Two-dimensional quantum percolation on anisotropic lattices

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In a previous work [Dillon and Nakanishi, Eur. Phys. J B 87, 286 (2014)], we calculated the transmission coefficient of the two-dimensional quantum percolation model and found there to be three regimes, namely, exponentially localized, power-law localized, and delocalized. However, the existence of these phase transitions remains controversial, with many other works divided between those which claim that quantum percolation in 2D is always localized, and those which assert there is a transition to a less localized or delocalized state. It stood out that many works based on highly anisotropic two-dimensional strips fall in the first group, whereas our previous work and most others in the second group were based on an isotropic square geometry. To better understand the difference in our results and those based on strip geometry, we apply our direct calculation of the transmission coefficient to highly anisotropic strips of varying widths at three energies and a wide range of dilutions. We find that the localization length of the strips does not converge at low dilution as the strip width increases toward the isotropic limit, indicating the presence of a delocalized state for small disorder. We additionally calculate the inverse participation ratio of the lattices and find that it too signals a phase transition from delocalized to localized near the same dilutions.

I. INTRODUCTION

Quantum percolation (QP) is one of several models used to study transport in disordered systems. It is an extension of classical percolation, in which sites/bonds are removed with some probability q. In the classical percolation model, transmission on a disordered lattice is dependent solely on the connectivity of the lattice: the lattice is transmitting only if there exists some connected path across the lattice. As the dilution increases, the probability of finding a connected path between any two arbitrarily chosen points decreases while there is still a 100% guarantee of finding some connected path through the lattice; at some critical dilution (q ≈ 41% in site percolation and q = 50% in bond percolation, on the square lattice) there is zero chance of finding any connected path across the lattice and the system is insulating. In the quantum percolation model, the particle traveling through the lattice is a quantum one, and thus quantum mechanical interference also influences transmission; in fact, even in a perfectly connected lattice (q = 0) one may have partial transmission depending on the energy of the particle and the boundary conditions of the lattice. Because of these interference effects, localization will occur at a lower dilution than in the classical model, if at all.

The question of whether disorder prevents conduction, especially in two dimensions, is one which spans decades, beginning with the introduction of the Anderson model in 1958. A few decades later, Abrahams et al used one-parameter scaling theory to show that in the Anderson model, any amount of disorder prevents conduction for d ≤ 2.2 This result was confirmed through various studies in the years following, with some exceptions for special cases (see for example Refs 3 and 4 and references therein).

Due to its similarities with the Anderson model, it was initially believed that the quantum percolation model would likewise lack a transition to a delocalized state in two dimensions. However, this proved to not necessarily be the case, and some controversy arose over what phase transitions may exist for the 2D QP model. Some found there to be only localized states, while others found a transition between strongly and weakly localized states but no delocalized states. More recent work, including previous work by this group, has found that a localized-delocalized phase transition does in fact exist for the quantum percolation model at finite disorder in two dimensions. Most recently, present authors determined a detailed phase diagram showing a delocalized phase at low dilution for all energies 0 < E ≤ 1.6, with a weak power-law localized state at higher dilutions and an exponentially localized state at still higher dilutions.

Among the various calculations employed to study the quantum percolation model, it stands out that most works based on two-dimensional, highly anisotropic strips yield results supporting one-parameter scaling’s prediction of only localized states, whereas our calculations in Ref. 17 and most others finding a delocalized state were based on an isotropic square geometry. One of the studies in the first group was by Soukoulis and Grest, who used the transfer matrix method to determine the localization length λ_M of long, thin, quasi-one-dimensional strips of varying width M, after which they used finite size scaling to determine the localization length λ in the two-dimensional limit and thus the phase of the system (Ref. 6 see Ref. 13 for more detail on the transfer matrix method in two dimensions). It is worth noting that Daboul et al., who found at most weakly localized states on isotropic lattices, also found disagreement with Soukoulis and Grest’s results;

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they noted that the extreme anisotropy of the strips used in the transfer-matrix method might overly influence its results toward a more 1-D geometry than 2-D. Aside from geometry, Soukoulis and Grest also differ from our previous work in that they only examined dilutions within the range \(0.15 \leq q \leq 0.50\), the lower limit of which is very close to the delocalization phase boundary we found in Ref. \(^{17}\) which could explain why they did not find any delocalized states. To better understand the differences between our results and theirs, in this work we apply our direct calculation of the transmission coefficient to the quasi-1D scaling geometry used by Soukoulis and Grest over the same energies \(E\) and widths \(M\) they used, but over a larger range of dilutions extending into lower dilutions than those they examined. We additionally examine the inverse participation ratio of the lattices, which, when extrapolated to the thermodynamic limit, provides another indicator of localization.

We start from the approach used by Dillon and Nakanishi\(^{13}\), using the quantum percolation Hamiltonian with off-diagonal disorder and zero on-site energy

\[
H = \sum_{<ij>} V_{ij} |i\rangle \langle j| + h.c
\]  

where \(|i\rangle\) and \(|j\rangle\) are tight binding basis functions and \(V_{ij}\) is a binary hopping matrix element between sites \(i\) and \(j\) which equals a finite constant \(V_0\) if both sites are available and nearest neighbors and equals 0 otherwise. As in previous works, we normalize the system energy and use \(V_0 = 1\).

We realize this model on an anisotropic square lattice of varying widths \(M\) and lengths \(N\) to which we attach semi-infinite input and output leads at diagonally opposite corners and which we randomly dilute by removing some fraction \(q\) of the sites, thus setting their corresponding \(V_{ij}\) to zero. \(N\) is chosen such that \(N = 10 \times M\) at minimum to obtain quasi-one-dimensional geometry, and such that the diagonally opposite sites have the same parity in order to maintain the symmetry of the input and output leads as \(N\) is varied for the same \(M\) (i.e., the leads are always on the same sublattice). The wavefunction for the entire lattice plus input and output leads can be calculated by solving the Schrödinger equation

\[
H\psi = E\psi
\]

where, \(\psi = \begin{bmatrix} \psi_{in} \\ \psi_{\text{cluster}} \\ \psi_{out} \end{bmatrix}\) (2)

and \(\psi_{in} = \{\psi_{-(n+1)}\}\) and \(\psi_{out} = \{\psi_{+(n+1)}\}\) are the input and output lead parts of the wave function, respectively. Using an ansatz by Daboul et al.,\(^{11}\), we assume that the input and output parts of the wavefunction are plane waves

\[
\psi_{in} \rightarrow e^{-i\kappa} + re^{i\kappa} \\
\psi_{out} \rightarrow e^{i\kappa}
\]  

where \(r\) is the amplitude of the reflected wave and \(t\) is the amplitude of the transmitted wave. This ansatz reduces the infinite-sized problem to a finite one including only the main \(M \times N\) lattice and the nearest input and output lead sites, for the wavevectors \(\kappa\) that are related to the energy \(E\) by:

\[
E = e^{-i\kappa} + e^{i\kappa}
\]  

Note that the plane-wave energies are thereby restricted to the one-dimensional range \(-2 \leq E \leq 2\) rather than the full two-dimensional energy range \(-4 \leq E \leq 4\); nonetheless this energy range has been sufficient for us to observe the localization behavior of the wavefunction in prior work.

The reduced Schrödinger equation after applying the ansatz can be written as a \((M \times N + 2) \times (M \times N + 2)\) matrix equation of the form

\[
\begin{bmatrix}
-E + e^{i\kappa} & c_1^t & 0 & 1 + r & e^{i\kappa} - e^{-i\kappa} \\
c_1 & A & c_2 & \psi_{\text{cluster}} & 0 \\
0 & c_2^t & -E + e^{i\kappa} & t & 0
\end{bmatrix}
\]  

where \(A\) is an \(M \times N \times M \times N\) matrix representing the connectivity of the cluster (with \(E\) as its diagonal components), \(c_i\) is the \(M \times N\) component vector representing the coupling of the leads to the cluster sites, and \(\psi_{\text{cluster}}\) and \(\bar{0}\) are also \(M \times N\) component vectors, the former representing the wavefunction solutions (e.g., on sites \(a-h\) in Fig. 1). The cluster connectivity in \(A\) is represented with \(V_{ij} = 1\) in positions \(A_{ij}\) and \(A_{ji}\) if \(i\) and \(j\) are connected, otherwise 0.

Eq. 5 is the exact expression for a 2D system connected to semi-infinite chains with continuous eigenvalues within the range \(-2 \leq E \leq 2\) as discussed above. The transmission \((T)\) and reflection \((R)\) coefficients are determined by \(T = |t|^2\) and \(R = |r|^2\).
From the wavefunction solutions of Eq. 5 we also calculate the Inverse Participation Ratio (IPR), which measures the fractional size of the particle wavefunction across the lattice and gives a picture of the transport complementary to the picture provided by the transmission coefficient alone. The IPR is defined here by:

$$ \text{IPR} = \frac{1}{\sum_i |\psi_i|^4 (M \times N)} \quad (6) $$

where $\psi_i$ is the amplitude of the normalized wavefunction for the main-cluster portion of the lattice on site $i$ and $M \times N$ is the size of the lattice. (For our model, we have chosen to normalize the IPR by the lattice size rather than connected cluster size, as is sometimes done, since the lattice size is the fixed parameter and doing so allows better comparison between different sizes when extrapolating to the thermodynamic limit.) It should be noted that our $\psi$ for given $E$ is a continuum eigenstate of the system containing the 1D lead chains, and $\psi_{\text{clust}}$ is expected to correspond to a mixed state consisting of eigenstates of the middle square portion of the lattice. We see that given two lattices of the same size, the one with the smaller IPR has the particle wavefunction residing on a smaller number of sites, though the precise geometric distribution cannot be known from the IPR alone. The IPR is often used to assess localization by extrapolating it to the thermodynamic limit: if the IPR approaches a constant fraction of the entire lattice, this ensures that the transport symmetry is not disturbed as $N$ is changed for the given $M$. In our case only even widths $M$ were examined. The upper limit of $N$ was determined by computational limitations, since for large $N$ and $q$ the transmission was small enough to result in an underflow 0. For most dilutions this occurred for $N \geq 200M$, though for larger energies the cut-off was lower. Despite these computational limitations in calculating $T$, we found that the transmission dropped off with $N$ sufficiently smoothly and quickly that an accurate fit of the transmission was able to be found for all but the highest dilutions ($q \geq 30\%$), all of which fall well above the delocalization-localization phase boundary found in Ref. 17.

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From the transmission coefficients for lattices with the above parameters we are able to determine the localization length $\lambda_M$ of the various strips of width $M$, and extrapolate the results in the isotropic limit to find the 2D localization length $\lambda$. First, we plot transmission $T$ vs lattice length $N$ for each width $M$ and energy $E$, for each dilution $q$ that had a sufficient number of points to establish a fit for the transmission ($2\% \leq q \leq 25\%$ for smaller $M$ and larger $E$). All dilution curves decay exponentially ($T = a \times \exp(-bN)$), as is to be expected given the highly anisotropic quasi-1D lattices. An example of the fitted $T$ vs $N$ curves for $E = 1.05$ and $M = 64$ at selected dilutions is given in Fig. 2. The other $(E,M)$ pairs have similar transmission curves.

To determine the inverse localization length $b_M \propto 1/\lambda_M$ in the quasi-one-dimensional thermodynamic limit of a strip of width $M$ and length $N \to \infty$, we use the successive fitting procedure described in Ref. 17. In Section III, for each $T$ vs $N$ curve, we fit just the first 6 points, then the first 7 points, etc until all points have been added, saving the parameter $b$ from each exponential fit. We then plot the saved $b$ vs $N_{\text{max}}$, where $N_{\text{max}}$ is the maximum length included in the fit result.
FIG. 3. Inverse localization length $b_M$ of quasi-1D strips of width $M$ plotted vs. $M$ for selected dilutions $q$ at an energy of $E = 1.05$. At low dilutions the best fit is one which decays to zero, indicating delocalization (dashed line); for higher dilution the best fit is one with an offset term corresponding to the inverse localization length of the system (dotted line).

Extrapolating $b_M$ to the 2D isotropic limit determines the localization of the system: for $b_M \to 0$ ($\lambda_M \to \infty$) as $M \to \infty$, the system is delocalized, but if $b_M \to b_\infty$ ($\lambda_M \to \lambda$), where $b_\infty$ is some finite constant, then the system is localized. We fit $b_M$ vs $M$ for each energy and width and find that for $E = 1.05$ and $q \leq 12\%$, $E = 0.25$ and $q \leq 15\%$, and $E = 0.05$ and $q \leq 8\%$, a fit which decays to zero is the best fit, whereas above these dilutions a fit with a constant offset $b_\infty$ fits the $b_M$ vs $M$ curves better, as shown for example at $E = 1.05$ in Fig. 3.

Thus there is in fact a delocalized phase at each energy for these low values of disorder. Moreover, while our prior work did not study these energies specifically, the upper bounds for delocalization found here correspond roughly to those found in Ref. 17; an exact match is not expected due to the different geometry. At the dilutions and energies for which $b_M$ stabilizes to a non-zero value $b_\infty$, we calculate the localization length by $\lambda = 1/b_\infty$.

To most easily compare our results with those of Soukoulis and Grest, we plot $\lambda_M/M$ vs $\lambda/M$ (see Fig. 4a) as in their Fig. 1 from Ref. 5. There are two noticeable differences and one important similarity between their results and ours. First, our figure has no points in the lower left for the smaller values of $\lambda$ and $\lambda_M$. This area is where the small localization lengths at high dilution should be, and their absence is simply a result of the computational limitations of our transmission fit technique, described at the beginning of this section. Secondly, the localization lengths we do have do not exactly overlap in their values with those of Soukoulis and Grest, nor do they all collapse neatly onto one curve. These might partially be explained by a missing factor in our transmission fits; when determining the localization length, we assumed that in the fit $T = a \exp(-b_M N)$, $b_M = 1/\lambda_M$, when it may be that $b_M = c/\lambda_M$, where $c$ is another constant which may depend on $M$. If there is such a constant, the vertical position of our localization points may be shifted from their true values. Additionally, the $\lambda$ determined by Soukoulis and Grest were a fitting parameter chosen to induce the points to collapse onto one curve, following the scaling procedure outlined in Refs. 13 and 18, whereas our values of $\lambda_M$ were determined independently. Our $\lambda$ do have error bars (omitted from Fig. 4) to avoid cluttering the figure and choosing different $\lambda$ within the bounds of our fit estimates at $E = 1.05$ and $E = 0.25$, for instance, yields a somewhat better collapse of those energies’ localization lengths onto one curve (see Fig. 4b).

Despite the differences in our two figures, however, there is one significant similarity. That is, in the dilution range $15\% \leq q \leq 20\%$ for which our work does have overlap with the dilutions studied by Soukoulis and Grest, our localization lengths fall within the same or-
III. INVERSE PARTICIPATION RATIO CALCULATIONS

To corroborate our finding delocalized states at small disorder on the anisotropic quasi-1D strips, we also examined the Inverse Participation Ratio (IPR) as the system size increases. We observe that even at the largest and most anisotropic lattice studied, $M = 128, N = 200M$, the IPR distribution of all realizations at small dilution has a distinct peak at $IPR \neq 0$, and the average value is greater than $1/M$, which is the minimum fraction required to span the lattice, whereas at large dilution the peak is near zero (Fig. 5). This seems to hint at the transition we observed in the previous section. When we plot the average IPR vs $N$ for fixed width (as in Fig. 6), we also see that the average IPR decreases much less rapidly than the corresponding transmission $T$ (compare Fig. 2), with the IPR at large $N$ remaining well above zero (in fact, the average IPR does not have the problem with computational underflow that the transmission does at large dilution). This illustrates the fact that while the transmission and IPR are related, they do represent different ways of examining localization. It is entirely possible to have many realizations with clusters spanning the lattice that are connected to the input site and to an edge site on the opposite end that is not the output site, as illustrated in the hypothetical example in Fig. 7. If this is the case, the average IPR (which is measured over the entire lattice irrespective of the input) would be nonzero while the transmission (which is measured only corner-to-corner) would be very close to zero.

When we fit the average $IPR$ vs $N$ curves at fixed $M$, we observe an interesting trend in the curves as dilution increases. Surprisingly, the $IPR$ vs $N$ at low dilution can be fit very well to a curve with a nonzero offset that we call $IPR_M$. An example at $E = 1.05$ and $M = 64$...
crease the dilution, the isotropic 2D limit. On the other hand, as we in-
to a nonzero fraction of the lattice as we scale toward
the IPR grows in proportion to the width and stabilizes
an offset (in this case, a power-law with offset), meaning
lution the IPR → ∞ at energy E higher dilutions
IPR→ ∞ M
To capture the latter situation, we plot the offset terms
for those dilutions at which we found delocalization.
we should see the average IPR approach a finite value
calized, but if we extrapolate toward an isotropic case,

FIG. 8. Inverse participation ratio IPR_M for fixed-width
lattices plotted vs lattice width M for selected dilutions q
at energy E = 1.05. For low dilution, IPR_M → IPR_∞ as
M → ∞ (dashed lines), indicating delocalization, while at
higher dilutions IPR_M → 0, indicating localization (dotted line)
is shown in Fig. 7. This is unexpected, since in the 1-D
limit we know the states are localized, but can be ex-
plained as being a result of our including lengths only
up to N = 200M due to the computational limitations
in T. However, as q increases to large disorder, we find
that IPR vs N is best fit by a curve decreasing smoothly
to zero. This change hints at the phase transition we
observed in the 2D isotropic limit in Section II: if we
included still longer lengths N toward the 1-D limit, we
should see the IPR → 0 since the 1D limit is purely lo-
calized, but if we extrapolate toward an isotropic case,
we should see the average IPR approach a finite value
for those dilutions at which we found delocalization.
To capture the latter situation, we plot the offset terms
IPR_M from the lower dilution fits vs M (see Fig. 8 for
example at E = 1.05). Again, we find that at small di-
lution the IPR_M vs M curve is best fit by a curve with
an offset (in this case, a power-law with offset), meaning
the IPR grows in proportion to the width and stabilizes
to a nonzero fraction of the lattice as we scale toward
the isotropic 2D limit. On the other hand, as we in-
crease the dilution, the IPR_M vs M curves eventually
are better fit by a pure power law, meaning that al-
though the anisotropic lattices may have had spanning
clusters, these clusters do not grow proportionally with
M and eventually become disconnected from the output
due to the computational limitations
b_M = λ_M^1
in T. Although the transmission calculations
only allow us to study a limited range of dilutions ef-
fectively due to computational limitations, we none-
thless were able to detect a phase transition at specific
dilutions, above which the M-width strip inverse local-
ization lengths b_M converged to a finite value, and be-
low which they decayed to zero, indicating an infinite,

FIG. 7. An example of a lattice with a connected cluster spanning the lattice but not attached to the output corner.

IV. SUMMARY AND CONCLUSIONS

We have studied the quantum percolation model on

highly anistotropic two-dimensional lattices, scaling to-
ward the isotropic two-dimensional case (studied in pre-
vious works) to determine the localization state and
localization length in the thermodynamic limit. We
determined the localization length by a two-step pro-
cess in which we first determined the inverse localiz-
tion lengths N → ∞ (dashed lines), indicating delocalization, while at
higher dilutions IPR_M → 0, indicating localization (dotted line)

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prior work. The localization lengths found in this work for dilutions within the localized region fall within the same order of magnitude of those found by Soukoulis and Grest at the lower end of the range of dilutions they studied, leading us to believe that they simply did not look at small enough dilutions, thus missing the phase transition.

We additionally checked the localization state of the anisotropic strips by studying the inverse participation ratio of the lattices, which tells us what fraction of sites sustain the particle wavefunction. We find that even on narrow anisotropic strips, at small dilution the average IPR shows a distinct peak away from zero at a value large enough to span the lattice, while at large dilutions the peak is near zero. When we scale toward the isotropic limit, we find that the IPR vanishes for large dilution, indicative of localization, while it approaches a finite value for low dilution, indicative of a delocalized state. Furthermore, the dilutions above which the inverse participation ratio vanishes in the isotropic limit match the phase boundaries found in the first part of the paper.

The results of our work in this paper serve two purposes. First, by using the same basic technique (transmission coefficient and inverse participation ratio measurements) as our previous work on a different geometry - that is, highly anisotropic lattices scaled to the 2D thermodynamic limit - we obtain the same delocalization-localization phase boundary results, showing that the phase transition found previously was not dependent on using isotropic geometry. Secondly, by using the same geometry as Soukoulis and Grest (and other works that use the transfer matrix approach), we found overlap between our localization length results and theirs at higher dilutions, but also examined smaller dilutions and found a delocalized state, leading us to suspect that their extrapolation of the results from 15% ≤ q ≤ 50% toward even smaller dilutions was not warranted. Had our localization lengths within their range dramatically differed from theirs, we would perhaps conclude that the differing techniques used led to the difference in whether a delocalized state was found, but as we have shown, this seems not to be the case.

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