron's wavefunction is defined at each point in the lattice. The Hamiltonian

for this system is defined to be

$$\hat{H} = -\sum_{(n,n')} a_n^\dagger a_{n'} + \sum_n \epsilon_n a_n^\dagger a_n. \tag{1}$$

n sums over all sites, and(n, n') sums over all nearest neighbors. $a_n^\dagger$ and a_n are the creation and annihilation operators respectively. ϵ_n is a small energy associated with the site n, and which introduces the disorder into the system. In our model, the ϵ_n are randomly distributed over some finite range for a disordered system. The more disordered the system, the wider that range is. For a system with no disorder, $\epsilon_n = 0$ for all n.

To illustrate how this Hamiltonian operates, consider figure 1.

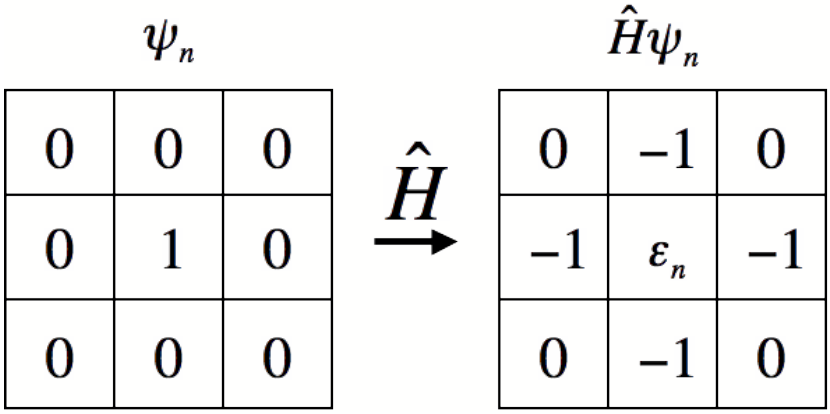

Figure 1: An illustration of how the Hamiltonian operates.

This Hamiltonian is known as the hopping matrix for this system, because it gives a negative energy for the electron "hopping" from one site to an adjacent site in the first term of the Hamiltonian. The fact that the energy is negative tells us that the electron typically tries to spread out to it's nearest neighbors, diffusing through the system. If there was no disorder, and the ϵ_n were zero, then the electron would diffuse outwards in a Bloch wave state. However, behavior is more complicated when we introduce disorder, which randomizes the energy associated with the electron staying in the same site.

3 Lanczos Algorithm

If you have the matrix $\hat{H}$, and you have an orthonormal set of electron states $\psi_0, \psi_1, \psi_2, ..., \psi_m$, which spans the subspace S_m then the best approximation of the eigenvalues of $\hat{H}$, $(\lambda_0, \lambda_1, ..., \lambda_m)$, which correspond to eigenstates in S_m are given by the eigenvalues of the matrix $T_m = L^T \hat{H} L$, where $L = (\psi_0, \psi_1, \psi_2, ..., \psi_m)$. If S_m is the subspace spanned by $\psi_0, \hat{H}\psi_0, \hat{H}^2\psi_0, ..., \hat{H}^{m-1}\psi_0$,

then T_m is tridiagonal of the form

$$\begin{pmatrix} a_1 & b_1 & \cdots & 0 & 0 \\ b_1 & a_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a_{m-1} & b_{m-1} \\ 0 & 0 & \cdots & b_{m-1} & a_m \end{pmatrix} \tag{2}$$

From the relation $T_m = L^T \hat{H} L$, we get the expressions

$$a_i = \psi_i \hat{H} \psi_i \tag{3}$$

$$b_{i-1} = \psi_{i-1} \hat{H} \psi_i. \tag{4}$$

Also, since $L^T = L^{-1}$, we get that $LT^m = \hat{H}L$, and since T^m is diagonal, we get the relation

$$\hat{H}\psi_i = b_{i-1}\psi_{i-1} + a_i\psi_i + b_i\psi_{i+1}. \tag{5}$$

Note we can also flip the signs on equations (3), (4), and (5) and they would still be true.

If we know ψ_{i-1}, ψ_i, and $\hat{H}$, then, since a_i and b_{i-1} are determined in terms of those objects, it is possible to determine $b_i\psi_{i+1}$. Then, since we know that the electron's wavefunction ψ_{i+1} is normalized, we can also find ψ_{i+1} and b_i.

Thus, we have a method by which we can generate any sized tridiagonal matrix whose eigenvalues approximate those of $\hat{H}$. All we need are two initial wavefunctions to start the process. We choose the initial two states to be ψ_0, which represents the absence of an electron, with all entries in the lattice being zero, and ψ_1, which represents the state where the electron's wavefunction is completely located at the origin. We can carry out the process of finding new elements of the tridiagonal infinitely using these two states.

4 Results With No Disorder

When we don't include any disorder in our Hamiltonian, and we carry out the Lanczos Algorithm, we see some very consistent behavior. The region in which the wavefunction is nonzero is called the support. The support of each sequential wavefunction expands by one unit along the edges of the lattice, producing a square. However, the wavefunction behaves differently as you go away from the origin, depending on the angle you have with the axis. For example, along the diagonal of the lattice, the wavefunction is an oscillating, analytically derivable function. It's maximum occurs at the edge of the support as shown in Figure 2. While, along the axes, the function is not analytically derivable, and the maximum comes at approximately $1/\sqrt{2}$ times the distance to the edge of the support, and you can see in figure 3.

To get a better picture of the system as a whole, consider the three dimensional plot of the wavefunction, provided in Figure 4. The maximum we

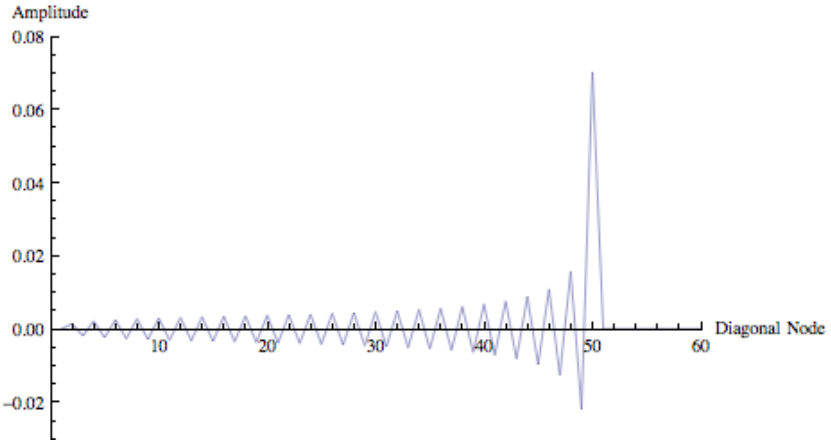

Figure 2: The wavefunction along the diagonal for the 100th iteration of the Lanczos method.

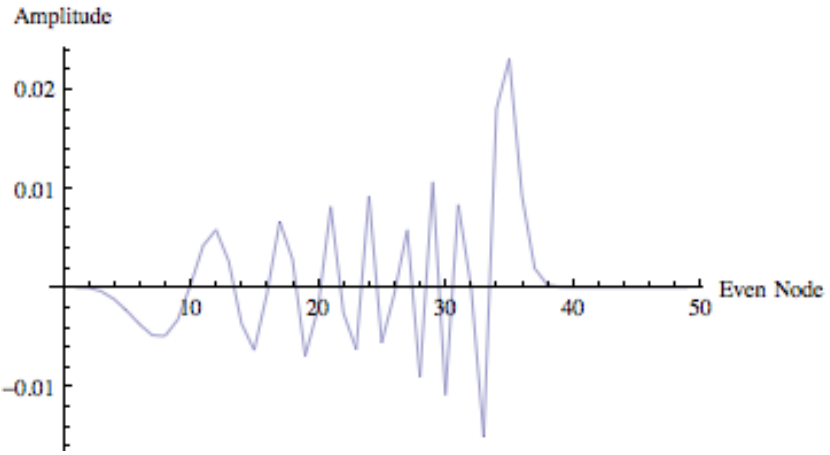

Figure 3: The wavefunction along the axis for the 100th iteration of the Lanczos method.

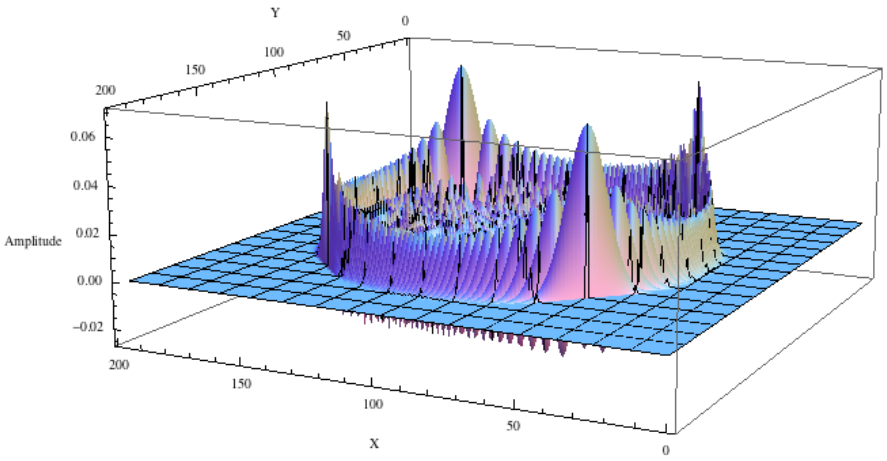

Figure 4: The wavefunction with no disorder after 100 iterations.

mentioned earlier appears to have a circular shape, and its height appears to decrease as $1/n$. These wavefunctions are like a wavefront which is propagating outwards at a constant speed with every sequential iteration. In the resulting tridiagonal matrix $b_n = 2$ and $a_n = 0$ for all n.

5 Results With Disorder

To begin the investigation of disorder, we examined the simple case of a single impurity. We simulate a single impurity in the lattice by introducing a small energy ϵ_i at a single site. The result of this impurity can be viewed as the scattering of the wavefront shown in figure 4 off of the impurity. This is illustrated in Figure 5. You have multiple wavefronts propagating from the source, and

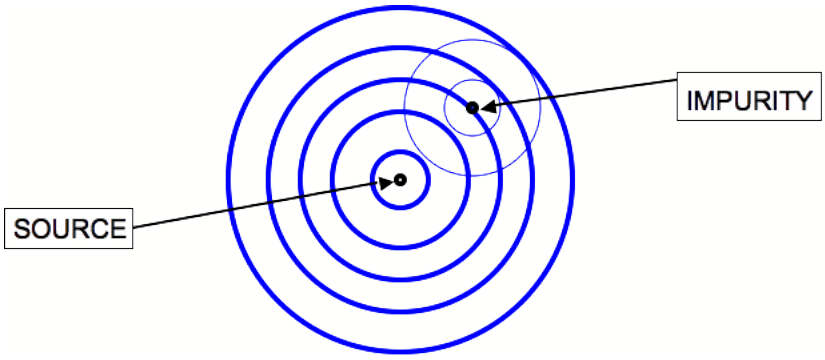

Figure 5: Scattering of wavefronts off of an impurity.

when they interact with the impurity, wavefronts of a much smaller amplitude propagate out from the impurity with the same speed as the original wave.

It should be noted that we can see the diagonal element of the Tridiagonal as a measure of the disorder that is caused by the impurity. When we run the calculations with a single impurity, we find that the diagonal element a_n spikes when the wavefront reaches it, and then decreases over sequential iterations, as shown in Figure 6.

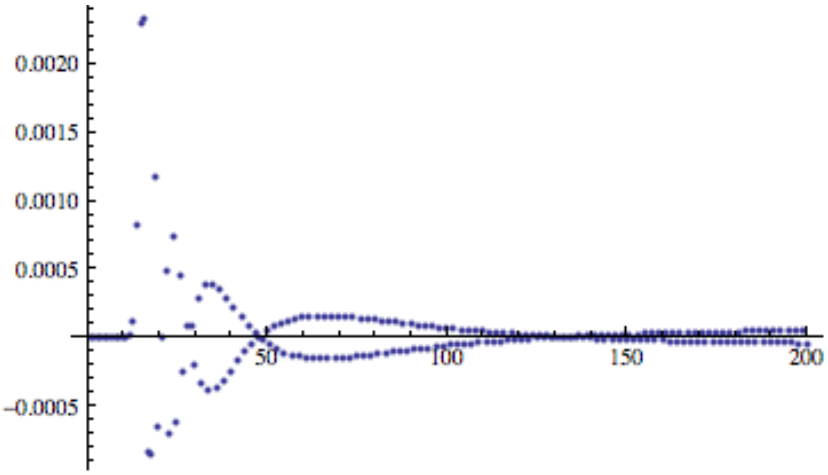

Figure 6: Result of one impurity on the diagonal element of the tridiagonal.

This helps us understand what happens when we consider the case of uniform random disorder. In this case, at every point we have an energy ϵ_n which is selected randomly from a finite range. When ϵn is selected from a small range, we can view the disorder in the system as being caused by the sum of disorder of each individual point. With each iteration, the wavefront propagates outwards, encountering new disorder at each site, which is uncorrelated with the previous disorder. Because the height of the wavefunction at the wavefront is $1/n$, each term at the wavefront contributes approximately w^2/n^2 to the variance of the system, where w is the standard deviation of the energies at each site. Since there the number of sites at the wavefront goes as n, we get that the sum of the variance should go as

$$w^2/n. \tag{6}$$

When we carry out the calculation with ϵ_n selected from the range $(-.1, .1)$, we get that the diagonal element of the tridiagonal has the behavior, which is shown in figure 8.

The variance of this function has the expected behavior, because the variance appears to match the function we derived, as shown.

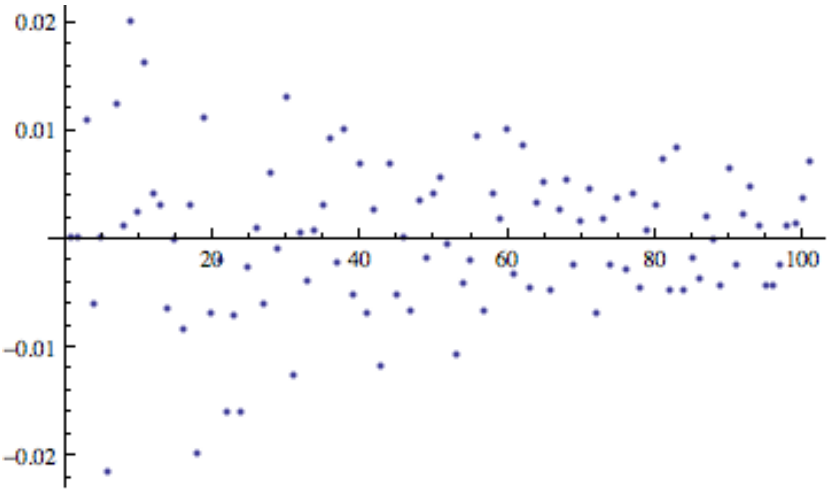

Figure 7: Result of uniform random disorder on the diagonal element of the tridiagonal.

6 Analysis

With our calculated tridiagonal matrix, it is possible to attempt to answer the question of whether or not we have localization for various disorders. However, to do this, we need to introduce the Green matrix for the tridiagonal T_m, which is defined $R(E) = (EI - T_m)$, and for which the corner element $R_{1,m}$ is the probability of the electron jumping from the across the support of the lattice.

$$R(E)_{1,m} = \frac{\prod_{i=1}^{m-1} b_i}{det(EI - T_m)} \tag{7}$$

For extended states, $\sqrt[m]{R(E)_{1,m}} \to 1$ as $m \to \infty$. For localized states $\sqrt[m]{R(E)_{1,m}} \to$ goes to a number less than one as $m \to \infty$. The Lyapunov exponent is defined to be $\lambda = -ln|\sqrt[m]{R(E)_{1,m}}|$, or

$$\lambda = -\frac{1}{m}(\sum_{i=1}^{m-1} ln|b_i| - \sum_{i=1}^{m} ln|E - E_i|), \tag{8}$$

where E_i are the eigenvalues of T_m. We get the condition that for localized states, λ approaches a number greater than zero as $m \to \infty$, and $\lambda \to 0$ as $m \to \infty$ if the state is extended.

When we calculate the lyapunov exponent for sequential iterations, we get figures 9-11.

The results are difficult to interpret. For instance, it is difficult to distinguish qualitatively between the case where $disorder = .1$ and the case where $disorder = 1$. This is odd, because a disorder of one seems like it would be

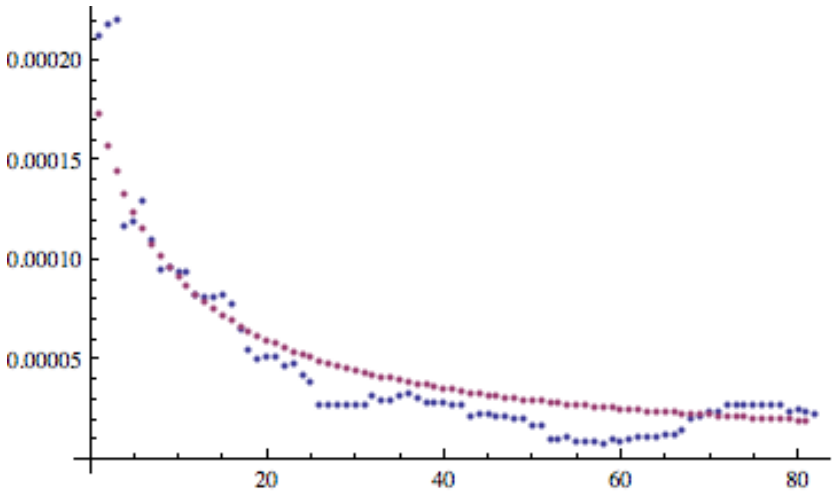

Figure 8: The blue points are the calculated variance from the iteration, and the purple points describe the theoretically derived variance.

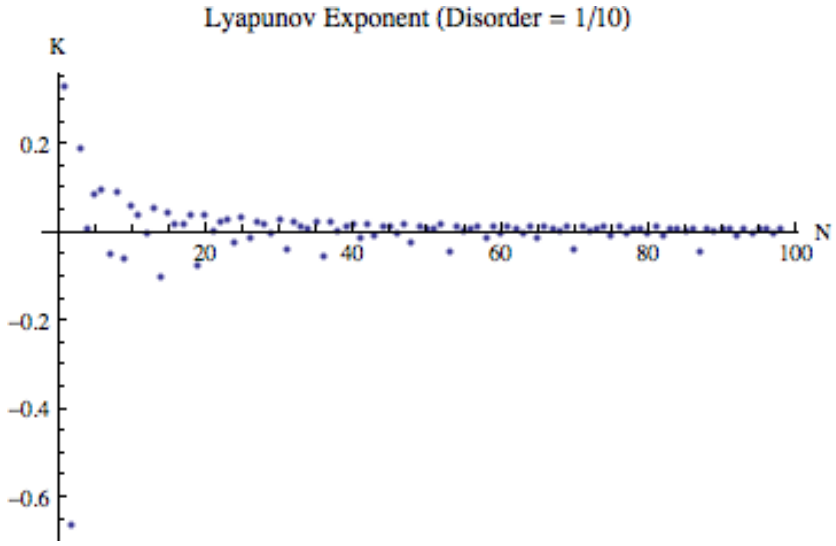

Figure 9: Lyapunov exponent for the system with disorder=.1.

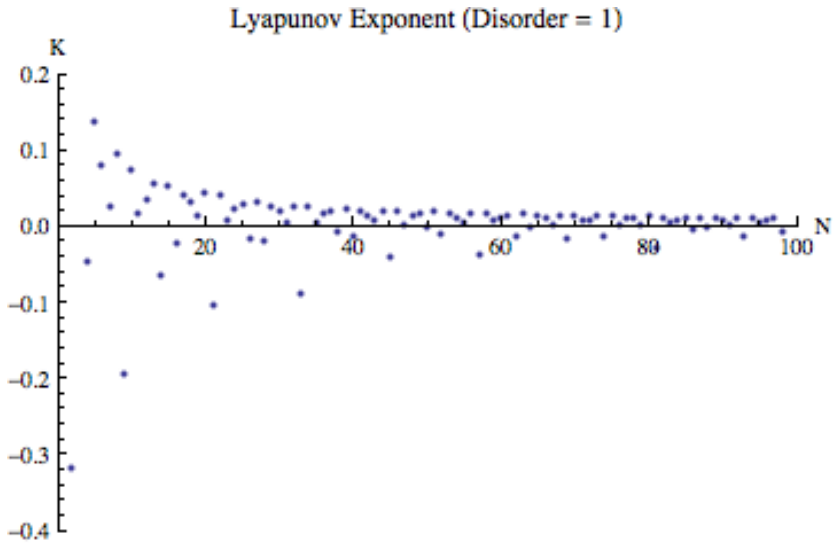

Figure 10: Lyapunov exponent for the system with disorder=1.

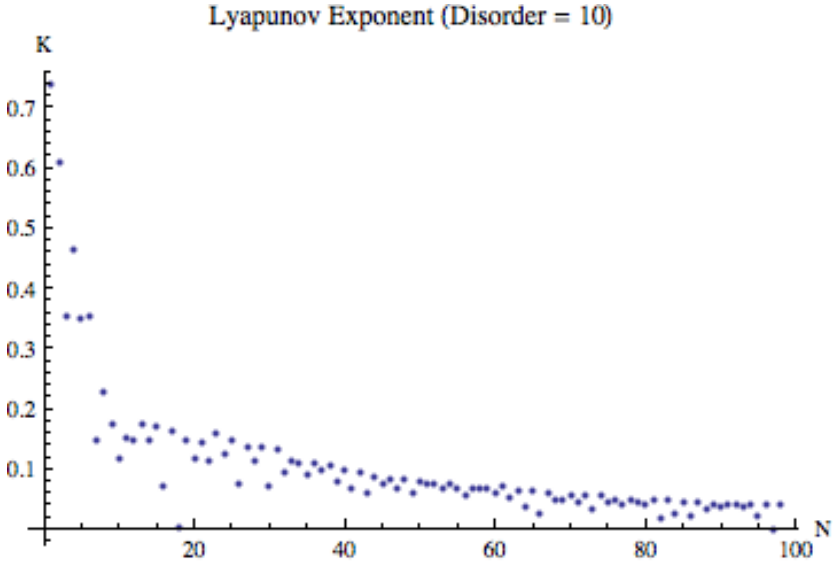

Figure 11: Lyapunov exponent for the system with disorder=10.

close to the case of strong disorder, where the wavefunction should be localized. However, if there is a distinction, it's hard to tell. All the cases appear to be converging to some limit, but it is difficult to tell from these results whether or not the Lyapunov exponent is converging to zero, or a positive number.

So, in terms of answering our original question, of whether or not any amount of disorder yields localization, we need to do more work. We have the tools to generate the data necessary to answer the question, but we still need to find out how we can analyze this system.

7 Acknowledgements

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References

[1] P.W. Anderson, *Phys. Rev.* **109**, 1492 (1958)

[2] D. C. Herbert and R. Jones, *J. Phys. C : Solid St Phys.* **4**, 1145 (1971)

[3] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, *Phys. Rev. Lett.* **42**, 673 (1979)