Study of localization in site-dilute systems by tridiagonalization

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A site-dilute model with nearest-neighbor interactions is examined by reduction to tridiagonal form. The statistical behavior of the tridiagonal coefficients is argued to imply localization for $x_c \approx 0.05$ and 0.62 in square and cubic lattices, respectively, with considerable ambiguity in the former value. The limitations of the method are discussed, and the present study extends and corrects an earlier one.

I. INTRODUCTION

The study of both localization phenomena in disordered systems[1] and of the recursion method of converting a matrix to tridiagonal form has attracted much attention.[2] The suitability of the latter method for the study of the former has also been argued for.[3]

In this paper I present the results of a study of the behavior of the tridiagonal coefficients of the Hamiltonian closely analogous to the problem of site percolation in classical physics. In Sec. II the Hamiltonian and the method of tridiagonalization are recapitulated. A brief introduction is made to a connection between the effective dimensionality of the tridiagonal form and the approach to unitarity of the transformation. In Sec. III, a preliminary study is made of the difficulties of interpretation of the tridiagonal coefficients. The points introduced in Sec. II are amplified and the misleading nature of comments in the literature, including our own previous work,[4] are pointed out. Nevertheless, the tridiagonal coefficients are claimed to contain information on localization. This is examined in the following sections. Sections IV and V present the results for simple square and cubic lattices, respectively, and it is concluded that localization occurs earlier than classical percolation in both cases, as the fraction x of sites absent increases. Estimates of x_c are given. Finally, in Sec. VI a few remarks are made to compare with previous work and towards future problems.

II. REVIEW OF THE METHOD

The Hamiltonian studied is of the form

$$H=\sum_{\vec{l},\vec{l}'} |\vec{l}\rangle\langle\vec{l}'| \xi_{\vec{l}}\xi_{\vec{l}'}, \tag{1}$$

where sites $\vec{l},\vec{l}'$ are to be regarded as nearest neighbors in a square or cubic lattice. $\xi_{\vec{l}}$ are site-occupation indices, i.e., $\xi_{\vec{l}}=0$ or 1 with probabilities x and $1-x$, respectively, so that a fraction x of sites is absent in a large lattice.

The above Hamiltonian has been chosen to compare the results with those of classical site-percolation problems in this case. A previous similar study was made of bond-percolation problems.[4]

The Lanczos method for reducing an operator H to tridiagonal form, as is well known,[2] starts with the (arbitrary) vector $\vec{V}_0$ and performs a Schmidt orthonormalization on the sequence

$$\vec{V}_0, H\vec{V}_0, H^2\vec{V}_0, \ldots, H^n\vec{V}_0, \ldots \tag{2}$$

in that (left-to-right) specific order. When this is done, the process requires only two vectors at each stage of the orthonormalization. For symmetric H this becomes

$$\beta_{n+1}\vec{V}_{n+1}=H\vec{V}_n-\alpha_n\vec{V}_n-\beta_n\vec{V}_{n-1}, \tag{3a}$$

where

$$\alpha_n=\langle\vec{V}_n, H\vec{V}_n-\beta_n\vec{V}_{n-1}\rangle \tag{3b}$$

and β_{n+1} is determined by

$$||\vec{V}_{n+1}||=1. \tag{3c}$$

Since $\langle\vec{V}_n,\vec{V}_{n-1}\rangle=0$, Eq. (3b) contains a redundancy but we use it in numerical computations. Also, throughout this study $\vec{V}_0$ is chosen to be localized on a given site (the central site).

When applied to Eq. (1), H becomes, in the basis defined by the $\vec{V}$'s, a tridiagonal (TD) (infinite) matrix, i.e.,

$$H_{\mathrm{TD}}=\sum_{n=0}^{\infty}\beta_{n+1}|\vec{V}_n\rangle\langle\vec{V}_{n+1}| + \mathrm{H.c.}. \tag{4}$$

The diagonal elements are zero because of the special form of (1): In general of course, a term $\sum_{n=0}^{\infty}\alpha_n|\vec{V}_n\rangle\langle\vec{V}_n|$ must be added to (4).

The use of the tridiagonalization method in studying random systems is well documented.[3] In particular, Haydock[3] has argued that the results expected in the strong-disorder limit are well reproduced.

All previous studies (with the exception of Ref. 4) of random systems by tridiagonalization have focused on the "disorder" problem. That is the coupling coefficients in a tight-binding-type Hamiltonian were regarded usually as Gaussian random variables. While the "dilution" problem considered here is simply a particular bimodal form of the distribution functions of $\xi_{\vec{l}}$, it has its own special features, especially with regard to the convergence of the

coefficients β_n, as mentioned below.

We have stated H_{TD} to be an infinite matrix. Obviously, for the dilution problem considered here β_n could be zero and H_{TD} truncates. The statistics of this occurring is directly related to classical results, but in discussions of the convergence behavior of β_n, we shall only consider cases where H_{TD} does not truncate. This occurs in the overwhelming probability of cases as one approaches the classical percolation threshold, i.e., when the fraction x of sites absent is less than at threshold.

In the basis of the $\vec{V}_n$'s the Hamiltonian matrix is that of a one-dimensional nearest-neighbor system. Unless we know how the $\vec{V}_n$'s are related to the original basis functions, i.e., the site-localized $\vec{l}$'s, this does not help us to infer the behavior of the eigenfunctions of the original system if we known the behavior of the corresponding eigenfunctions of the one-dimensional system. The problem is related to the unitarity of the transformation. If one writes $U^\dagger=(\vec{V}_0,\vec{V}_1,\vec{V}_2,\ldots)$ where the $\vec{V}$'s are as usual regarded as column vectors, then

$$H_{TD}=U^\dagger H U \ . \tag{5}$$

If H is a finite-dimensional matrix, then U is obviously unitary. If H is infinite dimensional, then the vectors $\vec{V}$, while being complete in the space spanned by (2), may not be so in the original space of (1): In particular, if $\vec{V}_0$ has a special symmetry of the Hamiltonian, this will be respected by the recursion vectors. Of course, in a disordered system, if $\vec{V}_0$ is chosen to be a particular site $|\vec{l}_0\rangle$ one may expect that $|\vec{l}_0\rangle$ has no special symmetry so almost all members in an ensemble of $\{\xi_{\vec{l}}\}$ will be such that the corresponding recursion vectors will approach a complete set, however, slowly, for all lattice points with $\xi_{\vec{l}}=1$. This fact, i.e., the lack of any point-group symmetry, is often used to justify the application of the tridiagonal method to disordered systems. Any site is statistically equivalent to another so that the projected density of states, for example, will be the same (with probability one).

When the transformation U is *not* unitary, as in a periodic system, and the $\vec{V}_n$'s are spherically symmetric, one can reasonably infer that the $\vec{V}_n$'s may be labeled by radial coordinates in the original space. If this is so, any given behavior of the eigenfunctions in the one-dimensional system may be directly interpreted for the original lattice. In the disordered system, however, U is unitary in the full space, as is argued in Sec. III, and the Hamiltonian (4) retains the full dimensionality of the original problem. The nature of the $\vec{V}_n$'s is more problematic, and they are not localized on a given shell. Then the tridiagonal matrix of coefficients α_n,β_n *cannot* be used (without additional knowledge) to correctly determine the nature of the eigenfunctions of (1) and (4). This will be clearer from Sec. III below. Despite the problems of interpretation, which constitute an important theoretical problem, the statistical behavior of the β_n's is used in the following sections to infer localization.

We conclude this section by stating that we shall *not* be concerned with the spectral distribution (density of states) of H in this paper. The tridiagonal form can be used to obtain the density of states projected on to the central site,[2] but our concern here is entirely with the nature of the eigenfunctions. A more detailed study would use the spectral density to infer the behavior of eigenfunctions at different energies: Here we can only infer grosser features, e.g., the onset of localization for all energies. A more detailed study as a function of energy is a subject for the future.

III. PRELIMINARIES

We may begin our study of the quantum-percolation problem by looking at questions of dimensionality and completeness. Weaire has in particular pointed out some of the difficulties in the interpretation of the tridiagonal form and I am indebted to him for stimulating discussions on this subject.

In Fig. 1 a plot is given of $\sum_{n'=0}^{n} |\langle \vec{l} | \vec{V}_{n'} \rangle|^2$ as a function of the iteration index n in a square lattice for zero, 5% and 50% of sites absent and for $\vec{l}-\vec{V}_0=(0,1)$. The results are not surprising. The perfect lattice displays the sum to be $\frac{1}{4}$ (equal amplitude on the four neighbors of the central site) for all n. This is a reflection of the symmetry of the square. The 5% case shows a very slow completion and 50% case a fairly rapid completion and would undoubtedly be complete for practical purposes by $n=100$. It may be mentioned that no boundary effects occur anywhere in this study: The lattices are always taken large enough so that the iterations do not reach the boundary. Also, choosing a different $\vec{l}$ would display qualitatively similar results.

For the perfect lattice the recursion vectors have spherical symmetry. A parametrization used by Weaire[5] is that of the center of gravity of V_n. One may define (with $\vec{l}_0$ as the origin)

$$R(n)=\sum_{\vec{l}} |V_n(\vec{l})|^2 R(\vec{l})$$

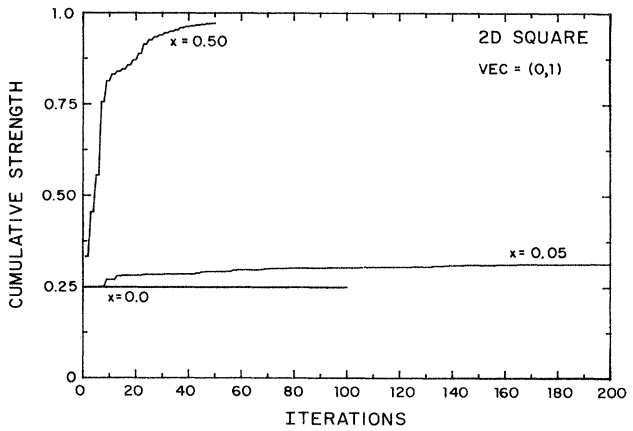

FIG. 1. Cumulative total of the square of the projection of successive recursion vectors onto a site neighboring the central one. Curves are for a square lattice and the fraction of sites missing is denoted x.

and

$$\rho^2(n)=\sum_{\vec{l}} |V_n(\vec{l})|^2 R^2(\vec{l}),$$

where $R(l)$ is the radius of the site $\vec{l}$. For the pure case, Weaire has calculated these.[5] I obtained $R(n)\sim 0.648n$ and $\rho(n)\sim 0.655n$. This shows that the mean radius, the root-mean-square radius, and the standard deviation are all proportional to n so that the recursion vectors propagate radially outward in step with the shell number. If we choose to parametrize $R(n)=Cn^{\delta}$ so that δ is a measure of the effective dimensionality of the propagation of the fronts of the recursion vectors, then Table I lists approximate values of this as a function of the dilution fraction. Actually, the relation $R(n)=Cn^{\delta}$ is not well obeyed for $x\neq 0$; both C and δ fluctuate quite a bit: Nevertheless, some (expected) trends are apparent. Also $\langle R^2\rangle-\langle R\rangle^2$ continues to increase with x, and even for small values of x the recursion vectors are spread over many shells and by no means confined to a thin spherical shell. The above parametrization is really inadequate except in the ordered limit. Although one would imagine the results for the periodic lattice to be derivable analytically, I have not been able to do so.

From the foregoing we may conclude that the tridiagonal form can be interpreted as a one-dimensional chain only for $x=0$ (because the spherically symmetric $\vec{V}_n$'s propagate along one-dimensional channels). This interpretation becomes increasingly untenable as x increases from zero, and rigorously speaking, no one-dimensional theorems on disorder can be invoked for $x\neq 0$. Weaire and others[6] have been vigorous in pointing out such difficulties of interpretation. Nevertheless, I disagree with him on an apparent paradox. He has stated that if $R(n)\sim n^{\delta}$ then exponential localization on the chain implies an $e^{-r^{\delta}}$ localization on the original lattice. The argument is that a length unit on the chain corresponds to the δth power of the length unit on the original lattice. This is not so: For a disordered system, U in (5) is unitary (with probability 1) and, of course, unitary transformations do not change dimensionality. The argument that u is unitary is based both on empirical (Fig. 1) and symmetry considerations [following Eq. (5)]. In particular if $\hat{x}$ is the position operator in the original space and $\hat{q}=U^{\dagger}\hat{x}U$, $\langle x\,|\,q\rangle$ is rather delocalized and merely using the exponent δ to guess the behavior in the original space would be incorrect. The $\vec{V}_n$'s are spread throughout the lattice even in the strong-disorder limit. There is no paradox but a difficult analysis must be employed to reveal the nature of the eigenfunctions in the original space. So, one cannot in any rigorous way infer localization from a disorder in the recursion coefficients α_n,β_n as $n\to\infty$. This was pointed out at the end of the preceding section.

TABLE I. Some values of the effective dimensionality δ of propagation of the center R of the recursion vectors for various dilution percentages x. Amplitude A defined by $R=An^{\delta}$ is also given. See text for explanation.

x	A	δ
0	0.648	1
5	1.1	0.72
10	1.2	0.66
20	1.09	0.61
30	1.1	0.6
50	1.76	0.2

The common way out of this dilemma is to look at the eigenfunctions and not just the coefficients. It is incorrect to examine only the eigenfunctions of the tridiagonal matrix formed by the α's and β's since information has been lost in the process (assuming we do not know the $\vec{V}$'s): This is simply the one-dimensional interpretation all over again. In the following two sections I show in a frankly experimental way that the statistical behavior of the β's alone ($\alpha_n=0$ in the work here) does display clear trends that allow us to infer the onset of localization. I do not have a rigorous justification for this and such theoretical considerations are for the future. Also, it is important to compare the tridiagonal method with brute-force-diagonalization schemes.

To conclude this section, Fig. 2 shows how the recursion vectors proceed to complete $\vec{l}=\vec{V}_0+(0,0,1)$ in three dimensions. It is obvious that the procedure is slower in three dimensions, a fortunate occurrence for localization studies that proceed from the extended-state regime.

IV. TWO-DIMENSIONAL SITE DILUTION

The perfect-lattice results are well known and the recursion coefficients display oscillations related to the van Hove singularities.[7] In Fig. 3 is displayed the mean [over 18 realizations of (1)] of β_n as a function of n for $x=0.05$, 0.25, and 0.50. It may be seen that for small values of x the mean $\bar{\beta}_n$ decreases in its fluctuations as a function of n and then settles to a more or less constant-amplitude

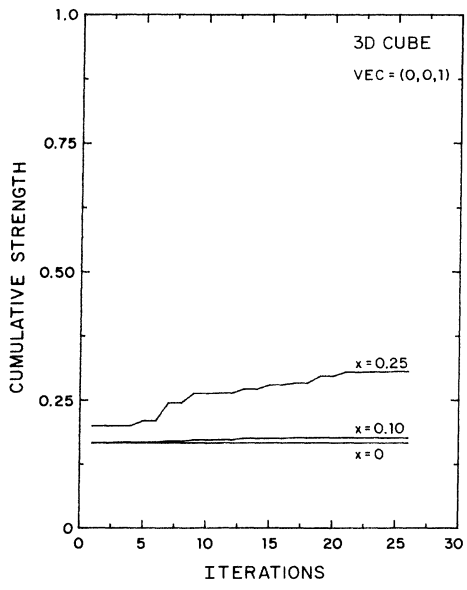

FIG. 2. Curves analogous to Fig. 1, but for a cubic lattice.

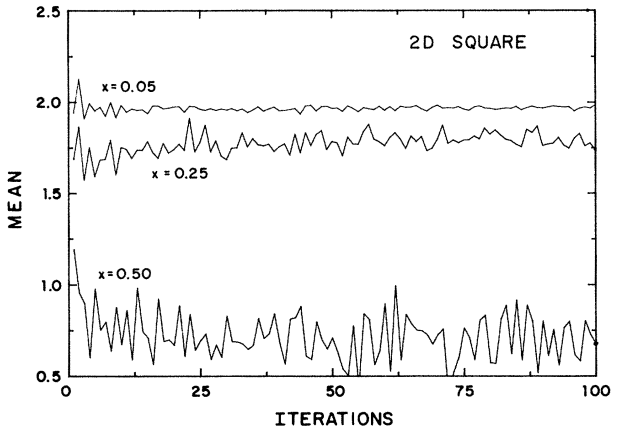

FIG. 3. $\langle \beta_n \rangle$ as a function of n. β_n is the nth off-diagonal coefficient [Eq. (4)] and $\langle\ \rangle$ is an average over (18) different realizations of a square lattice with a given fraction (x) of sites absent.

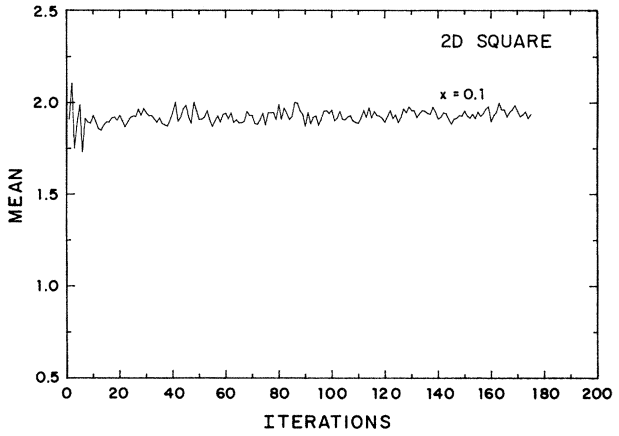

FIG. 5. $\langle \beta_n \rangle$ up to $n=175$, $x=0.1$ (six realizations). Again the existence of $\lim_{n\to\infty}\langle \beta_n \rangle$ cannot be inferred.

fluctuation. This is in contrast to the results of Stein and Krey[8] in which, in fact, they infer localization in a disorder problem according to how rapidly the means approach a hypothetical asympototic value. We shall return to this point later, but here we point out that the behavior is neither the result of computer error nor a question of not having gone sufficiently far in n. In Figs. 4 and 5 are displayed the results of double-precision calculations of the means over six realizations of a larger lattice. We note that the variation persists out to large n; furthermore the variation is not enhanced by $\sqrt{18/6}$ as one might expect from sampling errors. It is hard to infer localization from these results (and here I retract the "one-dimensional" thinking displayed in earlier work), unless we use the criterion that for $x \geq 0.1$ the means do not approach regular oscillations as fast as the recursion vectors fill up the space (with exponent δ).

If we proceed to a study of the variance, i.e., $\langle \beta_n^2 \rangle - \langle \beta_n \rangle^2$, where the $\langle\ \rangle$ refer to averages over 18 realizations most of the time, the results are shown in Fig. 6. Clearly the variance does not approach zero as $n \to \infty$, in agreement with the result on the means. Again the variances for a large lattice, but fewer (six) realizations are shown (Fig. 7) to demonstrate that the results are not simply a sampling error. From one-dimensional thinking one would suggest localization for $x \geq 0.1$. The results seem ambiguous for $x = 0.05$.

A more revealing picture is obtained by plotting the variances averaged over iterations as a function of the dilution percentage (Fig. 8). There is a plausibility argument connecting these variances to a weighted average of the inverse participation ratio.[9] An extrapolation of the initial slope of the curve (from the region of larger x to smaller x) would indicate an $x_c \cong 0.25$ while the final slope indicates $x_c \lesssim 0.05$. Since the bend of the curve is gradual we can only infer $0 \leq x_c \leq 0.3$. Nevertheless, there is a clear indication of the onset of localization before the classical limit.

The large variances encountered and their persistence for large n may be connected with the percolation problem

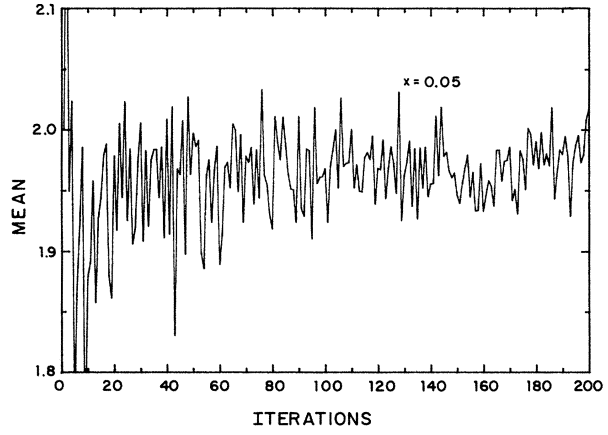

FIG. 4. Amplified picture of $\langle \beta_n \rangle$, $x=0.05$, up to $n=200$. No limiting value is apparent. Here the average is over only six realizations.

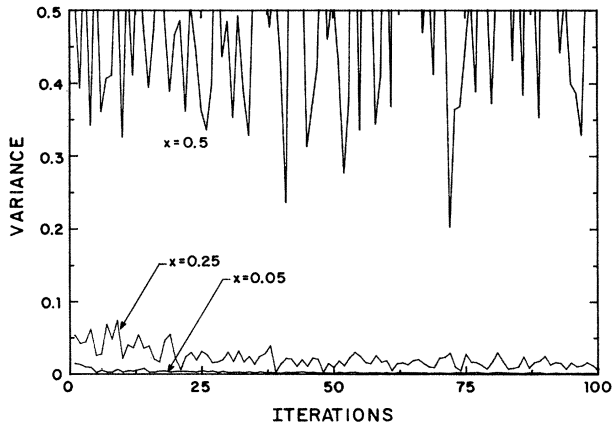

FIG. 6. Varβ_n ($\equiv \langle \beta_n^2 \rangle - \langle \beta_n \rangle$) as a function of n for various x. Symbols are defined in the caption of Fig. 3 and in the text.

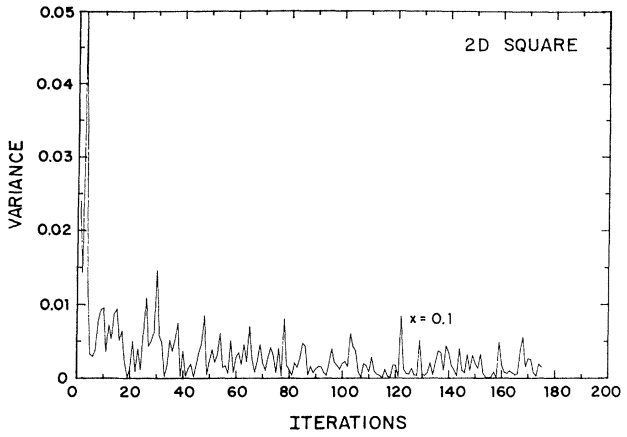

FIG. 7. Varβ_n for $x=0.1$ up to $n=175$ and for six realizations. Variance is not approaching zero nor is it increased for the same n by $\sqrt{18/6}$ over the corresponding case for 18 realizations.

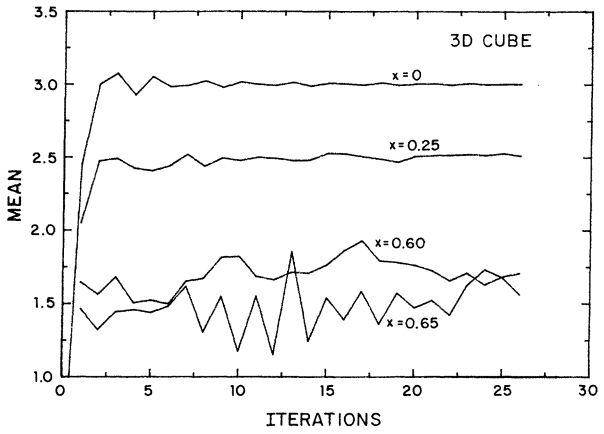

FIG. 9. $\langle \beta_n \rangle$ for the cube. See caption of Fig. 3 for definitions. Here $\lim_{n\to\infty} \langle \beta_n \rangle$ for $x \lesssim 0.60$ seems more apparent.

and associated localized states in the infinite cluster.[10] Such behavior has not been encountered in studies on disordered[8] as opposed to dilute lattices.

The coefficients of the tridiagonal form are incapable of estimating the fraction of localized states for $x < x_c$ in the present form. Whether estimates can be made by examining the changes of the density of states (which may be directly computed from α_n, β_n) under differing boundary conditions is a matter for future investigation, but the problem is expected to be difficult.

The fact that the curve of variance bends over and does not vanish for finite x is an inevitable consequence of not examining states in a small energy range. Weighting functions for such purposes may be constructed but have not been used here.

It may also be mentioned that variances for individual iteration numbers are remarkably similar for $x > 0.25$. The averaging over iterations serves primarily to smooth the curve for small x where the bending over becomes more pronounced. Also, the results for small iteration numbers is not markedly different: One would arrive at similar conclusions by looking at $50 < n < 75$. This is a worthwhile point to bear in mind: There is probably not much necessity to use very large lattices except for refinements that are questionable, to say the least, at the present state of the theory.

The conclusion is that localization does not occur below $x=0.25$ and perhaps below $x \approx 0.05$. Unlike in earlier work, we cannot infer localization for all $x > 0$.

V. THREE-DIMENSIONAL SITE DILUTION

The three-dimensional (3D in figures) case shows interesting differences. Both the curves of mean and variances (Figs. 9 and 10) taken over nine samples show a smoothing for small x not exhibited by the two-dimensional (2D in figures) case. One may suspect from the curves that the onset of localization is between $x=0.60$ and 0.65; certainly the latter curve looks strongly disordered. Figure 11 shows the $x=0.5$ case pushed out to $n=30$, i.e., the number of sites involved is

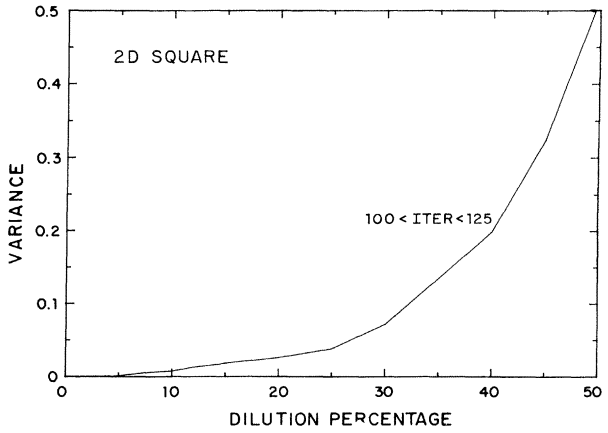

FIG. 8. Varβ_n averaged from $n=100$ to 125 as a function of x. Owing to the gradualness of the curve, x_c can lie anywhere between 0 and 0.25 according to the interpretation in the text.

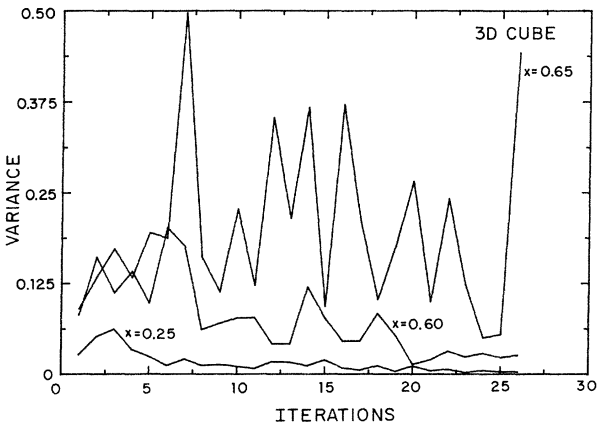

FIG. 10. Varβ_n for the cube. Again $\lim_{n\to\infty}$ Var$\beta_n = 0$ and $x_c \lesssim 0.60$ seems justifiable by extrapolation.

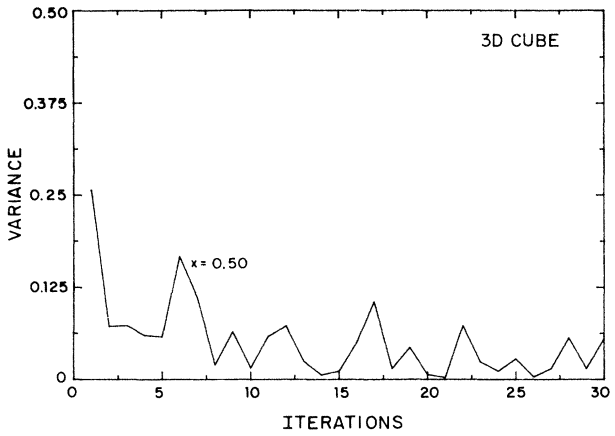

FIG. 11. Varβ_n up to $n=30$ for $x=0.50$ showing that the variance continues to decrease somewhat.

$$\left[4\sum_{m=0}^{n} m^2\right]+2n\approx 38\,000\ ,$$

and the variance continues to decrease. Figure 12 demonstrates, I believe, the most convincing evidence for localization at or near $x=0.62$ from an extrapolation of the curve for $x>0.62$. The fluctuation for smaller x will, I am sure, be smoothed out if more samples were to be taken. (This is analogous to the two-dimensional case where 18 samples were taken.) On the basis of these curves $x_c\cong 0.62$.

It is amusing to note that by keeping count of the percentage of terminations (in the sense $\beta_n=0$ for $n<12$) in the recursion procedure and extrapolating the (quite linear) curve from large x, one obtains a good estimate of the classical percolation threshold. This classical threshold $x_{\rm cl}$ is 0.5 for the square and approximately 0.68 for the cubic lattice.[11] This is shown for the cubic lattice in Fig. 13 where the count was kept in 15 runs of length

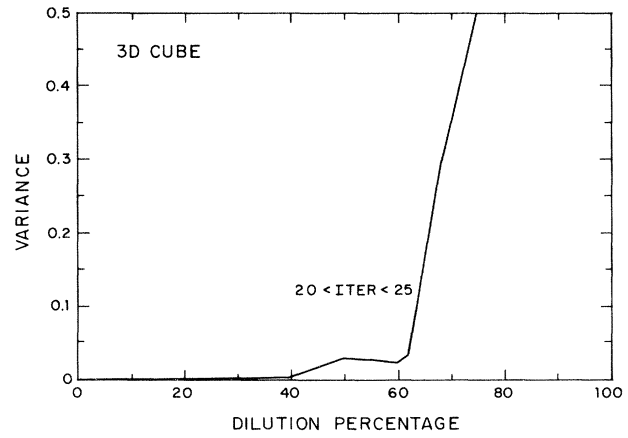

FIG. 12. Varβ_n averaged over the region $n=20$—25 as a function of x. Curved for $x>x_c\cong 0.62$ is steeper than in two dimensions, leading to greater confidence in predicting the localization limit.

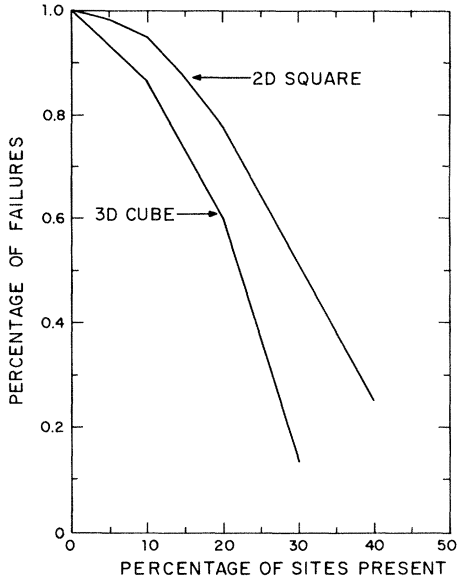

FIG. 13. Fraction of cases for which $\beta_n=0$, $n\lesssim 10$, as a function of $1-x$. Plot is terminated above $x_{\rm cl}$. Extrapolation of the curve leads to $x_{\rm cl}\approx 0.68$ for the cube, in good agreement with standard results.

$N=12$. In fact, one out of the 15 recursions terminated even at $x=0.68$, but the extrapolation of the curve from $x\geq 0.7$ intersects quite closely to the classical value. Similar results were obtained for the square lattice. This characterization of the classical percolation is quite different from that of the quantum localization phenomena described above, i.e., it has nothing to do with the statistical behavior of β_n except for keeping track of when $\beta_n=0$. Such terminations of course were not included in the statistical averagings shown in the earlier figures.

VI. COMPARISON WITH PREVIOUS WORK

In an earlier publication on a bond-dilute model,[4] the claim was made that in two dimensions $x_c=0.0$. While the present model and method is a little different, I do not believe that the claim can be sustained. It was partly based on an incorrect one-dimensional analogy already discussed. What is interesting, however, is that the ensemble variances used in this work, which one might suspect to be more sophisticated, give roughly similar results to variance with shell number used in the earlier work. The different definitions seem to be in approximate correspondence.

Recently, Shapir, Aharony, and Brooks Harris have examined the bond-dilute model and obtained results for various dimensionalities.[12] It would be fruitful to work out the consequences of their technique on the site-dilute case as a check on the present calculations and perhaps a mutual check on both.

ACKNOWLEDGMENTS

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