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LETTER TO THE EDITOR

On the density of states for the quantum percolation problem

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Abstract. For the site dilution model on the hypercubic lattice $\mathbb{Z}^d$, $d \geq 2$, we examine the density of states for the tight-binding Hamiltonian projected onto the infinite cluster. It is shown that, with probability one, the corresponding integrated density of states is discontinuous on a set of energies which is dense in the band. This result is proved by constructing states supported on finite regions of the infinite cluster, analogous to the Kirkpatrick and Eggarter zero-energy molecular state.

The electronic properties of disordered media are often described by the tight-binding Hamiltonian, defined on the square integrable functions $l^2(\mathbb{Z}^d)$, by

$$\mathcal{H} = -\Delta + \sum_i v_i \tag{1}$$

where Δ is the lattice Laplacian (i.e. the hopping operator) and the v_i are (independent and identically distributed) random potentials with distribution $g(dv)$. Models of this form were first considered by Anderson (1958) for the case of a uniform distribution.

For general $g(dv)$, two related quantities of fundamental interest are the density of states, $\rho(E)$, and the integrated density of states, $n(E)$. The latter is defined by considering a finite rectangle $\Lambda \subset \mathbb{Z}^d$ and computing

$$n(E;\Lambda) = |\Lambda|^{-1} \text{ (number of eigenvalues of } \mathcal{H}_\Lambda \leq E) \tag{2}$$

where $\mathcal{H}_\Lambda$ is the restriction of $\mathcal{H}$ to the rectangle Λ with (say) Neumann boundary conditions. Sub-additive arguments may be applied to show that, with probability one, a thermodynamic limit, $n(E)$, exists and is independent of the realisation (see, e.g., Benderskii and Pastur 1970). Then $\rho(E)$ may be 'defined' as $dn(E)/dE$.

There have been many results demonstrating varying degrees of smoothness for $n(E)$ depending on the behaviour of the potential distribution $g(dv)$. Under rather general circumstances, Craig and Simon (1983) proved log-Hölder continuity of $n(E)$, while by a quite different argument Delyon and Souillard (1984) established the continuity of $n(E)$. Wegner (1981) proved that if g is bounded, then so is $\rho(E)$, a

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result extended by Maier (1985) to the case in which $g \in L^P$, $P > 1$. Very strong results for one dimension have been obtained by Simon and Taylor (1985) and Campanino and Klein (1986). For special distributions, e.g., a Cauchy distribution or a Gaussian of sufficiently large width, $\rho(E)$ turns out to be analytic at all energies (Lloyd 1969, Edwards and Thouless 1971, Constantinescu *et al* 1984). For an excellent review of these and other mathematical aspects of localisation theory, the reader is referred to the lecture notes of Spencer (1986).

In cases where $g(\mathrm{d}v)$ is not particularly smooth, some negative results have been discovered. Halperin (1967) (see also Simon and Taylor (1985)) showed that if a one-dimensional chain has a random potential which can take on only two values (i.e. substitutional disorder), then $\rho(E)$ will fail to be continuous.† Somewhat more disturbing are the zero-energy 'molecular states' found by Kirkpatrick and Eggarter (1972) for the case of dilution disorder—sometimes known as quantum percolation.

Quantum percolation, first studied by de Gennes *et al* (1959a, b), can be formally regarded as a tight-binding model of the form (1) where $v_i = 0$ with probability p and is infinite otherwise. (For convenience, the diagonal portion of the lattice Laplacian has also been set to zero.) It is straightforward to show that the spectrum of this model is $[-2d, +2d]$, and that the total number of states per volume (i.e. $n(2d)$) is p. In general, there are two types of states: For any p, some states are isolated on finite clusters of $v = 0$ (active) sites; if p exceeds the percolation threshold, there are also states supported on an active infinite cluster. The first class is both uninteresting, in the sense that it does not contribute to transport, and pathological in the sense that it creates spurious discontinuities in the integrated density of states. We therefore take p above the percolation threshold (which necessitates $d \geqslant 2$) and confine attention to sites which are part of an infinite cluster; indeed, as we will later discuss, it is straightforward to define an $n(E)$ on the restriction of configurations to their active infinite components.

The observation of Kirkpatrick and Eggarter (1972) was that even if one removes the finite clusters, there are still discontinuities in $n(E)$—most notably at $E = 0$—arising from compactly localised (molecular) states on the infinite cluster. Kirkpatrick and Eggarter identified states contributing to discontinuities at both $E = 0$ and $E = \pm 1$; their zero-energy state is illustrated in figure 1. Since configurations allowing these states occur with non-zero probability, a positive fraction of the spectral measure will be concentrated at these energies. It should be noted that these states are localised in a much stronger sense than the typical exponentially localised states; these molecular states *vanish* outside a finite region, and hence have zero localisation length. On the basis of numerical observations, which have since been confirmed and extended by other groups (Jonson and Franz 1980, Franz 1985), Kirkpatrick and Eggarter concluded that such molecular states should occur at several additional energies. Some further results along these lines have been reported in Shapir *et al* (1982).

The purpose of this letter is to demonstrate just how bad a density of states is capable of being. In particular, we will show that for the quantum percolation model, molecular states can be constructed arbitrarily close to any energy in the band, with positive density (so that, by equation (2), $n(E)$ has discontinuities on a *dense* subset of $[-2d, +2d]$). If one assumes that the quantum percolation model has extended states (which is presumably the case for $d \geqslant 3$ and $1 - p$ sufficiently small), this indicates

† For such systems, Carmona *et al* (1986) have recently shown that $n(E)$ can have a non-trivial singular component.

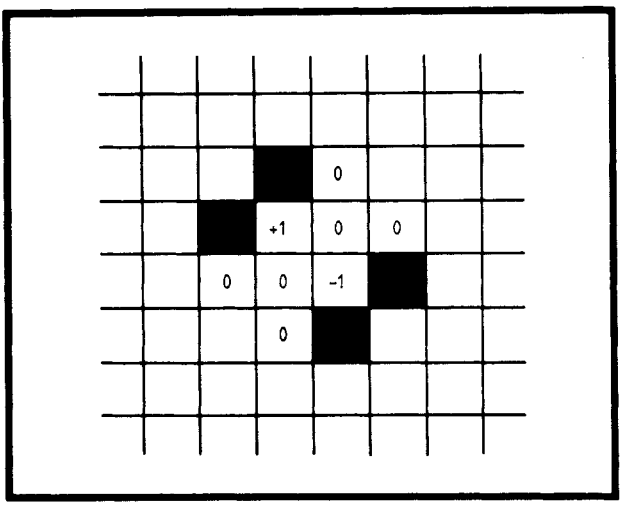

Figure 1. An example of Kirkpatrick and Eggarter (1972). The values of the (unnormalised) molecular wavefunction are depicted; □: active sites ($v=0$); ■: vacant sites ($v=+\infty$).

the coexistence of localised and extended states, contrary to what is expected for models with less pathological potentials. While certain aspects of this seem to have been understood by Shapir *et al* (1982), it is hoped that our results will provide a useful counterexample in formulating extensions of the regularity theorems discussed above.

We begin by defining the relevant density of states, $n_\infty(E)$, for the quantum percolation problem. Suppose then that $\Lambda \subset \mathbb{Z}^d$ is a finite rectangle. Define $\mathscr{H}^*_{\Lambda,\partial\Lambda}$ to be the Hamiltonian, with Neumann boundary conditions, restricted to (active) sites which are in the connected components of the boundary, $\partial\Lambda$. It is not hard to show that $N_{\partial\Lambda}(E;\Lambda)$, the number of eigenvalues of $\mathscr{H}^*_{\Lambda,\partial\Lambda}$ of energy not exceeding E, satisfies the usual sub-additivity condition. Thus, by the sub-additive ergodic theorem (Ackoglu and Krengel 1981), the quantities $n_{\partial\Lambda}(E;\Lambda) \equiv \Lambda^{-1} N_{\partial\Lambda}(E;\Lambda)$ converge almost surely to a (realisation-independent) function which we denote by $n_\infty(E)$. We will call $n_\infty(E)$ the infinite component integrated density of states.

Remark. The spectrum of this model again lies in the interval $[-2d, +2d]$. Morally, the analogue of the statement $n(2d)=p$ is simply $n_\infty(2d)=P_\infty(p)$, where $P_\infty(p)$ is the infinite cluster density for Bernoulli percolation on $\mathbb{Z}^d$ at site density p. However, a proof of this statement requires that the percentage of sites connected to the boundary, $\partial\Lambda$, which are *not* in the infinite cluster, tends to zero as $\Lambda \uparrow \mathbb{Z}^d$. A sufficient condition for this is that $\chi'(p)$, the expected size of finite clusters, is not infinite. It should be noted that there are models for which $P_\infty(p)>0$, but $\chi'(p)=\infty$ (Aizenman *et al* 1986*a*). However, it is anticipated that for standard (i.e. short-range) percolation models, $\chi'(p)<\infty$ whenever $P_\infty(p)>0$. This is known to be true in two dimensions (Kesten 1982); for general dimension, the strongest results along these lines have been obtained by Chayes *et al* (1986).

We now derive our principal result.

Proposition. For the quantum percolation model on $\mathbb{Z}^d$, the infinite component integrated density of states, $n_\infty(E)$, has discontinuities on a dense subset of the band.

Proof. Our strategy is to find active site configurations, $\mathscr{C}$, which occur along the active infinite component†, and which are capable of supporting molecular states $\{\Psi_j(\mathscr{C})\}$ with eigenvalues $\{E_j(\mathscr{C})\}$ such that $\bigcup E_j(\mathscr{C})$ is dense in $[-2d, +2d]$. For clarity of exposition (principally pictorial), we will first focus on two dimensions.

Let c be a finite, connected cluster, assumed for simplicity to lie above the line $x=0$ and contain the point $(0, 1)$. Let c^R be the mirror image of c reflected through the x axis and let $\mathscr{C} \equiv c \cup c^R$ (see figure 2). We claim that even when $\mathscr{C}$ is 'attached' to a segment of an infinite cluster (e.g. a straight portion running along the x-axis), there are eigenfunctions which vanish on the complement of $\mathscr{C}$. Indeed, let $\{\psi_j \mid j = 1, 2, \ldots, |c|\}$ be the finite cluster wavefunctions of c with energies $\{E_j\}$, and ψ_j^R the associated (mirror) wavefunctions of c^R. Then the wavefunctions $\Psi_j \equiv (1/\sqrt{2})[\psi_j - \psi_j^R]$ satisfy the Schrödinger equation and have energy E_j.

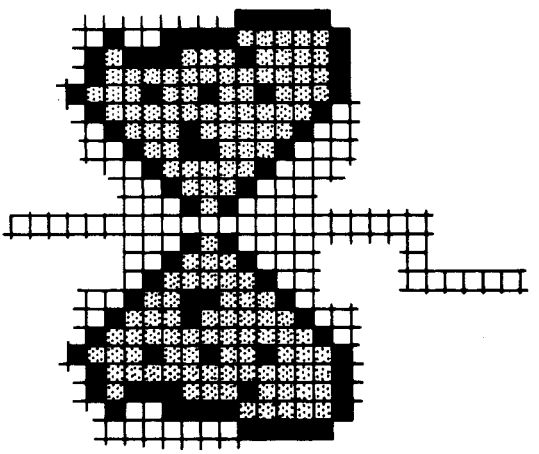

Figure 2. Construction of molecular states with matching clusters; □: active sites ($v=0$); ■: vacant sites ($v=\infty$); ▩: support of Ψ.

The above argument is easily carried to higher dimensions; one need only reflect any finite cluster across the $(d-1)$-dimensional hyperplane just below its lowest point and construct the antisymmetric modes. Since these wavefunctions automatically vanish on the symmetry plane (whether or not these sites are active) such mirror pairs can easily be attached to an infinite cluster.

Since any given mirror pair $\mathscr{C} = c \cup c^R$ is a finite configuration, it occurs with a (well defined, non-zero) density along the infinite cluster with probability one; this density provides a lower bound on the discontinuity of $n_\infty(E)$ at the energies $E = E_j(\mathscr{C})$. Furthermore, since the clusters we employ are arbitrary, such discontinuities occur at all possible finite cluster energies. Thus for any fixed energy E_0 in the band, one can always find a cluster $\mathscr{C}$ supporting a wavefunction $\psi(\mathscr{C})$ with an energy $E(\mathscr{C})$ such that $|E_0 - E(\mathscr{C})|$ is as small as desired.

† It should be remarked that for all these site percolation models on $\mathbf{Z}^d$, whenever p is above threshold, the infinite cluster is unique (Aizenmann *et al* 1986b). This is not relevant to our argument, which holds just well on the Bethe lattice (with either Dirichlet or Neumann boundary conditions) where it is known that there are infinitely many infinite clusters. It is worth pointing out that the Bethe lattice is, in fact, where many of the molecular states have been observed numerically (Jonson and Franz 1980, Franz 1985).

We conclude with the following remarks.

1. It is worth noting that the construction as described above is not the only mechanism for producing molecular states and, indeed, that there are others which do not require the full mirror symmetry. In fact, such other mechanisms are quite important in obtaining any estimate on the contribution of molecular states to the total spectral measure.

2. It is clear that, unless the finite cluster energies $E_j(\mathscr{C})$ are somehow removed from the spectrum, there can be no sharp mobility edge for quantum percolation. The traditional arguments against the coexistence of localised and extended states do not apply to this model. Of course, unlike the states supported on finite clusters, these states are on branches of the infinite cluster which cannot be pruned. It is an open question whether these compactly localised states induce complicated structure into the rest of the spectrum, or whether the 'remainder' of the spectrum has a smooth density of states and meaningful mobility edges.

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