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## LETTER TO THE EDITOR

# A study of the two-dimensional bond quantum percolation model

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**Abstract.** The nature of the electronic states of the two-dimensional bond quantum percolation model is investigated using the finite size scaling method. The results indicate that at all concentrations above the percolation concentration the states are exponentially localised. There is no delocalisation transition. The scaling behaviour of the model is found to be the same as for the normal Anderson model in two dimensions.

Recently there has been a report (Meir *et al* 1989) claiming clear evidence of a delocalisation transition in the 2D quantum percolation model (QPM) (Kirkpatrick and Eggarter 1972). The implications of such a transition for a single-parameter scaling theory of localisation (Abrahams 1979) and the associated universality ideas motivated this work on the model using an alternative technique.

We treat the model, defined below, numerically using the finite size scaling method (MacKinnon and Kramer 1983), which has proven very powerful in earlier studies of the Anderson model. We find no evidence of a delocalisation transition at any concentration. Our results show a single-parameter scaling which is similar to that of the normal Anderson (NA) model.

We will now consider our model. The QPM is a nearest neighbour (NN) tight-binding Hamiltonian (TBH) defined on a square lattice.

$$H = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{i,j} |i\rangle V_{ij} \langle j|. \quad (1)$$

$\{|i\rangle\}$  are a basis of wavefunctions centred on each site,  $i$ . The site energies  $\varepsilon_i$  are constant and taken to be zero. The hopping integrals  $V_{ij}$  are taken to be either 1, with probability  $p$ , or 0, with probability  $1 - p$ , depending on whether the *bond* is present or absent; i.e. they are distributed randomly with probability distribution

$$P(V_{ij}) = p\delta(V_{ij} - 1) + (1 - p)\delta(V_{ij}). \quad (2)$$

The analogy between the value of the hopping element and the presence or absence of a bond leads to the name *quantum percolation*. The model can equally well be thought of as a NN TBH model with an underlying lattice structure given by percolation clusters rather than say, a square lattice. The disorder in the problem is that due to the irregularity of the percolation cluster and so a higher concentration of bonds means a lower disorder.

Our work involved the use of the finite size scaling method, whereby a quasi-1D system is generated by coupling isolated slices of width  $M$  to a stem to build up a strip of arbitrary length  $N$ .

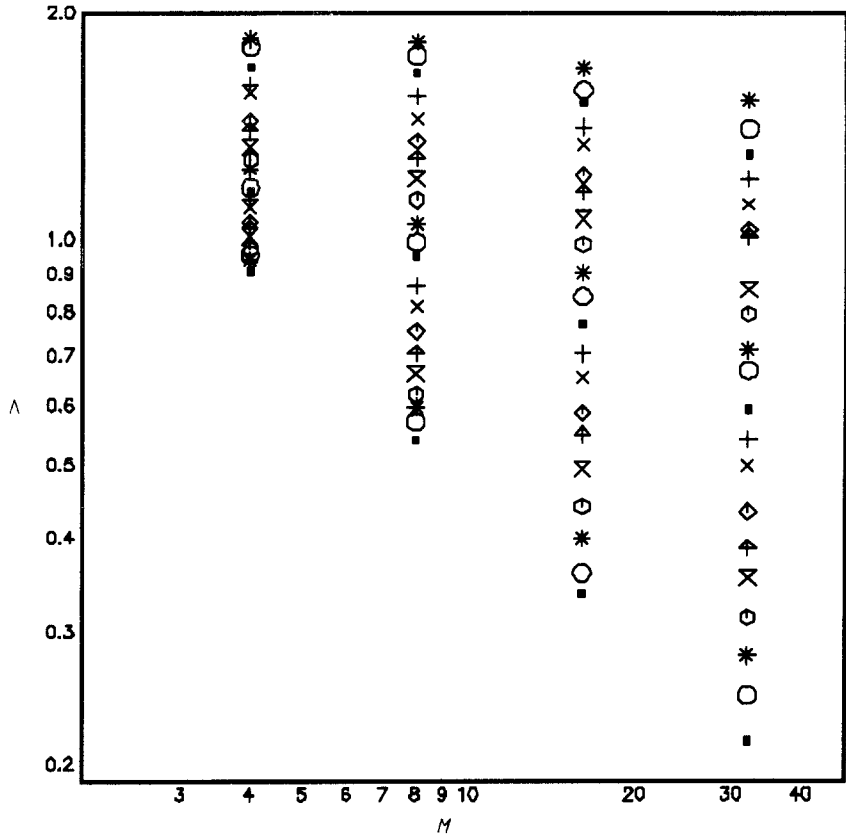


Figure 1. Double-logarithmic plot of the renormalised exponential decay length  $\Lambda = \lambda/M$  of the transmission coefficient of strips of width  $M$  as a function of  $M$  for concentrations from  $p = 0.79$  at the top to  $p = 0.58$  at the bottom in steps of 0.01.

The submatrix, of the systems Green's function, relating the 1st slice and the  $N + 1$ th slice,  $\mathbf{G}_{1,N+1}$  can be calculated iteratively.

If  $\mathbf{H}^{(N)}$  is the Hamiltonian of a strip of length  $N$ , then the Hamiltonian of the new system resulting from the addition of a slice can be written as

$$\mathbf{H}^{(N+1)} = \mathbf{H}^{(N)} + \mathbf{V}_{N,N+1} + \mathbf{H}_{N+1}^0 \tag{3}$$

where  $\mathbf{V}_{N,N+1}$  is the matrix of hopping elements coupling the  $(N + 1)$ th slice to the system through the  $N$ th, and  $\mathbf{H}_{N+1}^0$  is the Hamiltonian of the  $(N + 1)$ th slice in isolation.

The Green's function for the system of size  $N + 1$ ,  $\mathbf{G}^{N+1}$ , can then be determined from the Green's function for the system of size  $N$ ,  $\mathbf{G}^{(N)}$ , and the Green's function for the isolated slice,  $\mathbf{G}^0$ , by treating  $\mathbf{V}_{N,N+1}$  as a perturbation and using Dyson's equation:

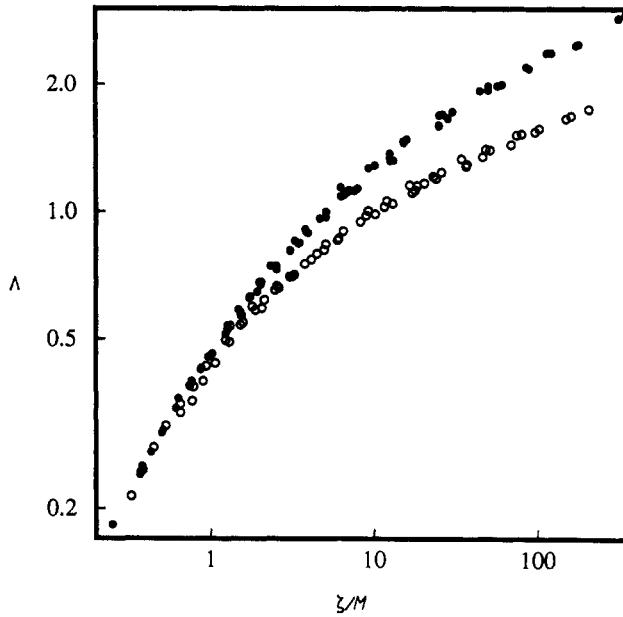
$$\mathbf{G}^{(N+1)} = (\mathbf{G}^{(N)} + \mathbf{G}^0) + (\mathbf{G}^{(N)} + \mathbf{G}^0)\mathbf{V}\mathbf{G}^{(N+1)} \tag{4}$$

It can then be seen that the only non-zero terms required to determine the submatrix relating the 1st slice and the  $(N + 1)$ th slice are given by the equations

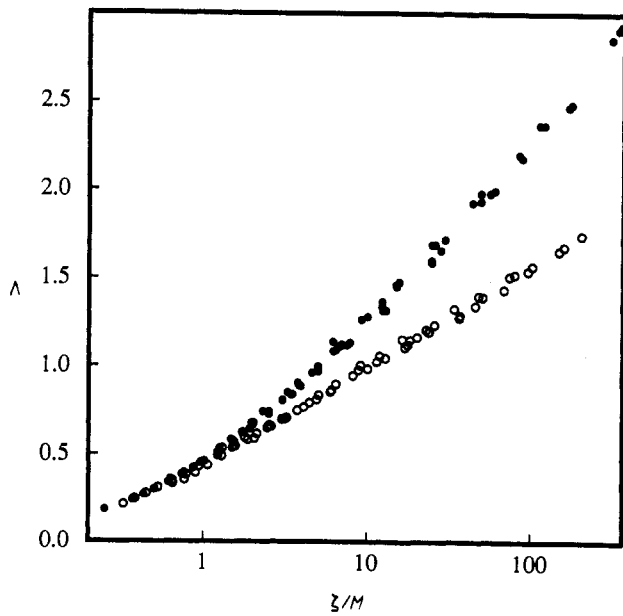
$$\mathbf{G}_{1,N+1}^{(N+1)} = \mathbf{G}_{1,N}^{(N)} \mathbf{V}_{N,N+1} \mathbf{G}_{N+1,N+1}^{(N+1)} \tag{5}$$

$$\mathbf{G}_{N+1,N+1}^{(N+1)} = (\mathbf{E}_F \mathbf{1} - \mathbf{H}_{N+1,N+1}^0 - \mathbf{V}_{N+1,N} \mathbf{G}_{N,N}^{(N)} \mathbf{V}_{N,N+1})^{-1} \tag{6}$$

$$\mathbf{G}_{1,1}^{(1)} = \mathbf{1} \tag{7}$$



**Figure 2.** Double-logarithmic plot of the renormalised exponential decay length of the transmission coefficient  $\Lambda$  of strips of width  $M$  as a function of  $\zeta/M$ .  $\zeta$  is the scaling parameter, which is chosen to fit all data onto one and the same curve. Normal Anderson model:  $\bullet$ ; QPM:  $\circ$ .



**Figure 3.** Plot of the renormalised exponential decay length of the transmission coefficient  $\Lambda$  of strips of width  $M$  as a function of the logarithm of  $\zeta/M$ .  $\zeta$  is the scaling parameter. Normal Anderson model:  $\bullet$ ; QPM:  $\circ$ .

$$\mathbf{G}_{0,0}^{(0)} = \mathbf{0} \quad (8)$$

where  $E_F$  is the Fermi energy. Periodic boundary conditions are imposed across the strip to remove surface effects.

This procedure must be used instead of the usual transfer matrix approach (MacKinnon and Kramer 1983), as the latter requires the inversion of the matrix  $\mathbf{V}_{N,N+1}$  which is singular in the QPM case.

The resolvent  $\mathbf{G}_{1,N}^{(N)}$  can be used to define the localisation length of the system through

$$\frac{2}{\lambda_M} = - \lim_{N \rightarrow \infty} \frac{1}{N} \ln \text{Tr} |\mathbf{G}_{1,N}^{(N)}|^2. \quad (9)$$

For the QPM, care must be taken with this method since after some finite number of slices have been added there will no longer be a pathway of bonds connecting the 1st slice with the new  $N$ th one, implying that  $\mathbf{G}_{1,N}^{(N')} = \mathbf{0}$  for all  $N' \geq N$ .

This meant that it was not possible to take  $N$  to be arbitrarily large as is the case in the NA problem and so the self-averaging of  $\lambda_M$  that this limit invokes was no longer accessible. Instead, provided that  $N > \lambda_M$ , the average can be done explicitly by considering many smaller systems. This was done using a chi squared fit of

$$- \ln \text{Tr} |\mathbf{G}_{1,N}^{(N)}|^2 = (2/\lambda_M)N + B \quad (10)$$

with a total of 300 000 slices making up the systems. The equivalence of these two approaches has been tested numerically for the NA.

Finite size scaling was then used to extrapolate the full 2D behaviour from the trend as the strip width is increased. The validity of the scaling *ansatz*

$$\lambda_M(p)/M = f(\zeta(p)/M) \quad (11)$$

was tested by mapping the data for different concentrations onto a single curve by fitting  $\zeta(p)$ .

The method outlined above was applied over the concentration range  $p = 0.55$ – $0.81$  with systems of width 4 sites to 32 sites. The Fermi energy was taken as the constant  $E_F = 0.3$  in units of the hopping integral, i.e. close to the band centre. The site energies were taken to have a small disorder, width  $W = 0.01$ , to remove any accidental degeneracies.

We found that the width  $M = 4$  data showed anomalous behaviour at both the low and high concentrations. At concentrations above  $p = 0.78$ , the  $M = 4$  systems were found to be sensitive to a change from periodic to anti-periodic lateral boundary conditions. This can be attributed to the phase coherence length being of the same order as the system width (MacKinnon and Kramer 1983). The data for the higher concentrations were thus not considered in the scaling analysis. The behaviour at concentrations below  $p = 0.60$  will be discussed later. The remainder of the data behaved as follows.

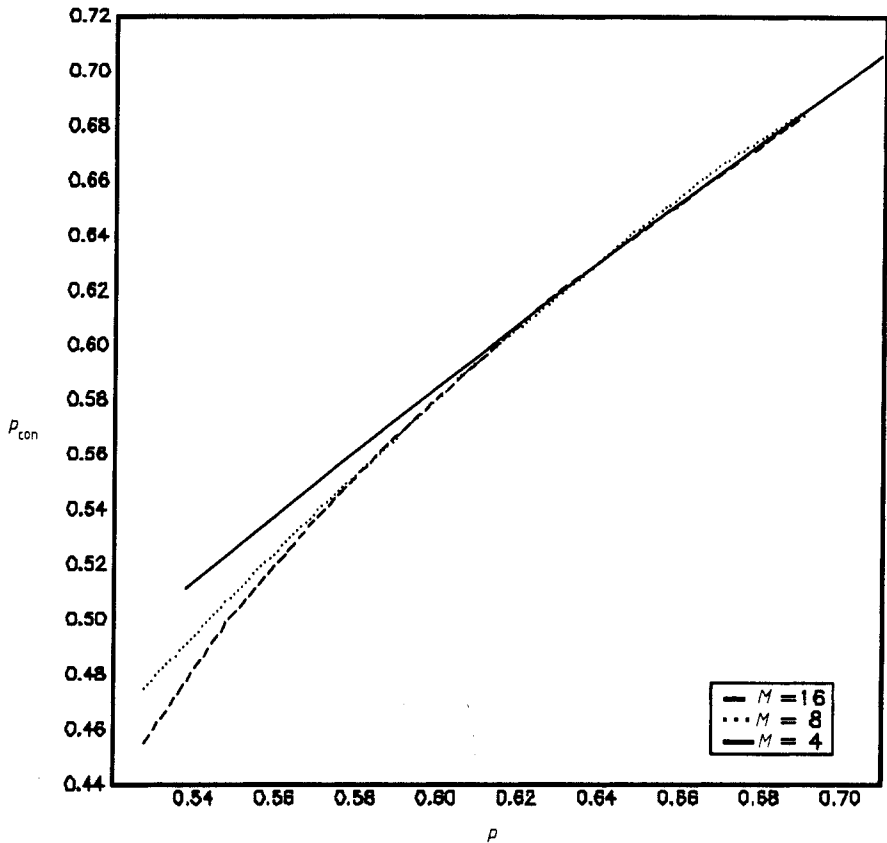
The plots of  $\ln(\lambda_M/M)$  versus  $\ln M$  over the above range of concentrations, figure 1 never have a positive gradient—indicating that the states remain localised.

Using the fitting procedure described by MacKinnon and Kramer (1983) a single-parameter scaling is obtained, figure 2.

The scaling curve for the QPM has the same form as that of the NA model. In the weak disorder region  $\Lambda = \lambda_M/M$  is increasing logarithmically with the localisation length in both cases:

$$\Lambda = A \ln(\zeta(p)/M) + C. \quad (12)$$

However, the resulting straight lines for these two models, figure 3, do have somewhat different gradients.



**Figure 4.** Plot of the average concentration of bonds in the cluster connecting the 1st slice to the  $N$ th slice as a function of the generating concentration,  $p$ , for systems of width  $M = 4, 8, 16$ .

The anomalous behaviour of the  $M = 4$  data can be understood as a cross-over effect caused by the change with concentration of the length scale on which the underlying percolation structure appears to be fractal.

Gefen *et al* (1983) proposed a theory of the QPM that accommodates the effect of the fractal character of the clusters on length scales less than the percolation correlation length  $\xi_p$ . They introduced a parameter  $x = L/(\xi_p + L)$ . For  $x < 0.5$  the fractal character dominates the behaviour of the conductance. This crosses over to a single-parameter scaling equivalent to the NA in the limit  $x \rightarrow 1$ .

The average concentration of bonds in the cluster connecting the 1st slice to the  $N$ th slice was determined as a function of the generating concentration for systems of width  $M = 4, 8, 16$ , figure 4. A width dependence is evident at concentrations below  $p = 0.60$ , the concentration of the connecting cluster being significantly higher in the width  $M = 4$  systems. This effect can be attributed to the pair connectedness length,  $\xi_p$  being comparable with the system width; i.e.  $x \approx 0.5$  and a single-parameter scaling should not be expected. However, for larger widths or higher concentrations the system will appear homogeneous and the single-parameter scaling should be applicable, as is found. The increased processing power required for the treatment of 3D systems means that in

the critical region it is not possible to take this homogeneous systems limit and the cross-over effects themselves must be treated in order to determine the transition point. Results for the 3D site quantum percolation model will be published elsewhere.

In conclusion, our results show no evidence of a delocalisation transition in the 2D bond quantum percolation model. They do show that a single-parameter scaling is valid over a large range of concentrations. The small system widths, however, appear to be strongly affected by the structural correlations of the supporting percolation clusters and require a more complex scaling analysis to be incorporated correctly. The scaling curve obtained differs only slightly from that obtained for the normal Anderson model by this technique and retains the same weak disorder trend.

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