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LETTER TO THE EDITOR

Quantum percolation thresholds and random walk fractal dimensions

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Abstract. We present an empirical, novel relationship between the quantum percolation threshold, p_q^*, the lattice coordination number, Z, and the random walk fractal dimension, d_w'. The values of p_q^* obtained from this relationship are in good agreement with literature results from numerical simulations on the cubic lattice and its higher dimensional variants. Comparisons with the perturbative theory of Harris are discussed. The impact of the approximate nature of the Alexander-Orbach conjecture on our results has been found to be minimal. We present estimates of p_q^* for several common three-dimensional lattices for which no simulation data exist. Our result is expected to contribute toward estimating p_q^*, particularly in systems for which the underlying lattice structures are either non-trivial or non-existent. The physical implications of our results are discussed.

The question of Anderson localisation has been the subject of intense research interest [1, 2]. One research area involves the so-called off-diagonal disorder in the following tight-binding Hamiltonian:

$$H = \sum_{i \neq j} (v_{ij} a_i^+ a_j + \text{complex conjugate}). \tag{1}$$

Here v_{ij} is the hopping matrix element between site i and site j, and a_i^+ and a_j are, respectively, the creation and annihilation operators for the quantum mechanical particle at site i and j. One imposes a probability distribution on v_{ij} such that $v_{ij} = v \neq 0$ with probability p_q and $v_{ij} = 0$ with probability $1 - p_q$. This is the quantum analogue of the classical bond percolation problem [3-10]. One can study the nature of the eigenstates of the Hamiltonian described by equation (1) as a function of probability, p_q, the Euclidean dimension, d, and the underlying lattice structure. One of the major issues is the critical value of p_q, p_q^* below which no extended eigenstate of equation (1) exists. Extensive calculations [3-10] on p_q^*, based on a variety of numerical techniques, have been reported for values up to $d = 8$. One general result of this effort is the finding that $p_q^* > p_c^*$, the critical threshold for the corresponding classical bond percolation problem [11-13]. The most comprehensive results reported so far have been obtained for the square lattice ($d = 2$) and its higher dimensional equivalence. It is not known what effect the topology of the underlying lattice structure has on p_q^*.

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The purpose of this letter is to introduce a relationship that is approximately dimensionally invariant for quantum percolation and to demonstrate its empirical validity. This relationship is obtained by exploiting the similarity, as well as the differences, between quantum and classical percolation theory. For classical bond percolation, the value of p_c^* depends on the lattice types and the Euclidean dimension [14-16]. However, the quantity $p_c^* Z$ (where Z = coordination number of the lattice) has been known for some time to be approximately dimensionally invariant. In fact, one finds that the relation

$$p_c^* Z \sim d/(d-1) \tag{2}$$

[14-16] agrees quite well with the numerical simulation for $Z = 3$ to 12 in two and three dimensions. An important question is whether a corresponding relationship exists for quantum percolation.

We have discovered an empirical quantum analogue to equation (2) having the following form:

$$p_q^* Z = d_w'/(d_w' - 1) \tag{3}$$

where p_q^* is the critical threshold for quantum percolation and d_w' is the random walk fractal dimension, which is defined such that the mean square displacement $\langle R(t)^2 \rangle$ of a random walker on a fractal is proportional to $t^{1/d_w'}$ for 'short' time t [17-19]. Note that equation (3) has exactly the same form as the corresponding classical relationship. The one crucial difference is the replacement of the Euclidean dimension, d, by the random walk fractal dimension, d_w'.

In looking for a quantum analogue of equation (2) one is guided by the expectation that $p_q^* Z$ is (at least approximately) a dimensionally invariant quantity. However, the effective dimension that enters into the RHS of equation (3) would have to include the effect of the Euclidean dimension as well as the particular features of quantum propagation that would lead to localisation on a percolation cluster. In classical bond percolation, the threshold is determined by the geometrical connectivity of the cluster. In quantum bond percolation, one needs to go beyond purely geometrical effects. We shall present physical arguments suggesting that, due to interference effects and the Alexander-Orbach conjecture, d_w' is the crucial parameter that contains the dimensional dependence as well as the peculiar features of the quantum percolation process [20]. However, before one embarks on these discussions, let us examine how well equation (3) works out in practice.

Calculated results using equation (3) are shown in table 1. The lattices are the simple cubic and its higher dimensional variants. The results from our empirical relationship agree well with numerical data obtained from a variety of simulation techniques. For $d = 5$, 6, 7 and 8, the results agree very well with available data [8]. For $d = 3$, there is scatter in the literature numerical simulation data [5, 7, 8]. To gain a better perspective, we have plotted in figure 1 all the available numerical data from the literature, together with our results from equation (3). The full curve is the best fit drawn through the literature data and is intended to give an indication of likely values of p_q^* for $d = 3$ and 4, as suggested by the data trend. The literature results indicate favourable agreement with equation (3), including $d = 3$ and 4. We have computed d_w' from the fractal dimension, d_f, by using the Alexander-Orbach (AO) conjecture [20]. The AO conjecture is expected to be sufficiently accurate that it is numerically useful for $d \geqslant 3$, as the present application illustrates. Like its classical analogue, equation (3) has no known rigorous justification. It is probable that equation

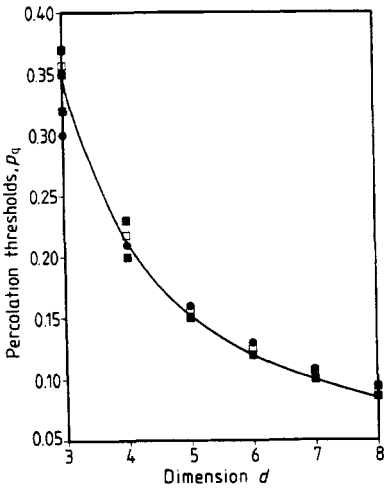

Figure 1. Quantum bond percolation thresholds (p_q^*) against Euclidean dimension (d). The numerical simulation data (■) are from references [3–10], □ is from equation (3) and ● from [26] and [27]. The full curve is a best fit of the numerical simulation data.

(3) is a leading-order approximation that works well in practice. However, the physical reasons for the significance of d'_w can be understood as follows.

The mean square displacement $\langle R^2 \rangle$ of a random walker on a fractal structure (such as a percolation cluster near the critical threshold) scales with time t as $\langle R^2 \rangle \sim (t)^{1/d'_w}$. This relationship holds for time short enough that $\langle R^2 \rangle$ is less than ξ, the correlation length of the percolation network [18]. Note that $d'_w > 1$ [18, 19]. This is contrary to the situation on a Euclidean lattice in which $\langle R^2 \rangle \sim t$. The physical reason that $d'_w > 1$ is because in the fractal regime the walker spends a lot of time in revisiting previously visited sites. In fact, the probability of return to an arbitrarily chosen starting point with excursion up to a distance R away from this starting point can be estimated as

$$\begin{aligned} P_r(R) &\sim \int^{\tau} \frac{1}{t^{\tilde{d}/2}} \, dt \\ &= \tau^{1-\tilde{d}/2} \\ &\propto R^{d'_w(2-\tilde{d})}. \end{aligned} \tag{4}$$

The last line follows from $R^2 \sim \tau^{1/d'_w}$ where τ is the time necessary to undertake a root mean square displacement of R. $\tilde{d}$ is the ratio d_f/d'_w. According to the AO conjecture $\tilde{d}$ has the 'superuniversal' value of $\frac{4}{3}$ [20]. This implies that $P_r(R)$ increases as R increases. Furthermore, within the accuracy of the AO conjecture, the exponent $\beta'_L = d'_w(2-\tilde{d})$ for R in equation (4) becomes directly proportional to d'_w. The dimensional dependence of β'_L enters only through d'_w. In addition, note that β'_L is related to the parameter β_L in the scaling theory of localisation on fractals via $\beta'_L + \beta_L = 0$ [19]. Thus, d'_w is the effective dimensional exponent that characterises $P_r(R)$ in the fractal regime.

The significance of $P_r(R)$ lies in the fact that it determines the probability of forming closed loops (i.e. self-intersecting pathways) of linear extent R. Quantum propagation amplitudes along closed loops in opposite direction (i.e. pairs of time-reversed paths) are phase coherent. These successive multiple return scatterings give rise to constructive

interference [21-23]. They lead to a peak in the scattering intensity in the back-scattering direction. If the disorder is large enough then the accumulation of correlation through successive multiple return scatterings could lead to localisation of the particle. The physical basis of the argument is similar to the theory of diffusional correction to the transport coefficients in weak localisation phenomena [21-23]. Although the thresholds for quantum percolation involve a strong localisation phenomenon, we believe that, for the present system, with strict time reversal invariance, at least the physical basis of the argument should remain applicable [23]. The overall effect is to lead to termination of the propagation of the quantum particle and localisation if the disorder is great enough. These physical arguments suggests that the random walk fractal dimension d'_w rather than the Euclidean dimension is the significant parameter here. Furthermore, the explicit form of equation (3) suggests that the parameter $d'_w/(d'_w-1)$ is in fact the average number of open bonds leading from any given node necessary for the establishment of an extended state in quantum percolation. Note that d'_w only becomes relevant if localisation takes place within the fractal regime (i.e. within a region of linear size $\sim\xi$). This we believe to be the case for $d \geqslant 3$ [24, 25]. In fact, if the excursion distance R is much larger than ξ then one is in the Euclidean regime. The probability of return $P_r(R)$ is given by

$$\begin{aligned} P_r(R) &\sim \int^{\tau} \frac{1}{t^{d/2}}\,dt \\ &= \tau^{1-d/2} \\ &\propto R^{2-d} \qquad \text{if } d \geqslant 3. \end{aligned} \tag{5}$$

The last line follows from $\langle R^2\rangle \sim \tau$ in the Euclidean regime. Note that equation (5) is valid only for $d \geqslant 3$ and that in those cases $P_r(R)$ decreases as R increases. This is qualitatively different from the situation in the fractal regime. A semi-quantitative sketch of the behaviour of P_r as a function of R/ξ for $d=3$ is shown in figure 2. The detailed behaviour of $P_r(R)$ in the region close to ξ cannot be accounted for with the simple power law behaviour as indicated in equations (4) and (5). Nevertheless, the

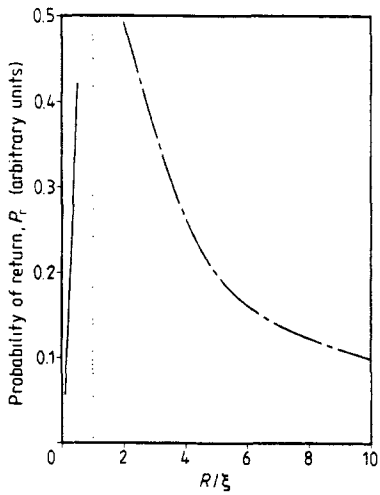

Figure 2. Probability of return P_r as a function of R/ξ at $d=3$: ——, equation (4), fractal regime; - - -, equation (5), Euclidean regime; · · · · ·, the boundary $R=\xi$.

two equations taken together imply that $P_r(R)$ (for $d \geqslant 3$) reaches some maximal behaviour somewhere in the vicinity of the percolation correlation length ξ. One expects that the localisation length $\leqslant \xi$. Since the quantum percolation threshold p_q occurs substantially above p_c it implies that, near p_q, ξ is at most several lattice constants in length. Consequently, localisation is expected to be exponential for quantum percolation in $d \geqslant 3$. However, if the localisation length is longer than ξ (as expected for $d = 2$), then d'_w would not be the relevant parameter for two-dimensional quantum percolation [26]. For this reason, our dimensionally invariant relationship is not expected to be applicable for $d = 2$.

The above discussion is heuristic and physical rather than rigorous. Nevertheless, further support to the above ideas is provided by comparing our results to the perturbative theory of Harris [26] on quantum percolation. It can be seen from table 1† and figure 1 that, except for $d = 3$, the two approaches compare very favourably. The key element in the theory of Harris is a perturbative representation of hypercubic lattices in terms of addition of closed loops to a Cayley tree. The fact that the theory of Harris gives satisfactory results attests to the importance of closed loops (i.e. self-intersecting paths) leading to multiple return scatterings and subsequent localisations. For $d = 3$, our results seem to be in better agreement with the numerical simulation data. The threshold seems to have been underestimated with the Harris result. This may be because the perturbation parameter in the theory of [26] is $1/\sigma$, where $\sigma + 1$ is the lattice coordination number Z. Thus, the theory of Harris is expected to be more satisfactory at higher dimensions, as can be seen from table 1 and figure 1.

Table 1. Values for p_q^* against dimension d.

d	p_q^* numerical experiments	p_q^* equation (3)	p_q^*[26] (Harris)
3	0.37[5], 0.32[8], 0.35[7]	0.357	0.30
4	0.23[5], 0.20[8]	0.218	0.21
5	0.15[8]	0.157	0.16
6	0.12[8]	0.125	0.13
7	0.10[8]	0.107	0.108
8	0.086[8]	0.094	0.095

Using equation (3) and assuming its general validity, we have estimated the quantum bond percolation thresholds, p_q^*, for the diamond lattice ($p_q^* = 0.536$), the BCC lattice ($p_q^* = 0.268$), and the FCC lattice ($p_q^* = 0.179$). As far as the authors are aware, this is the first time that estimates of p_q^* for these three-dimensional lattices have been made. It would be interesting to compare these estimates with those from detailed computer simulations. This would serve to better determine the regime where our dimensionally invariant relationship is valid. The above discussion leads to an interesting question. Our heuristic argument rests mainly on two points. Firstly, the use of $P_r(R)$ if the mode of propagation can be described as diffusive (in both fractal and Euclidean domain), and secondly the possibility of constructive interference for propagation

† These results were obtained by us using the theory in [26].

along pairs of time-reversed paths. Thus, one might expect similar phenomena occurring for wave propagation in general (classical or quantum) on percolation clusters†. In particular threshold behaviour characterised by d'_w and equation (3) might be anticipated. One may gain important insight into these questions as well as the problems of quantum percolation and localisation by exploring further the theoretical implications of the present results.

In conclusion, we have discovered an empirical relationship between p_q^*, Z and d'_w. The physical significance of d'_w is discussed in terms of self-intersecting pathways and multiple return scatterings. The relationship gives results that compare very favourably with existing numerical experiments and analytical theory. It identifies an important parameter, $d'_w/(d'_w-1)$, which is the average number of open bonds leading from any given node necessary for the establishment of an extended state in quantum percolation. If our relationship for quantum percolation has general applicability similar to its classical counterpart, then it could provide rapid and useful estimates for the critical thresholds. It would be particularly useful for many applications in which either the underlying lattice structures are too complex for efficient simulations or else there is only local short-range order. Even in systems that are more amenable to numerical simulations, it would be useful to have a good idea of the general location of the critical threshold. More importantly, our dimensionally invariant relationship would suggest a deep and hitherto unsuspected connection between quantum percolation and fractal random walk.

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† The present discussions relate to strong localisation on percolation clusters. For classical weak localisations on disordered media generated by diffusion-limited aggregation, see e.g. [27].

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