

## Corrections to Scaling at the Anderson Transition

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We report a numerical analysis of corrections to finite size scaling at the Anderson transition due to irrelevant scaling variables and nonlinearities of the scaling variables. By taking proper account of these corrections, the universality of the critical exponent for the orthogonal universality class for three different distributions of the random potential is convincingly demonstrated. [S0031-9007(98)08164-2]

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The possibility of the Anderson localization of electron states as a result of disorder was first suggested four decades ago [1]. Following the proposal of the scaling theory of localization [2] attention has focused on understanding the critical properties of the Anderson transition (AT), the quantum phase transition which occurs at a critical disorder separating a diffusive metallic phase from an insulating localized phase [3].

Our current understanding of the AT is based on the nonlinear  $\sigma$  model (NL $\sigma$ M) [4]. This has been analyzed using an expansion in powers of  $\epsilon$ , where  $d = 2 + \epsilon$  is the dimension of the system. According to the NL $\sigma$ M it should be possible to classify the critical behavior using three universality classes: orthogonal, unitary, and symplectic depending on the symmetry of the Hamiltonian with respect to time reversal and spin rotation. Here we focus on the orthogonal universality class corresponding to systems with both time reversal and spin rotation symmetries.

Beyond the suggestion of the appropriate universality classes, there has not been much success in making detailed predictions about the critical behavior with the NL $\sigma$ M. The problems are well illustrated by attempts to estimate the critical exponent  $\nu$  which describes the divergence of the correlation length  $\xi$  at the AT. In early work it was found that  $\nu = 1/\epsilon$  [5] which gives  $\nu = 1$  when extrapolated to  $d \equiv \epsilon + 2 = 3$ . When combined with the Wegner scaling law  $s = \nu\epsilon$  [6] this leads to a conductivity exponent  $s = 1$ . Measurements on some, but not all, materials do indeed yield  $s = 1$  [7]. However, calculations at higher orders in  $\epsilon$  produced strong corrections to the leading order when extrapolated to  $\epsilon = 1$  [8,9], showing that this agreement is fortuitous. There is now no accepted estimate of the exponent based on the  $\epsilon$  expansion or any other analytic technique.

While the preceding problem can be regarded as a rather unfortunate technical difficulty, fears have also been expressed that there may be an infinite number of relevant operators in the NL $\sigma$ M [10] and that the theory may be unsound. While it now seems unlikely in view

of [11] that this is actually the case, in this context it is nevertheless important to have independent confirmation that our understanding of the AT is correct. At the present time, numerical simulations [3,12–14] offer the only viable alternative.

In this paper we demonstrate an important basic principle underlying our understanding of the AT: the universality of the critical properties of the AT. To do this has required us to address the principle uncertainty in previous numerical studies of the critical properties of the AT, the presence of systematic corrections to scaling in the numerical data due to the practical limitations on the sizes of the system which can be studied.

The computer time required in numerical studies of the AT increases very rapidly with increasing system size (as  $L^7$  for the method used here). This sets a severe limitation on the system sizes which can be simulated. However, systematic corrections to scaling are expected in smaller systems, and their neglect leaves important questions about the validity of any conclusions drawn from the analysis of the numerical data. Here we consider two ways in which such corrections can arise: the presence of irrelevant scaling variables and nonlinearity of the scaling variables [15]. These effects lead to systematic rather than random deviations from scaling and must be taken into account when estimating both the critical parameters and the likely accuracy of their estimation.

Our work has also been inspired by the successful analyses of corrections to scaling in the quantum Hall effect (QHE) transition [16,17]. The present problem is, however, more difficult since, unlike the QHE, the critical point is not known *a priori* on grounds of symmetry.

The universality of the exponent for the box and Gaussian distributions of random potential was demonstrated to a limited extent in [12] by taking account of corrections to scaling in an *ad hoc* manner. Here, taking account of corrections systematically, we confirm that result and extend its validity to include the Lloyd model [18].

The Hamiltonian used in this study describes noninteracting electrons on a simple cubic lattice with nearest

neighbor interactions only

$$\begin{aligned}\langle \vec{r} | H | \vec{r} \rangle &= V(\vec{r}), \\ \langle \vec{r} | H | \vec{r} - \hat{x} \rangle &= -1, \\ \langle \vec{r} | H | \vec{r} - \hat{y} \rangle &= -1, \\ \langle \vec{r} | H | \vec{r} - \hat{z} \rangle &= -1.\end{aligned}$$

Here  $\hat{x}$ ,  $\hat{y}$ , and  $\hat{z}$  are the lattice basis vectors. The potential  $V$  is independently and identically distributed with probability  $p(V)dV$ . We studied three models of the potential distribution: The box distribution

$$p(V) = 1/W \quad |V| \leq W/2, \\ = 0 \quad \text{otherwise,}$$

the Gaussian distribution

$$p(V) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{V^2}{2\sigma^2}\right),$$

with  $\sigma^2 = W^2/12$ , and the Lloyd model in which  $V$  has a Lorentz distribution

$$p(V) = \frac{W}{\pi(W^2 + V^2)}.$$

For this distribution all moments higher than the mean are divergent and the parameter  $W$  is proportional to the full width at half maximum of the distribution. For these three models we analyzed the finite size scaling [15] of the localization length  $\lambda$  for electrons on a quasi-1d dimensional bar of cross section  $L \times L$ . The length  $\lambda$  was determined to within a specified accuracy using a standard transfer matrix technique [19,20].

The starting point of our analysis is the renormalization group equation which expresses the dimensionless quantity  $\Lambda = \lambda/L$  as a function of the scaling variables

$$\Lambda = f\left(\frac{L}{b}, \chi b^{1/\nu}, \psi b^y\right).$$

In this equation  $b$  is the scale factor in the renormalization group,  $\chi$  is the relevant scaling variable, and  $\psi$  is the leading irrelevant scaling variable. We should find  $y < 0$  if  $\psi$  is irrelevant. An appropriate choice of the factor  $b$  [15] leads to

$$\Lambda = F(\chi L^{1/\nu}, \psi L^y), \quad (1)$$

where  $F$  is a function related to  $f$ .

For  $L$  finite there is no phase transition and  $F$  is a smooth function of its arguments. Assuming the irrelevant scaling variable is not dangerous, we make a Taylor expansion up to order  $n_I$

$$\Lambda = \sum_{n=0}^{n_I} \psi^n L^{ny} F_n(\chi L^{1/\nu}), \quad (2)$$

and obtain a series of functions  $F_n$ . Each  $F_n$  is then expanded as a Taylor series up to order  $n_R$

$$F_n(\chi L^{1/\nu}) = \sum_{m=0}^{n_R} \chi^m L^{m/\nu} F_{nm}. \quad (3)$$

To take account of nonlinearities in the scaling variables we expand both in terms of the dimensionless disorder

$w = (W_c - W)/W_c$  where  $W_c$  is the critical disorder separating the insulating ( $w < 0$ ) and conducting phases ( $w > 0$ ).

$$\chi(w) = \sum_{n=1}^{m_R} b_n w^n, \quad \psi(w) = \sum_{n=0}^{m_I} c_n w^n. \quad (4)$$

The orders of the expansions are  $m_R$  and  $m_I$ , respectively. Notice that  $\chi(0) = 0$ . The absolute scales of the arguments in (1) are undefined; we fix them by setting  $F_{01} = F_{10} = 1$  in (3). The total number of fitting parameters is  $N_p = (n_I + 1)(n_R + 1) + m_R + m_I + 2$ .

The qualitative nature of the corrections can be understood by looking at some special cases. First, let us suppose that nonlinearities are absent ( $m_R = 1$  and  $m_I = 0$ ) and truncate (2) at  $n_I = 1$

$$\Lambda = F_0(\chi L^{1/\nu}) + \psi L^y F_1(\chi L^{1/\nu}).$$

From this equation we can infer that the estimate of the critical disorder, and possibly also the critical exponent, will appear to shift in a systematic way as the size of the system increases. To exhibit scaling it is necessary to subtract the corrections due to the irrelevant scaling variable. When  $n_I = 1$  we define

$$\Lambda_{\text{corrected}} = \Lambda - \psi L^y F_1(\chi L^{1/\nu}), \quad (5)$$

with the obvious generalization when  $n_I > 1$ . We then have

$$\Lambda_{\text{corrected}} = F_{\pm}\left(\frac{L}{\xi}\right). \quad (6)$$

The functions  $F_{\pm}$  are defined by  $F_{\pm}(x) = F_0[\pm(\xi_{\pm}x)^{1/\nu}]$ . In this case the correlation length  $\xi$  has a simple power law dependence on the dimensionless disorder  $\xi = \xi_{\pm}|w|^{-\nu}$ . The constants  $\xi_{\pm}$  are not normally determined in finite size scaling studies.

On the other hand, if we neglect the irrelevant variable and consider only nonlinearity in the scaling variable we find  $\Lambda = F_{\pm}(L/\xi)$  without the need to subtract any corrections. No systematic shift of the estimated critical point should occur as the system size is increased. However, the correlation length  $\xi$  no longer has a simple power law dependence on  $w$  but behaves as  $\xi = \xi_{\pm}|\chi|^{-\nu}$ .

The critical exponent  $\nu$ , the irrelevant exponent  $y$ , and the functions  $F_n$  are expected to be universal, while the coefficients  $\{b_n\}$  and  $\{c_n\}$  are not. Though we have explicitly considered corrections due to the leading irrelevant scaling variable only, the analysis can easily be extended to several such variables.

In the simulation  $\lambda$  was evaluated as a function of disorder  $W$  for a range of system sizes  $L$ . The best fit was determined by minimizing the  $\chi^2$  statistic [21]. This is justified if we suppose a uniform prior probability for all parameters, that the deviations between the model and the simulation data are purely random in origin and distributed following a Gaussian distribution [21]. This last

TABLE I. The disorder distribution (B: box; G: Gaussian; L: Lorentz), the type of fit, the range of disorder  $W$ , the number of data  $N_d$ , the number of parameters  $N_p$ , the value of  $\chi^2$  for the best fit, and goodness of fit  $Q$ . The system sizes used were  $L = 4, 5, 6, 8, 10, 12, \text{ and } 14$ .

Disorder	$n_R$	$n_I$	$m_R$	$m_I$	$W$	$N_d$	$N_p$	$\chi^2$	$Q$
B	3	1	2	0	15, 18	224	12	214	0.5
G	2	1	2	0	20.2, 22.2	175	10	174	0.3
L	2	2	1	0	4.1, 4.5	224	12	203	0.7

assumption is also important in determining the likely accuracy to which the critical parameters have been estimated. Since the inclusion of corrections to scaling allows for systematic rather than just random deviations from scaling in the numerical data, this assumption is more reasonable here than when corrections to scaling are neglected. Therefore we expect the estimates of the accuracy of the critical exponent, etc., to be more reliable. The model (2)–(4) is nonlinear in some parameters so the goodness of fit  $Q$  has been checked using a Monte Carlo technique and the confidence intervals evaluated by re-sampling [22,23].

The inclusion of the corrections in (2)–(4) leads to a rapid increase in the number of fitting parameters, and high quality data are essential if meaningful fits are to be obtained. All data used here have an accuracy of either 0.1% or 0.05%. To achieve this accuracy between  $10^6$  and  $10^7$  iterations in the transfer matrix method were required. When deciding which correction terms to include we attempted to maximize the goodness of fit  $Q$  while keeping the number of correction terms to a minimum.

The details of the simulations and the types of fit used are listed in Table I. The estimated critical parameters and their confidence intervals are given in Table II. Some typical data are displayed in Fig. 1. To exhibit scaling the data are replotted after subtraction of the appropriate corrections in Fig. 2. The corrected data now fall on a single curve clearly exhibiting scaling in agreement with (6). The magnitude of the corrections needed to obtain the scaling shown in Fig. 2 are of the order of 2% or so for the smallest system size decreasing to around 0.3% for the largest system size.

The most important point to be drawn from Table II is that the estimates of the exponent  $\nu$  for the three different disorder distributions are in almost perfect agreement. The same is true for the estimates of the critical parameter

TABLE II. The best fit estimates of the critical disorder and the critical exponent and their 95% confidence intervals. The quantity  $\Lambda_c = F_0(0)$  is expected to be universal.

	$W_c$	$\Lambda_c$	$\nu$	$y$
B	16.54(53, 56)	0.576(74, 78)	1.57(55, 59)	-2.8(3.3, 2.3)
G	21.29(28, 31)	0.576(74, 77)	1.58(55, 61)	-3.9(5.9, 2.7)
L	4.265(52, 72)	0.579(76, 88)	1.58(47, 65)	-2.5(3.2, 1.3)

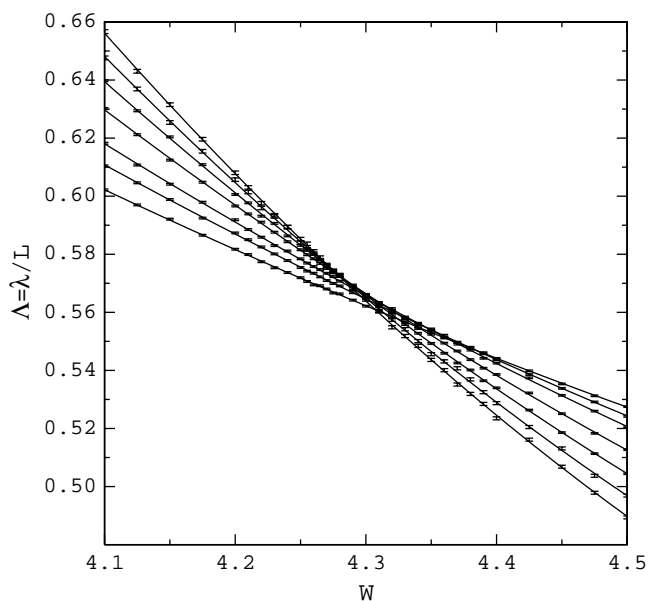


FIG. 1.  $\Lambda$  as a function of disorder for the three dimensional Lloyd model. The solid lines are the fit (2)–(4).

$\Lambda_c$ . This is strong evidence in favor of the universality of the critical exponent and other critical parameters.

How do the results of the present analysis compare with those obtained when corrections to scaling are neglected? In Table III we give the results obtained for the same potentials neglecting corrections. The first thing to notice is that the range of system sizes (and in the box distribution, the range of  $W$ ) for which an acceptable fit ( $Q > 0.1$ ) can be achieved is very limited. After discarding data for the smaller system sizes, reasonable agreement is obtained between Tables II and III. However, given the more

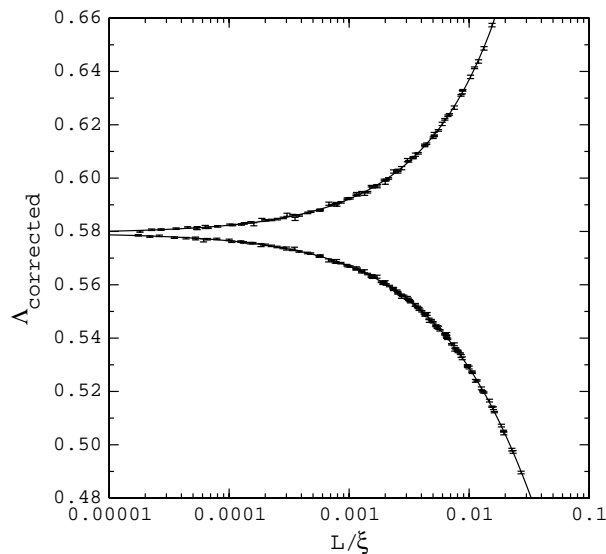


FIG. 2. The data in Fig. 1 after subtraction of corrections to scaling [see (5)] together with the scaling functions (6). Here  $\xi = \xi_{\pm} |\chi|^{-\nu}$ . The upper branch corresponds to the metallic phase and the lower branch to the insulating phase.

TABLE III. Best estimates of the critical parameters when corrections to scaling are neglected.

	$L$	$W$	$W_c$	$\Lambda_c$	$\nu$
B $\geq 8$	16, 17		16.514(07, 22)	0.579(78, 80)	1.58(53, 63)
G $\geq 8$	20.2, 22.2		21.28(26, 29)	0.577(76, 78)	1.58(54, 62)
L $\geq 10$	4.1, 4.5		4.275(72, 78)	0.574(73, 75)	1.58(53, 62)

limited range of system sizes, the estimates of the accuracy to which the critical parameters have been determined when corrections are neglected are too optimistic. The problem is more evident when looking at less accurate, e.g., 0.2% data [24] for the box distribution. Ignoring corrections to scaling, it was found that  $W_c = 16.45 \pm 0.01$ ,  $\Lambda_c = 0.586 \pm 0.001$ , and  $\nu = 1.59 \pm 0.03$ . The estimates of  $W_c$  and  $\Lambda_c$  are not consistent with Table II. The effect which gives rise to this inconsistency can also be seen in the data for the Lloyd model displayed in Fig. 1. A systematic shift of the apparent critical disorder to a lower value as the system size increases is evident. For the box and Gaussian distributions the shift was found to be in the opposite sense to higher disorder. It seems likely that any analysis which assumes that deviations from scaling are purely random origin, rather than allowing for systematic corrections such as considered here, will lead to an overoptimistic estimate of the accuracy to which the critical point has been determined and even to an incorrect determination of the critical point. In contrast, the estimate of the critical exponent is quite consistent with that in Table II. Of course, the precise location of the critical point in any particular model is not in itself very important, but any inaccuracy in its estimate also affects the estimate of the critical conductance distribution [24].

We should also mention that surface effects and the influence of boundary conditions may also give rise to corrections to scaling behavior. We have used periodic boundary conditions to minimize surface effects. Even so there may remain some influence of the boundary conditions. To quantify this we have evaluated  $\lambda$  for some representative values of the parameters for fixed (fbc), periodic (pbc), and antiperiodic (apbc) boundary conditions. A large statistically significant shift in the localization length  $\lambda$  was found between fbc and pbc. However, even when calculating at a higher accuracy of 0.02% no such difference between pbc and apbc was found. We therefore think it reasonable to neglect such corrections here.

We have presented a numerical study of the Anderson transition in three dimensions in which systematic corrections to scaling have been explicitly taken into account when estimating the critical disorder and other critical parameters. The universality of the critical exponent with respect to the choice of the distribution of disorder has been accurately verified.

While in this paper we have concentrated on the scaling of the correlation length in the three dimensional Anderson model, corrections of a similar nature may also be important in finite size scaling analyses of the conductance distribution and energy level statistics. The method we have described here is applicable in these cases and, indeed, to any continuous quantum phase transition.

Part of this work has been carried out on supercomputer facilities at the Institute for Solid State Physics, University of Tokyo.

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