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Critical exponent and multifractality of states at the Anderson transition

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Based on the assumptions of the existence of a one-parameter scaling law for a self-averaging scaling variable, and on a finite correlation length for the randomness, the lower bound for the critical exponent of the Anderson transition derived earlier by Chayes *et al.* [Phys. Rev. Lett. **57**, 2999 (1986)] for uncorrelated disorder is generalized to the case of *spatially correlated* disorder. The bound is determined by the system-size dependence of the number of the random variables that are necessary to describe the transition. It is speculated how to relate the critical exponent to the multifractal properties of the states near the critical point. Exponents of several models are estimated and compared with numerical scaling calculations.

There are three important results of the efforts of the past two decades towards the solution of the problem of the Anderson transition (AT). Consistent with analytical conjectures,[1–3] the numerical scaling work[4–6] indicated that for certain classes of models, and suffiently close to the AT, a universal, one-parameter scaling function can be established for an appropriately defined scaling variable, and by using a suitable scaling parameter. The former is related to the logarithm of the density-density correlation function, and depends on the specific disorder configuration, but is self-averaging. Its most probable value agrees with its mean in the limit of infinite system size. The scaling parameter corresponds to a correlation length that was identified with the localization length in the regime of large disorder and with the inverse of the dc conductivity for small disorder.

A rigorous lower bound for the critical exponent for models with independent bond or site disorder was found under the assumption that a one-parameter scaling law existed.[7] Not only that such a lower bound can be used for consistency checks of experimental[8] and theoretical[4,5,9] determinations of the exponents. There are certain aspects of the proof itself that may provide useful information about the quantities that eventually determine the AT.

Finally, it has been demonstrated that the quantum states at the AT do have multifractal properties.[10–13] It was possible to determine the complete set of generalized fractal dimensions characteristic for the statistical behavior of the density distribution of the states close to the singularity of the scaling correlation length for the three-dimensional (3D) Anderson model and the 2D disordered Landau model.

In this paper, the lower bound for the critical exponent obtained previously for uncorrelated disorder is generalized to the case of *statistically correlated disorder*. It is rigorously shown that the critical behavior is closely related to the system-size dependence of the number of the random variables that are necessary to describe the transition, provided that a one-parameter scaling law for a self-averaging scaling variable exists. Furthermore, as a speculation, a relation between the lower bound for the exponent and the generalized multifractal dimensions of the states at the critical point is suggested. It is argued that, since the multifractal property implies the information about the wave functions being concentrated only in subregions of the total Euclidean space, and the scaling variable contains all powers of the probability density corresponding to the states near a given energy, the lower bound for the exponent can be improved by considering only subsets of the random variables close to the transition. Using the suggested relation the critical behavior of those models is discussed for which both the critical exponents and the multifractal properties have been previously determined.

In order to generalize the lower bound it is assumed that a positive scaling variable $\Lambda(M) = \Lambda(M, \epsilon_1, \ldots, \epsilon_N)$ exists. It is supposed to depend on a set of $N = N(M)$ random variables. M denotes the size of the system. Physically, the random variables may represent the values of a potential energy at certain sites, the positions of impurities, the values of exchange or bond matrix elements, or, more generally, N of the matrix elements of the Hamiltonian of the system when taken in a complete orthonormal basis. The best lower bound is obtained when the orthonormal basis is chosen in such a way that N is smallest.

$\{\epsilon_1, \ldots, \epsilon_N\}$ are the members of a statistical ensemble described by a normalized distribution function $P(W, \epsilon_1, \ldots, \epsilon_N) = W^{-N} f(\epsilon_1/W, \ldots, \epsilon_N/W)$. W is the disorder parameter. P is assumed to be sufficiently rapidly decaying at infinity for each of the variables. For simplicity, it is also assumed that it is continuously differentiable, and bounded, i.e., $0 \leq P \leq C < \infty$, such that all of its moments exist. Furthermore, the odd moments are supposed to vanish, and the second moment of each of the variables is given by W^2. In cases where some of these assumptions are not valid, such as, for instance,

the box distribution and the random two-component alloy, one can always show explicitly that the result derived in the following is correct.[14]

The random variables may be statistically correlated. The correlation function

$$K(j,j') \equiv W^{-2} \int \cdots \int \prod_i d\epsilon_i \epsilon_j \epsilon_{j'} P(W,\epsilon_1,\ldots,\epsilon_N) \equiv W^{-2} \langle \epsilon_j \epsilon_{j'} \rangle \quad (1)$$

is assumed to be homogeneous, $K(j,j') = K(j-j')$, and to decay sufficiently rapidly for $\mid j-j' \mid \rightarrow \infty$ so that $\sum_{j'} K(j-j')$ exists. Consequently, $P(W,\epsilon_1,\ldots,\epsilon_N) = p_j(\epsilon_j) P_{N-1}(W,\epsilon_1,\ldots,\epsilon_{j-1},\epsilon_{j+1},\ldots,\epsilon_N)$, whenever $\mid \epsilon_j - \epsilon_i \mid \rightarrow \infty$ for $i = 1,\ldots,N$, $i \neq j$.

Consistent with experience from numerical scaling studies,[4-6] the scaling variable is assumed to be self-averaging, i.e., its configurational average

$$\Lambda(M,W) \equiv \langle \Lambda(M,\epsilon_1,\ldots,\epsilon_N) \rangle \quad (2)$$

is identical to its most probable value in the thermodynamical limit.

A further crucial assumption is that there is a one-parameter scaling function

$$\Lambda(M,W) = h(\xi(W)/M), \quad (3)$$

which can be expanded near the critical point, W_c, as

$$\Lambda(M,W) = \Lambda_c - a(W-W_c)M^y, \quad (4)$$

where Λ_c and a are positive constants. The scaling parameter $\xi(W)$ must diverge at W_c as $\mid W - W_c \mid^{-\nu}$, with $\nu = 1/y$.

From Eq. (2), $d\Lambda(M,W)/dW$ may be expressed by the derivative of the distribution function. Since Λ is positive, and self-averaging, an upper bound for $|d\Lambda(M,W)/dW|$ at W_c can be derived by using the Cauchy-Schwartz inequality. One obtains

$$\left| \frac{d\Lambda}{dW} \right|_{W=W_c} \leq \frac{\Lambda_c}{W_c} \left(N - \sum_{jj'} \left\langle \frac{\partial^2 \ln P}{\partial \epsilon_j \partial \epsilon_{j'}} \epsilon_j \epsilon_{j'} \right\rangle \right)^{1/2} . \quad (5)$$

The first term on the right-hand side results for independent random variables. The second is due to statistical correlations. If the latter does dot increase faster than N, then

$$\left| \frac{d\Lambda}{dW} \right|_{W=W_c} \leq B \Lambda_c (N)^{1/2}, \quad (6)$$

with a constant $B < \infty$. We have still to show now that the right-hand side of Eq. (5) does not increase faster than N. Homogeneity of the system ensures that the terms in the sum depend only on the difference between j and j'. Applying again the Cauchy- Schwartz inequality to the double sum one can show that they are proportional to the correlation function, Eq. (1). Convergence with respect to the sum over j is now guaranteed by the above requirements concerning the correlation function. The second summation yields the required factor of N.

Equation (6) establishes the central result of this paper, together with Eq. (5). The statement is that independent of the nature of the randomness, and of whether or not the system is interacting, there is an upper bound for the derivative of the scaling function at the critical point, if it exists. It is proportional to the square root of the number of the random variables, provided the distribution function is bounded, continuously differentiable, with all of its moments existing, and the correlations are of finite range.

Near the critical point the dependence of the scaling variable on the size of the system is given by M^y. On the other hand, the number of the random variables must increase with M, say as M^κ. In general, one cannot assume κ to be smaller than d, the dimensionality of the system, otherwise the "concentration" N/M^d would vanish in the thermodynamic limit. Because of Eq. (6) we have $y \leq \kappa/2$, or, equivalently, $\nu \geq \nu_0 \equiv 2/\kappa$, consistent with the earlier result for uncorrelated randomness and $\kappa = d$.

It should be noted that the above derivation is valid as long as $a|W-W_c|M^y \ll \Lambda_c$. This can be satisfied for the above bound close to W_c with the choice $M < M_W \equiv C|W-W_c|^{-2/\kappa}$, C being a constant of order 1.

For "normal" 3D Hamiltonians the disorder will be physically originating in the random fluctuations of a potential energy, and $\nu_0 = \frac{2}{3}$. The numerical scaling studies for diagonal disorder indicate a considerably higher exponent, $\nu = 1.5 \pm 0.2$.[4] For the Anderson model with bond disorder given by $V = \pm 1$, numerically $\nu = 1.0 \pm 0.05$ was found.[15,13] For the 3D case with a large homogeneous magnetic field applied $\nu = 1.3 \pm 0.3$ was estimated.[16]

In 2D without magnetic field $\nu_0 = 1$. No AT at finite critical disorder exists in this case. However, one may take the limit $W \rightarrow 0$ as the critical point. The localization length there has an essential singularity, i.e., $\nu = \infty$, for vanishing magnetic field B, trivially consistent with the bound. When $B > 0$ numerical evaluation of the random Landau model yields $\nu = 2.35 \pm 0.04$,[5,17] which is again consistent with the bound.

In 1D the localization length diverges as W^{-2} at $W = 0$, without or with statistical correlations of the randomness.[18] Here the bound is met.

An interesting further test would be the AT in fractal systems. One expects $\nu_0 = 2/d^*$, d^* being the fractal dimension. Unfortunately, no determinations of critical exponents are presently available for such models.

All of the numerically calculated exponents are consistent with, and most of them are considerably higher than, the lower bound, when $\kappa = d$. One may therefore ask whether or not this bound can be improved.

The speculation presented in the following is an attempt towards motivating an answer to this question. It is essentially based on two observations. The first is that the scaling variable used in the numerical calculations[4] is related to the average of the logarithm of the modulus of the Green's function $G(E,\mathbf{r},\mathbf{r}')$ between two sites $\mathbf{r},\mathbf{r}'$ that are separated by a distance M,

$$\Lambda^{-1}(M,W) = - \langle \ln \mid G(E,M) \mid \rangle . \quad (7)$$

Homogeneity guarantees again that Λ does not depend on the absolute position. Using the spectral representation one notices that the scaling variable contains all powers of the wave functions near energy E at the sites separated by M.

The second concerns the statistical properties of the wave functions, $\psi(\mathbf{r})$, near the critical point. According to recent numerical work[10–12] their spatial properties can be characterized by a set of generalized fractal dimensions, $D(q)$. These describe the dependence on the length scale of the qth powers of the quantum-mechanical probability density $|\psi|^2$. Using the "box probability"[19]

$$\mu_j = \int_{\Omega(j)} |\psi(\mathbf{r})|^2 \, d^d r, \tag{8}$$

where $\Omega(j) = \ell^d$ is the volume of a box-shaped region of the linear size ℓ with $a \ll \ell \ll M \ll \xi$ (a is the microscopic length, M is the system size), one can obtain $D(q)$ from the scale dependence of the average qth moment of the μ_j ($-\infty < q < \infty$), $\mathcal{P}^{(q)}(\lambda) = \sum_{j=1}^{Z} \mu_j^q$, where $\lambda \equiv \ell/M$ and $Z \equiv \lambda^{-d}$ is the number of the boxes,

$$\mathcal{P}^{(q)}(\lambda) \propto \lambda^{(q-1)D(q)}. \tag{9}$$

For a simple fractal $D(q)$ is independent of q. However, in general, there is no single length scale for the spatial distribution of the density but an infinite set. $D(0)(= d)$ is the dimension of the total support of the wave function. $D(1)$ is called the information dimension, and $D(2)$ the correlation dimension. The latter was formerly discussed in connection with the participation number.[20,21] Generally, $D(q)$ may be considered as characteristic of the distribution of the density at different levels of the amplitudes. $D(q \to \infty)$ provides information about the scaling properties of those regions where the the largest amplitudes are concentrated.

Spectra of generalized fractal dimensions were determined for the 3D Anderson model (without magnetic field) for specific states close to the singularity of the scaling correlation length[12] yielding $D(1) \approx 2.17$ and $D(2) \approx 1.68$. Since the Anderson transition is related to the scaling properties of the logarithm of the density-density correlation function, it is tempting to identify κ with $D(2)$ in order to obtain a better estimate of the lower bound, $\nu_2 = 2/D(2)$. One obtains $\nu_2 \approx 1.2$ for the 3D Anderson model which is still lower than the exponent obtained from the scaling calculations.

No results are available on the fractal properties of 3D models including a magnetic field.

For the 2D random Landau model in the one-band approximation (limit of large magnetic field)[10,11] similar statements as in the above 3D case can be made for wave functions close to the center of the band. Here $D(2) \approx 1.43$ and $\nu_2 \approx 1.4$.

In order to ensure the self-averaging property of the scaling variable, the *logarithm* of the density-density correlation function had to be considered, i.e., all of its moments are important. Therefore one might expect to improve the estimate for the bound by inceasing q. $\nu_\infty = 2/D(\infty)$ could then provide a "best" estimate for the exponent.[14] Since $D(\infty) \approx 1$ for the 3D Anderson model,[12] and $D(\infty) = 0.85$ for the random Landau model,[10,11] one obtains $\nu_\infty \approx 2$ and $\nu_\infty \approx 2.35$, respectively. While the latter of these is remarkably close to the result from numerical scaling, the former is seemingly too high. However, taking into account the numerical errors for the critical exponents, and $D(\infty)$, namely $\delta D(\infty)/D(\infty) \approx 10\%$, one can claim that ν_∞ provides at least a reasonable estimate for the exponent.

Given that the above-mentioned value of the critical exponent for the 3D Anderson model with bond disorder, $\nu = 1.0$,[15] was correct, and the suggested relation between critical behavior and statistical properties of the states near the transition was reasonable, one would expect $D(\infty) \approx 2.0$. For the 3D case with high magnetic field one would estimate $D(\infty) \approx 1.0$ as with $B = 0$.

In conclusion, the lower bound for the critical exponent of the Anderson transition obtained earlier[7] for uncorrelated randomness has been generalized to correlated randomness. The bound was related to the dependence of the number of random variables on the size of the system. All of the critical exponents obtained by the numerical scaling method for various models without and with statistical correlations of the randomness are consistent with the bound when assuming that the number of the random variables increases proportional to the system size.

As recent multifractal analyses of states in random systems show that it is only a fraction of the space which ultimately contains almost all of the information about the states in random systems close to a phase transition, it is speculated that it is only a fraction of the total number of the random variables of the model which eventually determines the critical behavior. If one assumes that the dependence of this fraction on the size of the system is given by the largest of the fractal dimensions of the states, quantitative estimates for the critical exponents can be obtained. They are, within the errors, consistent with the results of the numerical scaling calculations.

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