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Localization Length Exponent in Quantum Percolation

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Abstract
Connecting perfect one-dimensional leads to sites i and j on the quantum percolation (QP) model, we calculate the transmission coefficient $T_{ij}(E)$ at an energy E near the band center and the averages of $\Sigma_{ij}T_{ij}$, $\Sigma_{ij}r^2_{ij}T_{ij}$, and $\Sigma_{ij}r^4_{ij}T_{ij}$ to tenth order in the concentration p. In three dimensions, all three series diverge at $p_q=0.36^{+0.01}_{-0.02}$, with exponents $\gamma=0.82^{+0.10}_{-0.15}$, $\gamma+2\nu$, and $\gamma+4\nu$. We find $\nu=0.38\pm0.07$, differing from "usual" Anderson localization and violating the bound $\nu\geq 2/d$ of Chayes *et al.* [Phys. Rev. Lett. **57**, 2999 (1986)]. Thus, QP belongs to a new universality class.

Disciplines
Physics | Quantum Physics

Localization Length Exponent in Quantum Percolation

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Connecting perfect one-dimensional leads to sites i and j on the quantum percolation (QP) model, we calculate the transmission coefficient $T_{ij}(E)$ at an energy E near the band center and the averages of $\sum_{ij} T_{ij}$, $\sum_{ij} r_{ij}^2 T_{ij}$, and $\sum_{ij} r_{ij}^4 T_{ij}$ to tenth order in the concentration p. In three dimensions, all three series diverge at $p_q = 0.36^{+0.01}_{-0.02}$, with exponents $\gamma = 0.82^{+0.10}_{-0.15}$, $\gamma + 2\nu$, and $\gamma + 4\nu$. We find $\nu = 0.38 \pm 0.07$, differing from "usual" Anderson localization and violating the bound $\nu \geq 2/d$ of Chayes *et al.* [Phys. Rev. Lett. **57**, 2999 (1986)]. Thus, QP belongs to a new universality class.

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The localization (Anderson) transition in disordered materials has been studied intensively for a long time [1,2]. One parameter scaling theory [3] showed that the electronic wave functions are localized (i.e., they decay exponentially with distance) at and below two dimensions (2D) for any amount of disorder, while above 2D they become extended as the disorder (measured by λ) decreases below some critical value λ_c. On the insulator side ($\lambda > \lambda_c$), one expects the wave functions at energy E to decay with distance r as $\exp[-r/\xi(\lambda, E)]$ (apart from power-law prefactors), and the localization length ξ to diverge as $\xi \sim (\lambda - \lambda_c)^{-\nu}$. The value of the exponent ν has been the subject of much recent discussion. Particularly, Chayes *et al.* [4] proved that if ξ was defined as a finite size scaling correlation length, then ν must satisfy the bound $\nu \geq 2/d$. They argued that this bound applies in percolation, disordered magnets, and Anderson localization. However, they noted that in 3D both the four-loop ϵ expansion for $d = 2 + \epsilon$ and some experiments seem to violate this inequality. In the present Letter we present the first accurate numerical determination of ν for the quantum percolation (QP) model [5–7], which is a special variant of the general Anderson model, and find that in 3D $\nu = 0.38 \pm 0.07$, violating the Chayes *et al.* inequality.

The QP model is based on a tight binding Hamiltonian,

$$\mathcal{H} = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{\langle ij \rangle} t_{ij}(|i\rangle\langle j| + |j\rangle\langle i|), \quad (1)$$

where $\langle ij \rangle$ denotes a pair of nearest-neighbor sites, $|i\rangle$ represents a wave function localized near site i, and we assume a constant on-site energy, ϵ_i, which we arbitrarily take to be zero. The nearest-neighbor hopping matrix element t_{ij} is a random variable which assumes the values 1 or 0 with respective probabilities p and $1 - p$.

One of the natural and physical measures to probe the localization transition is the average sum over transmission coefficients [7],

$$T(p, E) = \left[\sum_{i,j} T_{ij}(E) \right]_p, \quad (2)$$

where $T_{ij}(E)$ is the transmission coefficient between sites i and j, the sum is over all pairs of points including $i = j$, and $[\cdots]_p$ represents a configurational average over the t_{ij}'s. To define $T_{ij}(E)$ we attach perfect one-dimensional leads (in which all nearest-neighbor t's are unity) to points i and j, insert an incoming wave with energy E on lead i, and calculate the amplitude of the outgoing wave on lead j by the QP model. Given the concentration p of "metallic" bonds, each realization of the system consists of clusters (Γ) of sites interconnected by metallic bonds. For $p \leq p_c$ the average $[\cdots]_p$ may be expressed as a sum over the clusters [8],

$$T(p, E) = \sum_\Gamma W_d(\Gamma) p^{n_b(\Gamma)} (1 - p)^{n_p(\Gamma)} \sum_{i,j \in \Gamma} T_{ij}(E), \quad (3)$$

where $W_d(\Gamma)$ is the embedding weight (per site) of Γ on the lattice, while $n_b(\Gamma)$ and $n_p(\Gamma)$ are the numbers of bonds in Γ and on its perimeter. If $T_{ij} = 1$ for all i and j on a given cluster, then Eq. (2) reduces to the mean cluster size (or "susceptibility") of classical percolation, which diverges at the classical percolation threshold p_c as $T \sim (p_c - p)^{-\gamma_p}$. In the quantum case, all states are exponentially localized for $p < p_q(E)$, where p_q is the threshold for "quantum percolation" and $p_q \geq p_c$. For $p < p_q$, the usual assumption that ξ is the only important length in the problem implies that in some average sense $[T_{ij}(E)] \sim r_{ij}^{-x} f(r_{ij}/\xi(p, E))$, where r_{ij} is the distance between sites i and j, and where $f(x)$ is a scaling function which approaches a constant as $x \to 0$ and decays strongly (e.g., exponentially) for $x \to \infty$. Therefore, $T(p, E) \sim \xi(p, E)^{d-x} \sim [p_q(E) - p]^{-\nu(d-x)} \sim [p_q(E) - p]^{-\gamma}$, with $\gamma = \nu(d - x)$. Three comments are in order. First, since we take E near the center of the band ($E = 0$), the values of $p_q(E)$ we quote should be close to the critical value p_q^* below which no extended states appear at any energy, studied, e.g., in

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Ref. [6]. Second, since we take E near $E = 0$, one might be worried about the singularities in the density of states which are known to arise at $E = 0$ due to many highly symmetric localized states [5]. To check this, we repeated our series derivation excluding the transmission channels through these states [9], and found that these states do not affect the divergence at p_q. Third, because all wave functions are localized for $p = p_c < p_q(E)$, we do not expect a power-law singularity at $p = p_c$. The absence of a singularity at $p = p_c$ was demonstrated in an exact solution [10]. In any event, our series analysis does not show such a singularity.

One way to obtain ξ uses moments of the distances between pairs of sites on the lattice,

$$A_k(p,E) = \left[\sum_{i,j} r_{ij}^k T_{ij}(E)\right]_p . \quad (4)$$

Given the above scaling *ansatz* about the behavior of $T_r(E)$, we expect these moments to diverge near $p_q(E)$ as $A_k(p,E) \sim [p_q(E) - p]^{-\gamma - k\nu}$. Stated more generally, the ratios A_{k+2}/A_k have dimensions of squared lengths. If the localization length ξ is the only relevant length near the transition, then we expect these ratios to be proportional to ξ^2, independent of the particular form of the scaling function $f(x)$. As we show below, both A_4/A_2 and A_2/A_0 diverge similarly to each other, and behave as $[p_q(E) - p]^{-2\nu}$. These results confirm and justify our scaling assumption. Since the sum in Eq. (3) contains polynomials in p, the averages in Eqs. (2) and (4) yield series in p. A calculation to order p^n involves all clusters with up to n bonds. We first generated three series, for $k = 0$, 2, and 4, exactly to all orders and for general E in 1D [11]. As expected, all the series diverge at $p_q = 1$, with exponents $\gamma = \nu = 1$. However, the analysis degraded as E increased, requiring more terms in the series to keep the same convergence. Since wave functions with small E (near the band center) have short waves ($E = 2\cos q$), their physics is already reflected by small clusters. Larger clusters seem to be needed for larger E. For this reason, and for comparison with earlier work [7], we present results at $E = 0.05$.

The series for $T(p,E)$, which requires only the topology of the clusters, were derived before [7] to order 13 for all d. In contrast to T, A_k depends on the explicit geometry of each cluster, which requires much more data. To obtain the new series A_2 and A_4, in $d = 2, 3$, we used data files for r_{ij}^2 and r_{ij}^4 on all clusters with $n \le 10$, which were constructed earlier for the study of the dilute quantum antiferromagnet [12]. For each cluster we calculated $T_{ij}(E = 0.05)$, and then generated the new 10-term series for A_2 and A_4. In the process, we realized that the series for T in Eq. (2), quoted in Ref. [7], did not include the contributions from the diagonal terms T_{ii}. These contributions are now included in our new series, whose behavior is thereby improved. The new 10-term series for $E = 0.05$ in 3D are given below [13].

The analysis of the series involved several processes. First we used a $d\log$ Padé analysis [14] for the three series, to identify the rough positions of poles (p_q) and residues ($\gamma + k\nu$). We found not only positive real poles, but also negative real poles which hampered the convergence of Padé approximants near the positive pole. In 3D, the smallest of these appeared at $p_x = -0.095$. In order to minimize this interference, we applied a conformal transformation of the series expansion variable $p = z/(1 + bz)$, where $b = 1/p_x$ is chosen so that the negative pole is pushed far away from the origin in the new complex plane. This transformation should not change the value of the leading critical exponent, but it generates an analytic correction to scaling [11]. The resulting series in z were then analyzed, using the recently developed efficient three-dimensional visualization methods [15] together with the M1 and M2 analysis algorithms [16], which allow a very accurate determination of the threshold p_q, leading critical exponent (denoted by h below), and confluent correction to scaling exponent Δ_1 simultaneously. Denoting the general series by $H(p)$, we assume the form

$$H(p) = A(p_q - p)^{-h}[1 + a(p_q - p)^{\Delta_1} + \cdots]. \quad (5)$$

In the M1 method, we study the logarithmic derivative of $B(p) = hH(p) - (p_q - p)dH(p)/dp$, which has a pole at p_q with residue $-h + \Delta_1$. For a given value of p_q we obtain graphs of Δ_1 versus input h for all Padé approximants, and we choose the triplet (p_q, h, Δ_1) where a selection of high, near-diagonal Padé approximants converge to the same point. In the M2 method, we first transform the series in p into a series in the variable $y = 1 - (1 - p/p_q)^{\Delta_1}$ and then take Padé approximants to $G(y) = \Delta_1(y - 1)d\ln[H(p)]/dy$, which should converge to $-h$. Here we plot graphs of h versus the input Δ_1 for different values of p_q and choose again the triplet (p_q, h, Δ_1), where the Padé approximants converge to the same point. In order to visualize the best converging point in the (p_q, h, Δ_1) space, we look at 2D plots at different trial p_q values, in perspective [15]. The effectiveness and preciseness of this series analysis method has been demonstrated in recent works [16–18].

To generate the numerical results presented below, we performed all these procedures on the series in the variable z, and only at the end plotted the graphs in terms of the original variable p. In Fig. 1 we present three slices from the M1 analysis of the $A_2(p, E = 0.05)$ series. The best convergence from different Padé approximants is achieved at $p_q = 0.36$. Figure 2 shows a slice at this value, from which we read the value of the leading critical exponent $\gamma + 2\nu \approx 1.58$ as well as the correction to scaling exponent $\Delta_1 \approx 1.05$. We repeated these analyses for T and A_4, and found a central value of $p_q = 0.36$ from all M1 and M2 analyses of all three series, except for M2 on T, which gave $p_q = 0.35$. The estimates of p_q quoted here are based on the intersection regions of the different

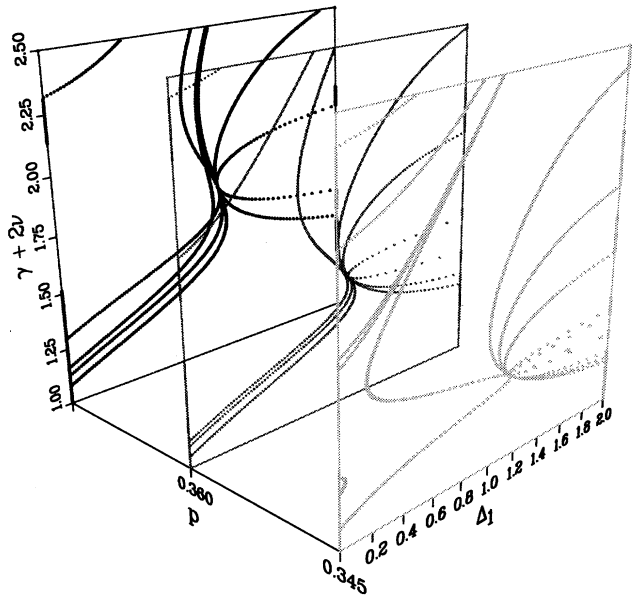

FIG. 1. Graphs of Padé estimates of Δ_1 as a function of $\gamma + 2\nu$ from the M1 analysis, at three values of p_q.

Padé approximants: If we look at the three slices of M1 graphs in Fig. 1, we see that at $p = 0.345$ the different approximants do not intersect in a symmetric way, but are skewed to the right. For $p = 0.375$ they are skewed leftward and in the region near $p_q = 0.36$ they are nicely balanced and meet at a single point. Convergence was found to degrade faster for $p > p_q$, compared to $p < p_q$. Given also the single central estimate (from M2 on T) of 0.35, we quote an overall estimate of $p_q(E = 0.05) = 0.36^{+0.01}_{-0.02}$. This estimate is close to but more precise than earlier series for the inverse participation ratio [6,7], and other studies [19,20]. [Note that the inverse participation ratio series should diverge at $p_q^* < p_q(E)$, since they contain a sum over all energies, and some energies have thresholds below $p_q(E)$.]

Having identified p_q, we proceeded to deduce overall exponent estimates. The gap exponents between T, A_2, and A_4 should give the estimates for 2ν. Indeed, within the window of $p_q = 0.36^{+0.01}_{-0.02}$ both M1 and M2 gave a constant gap exponent $2\nu = 0.76 \pm 0.14$ as well as $\gamma = 0.82^{+0.10}_{-0.15}$ and $\Delta_1 = 1.05^{+0.20}_{-0.05}$. We find it satisfactory that these three series gave practically the same value of p_q, a constant gap exponent, and moreover Δ_1 close to 1.0. Such an analytic correction to scaling was already expected, having resulted from the conformal transformation. This confirms that even with 10 terms our transformed series are well behaved and our analysis is reliable (Δ_1 was large for the analysis of the original series in p, which were less well behaved). Using $\gamma = \nu(d - x)$, our results imply that $x \approx 0.8$, with large error bars. Finally, we performed a self-consistent check for our results stated above. Namely, the term-by-term divided series [21,22] of A_4 by A_2 should diverge as $(1 - p)^{-(2\nu+1)}$, which is not biased by the value of p_q. Figure 3 shows the graphs from the M2 analysis of this term-by-term divided series, at $p = 1$, from which one reads $2\nu = 0.75$. The similar M1 analysis yielded $2\nu = 0.74$. Both agree excellently with our direct estimate.

Our main result, $\nu = 0.38 \pm 0.07$ in 3D, is surprising for two main reasons: First, it is quite different from values of ν found for the "usual" Anderson model, which are around 1.35 [23]. Assuming the latter values are reliable, we conclude that QP must belong to a different universality class. Our series definitely show no singularity near $\nu = 1.35$. In some respect, QP involves very strong randomness, as the electron is completely forbidden from hopping onto many sites. Our results indicate that such strong randomness is described by a new set of critical exponents. Second, our result violates the bound $\nu \geq 2/d$ by Chayes *et al.* [4]. Although our series are relatively short, and we cannot exclude the possibility of as yet unidentified systematic errors, we do not believe that these series can yield a value of ν above 2/3. Such a value appears only very rarely in our Padé tables, but then requires a much larger p_q (inconsistent with all other results) and different gaps between the three series. The internal self-consistency, the agreement of our p_q with other methods, and analysis of the 13-term

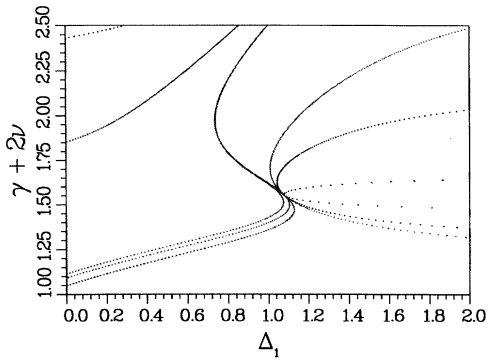

FIG. 2. Same as Fig. 1 at $p_q = 0.36$, which is the central slice from Fig. 1.

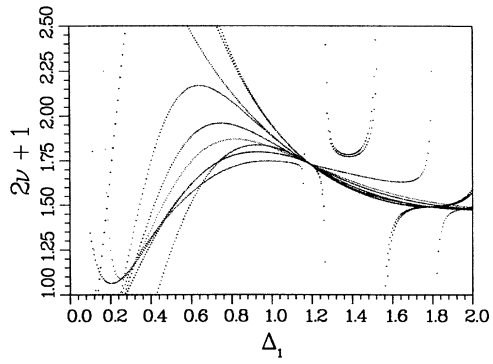

FIG. 3. Graph of Padé approximants at $p = 1$ to $2\nu + 1$ as a function of Δ_1 for the term-by-term divided series of A_4 by A_2 from the M2 analysis.

T series [11] all lead us to believe that longer series will not yield the large shift needed for obeying the inequality. Attempts to fit the series to essential singularities also failed [11]. The Chayes *et al.* proof is based on a particular finite size scaling correlation length, and they themselves agree that it might not apply to other lengths. Our ξ might indeed differ from theirs. Further, Fisher [24] recently presented a model in which the typical and the average correlation lengths scale differently, and the former violates the Chayes *et al.* inequality. Such a violation can occur when there is a very broad distribution of correlation functions. Returning to our data, we looked at series in which T_{ij} was replaced by a power T_{ij}^{α}, and found that for a wide range of $\alpha > 1$ they all diverged at the same p_q, with an exponent essentially independent of α. This is connected with the fact that for E near 0, most of the typical T_{ij}'s have values very close to 0 or to 1. This results from the fact that for such E, dangling ends tend to generate either full reflection or full transmission. Therefore, the distribution of the T_{ij}'s is extremely broad and this may affect the Chayes *et al.* inequality similarly to what was found in Ref. [24]. The validity of this inequality for QP thus remains in question, and we hope this Letter will stimulate more discussion of this issue.

In conclusion, we presented strong evidence that QP belongs to a separate universality class, in which the Chayes *et al.* inequality is violated. It would be useful to test these conclusions using alternative techniques. However, we are not sure if this can be achieved by realistic computer simulations: Experience (at least for simple classical spin problems) shows that n-term series yield information equivalent to simulations on lattices of size $(2n)^d$, and calculating the transmission coefficient on such sizes remains a computational challenge. Furthermore, simulations require repeating the calculations for many different realizations, and depend on the quality of the random number generators. Our series contain exact averages over *all* the random configurations.

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$T(p, E = 0.05) = 1 + 0.059369179264724\,p + 15.01853911937481\,p^2 - 74.34531602418894\,p^3 + 760.5161895506845\,p^4 - 6452.856516402639\,p^5 + 60185.76732793771\,p^6 - 559947.7643814172\,p^7 + 5311865.710968659\,p^8 - 50753977.66167882\,p^9 + 488216454.4491019\,p^{10}$,

$A_2(p, E = 0.05) = 6\,p + 12.59369179264723\,p^2 + 145.7767282576153\,p^3 - 309.7367650024585\,p^4 + 5958.584753455909\,p^5 - 44300.79379450257\,p^6 + 447994.9420215777\,p^7 - 4165093.042329666\,p^8 + 40552372.40381737\,p^9 - 395733428.8883613\,p^{10}$,

$A_4(p, E = 0.05) = 6\,p + 132.5936917926472\,p^2 + 642.4000984517376\,p^3 + 4150.660970827034\,p^4 + 7694.417728573961\,p^5 + 110181.6676560833\,p^6 - 354998.8902780859\,p^7 + 5761142.916124608\,p^8 - 46413682.89702190\,p^9 + 463242310.8309327\,p^{10}$.
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