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Abstract
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Exact Solution of a Model of Localization

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The exact solution is presented for the "susceptibility," χ (the number of sites covered by the maximally extended eigenfunction), for the zero-energy solutions of a hopping model on a randomly dilute Cayley tree. If p is the concentration, then $\chi \sim (p^*-p)^{-1}$ with $p^* \sim p_c e^{1/\xi_1}$, where p_c is the critical percolation concentration and ξ_1 the one-dimensional localization length. This result is argued to hold for the dilute quantum Heisenberg antiferromagnet at zero temperature.

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Recently much interest has been shown in the relation between classical[1] and quantum[2] percolation. The latter phenomenon is a model for the transition from localized to extended states that may occur for excitations in a random potential.[3] In these models bonds between nearest-neighboring sites are randomly present with probability p and absent with probability $1-p$. For both models we express the susceptibility, χ, in terms of the susceptibility, $\chi(\Gamma)$, of the cluster Γ of sites connected by occupied bonds:

$$\chi = \sum_\Gamma P(\Gamma)\chi(\Gamma), \tag{1}$$

where $P(\Gamma)$ is the probability of occurrence of a cluster Γ which intersects the origin. For classical percolation,[4] $\chi(\Gamma)$ is simply the number of sites in the cluster Γ.

To define $\chi(\Gamma)$ for quantum percolation one considers the eigenfunctions of the hopping Hamiltonian which obey

$$\sum_j t_{ij}\psi_E(j) = E\psi_E(i), \tag{2}$$

where t_{ij} assumes the value t if the bond between sites i and j is present and 0 otherwise. I consider only lattices which can be decomposed into two sublattices a and b such that t_{ij} is nonzero only when sites i and j are on different sublattices. Then, even in the presence of dilution, the density of states, $\rho(E)$, is an even function of E and is nonzero for $-zt < E < zt$, where z is the coordination number of the lattice. As the concentration p is decreased from unity the states near the edge of the band become localized (See Fig. 1). Thus there exist mobility edges at energies $\pm E_c$, such that states with $|E| > E_c$ are localized whereas for $|E| < E_c$ extended states appear (possibly coexisting with special localized states[5]). The mobility edges move towards $E=0$ as p approaches a critical value, p^*.

Under the reasonable assumption that extended states first appear at $E=0$, I locate p^* by an exact analysis of the eigenfunctions for $E=0$. To do this I introduce a localization susceptibility which diverges when extended states begin to form. Following the concept of the participation ratio introduced by Thouless[3] I define $\chi(\Gamma)$ by

$$\chi(\Gamma)^{-1} = \min \sum_i \psi(i)^4, \tag{3}$$

where the minimization is over ψ's such that $\psi(i)$ is a zero-energy eigenfunction with nonzero amplitude on the origin (which is on the a sublattice). To avoid any spurious effect of localized states, ψ must be connected, i.e., not decomposable into nonoverlapping eigenfunctions. It can be shown that such a connected eigenfunction is nonzero only on the a sublattice. The classical percolation problem can be obtained from Eq. (3) if, instead of solving Eq. (2), one sets $\psi(i) = n^{-1/2}$, where n is the number of sites in the cluster Γ. An important question is whether the concentration p^* is larger than the critical concentration p_c for percolation. Simulation[2] and series work[6] both suggest this to be the case, but the present work is the first to establish this conclusively and also leads to a simple intuitive picture for why p^* and p_c differ. These results follow from an exact solution for the quantum percolation susceptibility for a Cayley tree of

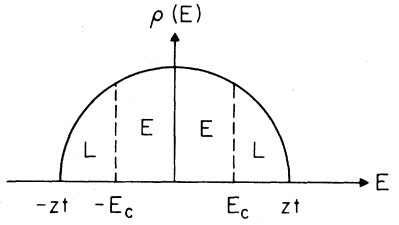

FIG. 1. The density of states for random hopping models. Here L denotes localized states, E_c the mobility edge energy, and E extended states (possibly coexisting with localized states).

coordination number 3 (see Fig. 2). The Cayley tree is a lattice for which the exact solution is expected to reproduce mean field theory.

To evaluate $\chi(\Gamma)$ from Eq. (3) note that a minimum value for a normalized $\psi(i)$ is obtained if it is possible to set $|\psi(i)|^2 = n(\Gamma)^{-1}$, in which case $\chi(\Gamma) = n(\Gamma)$, where $n(\Gamma)$ is the largest number of sites of the cluster which a zero-energy eigenfunction can cover. For $E = 0$ Eq. (2) is satisfied by choosing the phase of the wave function at sites j to be the complex nth roots of unity, where n is the number of neighbors over which the sum is taken. Thus, to evaluate χ one has to solve a modified percolation problem to find $n(\Gamma)$. Note that Eq. (2) forces any zero-energy wave function to vanish at a site adjacent to a free end. Thus $n(\Gamma)$ is not simply the number of a sites in the cluster Γ. To illustrate the construction of $\chi(\Gamma)$ Fig. 3 shows a cluster Γ for which a choice for $\psi(i)$ is given.

I now construct a generating function $F(q,p)$ such that

$$F(q,p) = \sum P(\Gamma) q^{n(\Gamma)}, \tag{4}$$

so that $\chi = [\partial F/\partial q]_{q=1}$. Since there are three statistically independent branches emanating from the origin, it is convenient to write

$$F(q,p) = q\Lambda(q,p)^3(1-p)^3, \tag{5}$$

where $\Lambda(q,p)$ is the generating function for a single branch. In a fuller paper the following result will be derived:

$$\Lambda(q,p) = x(q,p)/p(1-p), \tag{6}$$

where $x(q,p)$ satisfies

$$0 = p(1-p) - x(q,p) + q^2 x(q,p)^4 + 2qx(q,p)^2 x(1,p). \tag{7}$$

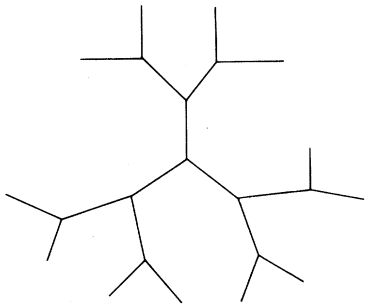

FIG. 2. Part of a Cayley tree with coordination number 3.

Equation (6) is obtained by summing contributions to $F(p,q)$ from all finite clusters.[7] Thus we find χ as

$$\chi = (x/p)(31 + 2x^2 + 2x^3)/(1 - 4x^2 - 4x^3), \tag{8}$$

where now $x = x(1,p)$ is the solution to Eq. (7) for $q = 1$ and is given by

$$(x + \tfrac{1}{2})^2 = \tfrac{3}{4} \pm |\tfrac{1}{2} - p|. \tag{9}$$

For small p the negative sign in Eq. (9) is the correct one to take and this solution obviously treats finite clusters. It would be incorrect to take the negative sign in Eq. (9) for $p > \frac{1}{2}$. So doing would yield a solution for x, and then for χp^3 which would be an even function of $\frac{1}{2} - p$. Since the probability of forming a finite cluster of n_b bonds is given by $(1-p)^3 y^{n_b}$, where $y = p(1-p)$ is an even function of $\frac{1}{2} - p$, I conclude that the negative sign in Eq. (9) corresponds for all p to treating only finite clusters. To describe the growth of the wave function within the infinite cluster, we analytically continue the low-p solution for $p > p_c = \frac{1}{2}$, i.e., we set

$$(x + \tfrac{1}{2})^2 = \tfrac{1}{4} + p, \tag{10}$$

for $p < p^*$, where p^* is the concentration at which χ diverges. I argue for Eq. (10) as follows.[8] Because of the blocking effect which effectively eliminates a finite fraction of free ends, the wave functions are localized near $p = p_c$. Thus near $p = p_c$ the distribution of sizes for wave functions is not anomalous and contributes analytically to χ. But in the absence of nonanalyticity, Eq. (10) must hold and yields

$$\chi = \varphi(p)/(1 + 4p - 16p^3), \tag{11}$$

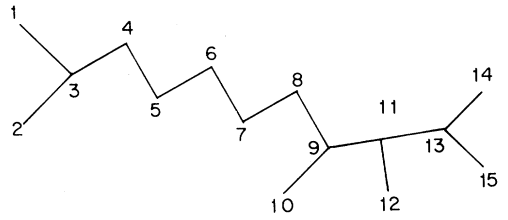

FIG. 3. A random cluster. If site 4 is the origin, then the only nonzero values of $\psi(i)$ resulting from the minimization in Eq. (3) are $\psi(1) = c\omega$, $\psi(2) = c\omega^2$, and $\psi(4) = -\psi(6) = \psi(8) = -\psi(10) = c$, where $c^{-2} = 6$ and $\omega = \exp(2\pi i/3)$. Note that the free ends at sites 10 and 12 prevent the wave function from reaching the right end of the cluster.

where

$$\varphi(p) = (2p^3)^{-1}[-1-p+12p^2+4p^3-24p^4+(1+4p)^{1/2}(1-p-8p^2+8p^3+8p^4)] = 1+p+3p^2\ldots . \quad (12)$$

Thus χ has a simple pole at a critical value of p denoted p^*, with $p^*/p_c = 1.191$, with $p_c = 0.5$. I have checked Eq. (11) by a diagrammatic evaluation of the low-p expansion for χ to order p^6.

The interpretation of the above result that $p^* > p_c$ is worth noting. For classical percolation on a Cayley tree with coordination number $\sigma+1$ the following argument gives p_c exactly. The average number of paths in continuing a branch is $p\sigma$. For infinite cluster growth one sets $p=1$ and obtains $p_c = \sigma^{-1}$. In the present case of quantum percolation the transmission coefficient of an occupied bond is not unity, because even if a bond is occupied, the wave function need not spread through it. For example, if an a site on a chain has a single dangling bond attached to it (cf. site 11 in Fig. 3), that bond will force the zero-energy eigenfunction to vanish on the a site and thereby the propagation of the wave function down the chain will be terminated. This blocking means that the average number of effective bonds is of order $2p[1-p(1-p)]$ for $\sigma=2$, since half the sites (i.e., the a sites) can be blocked by the appearance of a single free end which occurs with probability $p(1-p)$. For this effective number of bonds to be unity $p = p^* \times \frac{1}{2}(1+\frac{1}{8})$. This argument clearly underestimates p^*, since blocking can be caused by larger odd-parity groups. An intuitive way of stating this result is to say that the transmission probability is not simply p, but rather is $p\exp(-1/\xi_1)$, where ξ_1 is the one-dimensional localization length in units of lattice constants. For a homogeneous chain, the correlations will fall off with a power of distance so that $\xi_1 = \infty$ and the above argument is inappropriate. However, the proper ξ_1 to use is the localization length of a chain in the presence of the disordered medium. Here disorder is created by randomly attached side groups to the chain.

It remains to understand whether an alternative definition for χ would display more unambiguously a crossover[9] from percolation, for which $\chi \sim (p_c-p)^{-1}$, to dilute polymers,[10] for which $\chi \sim (p_c-p)^{-1/2}$. It seems plausible that my result should be interpreted as a crossover from percolation to animals.[10,11] Note that the animals exponent $\gamma = \frac{1}{2}$ is associated with the divergence in χ as the energy E is varied,[10,11] whereas here E is fixed but another variable, p, is varied. It is possible that the present solution is sensitive to the animals exponent at fixed order parameter for which γ assumes its usual mean-field value of unity.[10]

The implication of this work for some other problems is evident. For instance, one concludes that p^* for the emergence of long-range order in the dilute quantum Heisenberg antiferromagnet at zero temperature will be greater than p_c. One expects that $p^* \sim p_c \exp(1/\xi_1)$, where, as before, ξ_1 is the localization length for the Heisenberg antiferromagnetic chain in the presence of randomly placed side groups. Again, it would be wrong to ignore disorder and use the power-law decay of correlations for the Heisenberg chain. It seems clear that a crossover scaling theory like that given by Lubensky[12] for the dilute magnet can be formulated to describe the gradual introduction of quantum effects.

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[3]For a review of localization see D. J. Thouless, Phys. Rep. 13, 93 (1974).

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[5]S. Kirkpatrick and T. P. Eggarter, Phys. Rev. B 6, 3598 (1972).

[6]Y. Shapir, A. Aharony, and A. B. Harris, to be published.

[7]See Ref. 4 for elaboration of this point.

[8]It is crucial to argue that the appearance of the infinite cluster does not lead to terms in χ which are not analytic in p. One simple model for which this is obvious is the following. Consider the random cluster and associate a transmission coefficient for fluid flow, $\xi < 1$, with each bond. To find the volume which a fluid injected at the origin can reach, it is clear that one simply replaces p in the exact solution for the percolation problem by ξp and that the low-p form for χ is

valid for $\xi p < \frac{1}{2}$, even though an infinite cluster appears before the limit $\xi p = \frac{1}{2}$ is reached.

Another way to see that the present analytic continuation is correct is to consider the effect of attaching an arbitrary finite or infinite branch to a free end at the right end of the cluster in Fig. 3. Because of the complete blocking such an attachment will not affect $\chi(\Gamma)$. The exact effect on $P(\Gamma)$ is to replace the factor $p(1-p)$ for the free end by a factor p. This replacement is given by the infinite series for attachment of finite groups for $p < p_c$, and by the analytic continuation of this series for all $p \leq 1$. This argument only breaks down when the wave function becomes infinitely extended, i.e., when χ diverges.

[9]Crossover from percolation is discussed by A. B. Harris and T. C. Lubensky, Phys. Rev. B 24, 2656 (1981).

[10]"Lattice animals" is the name given to general cluster shapes, or equivalently, arbitrary dilute polymer configurations. See T. C. Lubensky and J. Isaacson, Phys. Rev. A 20, 2130 (1979).

[11]In high spatial dimension localization is closely related to lattice animals. See A. B. Harris and T. C. Lubensky, Solid State Commun. 31, 999 (1979), and Phys. Rev. B 23, 2640 (1981).

[12]T. C. Lubensky, Phys. Rev. B 15, 311 (1977). See also T. A. L. Ziman and R. J. Elliott, J. Phys. C 11, L847 (1978).