Band tails, length scales, and localization

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The one-parameter scaling theory of Anderson localization is discussed in the light of recent numerical results. It is argued that apparent violations of scaling can be understood as crossover phenomena, which should be expected to occur whenever the density of states varies rapidly near the mobility edge. The apparent existence of a sharp effective band edge for some two- and three-dimensional models with off-diagonal disorder, and the consequences for spin-glass models which follow from this, are also considered.

I. INTRODUCTION

The one-parameter scaling theory[1] of Anderson localization,[2] which is based on the idea that the behavior of the Thouless number,[3,4] as a function of length scale determines the localization length, has been enormously successful.[5,6] Recently, however, some numerical calculations have suggested[7–10] that this theory does not provide a complete classification of the mobility edge behavior of two- and three-dimensional systems. In addition, it has been known for several years that there exist one-dimensional models of smoothly varying potentials[11,12] which fall outside the scope of the simple scaling theory. In this work we will attempt to provide a framework with which we can understand the apparent exceptions to the scaling theory.

For definiteness, we consider a tight-binding Hamiltonian with one orbital per site and nearest-neighbor hopping:

$$H=\sum_i \varepsilon_i \mathbf{c}_i^\dagger \mathbf{c}_i+\sum_{\langle i,j\rangle} \nu_{ij}\mathbf{c}_i^\dagger \mathbf{c}_j+\nu_{ij}^*\mathbf{c}_j^\dagger \mathbf{c}_i\,, \qquad (1)$$

where we will assume that the sites form a (hyper)cubic lattice, and $\langle i,j\rangle$ indicates a sum over neighbor pairs. When all of the ν_{ij} are set equal to a constant V, and each ε_i is an independent random variable chosen from a rectangular probability distribution of width W, this becomes the standard Anderson model.[2] Due to gauge invariance, there is no loss of generality in choosing V to be real and positive. Another case which has received a great deal of attention is the random hopping model,[13] for which we choose all of the ε_i to be zero, and make the ν_{ij} independent, identically distributed random variables. The random hopping model is closely related to the Ising spin glass.[10] We will not explicitly consider the electron spin in this work.

II. ONE-PARAMETER SCALING

The one-parameter scaling hypothesis assumes that the properties of this model at some energy E are described by the function

$$\beta(g)=\frac{d\,\ln(g)}{d\,\ln(L)}, \qquad (2)$$

where $g(E,L)$ is the expectation value (averaged over the randomness) of the conductance at the energy E of a (hyper)cube of length L. The β function is claimed to be universal, meaning that it should be independent of E and of the probability distribution for the randomness.

We can rewrite the conductance as

$$g(E,L)=n(E,L)e\mu(E,L)L^{d-2}, \qquad (3)$$

where n is the electron density of states, e is the electronic charge, μ is the electron mobility, and d is the number of space dimensions of the lattice. In a metallic phase, μ rapidly converges to a finite constant as L increases, while in an Anderson-localized phase it behaves like $\exp[-2L/\lambda(E)]$ for large L, where $\lambda(E)$ is the localization length of the eigenfunctions. At the boundary between a metallic phase and an Anderson-localized phase, we find a mobility edge, where $\mu(E)$ falls to zero like a power of L as we take L to infinity.

The one-parameter scaling theory implicitly assumes that $n(E,L)$ can be approximated as $1/W$ in the energy region of interest. [Actually, it is clear from the form of Eq. (2) that it does not matter what n is, as long as it is well approximated by some positive constant.] When W is large, so that at most a small fraction of the eigenfunctions lying near the center of the band are extended, this approximation is justified, and Eq. (2) can be verified numerically.[6]

In this limit it has even been proven that n is an analytic function of E in the region of interest.[14] In general, however, it is only possible to prove that when the probability distribution for the randomness is continuous, then $n(E)$ is strictly positive everywhere inside the allowed energy band.[15] It can be demonstrated that there are cases[11,12,16] where $n(E)$ is nonanalytic precisely at E_c. It is not surprising that the one-parameter scaling theory, Eq. (2), fails to describe these special cases.

III. SMOOTH RANDOM POTENTIALS

Near the limits of the allowed eigenvalue spectrum, the eigenvectors are localized in rare, large fluctuations of the random potential.[17] The properties of these Lifshitz tail states are determined by the statistics of large fluctuations rather than by the localization length λ, because the size of a potential fluctuation which is strong enough to create a tail state is larger than λ. In a mean-field theory,[13,17] when the random potential is weak most of the eigenstates remain extended, and there is a sharp effective band edge E_c^*, where the Lifshitz tail states encounter the extended states.

Thus we see that there are two different mean-field theories of a mobility edge, which correspond to two different universality classes. For weak disorder[13,17] we see the Lifshitz transition: most of the states are extended and n is nonanalytic at E_c^*. For strong disorder[2] we have the Anderson transition: most of the states are localized and n is analytic at E_c. It would not be surprising if both types of transitions can contribute to behavior in three dimensions.

Harris and Lubensky[18] attempted a renormalization-group calculation for the Lifshitz transition. However, their treatment of the localized states must be incorrect, because it violates Wegner's theorem.[15] Thus, we do not yet understand how to go beyond mean-field theory for the Lifshitz transition.

The recent numerical calculations[7–10] show that the effective band edge $\tilde{E}$ seems to be well-defined in two or three dimensions for the random hopping model. Although we must treat this apparent numerical result cautiously, it is quite striking, and worthy of our attention. In three dimensions, E_c is not equal to $\tilde{E}$,[9,10] even in the weak disorder limit. However, in this case, the numerical results show that it resides in a region where $n(E)$ is varying rapidly. The states whose energies are between E_c and $\tilde{E}$ are Anderson states, localized by quantum interference. The sizes of these Anderson states, unlike the Lifshitz states, are characterized by the localization length $\lambda(E)$. Since the Lifshitz states become large as their energies approach the true band edge,[17] there must exist some energy where the size of a localized state is minimized. It is attractive to conjecture that this energy is $\tilde{E}$. The behavior of the transmission coefficient in the two-dimensional case[7] may also be explained by a rapid variation of $n(E)$.[8] Thus, it does not provide strong evidence for the existence of an anomaly in the mobility. It has been suggested by Godin and Haydock[7] that $\tilde{E}$ represents a true singular point of $n(E)$ even in two dimensions.

A theorem of Prange and Kadanoff,[19] which is an extension of Migdal's theorem,[20] requires that in the limit of weak, smoothly varying potentials the product $n\mu$ is independent of the random potential in the metallic phase. This arises from treating the random potential as a sum of long-wavelength zero-frequency phonons. This results in the existence of a Ward identity valid within a perturbation theory for the metallic phase, which breaks down at E_c. This breakdown of the Ward identity can be considered a symmetry-breaking phase transition, and it forces n to become nonanalytic at E_c.[11] Note that this picture is, in some sense, dual to the analysis of Kohn,[21] who argues that there is a broken symmetry and long-range order in the metallic phase.

It is to be expected that we will encounter cases where the potential is smooth, but not extremely smooth. For instance, we might be interested in a three-dimensional random potential whose wave-number power spectrum, $S(|\mathbf{k}|)$ is proportional to $(|\mathbf{k}|^2+k_0^2)^{-1}$, with $|k_0 a|\ll 1$ (where a is the lattice constant). When d is less than some critical dimension, the Prange-Kadanoff behavior, which is at the heart of the Lifshitz transition, is expected to be generically unstable. This critical dimension is not less than four,[18] but it may be even greater. Thus, a situation where the small-angle scattering is dominant should give rise to a crossover from the unstable Lifshitz-Prange-Kadanoff behavior to the stable fixed point described by Eq. (2).

Within perturbation theory we describe this by saying the small-angle scattering is not effective in changing the momentum of the electron, so that the length scale on which momentum conservation breaks down becomes much larger than the phase coherence length. The breakdown of momentum conservation under these conditions defines a new length scale L_p. The one-parameter scaling behavior can only be observed on length scales larger than L_p. As pointed out above, we can construct mathematical models for which L_p is infinite. Some readers may be interested in noting that the effect of smooth perturbations is related to the Kolmogorov-Arnold-Moser (KAM) theorem.

IV. SPIN GLASS

In the numerical simulations for the random hopping model in two[8] and three[9,10] dimensions, it turns out that the Lifshitz tail states are too rare to be seen on lattices of reasonable size. This has interesting consequences for the dynamics of spin-glass and gauge-glass models. The random hopping model with ν_{ij} chosen randomly from ± 1 can be identified as the high-temperature susceptibility matrix of the Ising spin glass.[10,22,23] When the ν_{ij} are chosen to be complex numbers of modulus 1 a similar identification can be made with the XY gauge glass.

It was claimed by Randeria, Sethna, and Palmer[24] that the long-time dynamics of the Ising spin glass, as seen in numerical simulations, was controlled by the Lifshitz tail states. In fact, the observed dynamical behavior[23,25] does not match the predictions of Randeria, Sethna, and Palmer. The predicted "Griffiths singularity"[26] presumably exists, since the Lifshitz states must exist in principle. However, this behavior is unobservably weak, and is not responsible for the observed behavior of the simulations and real experiments.[27]

The observed behavior must be coming from the Anderson states at the effective band edge. These states, which comprise perhaps 10^{-3} of the eigenstates in three dimensions,[9] are all very close to E_c. Therefore, the renormalization of these localized states of the susceptibility matrix across the mobility edge as the temperature is lowered, as proposed by Hertz, Fleishman, and Anderson,[22] becomes highly plausible. The density of these states gives a minimum length scale of somewhat more than ten lattice spacings for critical scaling behavior in the three-dimensional Ising spin glass, because we need to have several localized eigenstates in a sample to see the scaling behavior. A similar effect has been identified in other, related problems.[28–31] Since the number of Anderson states created by off-diagonal disorder is so small in $d=3$, one suspects that the susceptibility matrix for the spin glass does not have any such eigenvectors for $d\geqslant 4$.

We are left with a series of problems for future work. The first one is whether the effective band edge is truly well defined for the random hopping model in two and three dimensions. In other words, is it really possible to make a clear distinction between the Lifshitz tail states and the Anderson states for this case and, if so, why? An analysis by Soukoulis, Cohen, and Economou[32] argues for the existence of an energy like $\tilde{E}$, but it does not explain why $n(E)$ should be nonanalytic at this energy. The second one is convincingly identifying the critical dimension for the stability of the Lifshitz-Prange-Kadanoff behavior. And once we properly understand what is special about the random hopping model, we should finally be in a position to understand the Ising spin glass. Thus the third problem is working out the details of the renormalization of the localized Hertz-Fleishman-Anderson states in a three-dimensional system, and showing whether or not it leads to a true phase transition.

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