Localization and Quantum Percolation

Yonathan Shapir[a] and Amnon Aharony
Department of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel
and
A. Brooks Harris
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19174
(Received 14 May 1982)

Electronic wave functions are studied on dilute lattices, at dimensionalities $1 \leq d \leq 8$. Generalized average inverse participation ratios are expanded in powers of the bond concentration, p. Dlog Padé approximants indicate that these ratios diverge as $(p_q - p)^{-\gamma_q}$, signaling the appearance of extended states for $p > p_q$. These Anderson transitions occur above classical percolation. No divergence is detected at $d = 2$. These results are consistent with the existence of localized states at the center of the band.

PACS numbers: 71.30.+h, 71.55.Jv

The nature of the Anderson transition,[1,2] between localized and extended single-electron states in disordered materials, has been the subject of much recent research. A recent scaling approach[3] indicated that all states are localized at and below two dimensions of space, $d \leq 2$. For higher dimensionalities, $d > 2$, all the states are localized only for a large amount of disorder. As the amount of disorder is decreased, extended states appear (via the "Anderson transition") at the center of the allowed energy band, bounded by two *mobility edges*.[1,2] Recent field-theoretical models yielded expansions in $\epsilon = d - 2$ of the behavior near these mobility edges.[4] Related models gave a "mean-field theory," and indicated that the critical dimensionality above which it describes extended states is $d = 8$.[5] Although the predictions at $d = 2$ are confirmed by several calculations,[6] they are still disputed by others.[7,8] Very recently it was suggested[9] that at $d = 2$ the "extended" states decay algebraically, similarly to the spin correlations in the XY model. All these developments make it highly desirable to have a systematic study of localization at general dimensionalities.

The above-quoted studies mostly considered tight-binding Hamiltonians with *diagonal disorder*. It has recently been suggested[10] that purely *off-diagonal disorder* yields different results, i.e., no Anderson localization at the band center.

The simplest model with off-diagonal disorder is that of *quantum percolation*.[11,12] Bonds on the lattice are present, with probability p, or absent, with probability $1 - p$. The tight-binding Hamiltonian is then written as

$$\mathcal{H} = \sum_{\langle i,j \rangle} t_{ij} (a_i^{\dagger} a_j + \text{c.c.}), \tag{1}$$

where $a_i^{\dagger}$ creates the electron at site i, the sum is over nearest-neighbor bonds $\langle i,j \rangle$, and t_{ij} is equal to 1 (or 0) if the bond $\langle ij \rangle$ is present (or absent).

Classical percolation[13] occurs at a concentration p_c, below which all the connected clusters are finite. An infinite cluster first appears at p_c, and grows to cover the whole lattice as p approaches unity. Clearly, all the quantum states of Eq. (1) are localized (i.e., limited to a finite region of space) for $p < p_c$. However, Kirkpatrick and Eggarter[12] showed that localized states always exist on the infinite cluster, i.e., for all $p < 1$. Since all states are extended at $p = 1$ and no states are extended for $p < p_c$, one expects an Anderson transition from localized to extended states at some concentration p_q, with $p_c < p_q \leq 1$, such that no extended states occur for $p < p_q$. Such a transition was indeed found by Kirkpatrick and Eggarter,[12] and recently confirmed by Odagaki, Ogita, and Matsuda.[8]

An interesting result of Kirkpatrick and Eggarter[12] is that there is an infinite sequence of discrete energies at which localized states can be formed on the infinite cluster. These states require a symmetric subcluster and also seem to be specific to the quantum percolation model. Using the commonly accepted argument excluding the coexistence in energy of localized and extended states (due to mixing of these degenerate states by some coupling),[14] we would then conclude that the density of extended states has as infinite number of zeros throughout the band. Presumably if this were true, the usual concept of mobility edges would have to be discarded. However, a specific counterexample presented below shows that localized and extended states can indeed coexist in energy, and remain orthogonal to each other.

Similarly, the degenerate localized states do not mix to create extended states. These peculiar features are special to the present model because of its high symmetry.

The disagreement between various results at $d=2$, the general interest in the d dependence of localization, the question of universality (diagonal versus off-diagonal disorder), the curious role of the special localized states, and the relations of quantum to classical percolation[15] all motivated us to try a new approach to the model (1). In this communication we report on a series expansion of an appropriate measure of localization, χ, in powers of p, at general d. Our measure, related to the inverse participation ratio,[4] is expected to diverge when extended states first appear, i.e., as $p \to p_q^-$, in the form $(p_q - p)^{-\gamma_q}$. Indeed, analysis of our series indicates divergences at $p_q \simeq 0.32$, 0.20, 0.15, 0.12, 0.10, 0.086, with $\gamma_q \simeq 1.7$, 1.1, 0.96, 0.90, 0.87, 0.85, for $d=3$, 4, 5, 6, 7, 8. Comparing to[16,17] $p_c = 0.247$, 0.161, 0.118, 0.094, 0.079, 0.068, we see that indeed $p_q > p_c$. At $d=2$ the different approximants do not give any consistent results, probably indicating that $p_q = 1$. An attempt to fit χ with $\exp[C(p_q - p)^{-\gamma_q}]$, as predicted in Ref. 9, also failed.

After we finished the present work we learned about recent work by Raghavan and Mattis,[18] who studied the model (1) on the extended-states side ($p > p_q$), using the tridiagonalization method. They found $p_q = 1$, 0.37, and 0.23 at $d=2$, 3, and 4, in rough agreement with our estimates. Like Ref. 18, most of the earlier quantitative calculations were performed on the side of the extended states. Recently, Schäfer and Wegner[19] generated the first few terms in a perturbation expansion about the localized instanton states. However, our calculation contains many more terms and is the first to yield accurate quantitative results on the side of the localized states.

Our calculation is based on a generalization of the *inverse participation ratio*.[4] If we denote the g_E degenerate orthonormal eigenfunctions of (1) on the finite cluster Γ by $\{\psi_{E,\alpha}(i)\}$, this ratio is defined via

$$y_E(\Gamma) = \left[\sum_{i \in \Gamma} \left(g_E^{-1} \sum_{\alpha=1}^{g_E} |\psi_{E,\alpha}(i)|^2 \right)^2 \right]^{-1}. \qquad (2)$$

If all the states at energy E are extended, then $\psi_{E,\alpha}(i)$ is of order $1/\sqrt{N_S}$, where N_S is the number of sites on Γ. In this case $y_E(\Gamma) \sim N_S$. If all states at energy E are localized to regions of M sites, $y_E(\Gamma) \sim M g_E$. *The same result applies if both types of states coexist at energy E.* Since this last possibility rotates a commonly accepted argument,[14] we give an explicit example of it. Consider a chain with an even number of sites, 1, 2, ..., $2L$. To the end site ($2L$) attach bonds to n other sites, $i = 2L+1$, $2L+2$, ..., $2L+n$, as shown in Fig. 1(a). For $E=0$ there are n eigenvectors $\psi^{(0)}$, $\psi^{(1)}$, ..., $\psi^{(n-1)}$, where $\psi^{(j)}$ for $j>0$ are the $n-1$ eigenstates localized to the "tail" of n sites attached to site $2L$.[20] The state $\psi^{(0)}$ is an "extended" state, given by $\psi^{(0)}(i) = 0$ for $i = 2, 4, \ldots, 2L$, $\psi^{(0)}(i) = \alpha(-1)^{(i-1)/2}$ for $i = 1, 3, \ldots, 2L-1$, and $\psi^{(0)}(i) = (\alpha/n)(-1)^L$ for $i > 2L$, where α is a normalization constant. In the limit $L \to \infty$ we find $y_0(\Gamma) = n/(1-n^{-1})^2 \sim n$. Thus, $y_E(\Gamma)$ exhibits "localized" behavior in the case ($E=0$) when localized and extended states coexist. The other $2L$ eigenfunctions occur at nonzero energies and are extended, i.e., $y_E(\Gamma) \sim L$.

Since different finite clusters have different discrete energy levels, we chose to measure localization on the cluster Γ using $Y(\Gamma) = \sum_E y_E(\Gamma)$ (instead of a single y_E). If for the cluster Γ there exists a finite interval of energy where only extended states exist, then $Y(\Gamma)$ will grow with N_S as N_S^2, otherwise it will grow more slowly with N_S. In the example of Fig. 1(a), $Y(\Gamma)$ is of order L^2, in spite of the occurrence of the special energy $E=0$. Thus $Y(\Gamma)$ is not as sensitive to the existence of degenerate localized and extended states. Note also that $Y(\Gamma) \sim N_S$ if all the N_S states are localized and degenerate at the same energy E_0, when $Y = y_{E_0} \sim N_S$. We next average $Y(\Gamma)$ over all clusters, defining

$$\chi(p) = \sum_\Gamma Y(\Gamma) p^{N_b} (1-p)^{N_p}, \qquad (3)$$

where N_b and N_p are the numbers of bonds inside and adjacent to Γ. If $Y(\Gamma)$ is replaced by N_S^2 then

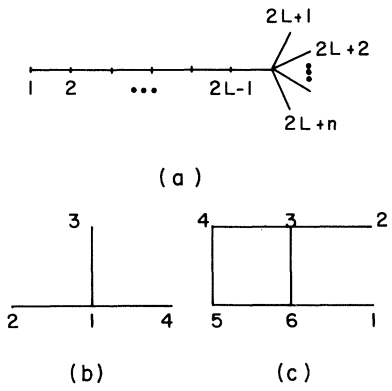

FIG. 1. Examples of graphs.

$\chi(p)$ reduces to the *classical mean cluster size* (Refs. 13, 16, and 17). In that case, $\chi \sim (p_c - p)^{-\gamma_p}$, similar to the susceptibility in magnetic phase transition problems. Because of quantum effects, $Y(\Gamma)$ measured only the "active" part of Γ, on which the wave function is nonzero. Thus, $Y(\Gamma) \lesssim N_s^2$ and we expect a weaker divergence at a higher value of p. If all states are localized then $Y(\Gamma) \sim N_s$, and χ behaves like the "magnetization," which never diverges.[13]

Equation (3) may now be rewritten as

$$\chi(p) = \sum_G m_d(G) Y^c(G) p^{N_b} = \sum_{k=0}^{\infty} a_k p^k , \qquad (4)$$

where $m_d(G)$ is the embedding factor of the graph G on the lattice (depending on d) and $Y^c(G)$ is the cumulant of Y,[21] $Y^c(G) = Y(G) - \sum_{G' \subset G} Y^c(G')$. The sum here is over all subgraphs of G. The coefficients a_k are thus simply given by

$$a_k = \sum_{\{G\}_{N_b = k}} m_d(G) Y^c(G).$$

In order to obtain a_k we thus have to calculate $Y(G)$, i.e., $\{\psi_{E,\alpha}(i)\}$, for graphs with k (or fewer) bonds. The solution of the Schrödinger equation, $\mathcal{H}\psi(i) = E\psi(i)$, on the graph G now amounts to a simple diagonalization of an $N_s \times N_s$ matrix, which is easily written down. For example, the graph of Fig. 1(b) corresponds to the 4×4 matrix $\{\mathcal{H}_{ij}\}$, with $\mathcal{H}_{i1} = \mathcal{H}_{1i} = 1$ for $i > 1$ and $\mathcal{H}_{ij} = 0$ otherwise. One of the eigenvalues is at $E = 0$, and is doubly degenerate ($g_0 = 2$). A possible choice of the basis for the degenerate eigenstates is $\psi_{0,1}(i) \equiv (0, 2^{-1/2}, -2^{-1/2}, 0)$, $\psi_{0,2}(i) \equiv (0, 6^{-1/2}, 6^{-1/2}, -2.6^{-1/2})$. The two remaining eigenvalues are $E = \pm\sqrt{3}$, with $\psi_{\pm\sqrt{3}}(i) \equiv (2^{-1/2}, \pm 6^{-1/2}, \pm 6^{-1/2}, \pm 6^{-1/2})$. Thus, $Y(G) = 9$. Note that our definition (2) is independent of the particular choice of the orthogonal basis for the degenerate states. Similarly, the graph of Fig. 1(c) yields $E = \pm 0.554\,96$, $\pm 0.801\,94$, and $\pm 2.246\,98$, and $Y(G) = 28$. It is useful to note that on lattices which can be divided into two interpenetrating sublattices, one has $y_E(G) = y_{-E}(G)$.

The coefficients a_k were calculated up to $k = 11$. For example, at $d = 6$ we find the coefficients, 1, 12, 22, 1496, $-11\,625\,\frac{2}{3}$, 344 247.2288, $-6\,355\,964.201$, 165 242 910.53, $-3\,379\,499\,799$, 32 335 825 765, $1.304\,059\,162\,6 \times 10^{12}$, $-8.057\,962\,542\,5 \times 10^{13}$. In general, the series are less regular than their classical percolation counterparts. This is due to the sensitivity of $Y(\Gamma)$ to the details of the graph (unlike N_s^2). For $d \geq 3$ our Dlog Padé analysis (aiming to find p_q and γ_q)[22] gave reasonably consistent values only for the high approximants [4/5], [4/6], and [5/5]. At $d = 6$, these respectively gave $p_q = 0.1194$, 0.1202, and 0.1202 and $\gamma_q = 0.891$, 0.911, and 0.910. For comparison, the [4/4] approximant gave $p_q = 0.169$ and $\gamma_q = 2.42$. Similar results were found for other dimensions. At $d = 3$, the three approximants gave $p_q = 0.2997$, 0.3454, and 0.3234 and $\gamma_q = 1.24$, 2.26, 1.60. At $d = 2$, there was no reasonable pole for the [4/6] approximant, and the other two gave $p_q = 0.653$ and 0.825, $\gamma_q = 2.21$ and 4.63. Dlog Padé approximants for logχ were even more erratic, and gave no reasonable poles.

In all dimensions we also found two pairs of unphysical complex singularities, very close to the origin. At $d = 6$, these were at $p \simeq -0.035 \pm 0.009i$, $-0.017 \pm 0.025i$. Apart from the fact that these may alter the values at the physical point, they might also have some physical significance which deserves further study.[23]

Note that the behavior of $\chi(p)$ for $p_c < p < p_q$ is based on an approach which does not take explicit account of the appearance of an infinite cluster at $p = p_c$. Since our results do not indicate any singularity in $\chi(p)$ at $p = p_c$ we hope that the extrapolation we use is justified.

In order to check the effect of the localized states at the center of the band, we tried two alternatives to Eq. (4), i.e., $Y(\Gamma) = [y_0(\Gamma)]^2$ and $Y(\Gamma) = [y_{E_m}(\Gamma)]^2$, where $E_m = \min|E|$.[24] The second was used in order to include the many clusters [like Fig. 1(c)] which do not have zero as an eigenvalue. Up to eleventh order, the series based on these choices gave erratic Padé approximants, from which no simple singularity could be identified. The states near $E = 0$ thus probably always remain localized!

It is interesting to note that the model is exactly solvable at $d = 1$. On a cluster with N_S sites, $\psi_E(i) = (2/N_S)^{1/2} \sin qi$, with $q = m\pi/(N_S + 1)$, $E = 2 \times \cos q$. Simple algebra then yields $\chi(p) = (1-p)^2 + 4p + \frac{4}{3}p^3/(1-p)$. Thus, $p_q = p_c = 1$ and $\gamma_q = \gamma_c = 1$. Our series program agrees with an expansion of this formula.

We expect similar series to arise in the *random site* problem (in which $t_{ij} \equiv 1$, but there is a diagonal energy term, equal to 0 or ∞). Since our results also agree qualitatively with those found for the Anderson model,[2-4] universality of diagonal and off-diagonal disorder seems to hold.

In conclusion, we have suggested a new tool to study localization in d dimensions, and found new results for the Anderson transition in quantum percolation. Since our results are based only on the three Padé approximants, it will be very in-

teresting to check higher-order terms in the series, and to study the model using alternative techniques. It will also be quite useful to relate the exponent γ_0 to other exponents (e.g., those of the localization length or the conductivity[2]), and identify its behavior at high dimensions (we have not identified any critical dimensionality above $d=2$). These questions remain for future study.

One of us (A.A.) is grateful to T. Odagaki, from whom he first learned about the quantum percolation model. We also acknowledge discussions with B. I. Halperin, E. Domany, S. Kirkpatrick, and T. C. Lubensky. This work was supported by grants from the U. S.–Israel Binational Science Foundation and the Israel Academy of Sciences and Humanities, and by the National Science Foundation under Grant No. DMR79-10153 and the U. S. Office of Naval Research under Grant No. N00014-76-C-01106.

[a]Present address: Physics Department, University of Illinois, Urbana, Ill. 61801.

[1]P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[2]For a review, see, e.g., D. J. Thouless, Phys. Rep. 13, 93 (1974); *Ill-Condensed Matter*, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, Amsterdam, 1979).

[3]E. Abrahams, P. W. Anderson, D. C. Liciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).

[4]F. J. Wegner, Z. Phys. B 36, 209 (1980); S. Hikami, Phys. Rev. B 24, 2671 (1981).

[5]A. B. Harris and T. C. Lubensky, Solid State Commun. 34, 343 (1980), and Phys. Rev. B 23, 2640 (1981).

[6]E.g., Domany and S. Sarker, Phys. Rev. B 20, 4729 (1979).

[7]E.g., P. A. Lee, Phys. Rev. Lett. 42, 1492 (1979).

[8]T. Odagaki, N. Ogita, and H. Matsuda, J. Phys. C 13, 189 (1980).

[9]J. L. Pichard and G. Sarma, J. Phys. C 14, L127, L617 (1981).

[10]P. D. Antoniou and E. N. Economou, Phys. Rev. B 16, 3768 (1977).

[11]P. G. de Gennes, P. Lafore, and J. P. Millot, J. Phys. Chem. Solids 11, 105 (1959), and J. Phys. Radium 20, 624 (1959).

[12]S. Kirkpatrick and T. P. Eggarter, Phys. Rev. B 6, 3598 (1972).

[13]For recent reviews, see, e.g., D. Stauffer, Phys. Rep. 54, 1 (1979); J. W. Essam, Rep. Prog. Phys. 43, 833 (1980).

[14]M. H. Cohen, in *Proceedings of the Tenth International Conference on the Physics of Semiconductors, Cambridge, Massachusetts, 1970*, edited by S. P. Keller, J. C. Hensel, and F. Stern, CONF-700801 (National Technical Information Service, Springfield, Va., 1970).

[15]E.g., G. Toulouse, C. R. Acad. Sci. Ser. B 280, 629 (1975).

[16]D. S. Gaunt and H. Ruskin, J. Phys. A 11, 1369 (1978).

[17]A. Aharony and K. Binder, J. Phys. C 13, 4091 (1980).

[18]R. Raghavan and D. C. Mattis, Phys. Rev. B 23, 4791 (1981).

[19]L. Schäfer and F. J. Wegner, Z. Phys. 39, 281 (1980).

[20]These states span the $(n=1)$-dimensional space for which $\psi^{(i)}(i)=0$ for $1\leq i\leq 2L$ and which are orthogonal to $\psi^{(0)}$.

[21]E.g., A. B. Harris and R. Fisch, Phys. Rev. Lett. 38, 796 (1977).

[22]The series for $d\ln\chi/dp$ was analyzed in search of a pole at p_q with residuum γ_q. See. e.g., *The Padé Approximant in Theoretical Physics*, edited by G. A. Baker, Jr., and J. L. Gammel (Academic, New York, 1970).

[23]Could these singularities relate to the instanton-like solutions of Ref. 19?

[24]One can construct series with any power $y_0{}^k$. We chose $k=2$ so that $Y(\Gamma)\sim N_s{}^2$ for extended states.