Localization with off-diagonal disorder: A qualitative theory

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I present a theory of localization for Hamiltonians with off-diagonal disorder in general dimension d. At $d=2$ for weak disorder the $E=0$ eigenstate decays as $\exp[-\gamma(\ln N)^{1/2}]$, with the coefficient γ varying with disorder. For strong disorder in all dimensions there is weak localization at $E=0$ and associated anomalies for $E\to 0$: the local density of states and rate of exponential decay are of the form found by Dyson in one dimension.

There has recently been an upsurge of interest in the Anderson localization of eigenstates of Hamiltonians with disorder in off-diagonal elements.[1,2] In part, this is motivated by the possibility that the fluorescing states in ruby, for example, may become localized at certain concentrations of the optically active ions owing to disorder in the exchange rather than the "diagonal" single-ion elements.[3] Theoretical work has been popular in models of "quantum percolation."[1,4] A related problem with correlated diagonal and off-diagonal disorder occurs in the theory of dilute ferromagnets.[5] I shall present a qualitative theory of the models considered which gives definite predictions for the localization at the center of the band. On a cautionary note, I also point out to what extent the anomalous behavior found is special to the class of models that have been proposed.

Consider the Hamiltonian for random nearest-neighbor bonds on a d-dimensional hypercubic lattice with coordinates $(n_1, n_2, \ldots, n_d)$ n_j integers:

$$\mathcal{H}=\sum_{NN} t_{ij} a_i^{\dagger} a_j \quad . \tag{1}$$

The t_{ij} are non-negative independent real random variables, $a_i^{\dagger}, a_j$ denotes annihilation and creation operators on nearest-neighbor sites i and j. For (bond) "quantum percolation" t_{ij} is 0 or 1 with probability p and $1-p$, respectively. We shall allow the distribution of t_{ij} to be more general, however. Raghavan and Mattis[1] showed, in a numerical study of quantum percolation, the utility of "tridiagonalization"[6]: a one-dimensional submanifold is found on which the Hamiltonian is isomorphic to that of nearest-neighbor overlap on a semi-infinite linear chain. Diagonalization of the Hamiltonian on this subspace is sufficient to calculate the site-diagonal Green's function. Consider first the regular Hamiltonian, t_{ij} constant. Starting with vector ϕ_0 for a particle at site 0 the procedure generates a sequence of orthonormal vectors ϕ_n, where for a Hamiltonian of the form (1), ϕ_n is a linear combination of wave functions at sites $(n_1, \ldots, n_d)$ (denoted $|n_1, \ldots, n_d\rangle$) of "generation number" $n = \sum_{i=1}^{d} |n_i|$. For large n there are $C(n) \cong A_d n^{d-1}$ such sites, with A_d a geometric constant. It is convenient to define a sequence of vectors which are not unit vectors but have modulus squared $\langle\tilde{\phi}_n|\tilde{\phi}_n\rangle = C(n)$:

$$\tilde{\phi}_n=\sum_n a_{n_1,\ldots,n_d}|n_1, \ldots, n_d\rangle$$

for the regular case $a=1$. We now introduce the crucial simplification of the theory: We make the approximation, which is accurate for weak disorder, that in the random case we can also write the vectors $\tilde{\phi}_n$ generated by tridiagonalization as linear combinations of wave functions at sites of generation number n only. That is, at each step we neglect the part of the projection of $\tilde{\phi}_n$ on the subspace of sites of generation $(n-1)$ that is orthogonal to the previous vector $\tilde{\phi}_{n-1}$. We therefore generalize the a's to be real variables satisfying $\sum_n a^2_{n_1,\ldots,n_d} = C(n)$, where $\sum_n$ denotes a sum over all sites of generation number n. For the regular Hamiltonian the diagonal elements are zero and the off-diagonal elements $b_{n+1} = \langle\tilde{\phi}_n|\mathcal{H}|\tilde{\phi}_{n+1}\rangle$ are 1. In the random case $\tilde{\phi}_{n+1}$ and b_n are defined iteratively by $\mathcal{H}\tilde{\phi}_n = b_{n-1}\tilde{\phi}_{n-1} + b_{n+1}\tilde{\phi}_{n+1}$ and the normalization $\langle\tilde{\phi}_n|\tilde{\phi}_n\rangle = C(n)$. Thus given the amplitudes a for the nth generation,

$$\begin{aligned} b_{n+1} &= \left[\sum_{n+1} (a'_{n_1,\ldots,n_d})^2\right]^{1/2} \Big/ C(n+1)^{1/2} \quad , \\ \tilde{\phi}_{n+1} &= \sum_{n-1} \frac{a'_{n_1,\ldots,n_d}}{b_{n+1}} |n_1, \ldots, n_d\rangle \quad , \end{aligned} \tag{2}$$

where $a'_{n_i,\ldots,n_d} = \langle n_1, \ldots, n_d|\mathcal{H}\tilde{\phi}_n\rangle$. Apart from atypical sites (corners and edges) the random variables a' are determined from an equation

$$a'_{n_1,\ldots,n_d} = \sum_{j-1}^{d} t_j a_n^{(j)} \quad , \tag{3}$$

where the t_j are independent random variables, $a_n^{(j)}$ are d amplitudes on sites in the nth generation. To give a specific example, for $n=6$ in $d=2$ the equation reads $a'_{(3,4)} = t_1 a_{(2,4)} + t_2 a_{(3,3)}$. For the atypical site (7,0) there is only one term: Such sites are rela-

tively few for large n and will be ignored.

Let us now construct a theory for weak disorder: We assume that for large n the variables $a_n^{(j)}$ can be considered statistically independent with mean 1 and variance σ_n^2. The t_j's by definition are independent and will be normalized to have mean $\langle t\rangle = 1/d$ and variance σ_t^2/d^2; the assumption of independent a's is not correct. We will return to this point later and argue why it is a good approximation for *weak* disorder. Now from (3) we find

$$\sigma_{n+1}^2 = \sigma_n^2(\sigma_t^2+1)/d + \sigma_t^2/d \quad . \tag{4}$$

The difference equation (4) with boundary condition $\sigma_0 = 0$ has the solution

$$\sigma_n^2 = \frac{\sigma_t^2}{d}\left[1-\left(\frac{1+\sigma_t^2}{d}\right)^n\right]\Bigg/\left[1-\left(\frac{1+\sigma_t^2}{d}\right)\right] \quad .$$

Thus for $\sigma_t^2 < d-1$, σ_n converges to

$$\sigma^* = \left(\frac{\sigma_t^2}{(d-1)-\sigma_t^2}\right)^{1/2} \quad . \tag{5}$$

For large n each a_n' has mean 1 and variance σ^*.[2] Again ignoring correlation and assuming σ^* small, since b_{n+1} is the r.m.s. of $\approx A_d n^{d-1}$ variables a, it will have mean 1 and standard deviation decreasing as

$$\sigma_{b_n} \simeq \sigma^* / A_d^{1/2} n^{(d-1)/2} \quad . \tag{6}$$

The localization properties of the semi-infinite chain so defined can be formulated in terms of the product of random transfer matrices just as for the homogeneously disordered chain.[7] While for general energy E the matrices do not commute, at the special point $E=0$ the difference equations for eigenstates $E\psi_n = b_{n-1}\psi_{n-1} + b_{n+1}\psi_{n+1}$ can be solved explicitly and the asymptotic properties depend on the product

$$\prod_{j=1}^{M}\left(-\frac{b_{2j}}{b_{2j-1}}\right) = (-1)^M \exp\left[\sum_{j=1}^{M}\ln\left(\frac{b_{2j}}{b_{2j-1}}\right)\right] \quad . \tag{7}$$

To study the convergence of the sum it can be approximated by its asymptotic form

$$S_M = \sum_{i=1}^{M_1} \frac{f_i(2\sigma^*/A_d^{1/2})}{(2i)^{(d-1)/2}} \quad ,$$

where f_i is a random variable of mean 0 and variance 1. Taking the f_j independent and approximating the sum by an integral, we find $\langle S_M\rangle = 0$

$$\langle S_M^2\rangle \sim \begin{cases} \dfrac{4\sigma^{*2}}{A_d}(2M)^{2-d}, & d<2 \\ \dfrac{4\sigma^{*2}}{A_d}\ln(2M), & d=2 \\ \dfrac{\zeta(d-1)}{2^{d-1}}, & d>2 \quad . \end{cases}$$

Thus with probability 1 either the product (7), or its inverse, diverges as $\exp[\sigma^*(2M)^{(2-d)/2}]x_M$ for $d<2$ and as $\exp[\sigma^*(\ln 2M)^{1/2}x_M]$ for $d=2$ (x_M is a random variable of order 1) and for $d>2$ it converges. For weak disorder, then, we predict that the eigenstate $\psi_N(E=0)$ decays as $\exp[-\sigma^* N^{(2-d)/2}]$ for $d<2$, with the law $\exp[-\gamma(\sigma_t)(\ln N)^{1/2}]$ at $d=2$, with coefficient

$$\gamma(\sigma_t) \simeq \{4\sigma_t^2/A_d[(d-1)-\sigma_t^2]\}^{1/2}$$

varying with the strength of disorder, and is extended for $d>2$. This new behavior predicted for weak disorder in $d=2$ is *not* the same as power-law localization but it may be difficult to distinguish numerically between the two.

Let us now pause to consider the range of validity of the results for weak disorder. The most glaring omission is the neglect of correlations, of which there are two major sources. The first is that while each bond t_j appears in only one equation of form (3), a single $a_n^{(j)}$ occurs in d distinct sums. Thus even if the a's of one generation are assumed to be independent, correlation develops in the next. We can, however, calculate the correlations that develop and show that for small σ_n correlations decay exponentially with separation. Such short-range correlations do not affect the scaling behavior (6) and consequently the predictions of localization, although the value of the coefficient $\gamma(\sigma_t)$ will be altered. Thus the weak regime so far considered is consistent with these correlations.

The second important correlation is implied by the normalization of $\tilde{\phi}_n$ which provides that for a given n, a particular $a_n^{(j)}$ cannot exceed $(A_d n^{d-1})^{1/2}$. For σ_t^2 large ($>d-1$ to the lowest-order approximation) the exponential growth implied by (4) must be incorrect. The expectation for this case of strong disorder is that a few of the individual a_n grow to dominate the sum, in contrast to the weak regime for which all the a_n are of the same order of magnitude. This argument can be made more plausible by noting that if initially the a's have mean 1 and variance σ_n^2, as σ_n increases to become comparable to the mean, the (non-negative) a_n must have an increasingly skew distribution. Unusually large values will tend to dominate in sums of squares. To estimate the scaling of the elements b_n take the most extreme case in which a single a_n is taken as having all the weight. In that case b_{n+1} has variance approximately σ_t^2/d^2, i.e., a constant. In this strongly disordered regime the problem is therefore reduced to that of homogeneous off-diagonal disorder as originally studied by Dyson.[8] The localization and spectrum close to the band center are well understood: The $E=0$ wave function decays as $e^{-\sigma_B N^{1/2}}$, where σ_B is $\langle \ln b_n\rangle$. The local density of states and rate of exponential decay are singular as $E\to 0$: $\rho_0(E) \sim 1/E|\ln E|^3$; $\lambda(E) \sim 1/\ln E$.[8] We find then that these singularities in the lo-

cal density of states and localization length persist in *any* dimension for a Hamiltonian of form (1) provided the disorder is sufficient.

At this point we should return to the initial simplification of the theory, that each $\tilde{\phi}_n$ has amplitudes only on the shell of generation n. For weak disorder the amplitudes neglected at each stage are weaker by a factor proportional to the disorder and, more importantly, it is straightforward to argue that if included to low order they do not affect the scaling behavior. Thus the conclusion for weak disorder should remain good, with corrections to $\gamma(\sigma_t)$. What is not clear is whether the transition from weak to strong disorder is properly described. The conclusion that the strongly disordered regime maps onto a homogeneously disordered chain should not be affected. One feature of the theory which is not approximate and which is essential to the behavior at band center is that the diagonal terms vanish. This is an exact symmetry of the model whose significance will be discussed later.

What does this picture imply for "quantum percolation"? In $d=3$ there should be a region of weak dilution bounded by P_Q (in the notation of Ref. 1), in which the eigenfunctions at band center, and presumably a finite range of energies, are extended. For $p_Q > p > p_c$, the geometric percolation threshold, the center eigenstates decay as $\exp[-\sigma(p)\sqrt{N}]$ and for small energies the rate of exponential decay and local density of states exhibit the Dyson anomalies. Note that the equivalence of "weak disorder" and "weak dilution" is not complete: Dilution gives strong local disorder leading to strongly localized states that contribute δ functions to the average local density of states at special energies (e.g., $E=0$) that we would not expect for a weak continuous distribution of bond strengths.[4] The definition of "generation number" of a site has to be modified to take into account missing bonds to make the present theory valid even for low dilutions, although again the scaling of asymptotic coefficients should be the same.

In two dimensions arbitrarily weak dilution is predicted to cause decay as $\exp[-\gamma(p)(\ln N)^{1/2}]$ at band center, i.e., more weakly than a power law. At stronger dilutions there should be a transition to a strong-disorder regime. In contrast to Ref. 5, in which the Dyson singularities were introduced to include the quasi one dimensionality of a nodes-and-links picture of the percolating cluster, here they appear independently of such an assumption. The theory presented is not detailed enough to predict the position or nature of the transition: Taken beyond its likely range of validity (5) would suggest that the coefficient $\gamma(\sigma_t)$ may diverge. It is possible that there is an upper bound to $\gamma(\sigma_t)$.

So far we have concentrated on the band center at which eigenstates can easily be found once the off-diagonal elements are determined. For finite energies localization depends on the product of transfer matrices that do not commute. As has recently been discussed for one-dimensional problems, the existence of weakly localized states at $E=0$ can be associated with anomalies in the densities of states and a divergent localization length as $E \to 0$.[7] It was found that the anomalies could be derived simply by supplementing perturbation theory with a scaling hypothesis: Perturbation theory alone does not take full account of the lack of commutation of the matrices.[9] For strong disorder the present problem is mapped onto a homogeneously disordered chain and thus the singularities first found by Dyson will also occur, although in the dilution problem they may be masked by the δ-function singularities mentioned earlier. For the case of weak disorder in $d=2$, it is still an open question whether for small energies the eigenstates are exponentially localized. Recent numerical studies of Soukoulis, Webman, Grest, and Economou[10] support the belief that they are exponentially localized except at band center. This is what one might expect from the scaling theory.[11]

While considering the significance of these results for experiment it is well to remember that a certain symmetry has been imposed on the model: The lattice can be decomposed into two sublattices such that the Hamiltonian applied to states of one sublattice generates nonzero amplitudes only on the other. This apparently innocuous restriction ensures that the tridiagonal Hamiltonian has zero diagonal elements and therefore that the central eigenstate is never exponentially localized. Addition of next-to-nearest-neighbor interactions, for example, breaks the symmetry and generates a Hamiltonian similar to that of diagonal disorder. For ruby, in particular, the symmetry may be broken.

In conclusion I have presented a perturbative theory of off-diagonal disorder which leads to predictions of anomalies in the localization and local densities of states—behavior that can be considered the higher-dimensional analog of the singularities found by Dyson in one dimension. Clearly many details of the problem remain to be elucidated: It is hoped this Communication will stimulate precise numerical studies, in particular.

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