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Eigenfunction localization in dilute lattices of various dimensionalities

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As a fraction of bonds p is removed from a lattice, we find a threshold p_Q above which all eigenstates are nonpropagating (Anderson localized). This occurs well before the classical percolation threshold. For example, in two dimensions where the classical threshold is $p_c=\frac{1}{2}$, we find $p_Q\approx 0$.

Anderson introduced the concept of disorder-induced localization of eigenstates of a wave equation.[1] Subsequently, Licciardello and Thouless[2] and Abrahams, Anderson, Licciardello, and Ramakrishnan[3] have given reasons for all such eigenstates to be localized in two dimensions ($d=2$) at arbitrarily small values of the random potential V. Such localization has long been known to be a feature of one dimension,[4] whereas in four or more dimensions, the disorder parameter $|V|$ must exceed a critical magnitude V_c before eigenstates become localized. The critical magnitude V_c depends, of course, on the number d of dimensions.

Now, a number of questions concerning localization in $d=2$ or 3 have not been definitively answered. For example, of the most recent various studies of the random potential model, we have on the one hand those of Soukoulis and Economou[5] and the renormalization-group (RG) analysis of Domany and Sarker[6] which confirm the predictions of Refs. 2 and 3, finding $V_c=0$ in $d=2$. While on the other hand, we find the accurate numerical analysis of Stein and Krey[7] and a variant RG analysis by Lee[8] which contradict Refs. 2 and 3, by obtaining a sizable V_c (of the order of one-sixth the bandwidth) for $d=2$. Considerations of the relative merits of the various calculations aside, it is entirely possible that in $d=2$ (and perhaps $d=3$) the behavior is "nonuniversal," hence sensitive to the precise method of solution as well as to the nature of the disorder. We believe this to be the case for $d=2$, as we apply the very methods of Stein and Krey[7] to a variant model, and obtain results quite different from theirs.

Our work centers on the random-bond-dilution model, well known in connection with classical percolation, diffusion, and conductivity,[9] having a host of applications to solids, liquids, gases, lasers, etc. It is desired to obtain the effects on eigenstates of removal, at random, of a fraction p of the bonds.[10] One would not expect any extended states to persist once p exceeds the classical percolation threshold p_c, and indeed, we find that the quantum threshold p_Q is lower. With an estimated uncertainty of ± 0.05, our results indicate $p_Q\approx 0$, 0.63, and 0.77 in $d=2$, 3, and 4 dimensions, respectively. This may be compared with $p_c\approx 0.50$, 0.75, and 0.80 in $d=2$, 3, and 4 dimensions.[11] For the trivial case $d=1$ where $p_c=0$, we also obtain $p_Q=0$ and have nothing to add to the known results.[4]

We base our analysis on a numerically efficient "trick," the tridiagonalization of a Hamiltonian which has interactions limited to nearest neighbors on a generalized cubic lattice [lattice sites at $R_i=a(n,m,\ldots)$ where $n,m,\ldots$ are integers]. Tridiagonalization was first applied to a related problem when Haydock[12] used it to study the mobility edge on a Cayley tree lattice, which is in some sense equivalent to infinite d. Recently, this method was chosen by Stein and Krey[7] for their previously noted analysis, and by Mattis and Raghavan[13] for a rederivation of Wigner's famous semicircular density

of states for a totally random matrix. Tridiagonalization requires far fewer steps than diagonalization, and often yields greater insights, as we shall see. We refer the interested reader to a rapidly evolving literature on the subject of tridiagonalization,[14] and limit explanatory remarks here to the few details necessary to describe the model. A fraction p of nearest-neighbor bonds is removed from the lattice; the remaining bonds have magnitude $\frac{1}{2}$. Let us introduce the parameter ϵ_{ij} which is [1,0] depending on whether the bond is [present, absent] and write the Hamiltonian as

$$H = -\frac{1}{2}\sum_{(ij)} \epsilon_{ij}(c_i^\dagger c_j + \text{H.c.}) \quad . \tag{1}$$

The distributions of ϵ_{ij} is "frozen in." We then consider an eigenstate propagating out from some initial site R_i. This connects to the shell of nearest neighbors through the extant bonds, thence to the next shell, etc. The (real) matrix element b_n connecting the nth shell to the $(n+1)$st is obtained after normalizing the operators at each shell. Our symmetric, tridiagonal matrix consists of the b_n above and below the main diagonal, and zero everywhere else.

As we vary the initial site R_i or vary the statistical sample for a given value of p, we find the b_n's change but asymptotic $(n \to \infty)$ properties do not. These properties will be the main focus of discussion in this paper. Our analysis is based on sample of well over 20 000 sites in $d=2,3,4$ dimensions and a large number of numerical experiments. The experiments could be run quickly, as tridiagonalization is a very rapid and efficient procedure[14] compared with other numerical procedures.

In $d=4$ (and $d=3$) at small dilution, the matrix elements b_n rapidly approach an asymptotic value b_∞ which we plot as a function of p in Fig. 1. Beyond a certain critical dilution, which is denoted p_Q and indicated by a star in the figure, oscillations persist out to the largest attainable shell index n and, presumably, b_∞ ceases to exist. However, when this occurs, we find that the amplitude of the oscillations—the *noise* in b_n—does approach an asymptotic, stable value. Figure 1 shows the dependence of b_∞ on p in the range, $p < p_Q$, for which an asymptotic value is obtained. Significantly, such a value is never obtained in $d=2$, however large the sample we have used and however large the shell index (up to $n=150$), whereas the "noise" parameter is always asymptotically stable in $d=2$. Thus, the appropriate curve for $d=2$ shrinks to a point at $p=0$, $b_\infty=2$.

The significance of the noisy asymptotic behavior is to be found in the nature of eigenfunctions in one dimension. Tridiagonalization is tantamount to the extraction of the one-dimensional manifold of states having nonvanishing amplitudes at the chosen initial site R_i. The eigenstates of the tridiagonal form are eigenstates of the total Hamiltonian. As the tridiagonal form is isomorphic to a semi-infinite linear chain, all the well-known theorems of one dimension[4] apply to it and, in particular, that which states that if $|b_{n+1} - b_n|$ does not vanish at large n, *all* the eigenstates are localized. The converse, however, is not true. For even if the b_n approach an asymptotic value, some or all the eigenstates could be localized. Thus, the threshold we shall calculate will be an upper bound.

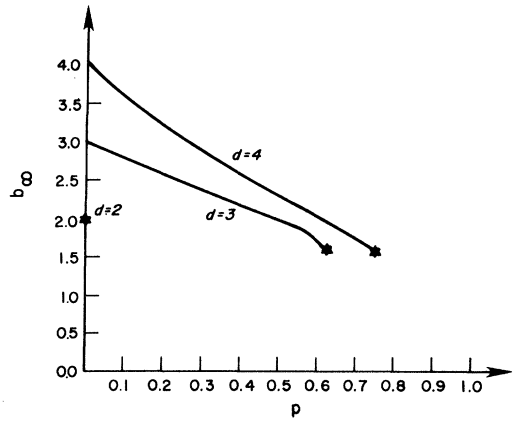

FIG. 1. Asymptotic b_∞ as a function of dilution p in the d-dimensional cubic lattices. For $p > p_Q$ (indicated by a star) the matrix elements b_n do not approach an asymptotic value b_∞, but continue to oscillate indefinitely. This occurs immediately for $d=1$ (not shown) and for $d=2$ (indicated by a star).

Figure 2, drawn from three dimensions, is an example which clearly shows the difference between the smooth approach to an asymptotic value at low dilution, and the noisy behavior for $p > p_Q$. It is in-

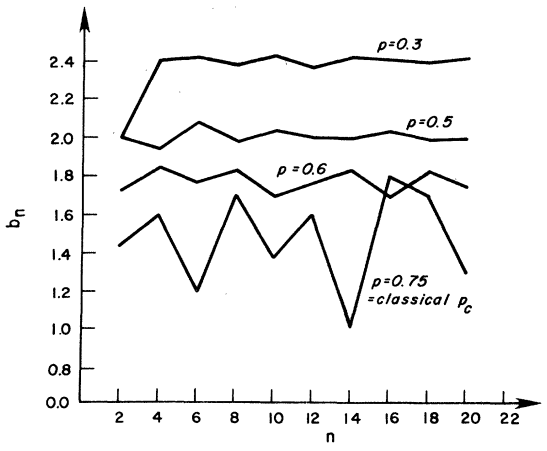

FIG. 2. Typical behavior of b_n as a function of shell index n. This example, in $d=3$ dimensions, shows the approach to asymptotic constancy at small dilution, the increasing "noise" with increasing dilution, and the lack of asymptotic constancy in b_n (tantamount to localization of all the eigenstates) at $p=0.75$.

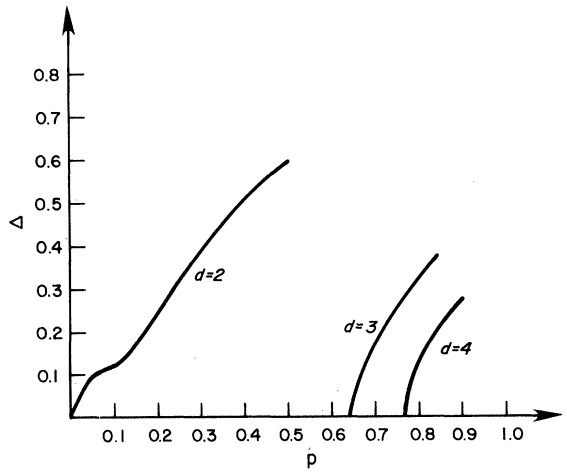

FIG. 3. Plot of the numerically computed parameter $\Delta(p)$ Eq. (2), for various d. Our data indicate p_Q (the value at which Δ vanishes) to be 0, 0.63, and 0.77 for $d=2,3,4$ as compared with classical $p_c=0.50$, 0.75, and 0.80. Thus for $d=2$ (as well as $d=1$), eigenstates are localized except when $p=0$.

teresting that the point $p=0.75$ which illustrates the noisy behavior is in fact the classical percolation threshold in $d=3$; we find the onset of noisy behavior to have occurred at $p_Q=0.63$ (not illustrated) for this case.

Finally, Figure 3 shows the noise parameter Δ we have chosen to calculate defined as follows:

$$\Delta \equiv \lim_{n\to\infty} \left| \frac{b_{n+1}-b_n}{b_n} \right| . \tag{2}$$

Error bars (omitted for clarity) would show an uncertainty in Δ of not more than ± 0.05. The "knee" seen in the $d=2$ figure at small p (the noise does not decrease rapidly as $p\to 0$) falls within this error bar, and could be an artifact. Nevertheless, it is clear that for $d=2$ the critical p_Q for localization is very much less than the classical $p_c=\frac{1}{2}$ and is either zero or very close to it. In $d=3,4$ we also find that p_Q is substantially below p_c. Clearly, the phenomenon of quantum percolation differs from the classical version and is deserving of further study.

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