Quantum localization near the classical percolation threshold

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(Received 21 May 92)

The effect of the fractal nature of a percolating cluster on the inverse participation number $\bar{\mathcal{P}}$, which is a direct measure of the size of localization domains, is discussed. As a function of composition, $\bar{\mathcal{P}}$ has a sharp jump at the classical percolation threshold, although the states are expected to be localized. We argue that the magnitude of this jump can be related to the fractal dimension of the percolation channel on a given lattice.

I. INTRODUCTION

In a calculation of the average inverse participation number, $\bar{\mathcal{P}}$, on square and cubic lattices with random bimodal distribution of atoms and vacancies (i.e., "infinite" disorder, the vacant sites being inaccessible to the spreading wave functions) Srivastava and Chaturvedi[1] (hereafter referred to as SC) reported a sharp jump at the classical percolation threshold, p_c. The number $\bar{\mathcal{P}}$, as calculated from the equation of motion method,[2] provides a measure of the inverse of the fraction of lattice sites participating in a wave function and is expected to be nonzero for $p \leq p_q$, which marks the "quantum" percolation threshold where the first extended state is formed. The cause for the jump in $\bar{\mathcal{P}}$ at p_c was not *a priori* obvious and simple scaling considerations[1] indicated that it might be caused by a sudden merger of a large number of large clusters at p_c to form the percolating channel, leaving the dominant contribution to $\bar{\mathcal{P}}$ to come from smaller clusters.

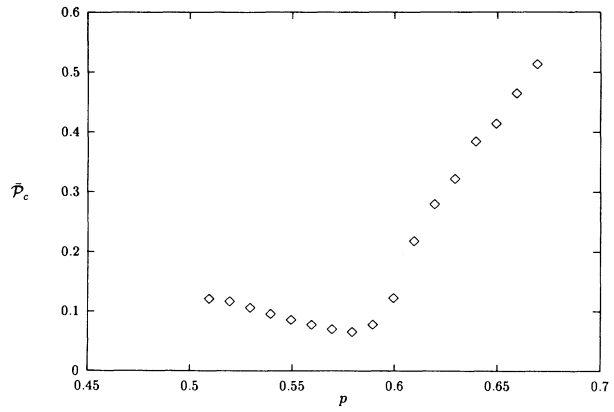

FIG. 1. Inverse of average cluster size, $\bar{\mathcal{P}}_c = < s >^{-1}$, vs concentration, p, of occupied sites *excluding* the percolating channel. This was expected in Ref. 1, to approximate $\bar{\mathcal{P}}$ and also to exhibit a local maximum at p_c similar to what was found in the $\bar{\mathcal{P}}$ vs p behavior (also shown in Fig. 2). The present calculation of $\bar{\mathcal{P}}_c$ is for a square lattice of dimensions 500×500 and an additional averaging has been done over 10 configurations.

We have performed a numerical test of the scaling hypothesis of SC to determine whether the jump in $\bar{\mathcal{P}}$ at p_c has the suggested classical origin. We find that the classical $\bar{\mathcal{P}}_c$, the inverse of the average cluster size, does not show the jump expected by SC at p_c — it decreases monotonically for increasing p, below p_c, and after a minimum at p_c it begins to rise for $p > p_c$ without ever coming down (see Fig. 1). A similar result is obtained if $\bar{\mathcal{P}}_c$ is calculated as the average of the inverse of cluster size as defined in Ref. 1. We suggest here that the reported sharp jump[1] in $\bar{\mathcal{P}}$ at p_c is attributable to the fractal nature of the percolating channel at $p = p_c$. The tortuous and ramified character of the percolating cluster is highly favorable for the states to be strongly localized on the cluster and, therefore, for large values of quantum mechanical $\bar{\mathcal{P}}$ at $p = p_c$ (the $\bar{\mathcal{P}}$ in SC is in fact calculated quantum mechanically). Thus, we suggest that the jump in $\bar{\mathcal{P}}$, although occurring at the classical percolation threshold, has a quantum-mechanical origin in that it arises as a result of the shrinking of the localization domain at $p = p_c$ when the percolation channel assumes a fractal nature; the simple calculation based on cluster-size scaling, which counts only the number of sites in the finite cluster, completely excludes the percolating cluster whose structural details we suggest here are crucial and are apparently responsible for the observed feature[1] in $\bar{\mathcal{P}}$.

II. SHORTCOMINGS OF THE CLASSICAL ARGUMENT

It may be important to understand why the scaling calculation of SC should have failed to explain the feature of $\bar{\mathcal{P}}$ in question, before proposing an alternative explanation.

Note that the calculation of $\bar{\mathcal{P}}$ is strongly weighted in favor of the energy at the center of the band.[1] Since these states are expected to be the most spread out compared with other energies in the band, it was suggested that these states will overlap all the clusters and on each clus-

ter their extent will be comparable to the cluster size. So it was suggested that $\bar{\mathcal{P}}$ would be an average of the inverse cluster size. We realize that this is not quite correct. The wave functions corresponding to the band center should overlap the largest clusters at a given value of p with the highest probability because the energy-level spacing on these clusters is the smallest. Consequently, at the outset, one should expect $\bar{\mathcal{P}}$ to decrease monotonically with increasing p since the size of the largest clusters grows continually as more and more atoms are added to the system. The distribution function for the finite cluster sizes and features such as having its weight shifting to the larger clusters for $p < p_c$, and to smaller clusters for $p > p_c$, etc., which were the basis of the SC calculation, do not seem to be important in view of the above argument.

If we do not restrict our consideration to the largest clusters at a given p but rather include some other large clusters also, for the sake of generality, then $\bar{\mathcal{P}}$ versus p should behave like $< s >^{-1}$ versus p with the average $< >$ taken from a probability distribution n_s, where s represents the cluster size and n_s is the number of s-clusters per lattice site.[3] Note that unlike what was done by SC in their calculation, we need not subtract out the percolating channel in the above calculation of $< s >^{-1}$. For $p > p_c$ the energies around the band center will have the maximum overlap on the percolating channel but because of the quantum interference arising due to the reflections from the infinitely high and torturous boundaries of the channel the wave function will be localized only to a part of it. Thus, although $< s >^{-1}$ will be zero for $p \geq p_c$, $\bar{\mathcal{P}}$ will still be nonzero for $p_c < p < p_q$. In fact, even for $p < p_c$, $\bar{\mathcal{P}}$ will be larger than $< s >^{-1}$ for the same reason.

III. JUMP IN $\bar{\mathcal{P}}$ AT p_c: QUANTUM NATURE

If the above understanding is correct, then the sharp feature of $\bar{\mathcal{P}}$ at $p = p_c$ reported by SC must arise because of a special property of the percolating channel which the clusters at $p < p_c$ do not possess. This special property evidently is the fractal nature of the percolating cluster.[3] We suggest that the fractality of the percolating cluster makes the localization stronger by restricting the wave function to a lesser number of sites. The value of $\bar{\mathcal{P}}$ should, therefore, jump to a higher value as soon as the above-described situation occurs and should then decrease steadily for $p > p_c$ as the gaps in the percolating cluster are filled in, which also reduces its fractal character. It turns out that, on the basis of this argument, the magnitude of the jump in $\bar{\mathcal{P}}$ at $p = p_c$ should be related to a measure of the fractality of the percolating cluster, which is its fractal dimension, d_f. The *dimensional reduction* from d to d_f is, in formal terms, the cause for stronger localization at a given energy.

Suppose the states in a narrow energy range, ΔE, around $E = 0$ spread over a volume R^d at a concentration p_c^-, just below p_c. The $\bar{\mathcal{P}}$ at $p = p_c^-$ will be inversely proportional to R^d since this measures the number of sites enclosed in that volume, assuming that the whole volume is almost entirely filled with sites and that there are very few gaps inside the region R^d. In addition, if we assume that the length (or the radius) of localization changes little as the concentration increases slightly to $p = p_c^+$, just above p_c, we note that now the region inside R^d has many gaps at different length scales and the actual mass (or the sites along which the wave function can spread) is much less than what it was at $p = p_c^-$; the reduced mass is now proportional to R^{d_f}, where d_f is the fractal dimension of the percolating cluster. Thus, the participation number changes from R^d, had the percolation channel not been a fractal, to R^{d_f}. So we can write $\bar{\mathcal{P}}|_{p_c^+} \approx [\bar{\mathcal{P}}|_{p_c^-}]^{d_f/d}$, from which we can estimate the fractal dimension as

$$d_f = d \frac{\ln \bar{\mathcal{P}}|_{p_c^+}}{\ln \bar{\mathcal{P}}|_{p_c^-}}. \tag{1}$$

Using the values of $\bar{\mathcal{P}}$ from Fig. 2, taken from the data of SC,[1] we find from Eq. (1) $d_f = 1.58$ for the square lattice and $d_f = 2.20$ for the cubic lattice. These should be compared with the fractal dimensions for the percolating clusters[3] $d_f = 1.896$ and $d_f = 2.53$ for two- and three-dimensional lattices, respectively.

The agreement between these values is to be considered reasonable since, first, there are finite-size effects to be taken into account in the calculation of $\bar{\mathcal{P}}$ and, second, the estimate from Eq. (1) is at best a lower bound to the true value of d_f in view of the following. At $p = p_c^+$, the fractal cluster inside the volume R^d may have more sites with reduced coordination than sites with full coordination. Consequently, there will be numerous reflections from the extremely tortuous, infinitely high boundaries of the cluster which will give rise to quantum interference and result in very strongly localized states. The radius of localization can reduce drastically below R, say, to a small value r. This would mean that the effective mass (i.e., the sites) over which the localized wave function is

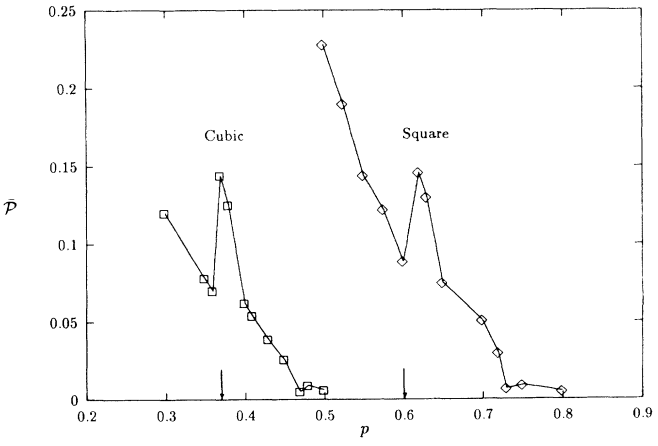

FIG. 2. $\bar{\mathcal{P}}$ vs p for square and cubic lattices as taken from the data of SC (Ref. 1). The straight lines joining the data points are guides to the eyes, and the vertical arrows mark the classical percolation threshold, p_c, for cubic and square lattices.

spread will actually decrease from R^d to r^{d_f} as p changes from p_c^- to p_c^+. So, instead of taking $\bar{\mathcal{P}}|_{p_c^\pm} \propto R^{-d_f}$, we should take $\bar{\mathcal{P}}|_{p_c^+} \propto r^{-d_f}$, which will increase the values of d_f obtained from Eq. (1), thus improving the agreement. A better agreement could also be obtained by averaging Eq. (1) over many configurations. More refined calculations of $\bar{\mathcal{P}}$ and d_f will be reported in a future publication.

IV. CONCLUSION

In summary, we argue that the fractal nature of the percolating channel should have a distinct effect on quantities measuring the localization domain, such as the inverse participation number $\bar{\mathcal{P}}$ discussed here, although the states are still expected to be localized on the percolating channel. The reported[1] nonmonotonic behavior of $\bar{\mathcal{P}}$ as a function of p which shows a sudden jump at $p = p_c$ has been related to the fact that localization is stronger (i.e., the wave function occupies fewer sites) in the percolating channel because of its fractal character. It is interesting to note that a refined $\bar{\mathcal{P}}$ vs p calculation can actually be used to determine the fractal dimension, since the latter is the only additional factor at $p = p_c$ that apparently affects the localization.

ACKNOWLEDGMENTS

One of us (V.S.) would like to thank Conselho Nacional de Pesquisas (CNPq), Brazil for financial support and Dr. Ivan C. da Cunha Lima for helpful discussions and hospitality at INPE, where this work was done. We are grateful to Dr. Tapio Ala-Nissila for numerous discussions on this work.

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