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Critical exponents for the metal–insulator transition

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Abstract. The critical exponents of the metal–insulator transition in disordered systems have been the subject of much published work containing often contradictory results. Values ranging between $\frac{1}{2}$ and 2 can be found even in the recent literature. In this paper the results of a long-term study of the transition are presented. The data have been calculated with sufficient accuracy (0.2%) that the calculated exponent can be quoted as $s = \nu = 1.54 \pm 0.08$ with confidence. The reasons for the previous scatter of results are discussed.

1. Introduction

The metal–insulator transition in disordered systems has been the subject of theoretical and experimental work at least since the article by Anderson (1958). The similarities with thermodynamic phase transitions had been noted by several authors (Thouless 1974, Wegner 1976) but it was not until 1979 that a usable formulation of the renormalization group or scaling theory became available (Abrahams *et al* 1979, Wegner 1979, Efetov 1983). The basic assumption of these theories, that the behaviour could be described by a single-parameter scaling theory, was confirmed in numerical calculations by the present author (MacKinnon and Kramer 1981, 1983). For a recent review of the area see the article by Kramer and MacKinnon (1994).

In spite of the progress made the exponents, s and ν, describing the behaviour of the conductivity and the localization length respectively, have proven difficult to calculate reliably. For some time there appeared to be a consensus between theory and experiment that both exponents were equal to unity, but more recently this has been called into question from both the theoretical (Kravtsov and Lerner 1984, Lerner 1991) and from the experimental (Stupp *et al* 1993) side.

Numerical results have been scattered at least between 0.5 and 2 with numerous attempts at developing alternative methods of calculation. A good example of the difficulties is given by the contrast between calculations for the Anderson model with rectangular or Gaussian disorder (Kramer *et al* 1990). Using identical methods the exponents obtained were about 1.5 and 1.0 for the rectangular and Gaussian distributions respectively. It is clearly unreasonable for the exponents for these two cases to be different. In fact if they were different then it would call into question the justification of the use of any simple model Hamiltonian to describe the transition and so undermine the whole foundation of the subject.

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In this paper the results of calculations carried out over several years are presented. All the basic results have an accuracy of at least 0.2%, which enables the critical exponents to be calculated much more accurately than when the conventional 1% is used.

2. Transfer matrix calculations

The transfer matrix method has been discussed in numerous papers (MacKinnon and Kramer 1983, Pichard and Sarma 1981) so only the brief outline will be attempted here.

The starting point is the usual Anderson (1958) Hamiltonian

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{i \neq j} V_{ij} |i\rangle\langle j| \tag{1}$$

where $V_{ij} = V_0$ between nearest neighbours on a simple cubic lattice and zero otherwise. In this work $V_0 = 1$ is chosen and will therefore not be mentioned explicitly. The diagonal elements ϵ_i are independent random numbers chosen either from a uniform rectangular distribution with $-\frac{1}{2}W < \epsilon_i < +\frac{1}{2}W$ or from a Gaussian distribution of standard deviation σ. For purposes of comparison between the two cases an effective W for the Gaussian case may be defined by equating the variances as $W^2 = 12\sigma^2$.

In terms of the coefficients a_i of the wavefunctions on each site the Schrödinger equation may be written in the form

$$Ea_i = \epsilon_i a_i + \sum_{j \neq i} a_j. \tag{2}$$

Consider now a long bar composed of L slices of cross-section $M \times M$. By combining the a_i values from each slice into a vector A_i (2) can be written in the concise form

$$EA_n = \mathsf{H}_n A_n + A_{n+1} + A_{n-1} \tag{3}$$

where the subscripts n now refer to slices and matrix H_n is the Hamiltonian for slice n. By rearranging (3) the transfer matrix is obtained

$$\begin{pmatrix} A_{n+1} \\ A_n \end{pmatrix} = \begin{pmatrix} E - \mathsf{H}_n & -\mathsf{I} \\ \mathsf{I} & 0 \end{pmatrix} \begin{pmatrix} A_n \\ A_{n-1} \end{pmatrix} \tag{4a}$$

$$= \prod_{m=1}^{n} \begin{pmatrix} E - \mathsf{H}_m & -\mathsf{I} \\ \mathsf{I} & 0 \end{pmatrix} \begin{pmatrix} A_1 \\ A_0 \end{pmatrix} \tag{4b}$$

$$= \mathsf{T}_n \begin{pmatrix} A_1 \\ A_0 \end{pmatrix}. \tag{4c}$$

A theorem attributed to Oseledec (1968) states that

$$\lim_{n \to \infty} \left(\mathsf{T}_n^{\dagger} \mathsf{T}_n\right)^{1/n} = \mathbf{M} \tag{5}$$

where $\mathbf{M}$ is a well defined matrix and T_n are product of random matrices. The logarithms of the eigenvalues of $\mathbf{M}$ are referred to as Lyapunov exponents and occur in pairs that are reciprocals of one another. By comparison with (4) the Lyapunov exponents may be identified with the rate of exponential rise (or fall) of the wave functions. In fact the smallest exponent corresponds to the longest decay length and hence to the localization length of the system.

In principle then it is necessary to calculate $\mathbf{T}_n$ for large n, and diagonalize $\mathbf{T}^\dagger\mathbf{T}$. Unfortunately, the calculation is not quite so simple: the different eigenvalues of $\mathbf{T}^\dagger\mathbf{T}$ rise at different rates so that the smallest, which we seek, rapidly becomes insignificant compared to the largest and is lost in the numerical rounding error. Typically this happens after about 10 steps.

2.1. Orthogonalization

In order to obtain the smallest Lyapunov exponent it is necessary to overcome this loss of numerical significance. This can be achieved in more than one way, the orthogonalization method is employed here.

After about 10 matrices have been multiplied together the columns of the product matrix are orthogonalized to each other and normalized. This is equivalent to multiplying the product from the right by an appropriate matrix. This orthogonalization process automatically separates the different exponentially growing contributions.

The process is repeated every 10 or so steps and the logarithm of the length of the vector closest to unity is stored. The Lyapunov exponent is given by the mean value of these logarithms divided by the number of steps between orthogonalizations. In practice it is necessary to use only 50% or $M \times M$ vectors rather than the full $2 \times M \times M$ as the required vector is invariably the $(M \times M)$th.

The error in the Lyapunov exponent can be estimated from the variance corresponding to the mean exponent. Although this estimate could be biased by correlations between the different contributions this is not found to be a serious problem in practice, at least when the localization length is short compared with the distance between orthogonalization steps.

The optimum frequency of orthogonalization steps can be estimated by comparing the length of the $(M \times M)$th vector before and after orthogonalization. The ratio should not be allowed to become close to the machine accuracy.

3. Scaling theory

The inverse of the smallest Lyapunov exponent is the localization length λ_M. The renormalized length $\Lambda = \lambda_M/M$ is found to obey a scaling theory (MacKinnon and Kramer 1981, 1983) such that

$$\frac{\mathrm{d}\ln\Lambda}{\mathrm{d}\ln M} = \chi(\ln\Lambda) \tag{6}$$

which has solutions of the form

$$\Lambda = f(M/\xi) \tag{7}$$

where ξ is a characteristic length scale, which can be identified with the localization length of the insulator, and which scales as the reciprocal of the resistivity of the metallic phase (MacKinnon and Kramer 1983).

In 3D (6) always has a fixed point $\chi = 0$ which corresponds to the metal–insulator transition. The behaviour close to the transition can be found by linearizing (6) and solving to obtain

$$\ln\Lambda = \ln\Lambda_c + A(\tau - \tau_c)M^\alpha \tag{8}$$

where τ is the disorder W or σ, Λ_c and τ_c represent the critical Λ and disorder respectively, and A and α are constants. By comparing (7) and (8) an expression for ξ can be obtained in the form

$$\xi \sim |\tau - \tau_c|^{1/\alpha} \tag{9}$$

so that the localization length exponent ν is given by $\nu = 1/\alpha$. Since it is well known (Wegner 1976, Abrahams *et al* 1979) that the conductivity exponent s is related to ν by $s = (d-2)\nu$ then by fitting (8) to the data and calculating α both exponents can be obtained.

Table 1.

	Rectangular	Gaussian
Exponent	1.515±0.033	1.484±0.048
Disorder range	$16.2 \leqslant W \leqslant 16.8$	$21.0 \leqslant W \leqslant 21.5$
System sizes	$4 \leqslant M \leqslant 12$	$4 \leqslant M \leqslant 12$
χ^2 (expected)	142	97
χ^2 (fitted)	126	75
W_c [a]	16.50±0.05	21.20±0.06
σ_c	4.763±0.015	6.120±0.018
Λ_c [a]	*0.580±0.005*	*0.580±0.005*

[a] The estimates of W_c and Λ_c are based on the values given by several different fitting procedures.

3.1. Deviations from scaling

One simple feature of (8) is that, when $\ln \Lambda$ is plotted against τ, the curves for different M intersect at a common point $(\ln \Lambda_c, \tau_c)$. In practice the data do not behave in exactly this way. There is a small deviation from scaling. This deviation could be taken into account by adding to (8) an extra term that depends on M but not on τ. Consider, however, the form

$$\ln \Lambda = A\tau M^{\alpha} + B(M) \tag{10}$$

which represents the most general form of such a correction. If a specific form for the correction were assumed it would require at least four independent fitting parameters to represent $B(M)$, including Λ_c and τ_c, and may still not represent the true deviation from scaling. It seems better therefore to fit an independent $B(M)$ for each value of M and therefore to make no assumption about the nature of the deviation from scaling, other than that it is non-critical, and therefore independent of τ, in the region of interest. By fitting the data to (10) in this way the exponent α is derived solely from the gradient of $\ln \Lambda$ versus τ and the intercept is allowed to float. The results of such fits are shown in figure 1.

3.2. Data fitting

The data can be fitted to (10) by iteratively using a standard least-squares procedure. Care is required with the non-linear parameter α. The quality of the fit can be tested by computing χ^2, defined as

$$\chi^2 = \sum_i \frac{(A\tau_i M_i^{\alpha} + B(M_i) - \ln \Lambda_i)^2}{\sigma_i^2} \tag{11}$$

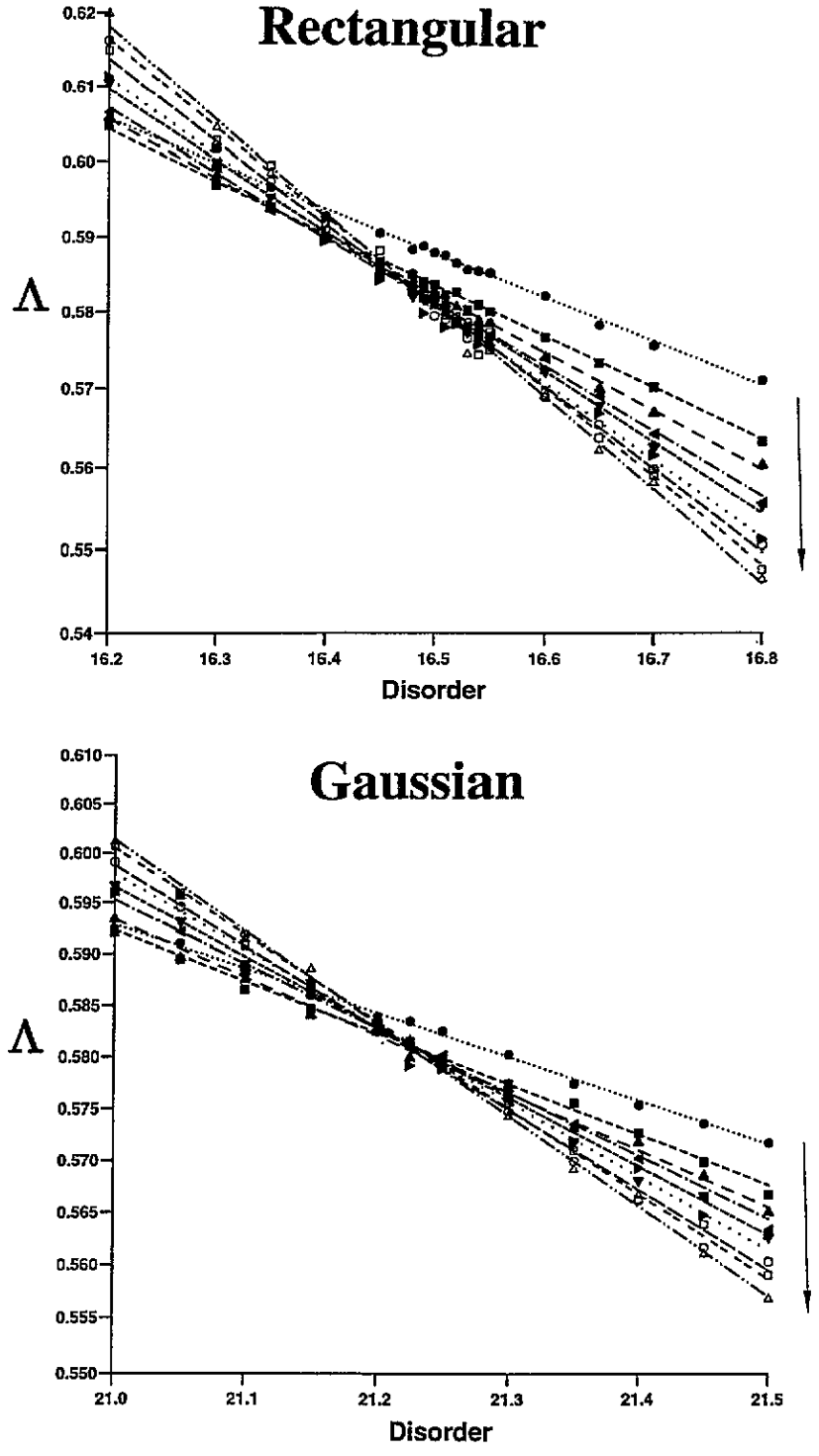

Figure 1. Λ versus W, for rectangular and Gaussian distributions. The data are represented by dots with differing symbols for different system sizes with $4 \leqslant M \leqslant 12$ increasing in the direction of the arrow. Each point is accurate to 0.2%. The lines are fitted using (10).

where i runs over all data points and σ_i is the error in point i. After fitting, χ^2 should be approximately equal to the number of data points minus the number of fitted parameters. Hence the value of χ^2 provides a measure of the quality of the fit. In the results presented here the range of values of disorder round the critical value was chosen such that χ^2 conforms to this condition. Then a large number of additional points was calculated inside this range. An important side effect of this procedure is that the apparently acceptable range of disorder around the fixed point becomes narrower as the calculations become more accurate. It is therefore important to test whether any apparent change in the fitted exponent is due to this narrowing.

The values of the ideal and the fitted χ^2 as well as the range considered are shown in table 1. Using $4 \leqslant M \leqslant 12$ and the widest range of disorder, $s = \nu = 1.53 \pm 0.04$ and $s = \nu = 1.48 \pm 0.05$ for rectangular and Gaussian cases respectively.

3.3. Statistical and systematic errors

The statistical error in the fitted critical exponent is easily estimated from the least-squares fitting procedure. Systematic errors are more difficult to take into account. In this work an attempt is made to consider three sources of systematic error, as follows.

(i) The limited range of system sizes: $4 \leqslant M \leqslant 12$ has been considered and the effect of ignoring the smaller system sizes tested.

(ii) The width of the critical region: the maximum range of disorder is imposed by χ^2 but may still be too large. The effect of narrowing this range still further has been tested.

(iii) The choice of distribution of random numbers: this has been tested by comparing the rectangular and Gaussian cases.

These tests are represented in figure 2. Unfortunately the general increase in the error bars due to ignoring data tends to mask any systematic changes. There does however appear to be a general increase in the exponents when the $M = 4$ data are eliminated and a tendency for the Gaussian data to lie below the rectangular. From these data $s = \nu \simeq 1.54 \pm 0.08$ has been estimated, where the error bar may be somewhat wider than necessary.

4. Results and conclusions

The results are summarized in table 1. All these results have been calculated in the middle of the band (i.e. $E = 0$), but there is ample evidence that for the models considered here, this point is not special and is truly representative of the whole band, at least in the range $-6 \leqslant E \leqslant 6$.

Unlike previous calculations (Kramer *et al* 1990) the exponents calculated for the two distributions now overlap well and are therefore consistent with the common assumption that simply changing the distribution does not change the universality class and hence the critical exponent. The discrepancy reported previously is presumably due to insufficient accuracy in the raw data and consequent assumption of a critical range of disorder that was too wide.

This may have consequences for experiment as it seems to suggest that it is possible to obtain an exponent of unity simply by using too wide a range of data around the critical disorder, energy, pressure, etc. It should also be borne in mind that the influence of interactions may also account for differences between experimental results and those based on a model of non-interacting electrons. For this reason it may be more realistic to compare the present results with photonic or acoustic rather than electronic experiments.

In summary, the critical exponent of the Anderson model of the metal–insulator transition is $s = \nu = 1.54 \pm 0.08$.

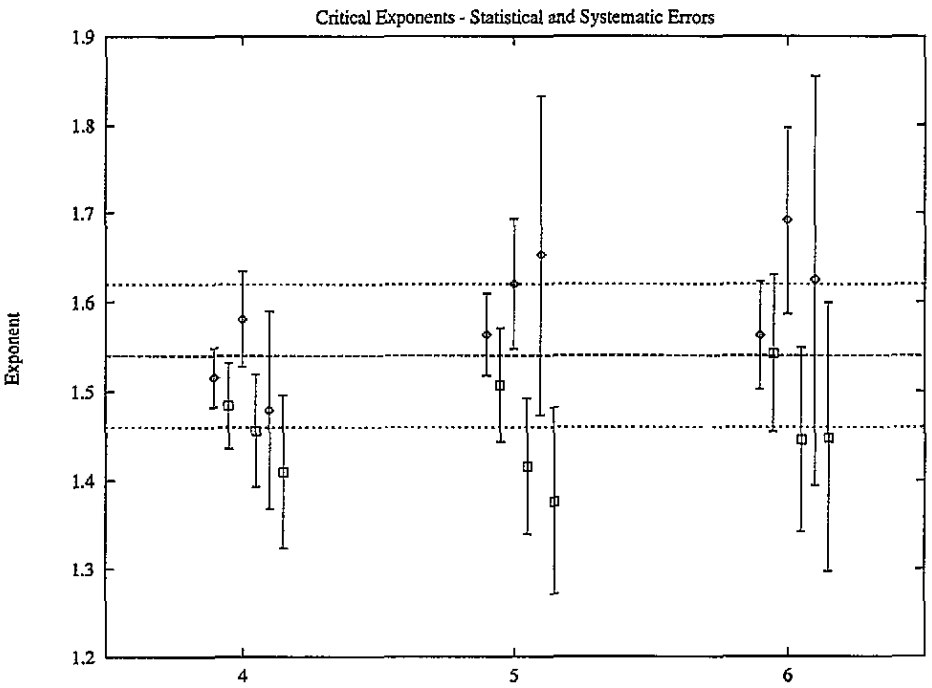

Figure 2. Fitted critical exponents for rectangular (diamonds) and Gaussian (squares) distributions. The abscissae represent the smallest system size taken into account (with small offsets for clarity). In each group the width of the fitted region is (from left to right) $(16.2 \leqslant W \leqslant 16.8) \rightarrow (16.3 \leqslant W \leqslant 16.7) \rightarrow (16.4 \leqslant W \leqslant 16.6)$ and $(21.0 \leqslant W \leqslant 21.5) \rightarrow (21.05 \leqslant W \leqslant 21.45) \rightarrow (21.1 \leqslant W \leqslant 21.4)$ for rectangular and Gaussian cases respectively. The dotted lines represent the range $s = \nu = 1.54 \pm 0.8$.

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