Correlation length and inverse-participation-ratio exponents and multifractal structure for Anderson localization

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(Received 22 November 1989)

We perform numerical finite-size-scaling calculations on a standard diagonally disordered tight-binding Hamiltonian, with a Gaussian site-energy distribution. We find that the localization-length exponent is $\nu=0.97\pm0.05$. We also find that $\pi_2/\nu=1.43\pm0.10$, where π_2 is the inverse-participation-ratio exponent. π_2/ν can also be interpreted as the fractal dimension of the critical eigenstates. Finally, by looking at higher moments of the critical wave functions, we show that they display a multifractal structure.

The problem of Anderson localization[1,2] has generated intense interest for over three decades. It can serve as a simple model for understanding the dynamics of vibrational or electronic excitons in molecular and inorganic crystals, as well as the transport of electrons in doped semiconductors. So far, most studies have been focused on determining the critical disorder and the correlation (localization) length exponent ν. Although initially there has been substantial disagreement about the value of the critical disorder for different model problems, more recently a consensus seems to have been reached, particularly for the original diagonally disordered Anderson model with a rectangular probability distribution of site energies,[3-5] and perhaps for the quantum site percolation model.[4,6] On the other hand, the case of the localization-length exponent is less clear. Using an ϵ-expansion technique ($\epsilon=d-2$, where d is the dimension of space), Wegner[7] found that $\nu=1/\epsilon+O(\epsilon^3)$, which gives $\nu=1$ in three dimensions. More recently, Wegner[8] discovered that this result is in error, and a correct calculation yields

$$\nu=1/\epsilon-(\tfrac{9}{4})\zeta(3)\epsilon^2+O(\epsilon^3)\ ,$$

where $\zeta(x)$ is the Riemann ζ function [$\zeta(3)=1.202\ldots$]. This result when evaluated for $\epsilon=1$ gives an (unphysical) value of $\nu<0$. Indeed, Chayes *et al.*[9] have shown that in three dimensions ν is bounded from below by $\frac{2}{3}$. In contrast, numerical work has led to widely varying results from 0.6 to 1.95.[4,10-18] Another interesting set of critical exponents, π_k ($k=2,3,4\ldots$), which will be described below, and which have received somewhat less attention, involve the inverse participation ratio and its generalizations.[7,19] In this paper, we present numerical calculations of ν, π_2, π_3, and π_4, and comment on the relationship among the different π_k, which in this case implies a multifractal structure to the critical wave functions.

We consider a modified Anderson model described by a tight-binding Hamiltonian defined on a three-dimensional (3D) simple cubic lattice:

$$H=\sum_i \varepsilon_i|i\rangle\langle i|+J\sum_{\langle i,j\rangle}|i\rangle\langle j|\ , \tag{1}$$

where $|i\rangle$ are orthogonal site states, J is the hopping matrix element, and the sum is over nearest neighbors only. The disorder is introduced by assuming that the site energies, ε_i, are uncorrelated random variables described by a Gaussian distribution with mean zero and variance Σ^2. A dimensionless disorder parameter, σ, is defined as $\sigma=\Sigma/J$. For a particular realization of the disorder one can diagonalize the Hamiltonian and express the eigenstates, $|\mu\rangle$, as

$$|\mu\rangle=\sum_i c_{i\mu}|i\rangle\ . \tag{2}$$

For the above Hamiltonian, the density of states is symmetric around the band center ($E=0$). For $\sigma>\sigma_c$ (σ_c is the critical disorder), all states are localized, and as σ is decreased below σ_c, extended states appear at the band center. Therefore, the localization length at the band center, $\xi(\sigma)$, diverges as $\sigma\to\sigma_c^+$ with a critical exponent defined by $\xi(\sigma)\sim(\sigma-\sigma_c)^{-\nu}$.

Focusing only at the band center, the inverse-participation ratio, $P^{(2)}(\sigma)\equiv P(\sigma)$, and its generalizations are defined as[19]

$$P^{(k)}(\sigma)=\frac{\left\langle\sum_{i,\mu}|c_{i\mu}|^{2k}\delta(E_\mu)\right\rangle_\sigma}{\left\langle\sum_\mu\delta(E_\mu)\right\rangle_\sigma}\ , \tag{3}$$

where E_μ are the eigenvalues, and the brackets indicate configurational averaging for a particular value of the disorder, σ. The inverse participation ratio is a measure of the inverse of the number of sites that "participate" in the eigenstates.[19] Let us consider a finite system with $N=b^3$ sites, and the corresponding $P_b^{(k)}(\sigma)$. It is clear that in the infinite cell limit $P_\infty^{(k)}(\sigma)$ are zero for extended states and finite for localized states; the critical exponents π_k are defined by[19]

$$P_\infty^{(k)}(\sigma)\sim(\sigma-\sigma_c)^{\pi_k}\ , \tag{4}$$

for $\sigma>\sigma_c$. Conversely, for a finite system, $P_b^{(k)}(\sigma)$ are finite for all σ. From the finite-size scaling argument,[20-22] one expects the finite and infinite system

values of $P^{(k)}(\sigma)$ to be related to each other by

$$P_b^{(k)}(\sigma)=P_\infty^{(k)}(\sigma)Y_k(b/\xi(\sigma)) , \tag{5}$$

where $\xi(\sigma)$ is the (infinite system) localization length mentioned above. Generally, the scaling functions Y_k are unknown, but the limiting behaviors are readily determined. Since $P_b^{(k)}(\sigma)$ for the finite system is always finite, the singularity of $P_\infty^{(k)}(\sigma)$ at $\sigma=\sigma_c$ must be canceled by $Y_k(b/\xi(\sigma))$, which implies that Y_k must behave like a power law for small argument. In particular, this implies that $P_b^{(k)}(\sigma_c)\sim b^{-\pi_k/\nu}$, which leads to a convenient method for determining π_k/ν, as will be discussed below.

For a fractal object such as a percolation cluster, the number of sites on the cluster inside a volume b^d goes like $N\sim b^D$, where D is the fractal dimension of the cluster. Since the inverse participation ratio is the *inverse* of the number of sites that participate in the eigenstates, from the above scaling of $P_b^{(2)}(\sigma_c)$ it is natural to associate a fractal dimension $D=\pi_2/\nu$ with the critical eigenstates.[23] There have been several suggestions as to the value of D for three-dimensional localization problems. It is believed[24] that for two dimensions or fewer, even with very small amounts of disorder, all states are localized, except under unusual circumstances.[25] This result leads to the conjecture that $D=2$.[26] In fact, numerical work by Soukoulis and Economou shows that $D=1.7\pm0.3$,[27] in agreement with this conjecture. Their approach, however, has recently been criticized.[28–30] Schreiber[23] also used the value $D=2$ as a criterion for localization in determining the critical disorder. Finally, the ϵ expansion gives[8]

$$D=2-\epsilon+3\zeta(3)\epsilon^4+O(\epsilon^5) ,$$

which in three dimensions leads to $D\approx4.6$.

Once π_2/ν is known, from the finite-size-scaling hypothesis one can define a generalized phenomenological renormalization transformation by[31]

$$\frac{P_b(\sigma)}{b^{-\pi_2/\nu}}=\frac{P_{b'}(\sigma')}{b'^{-\pi_2/\nu}} . \tag{6}$$

The fixed point of the above transformation gives an estimate of the critical disorder, and the correlation length exponent ν is obtained from

$$\nu=\frac{\ln(b/b')}{\ln(\lambda_b/\lambda_{b'})} , \tag{7}$$

where

$$\lambda_b=\frac{\partial}{\partial\sigma}\left[\frac{P_b(\sigma)}{b^{-\pi_2/\nu}}\right]\Bigg|_{\sigma=\sigma_c} . \tag{8}$$

For each pair of finite-sized systems with cell sizes b and b', this equation can be used to find an estimate for ν.

Our calculations are performed on five different cell sizes with $b=4$, 6, 8, 10, 12, and for $\sigma=4.5$, 5.0, 5.5, 6.0, 6.5, 7.0, and 7.5. For each value of σ, we generate many random configurations for the ϵ_i. For each configuration we diagonalize the Hamiltonian (assuming periodic boundary conditions) and then calculate the $P_b^{(k)}(\sigma)$, for $k=2$, 3, and 4 as defined above. For these calculations we replaced the δ function in Eq. (3) with a rectangular distribution centered at $E=0$ with unit area and width $2\Delta E$. We chose $\Delta E=0.8J$ for $b=4$, 6, and 8, and $\Delta E=0.6J$ for $b=10$ and 12, thus decreasing the energy range as the cell size increases, since in the infinite cell limit the rectangular distribution should become a true δ function.

From other numerical work, it is known that for this model $\sigma_c\approx6$ ($\sigma_c=6.03\pm0.14$[3]). We therefore calculated $P_b^{(k)}(6)$ for the cell sizes listed above; a plot of $\ln P_b^{(k)}(6)$ versus $\ln b$ is shown in Fig. 1. (In all figures and tables the error bars are two standard deviations.) For each value of k the data points lie on a straight line whose slope gives π_k/ν. In addition to the intrinsic uncertainty in these slopes from the linear fits, we can include a contribution to the error estimates from the uncertainty in σ_c. This analysis yields[32] $D=\pi_2/\nu=1.43\pm0.10$, $\pi_3/\nu=2.16\pm0.19$, and $\pi_4/\nu=2.62\pm0.27$. This value for D is in agreement with the numerical result of $D=1.7\pm0.3$,[27] but in strong disagreement with the conjecture that $D=2$,[26] and in stronger disagreement with the ϵ-expansion result of $D=4.6$.[8]

In fact, other numerical evidence supports the conclusion that $D<2$ exists. Schreiber[23] calculated the inverse-participation ratio for the same model, and plotted $\ln P_b$ versus $\ln b$ for different values of the disorder, finding straight lines in each case. However, in his analysis of the data he assumed that $D=2$ was the fractal dimensionality at criticality, from which he calculated that the critical disorder at the band center is $\sigma_c=4.79\pm0.10$. More recent work shows that this value of σ_c is substantially lower than the correct value.[3,33] Indeed, Schreiber found that D is a monotonically decreasing function of σ, so that at $\sigma\approx6$, D would be substantially less than 2. The disagreement of our value with the ϵ-expansion result[8] of $D=4.6$ is not altogether

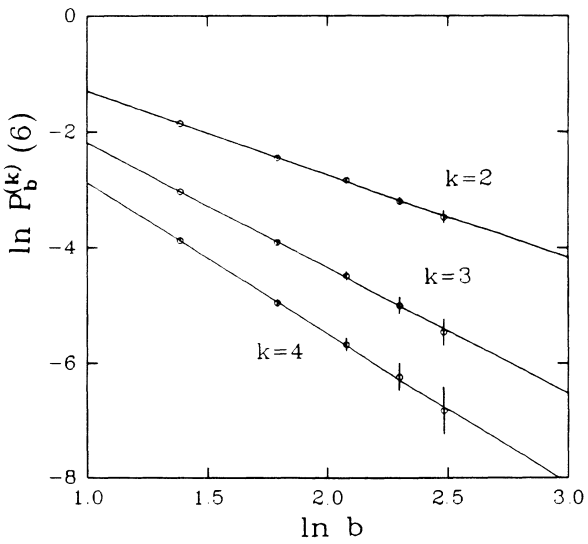

FIG. 1. The data points are $\ln P_b^{(k)}(6)$ vs $\ln b$ for $b=4$, 6, 8, 10, and 12, and $k=2$, 3, and 4. The solid lines are the best linear fits to the data.

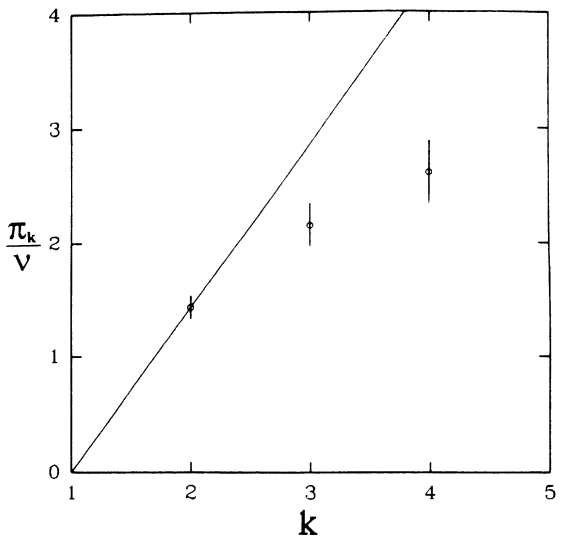

FIG. 2. π_k/ν vs k for $k=2$, 3, 4. The solid line is the relation $\pi_k/\nu=(k-1)D$, which would be valid for a homogeneous fractal.

surprising, since in this instance the expansion does not appear to be converging nicely. Expanding the series to first order in ϵ, one obtains (for three dimensions) $D=1+O(\epsilon^2)$, while retaining the quartic term, one obtains $D=4.6+O(\epsilon^5)$. However, a Padé-Borel resummation of the ϵ expansion as suggested by Paladin and Vulpiani,[34] but with the corrected fourth-order term,[8] yields a value close to our numerical result.

One can define generalized fractal dimensions by[34,35] $D_k=\pi_k/\nu(k-1)$, with $D_2=D$, as defined previously. For a homogeneous fractal $D_k=D$ for all k.[34,35] In Fig. 2, we have plotted π_k/ν versus k, as well as the line $\pi_k/\nu=D(k-1)$. One sees that this linear relation does not hold, implying a multifractal structure to the critical eigenstates.[34,35] One should also note that the ϵ-expansion results of Wegner[8]

$$\pi_k/\nu=2(k-1)-\epsilon(k-1)^2 +(\tfrac{1}{4})k(k-1)(k^2-k+4)\zeta(3)\epsilon^4+O(\epsilon^5)\ , \quad (9)$$

also predict a multifractal structure, although as in the case of D, the numerical estimates from the above ($\pi_3/\nu=18.0$; $\pi_4/\nu=54.7$) are not accurate. We also note that in the multifractal language D_2 is known not as the fractal dimension but the correlation dimension.[34]

An estimate for the exponent ν was calculated by employing the generalized phenomenological renormalization transformation defined in Eq. (6). $P_b(\sigma)$ was calculated for $b=4$, 6, 8, and 12 and the seven values of σ described above. For each cell size the data for different σ was fit to a second-order polynomial, which for each pair of cells crossed at $\sigma\approx 6$, as expected. The slopes of the fitted curves at the crossing were then used to determine ν for that pair from Eq. (7). These estimates are shown in Table I. The error in each value reflects the statistical uncertainty of the Monte Carlo sampling, and also has a contribution from the uncertainty in π_2/ν. Although there is some scatter in these values, they appear to be clustered near $\nu=1$. A weighted average of these values yields $\nu=0.97\pm0.05$. The error estimate of 0.05 must be considered a lower bound to the true error since it is conceivable that underlying the apparent random scatter in our values for ν lies a trend that would become manifest for larger cell sizes, and an extrapolation rather than an average would be appropriate. We also note that a recent numerical analysis by Schreiber has yielded a value of $\nu=1.0\pm0.1$.[18] Experiments on compensated or highly disordered doped semiconductors also suggest that $\nu\approx 1$.[36]

TABLE I. Estimates of ν for different pairs of finite cells.

b'	b	ν
4	6	0.92±0.07
4	8	1.03±0.09
6	8	1.19±0.30
4	12	0.98±0.09
6	12	1.01±0.16
8	12	0.89±0.21

At this point it is appropriate to comment on our previous work,[4,17] which used the concept of "quantum connectivity" to calculate critical thresholds and ν for various models—our values for the latter ranged between 1.63 and 1.95. We have subsequently used the same technique to study the model discussed in this paper, finding good agreement with other results[3] for the critical disorder. For small cells we also confirm our previous estimates for ν. However, for the largest pairs of cell sizes we have found that ν decreases systematically with cell size.[32] Thus our previous high estimates were apparently due to finite-size artifacts. From the above work, it would appear that finite-size corrections to scaling are less important for the inverse participating ratio than for the localization length, at least as determined from the quantum connectivity.

Note added in proof. A more thorough treatment of the material discussed herein and other numerical results for the Anderson localization problem are forthcoming.[32]

ACKNOWLEDGMENTS

J.L.S. thanks Ted Kirkpatrick for suggesting that it might be interesting to try to determine the participation ratio exponent numerically. J.L.S. also thanks Spiro Evangelou for bringing our attention to Refs. 8 and 34. This research is supported by the National Science Foundation under Grant Nos. CHE 89-10749, DMR 86-03394, and CHE 83-51207, and by the Camille and Henry Dreyfus Foundation.

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