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LETTER TO THE EDITOR

Multifractal wavefunctions at the mobility edge

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Abstract. I describe the critical behaviour of wavefunctions at the Anderson metal-insulator transition in terms of fractal measures. At the mobility edge the wavefunctions have structure on all lengths and they scale with a continuous set of non-related exponents D_q. The results are compared with field-theoretic calculations by Wegner in $d = 2 + \varepsilon$.

Electronic wavefunctions in disordered quantum tight-binding Hamiltonians above and below the Anderson transition [1] are geometrically simple. The localised wavefunctions display a single dominant maximum followed by an exponential decay of their amplitude. They are characterised by a localisation length which is related to the support of the wavefunction. Although the amplitude of the extended states remains constant on average they exhibit many peaks which indicate the presence of fluctuations. These fluctuations increase as one approaches the mobility edge. Precisely at the mobility edge the localisation length and the characteristic length describing the range of fluctuations diverge. The wavefunction shares the properties of both the extended and the localised states. One might expect in this case that the wavefunctions exhibit self-similar fluctuations on all length scales larger than the lattice spacing, and have a fractal character.

Critical wavefunctions of simple one-dimensional systems with an incommensurate modulation superimposed on the crystalline structure and models for quasicrystals have been studied before [2-4]. It was found that at the mobility edge the wavefunction is a curious intermediate between extended and localised states and is characterised by a continuous set of non-simply related multifractal exponents D_q, $\in [-\infty, +\infty]$. This means that in contrast to the usual critical phenomena the $(q+1)$th moment is described by a scaling exponent which cannot be related to that of the qth moment by a simple gap exponent. The one-parameter scaling idea [5] which is the simplest way to understand the predictions of the localisation theory, in this sense, must be reconsidered as was done in other examples such as aggregate structures and strange objects [6]. However, within the field theoretic framework of the Anderson transition pioneered by Wegner† the infinite set of D_q is not incompatible with the one-parameter scaling theory.

The behaviour of the wavefunctions at the critical point in the presence of a disordered potential is certainly more complicated. Indications come from several sources [8, 9] for the absence of conventional diffusive forms of eigenfunction correlations at the mobility edge. A properly defined autocorrelation function [8] which

† The beta and zeta functions are computed to four-loop order in $d = 2 + \varepsilon$ dimensions. A negative correction for the conductivity exponent s is found, i.e. $s = 1 - 9\zeta(3)\varepsilon^3/4 + O(\varepsilon^4)$ which gives $\nu = s/\varepsilon$ violating the inequality $\nu \geqslant 2/d$.

describes the spatial fluctuations and the two-particle spectral function $S(q, \omega)$ [9] have revealed novel dependences. They are characterised by power law divergencies described by one number also regarded as a fractal dimension. From a different viewpoint non-Gaussian sample-to-sample fluctuations, characterised by many unrelated generalised Lyapunov exponent [10], are seen in one-dimensional (localised) systems when the disorder is weak.

This numerical evidence combined with the field-theoretic results by Wegner [7] and more recent considerations [10, 11] might be interpreted as due to the fact that the wavefunctions at the mobility edge of disordered systems are described in terms of fractal measures. We will use the multifractal approach to investigate wavefunctions at the Anderson transition in the presence of a three-dimensional random potential. The method is commonly used in the theory of dynamical systems at the onset of chaos and has been used to describe strange attractors [12, 13] and aggregates [6]. We utilise the fact that one has to deal with scaling of distributions rather than simple averages. The different moments for the distribution of the wavefunction amplitude are considered and shown to scale in different ways at the modility edge. We find that an infinite set of non-related scaling exponents D_q is required for their description. We also study the local wavefunction amplitude distributions and their deviations from the approximate log-normal law which is approximately valid for strong disorder.

We have examined the discrete three-dimensional Schrödinger equation with a random potential at each lattice site, described by the Hamiltonian:

$$H = \sum_{\boldsymbol{r}} \varepsilon_{\boldsymbol{r}} |\boldsymbol{r}\rangle\langle \boldsymbol{r}| + \sum_{(\boldsymbol{r},\boldsymbol{r}')} |\boldsymbol{r}\rangle\langle \boldsymbol{r}'| + \mathrm{HC} \qquad (1)$$

using an orthogonalised site basis representation. The sums extend over all lattice sites $\boldsymbol{r}$ and $(\boldsymbol{r}, \boldsymbol{r}')$ denotes all nearest-neighbour pairs of sites in a three-dimensional lattice. The site energies $\varepsilon_{\boldsymbol{r}}$ are independent random variables chosen from a flat probability distribution on the interval $[-W/2, W/2]$. The parameter W describes the strength disorder and the metal–insulator transition is believed to occur at $W_c \approx 16.5$ [14]. For $W > W_c$ all states are localised and the conductivity is zero, while for $W < W_c$ mobility edges appear in the band separating localised states near the edges from extended states near the band centre. In the following we discuss (1) mostly at the critical region ($W = W_c$) when the mobility edges coincide at $E_c = 0$. Our method relies on numerical computations in finite samples and a finite-size scaling analysis. The complete eigensolutions are numerically obtained for many random samples of cubic lattices with periodic boundary conditions in all directions. The localisation length diverges at $E = 0$ which causes an uncertainty in determining E_c in finite samples, given by $\Delta E_c \propto L^{-1/\nu}$. In order to consider only critical states we restricted our study to a narrow window of energies near the band centre. In fact, we examined the states in a band of width ΔE_c centred at $E = 0$ whose number is proportional to $L^{d-1/\nu}$. As the system size increases one notices that the number of the critical states remains considerable in proportion to the total number of states (L^d) although the width of the energy window ΔE rapidly diminishes. This depends on the value of the critical exponent ν (e.g. $\nu^{-1} = \varepsilon + O(\varepsilon^3)$, in $d = 2 + \varepsilon^7$). The inequality $\nu \geqslant 2/d$ should be obeyed for disordered systems as proved by Chayes *et al* [15] and discussed in [16].

We have obtained numerical evidence that the critical wavefunctions have a multifractal character. In particular we have computed D_q which obeys

$$\sum_i p_i(l) \left(\frac{p_i(l)}{(l/L)^{D_q}} \right)^{q-1} = 1. \qquad (2)$$

The given lattice is partitioned into boxes of size l^3, the measure p_i is the amplitude squared on the ith box and the limit $l \to 0$ is taken. In a more straightforward approach we choose to vary instead the lattice size. We evaluate the critical wavefunction amplitudes $|\psi_n(\boldsymbol{r})|$ for energies E_n in the critical energy window for cubic lattices of size $N = L^3$. We view them as functions defined on cubes of linear size one and as N increases the lattice spacing proceeds towards zero. To compute (2) we first normalise the wavefunctions on every lattice size. By plotting $\log(\langle\Sigma_r|\psi_n(\boldsymbol{r})|^{2q}\rangle)$ against $\log(L)$ in figure 1 in accord with (2) we find D_q. The size of the critical energy window is chosen so that the number of eigenvalues is much less than L. For a given L, at most five critical eigenvalues were considered. Proper statistical averages of the moments are taken for fixed system size (up to $N = 20^3$) and the statistical ensemble consists of more that 500 samples in each case. Our procedure is very accurate for small and positive values of q. It becomes not so accurate for larger q and even worse for negative q. In the latter case a larger statistical ensemble is required.

In figure 2 is shown D_q, which may be interpreted as a generalised dimension of the set on which the qth moment of the squared wavefunction resides. One sees that at the mobility edge the wavefunction is characterised by a continuous set of scaling exponents. It is possible to obtain an $f(\alpha)$ spectrum of scaling indices by Legendre transforming D_q. Then $f(\alpha)$ indicates how much of a set is composed of regions that scale with an exponent α. For a more detailed discussion of the definitions and interpretations of D_q and the statistical mechanics of multifractals the reader is referred to [2, 6]. Our results for the critical indices are compared with the expressions given by Wegner [7]. They were derived from nonlinear σ models in $d = 2 + \varepsilon$ dimensions by studying the ensemble averaged moments of the localised wavefunction component

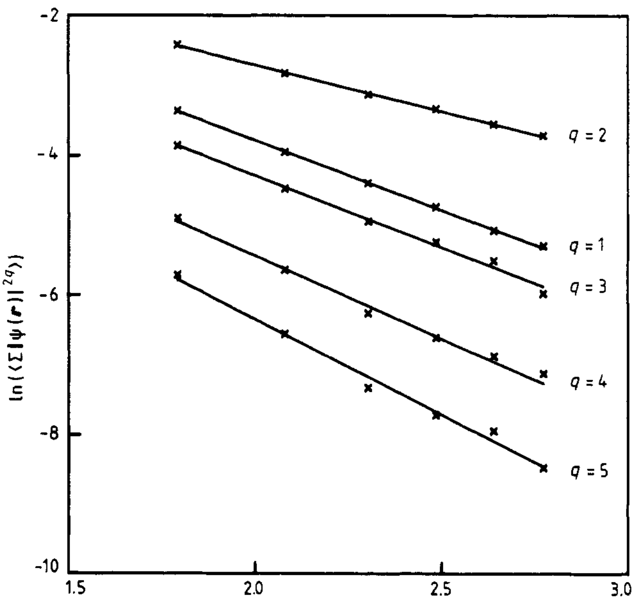

Figure 1. The log-log plots of the qth spatially averaged fluctuation moment $\langle\Sigma_r|\psi_n(\boldsymbol{r})|^{2q}\rangle$, for wavefunctions in the critical energy window ΔE, against the linear system size L. The slopes give $(q-1)D_q$ except when $q = 1$. Then $\langle\Sigma_r|\psi_n(\boldsymbol{r})|^2 \ln|\psi_n(\boldsymbol{r})|^2\rangle$ is plotted against $\ln(L)$ and the corresponding slope gives precisely the information dimension D_1.

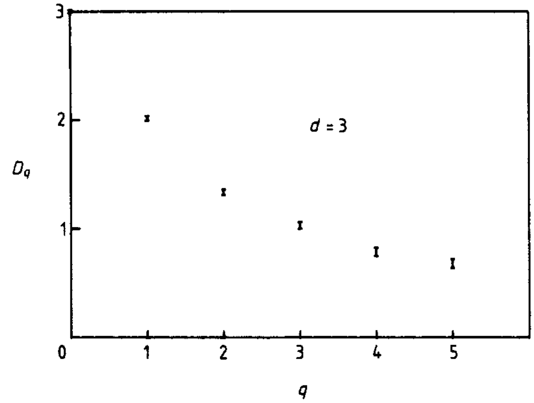

Figure 2. The main scaling exponents D_q are plotted against q for the wavefunction at the localisation threshold in three dimensions. The numerical results are indicated within their error bars arising from the least-squares fit. Note that $D_0=3$, $D_1=2.00\pm0.01$, $D_2=1.33\pm0.02$, $D_3=1.03\pm0.03$, $D_4=0.79\pm0.03$, $D_5=0.68\pm0.04$. For the correlation dimension the fractal exponent determined in [8] gives $D=1.7\pm0.3$, which should be compared with D_2. It should also be noted that the first order in ε gives the correct result for D_1 while the four-loop order yields large overestimates (especially for $q>1$).

$\psi_n(\boldsymbol{r})$ at energy E_n

$$P_q(E)=\left\langle\sum_n\left|\psi_n(\boldsymbol{r})\right|^{2q}\delta(E-E_n)\right\rangle\langle\rho(E)\rangle^{-1} \tag{3}$$

where $\langle\rho(E)\rangle$ is the averaged density of states. The anomalous scaling of P_q was related to the multifractal structure of the wavefunction [17]. Near the mobility edge E_c, $P_q(E)$ vanishes as $(E_c-E)^{\pi_q}$. We can easily identify, from π_q, the exponents D_q in powers of ε [7, 10]

$$\begin{aligned} D_q &= \nu^{-1}\pi_q/(q-1) \\ &= d-q\varepsilon+q(q^2-q+4)\zeta(3)\varepsilon^4/4+\mathrm{O}(\varepsilon^5) \end{aligned} \tag{4}$$

with $\zeta(3)\approx1.202$. In order to consider the case of $d=3$ we make the substitution $\varepsilon=1$. The result for the fractal dimension is now $D_0=d=3$ since the measure has compact support. The linear in ε terms imply a log-normal distribution law and the higher order nonlinear in q corrections a faster decay in the tails. For the information dimension $D_1=D_1$ and the correlation dimension D_2 the ε expansion up to fourth order gives overestimates. An improved result for D_q was given in [10] by means of a Borel resummation of the two-loop series. Our results must be seen in view of the more recent evaluations by Wegner [7] which allow a new Borel resummation which includes the four-loop terms. The D_q presented in this letter are in general less than both the Borel results. The corresponding $f(\alpha)$ spectrum of singularities can be also easily extracted [10] by Legendre transforming the D_qs.

Localised wavefunctions in the disordered Anderson model are self-similar only in a trivial way. In the inculating regime the distributions of many local quantities (wavefunction amplitude, current, local density of states, etc) become asymptotically log-normal [11, 18]. Consequently two-parameter scaling holds [18] for the first two cumulants which describe the distribution of $\log|\psi_n(\boldsymbol{r})|$ at site $\boldsymbol{r}$. This naturally leads to a kind of multifractal scaling described by a set of related in this case generalised

Lyapunov exponents $L(q) = \gamma q + (\mu/2)q^2$, $q \in [-\infty, +\infty]$†. The mean inverse localisation length γ is defined from the averaged logarithmic response of the wavefunction and μ is related to its statistical variance. For weak disorder, even in one dimension, deviations from the log-normal law have been found [10] which imply a set of unrelated $L(q)$. This can be seen as a precursor of the full critical fluctuation effects which are absent in one-dimension but studied in this letter. It was further argued [11] that the distributions in the metallic regime behave normally but have log-normal tails instead as a remnant of localisation. Then the variance of the conductance appears as a universal number. In order to check the suggested behaviour [11] we have studied the full distribution of the local wavefunction amplitudes. In figure 3 we present results for distribution function $n(p)$ where $n(p)\,\mathrm{d}p$ is the number of sites with squared wavefunction amplitude in the range $[p, p+\mathrm{d}p]$ for diperent values of the disorder. At the mobility edge the observed patterns indicate the presence of non-universal tails in the small amplitude (right-hand side of the figure) which cannot be fitted to a Gaussian law. The role of these tails becomes more pronounced as we enter the metallic regime (e.g. for $1 \ll L \ll \xi$, where 1 is the mean free path for elastic scattering). For the insulating regime the distributions broaden and approach an approximate

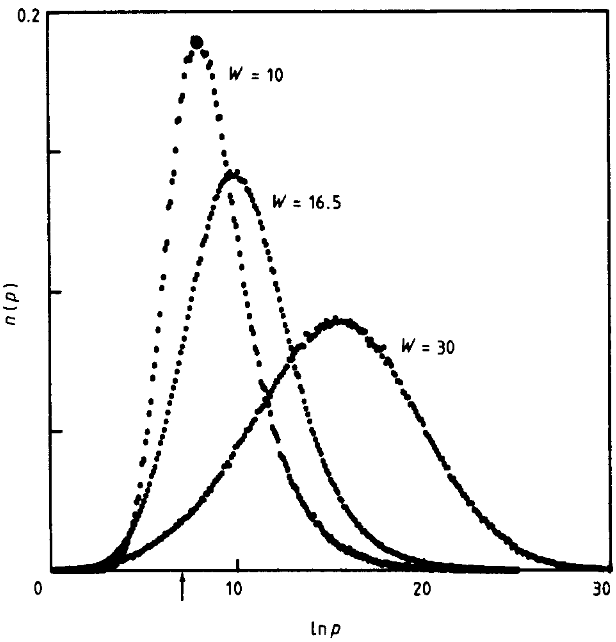

Figure 3. The normalised distribution of the wavefunction amplitudes above, below and at the mobility edge for many finite $(10 \times 10 \times 10)$ random samples. It can be seen that the role of the non-universal high $-\ln p$ tail increases as we move in the metallic regime $(L < \xi)$. The arrow indicates the position which corresponds to the amplitude of extended states for the given system size. In that case the distribution is centred closer to this value and has a longer tail while in the localised regime the distribution is centred at higher $-\ln p$ values, very broad and approximately Gaussian for the $\ln p$ (log-normal).

† The exponents $L(q)$ are defined in [11] and describe the sample to sample fluctuations for the moments of the wavefunction. Their Legendre transform leads to a parabolic $h(\alpha)$ spectrum, $\alpha \in [-\infty, +\infty]$. From the definitions $\gamma = \lim_{|r|\to\infty}(1/|r|)\cdot\langle \ln|\psi(r)|\rangle$, $\mu = \lim_{|r|\to\infty}(1/|r|)\cdot(\langle(\ln|\psi(r)|)^2\rangle - \langle \ln|\psi(r)|\rangle^2)$ the relative root mean square $\delta_{\gamma/\gamma}$ is proportional to $(\sqrt{\mu}/\gamma)(1/\sqrt{|r|})$, i.e. γ self-averages in the thermodynamic limit ($|r| \to \infty$).

log-normal form. No qualitative changes occur in the distributions of figure 3 by varying the system size N. In figure 4 we plot the critical distribution for two different values of N on the basis of an approximate scaling†. We have also checked our results by varying the number of critical states with no significant changes.

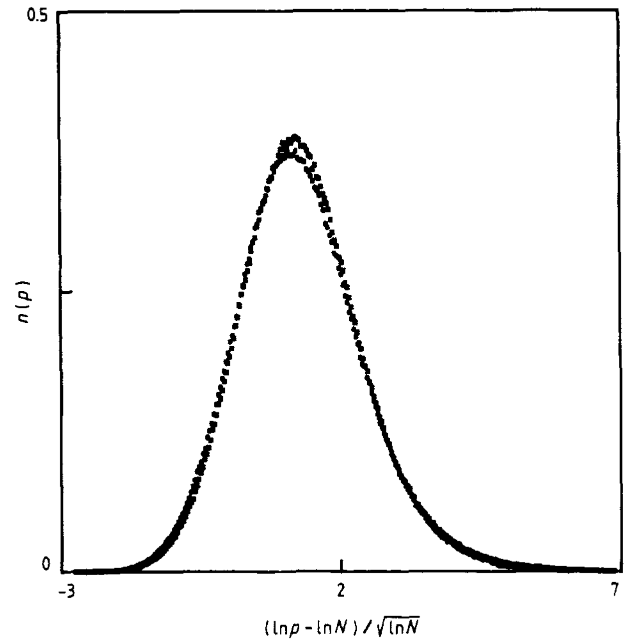

Figure 4. Approximate scaling of the normalised critical distributions for $L = 10, 14$ by assuming a log-normal distribution for $n(p)$.

In this letter we described the local eigenfunction probability distributions which arise in the study of the Anderson transition. The present work was initiated by Wegner's calculations [7] in $2+\varepsilon$ dimensions which showed for the first time an anomalous growth for the moments of the wavefunction. The simple hypothesis [5] that only one quantity, e.g. the length-dependent dimensionless conductance, characterises the critical behaviour at a given length scale L has been extremely useful. However, we have shown that the description of the critical distribution of the wavefunction amplitudes at the mobility edge requires an infinite set of unrelated exponents D_q, in accord with Wegner's predictions. These results may also be viewed as a step towards the necessity for scaling the whole distributions as it is implied by the high order gradient terms in the nonlinear σ-models discussed in [11]. We may now pose the question: do these non-Gaussian for the log exotic effects allow finding a properly defined quantity which self-averages in the thermodynamic limit? Such a quantity exists only in the strongly localised regime. From studies in one-dimensional disordered systems in the limit of infinite size a localisation length γ^{-1} can be defined [18]. This definition also extends to quasi-one-dimensional systems [19] but may be insufficient for the description of the mesoscopic regime (i.e. when L becomes comparable to γ^{-1}) due to fluctuations and it is still not clear whether it can uniquely describe the transition.

† By assuming an inherent multiplicative process we can approximate $n(p)$ by a log-normal distribution, i.e. $n(p) \propto \exp(-(\ln p - \langle \ln p \rangle)^2/2\Delta^2)$ with mean $\langle \ln p \rangle \propto \ln N$ and variance $\Delta^2 \propto \ln N$.

In summary, we have shown that critical wavefunctions are multifractals which confirms previous calculations by Wegner [7]. We have numerically demonstrated that the critical wavefunctions in three dimensions cover a space of lower dimensionality (e.g. bi-dimensional in the information sense since $D_1 \approx 2$). Moreover we show that the broad log-normal distributions valid in the insulating regime cross over to distributions with non-universal tails at the mobility edge. The existence of these tails is responsible for the rich scaling structure. This effect becomes even more pronounced in the region of mesoscopic fluctuations. Many questions in this area still remain, mostly concerning the identification of a proper scaling variable at the mobility edge. It is also natural to ask whether similar anomalous dimensions are likely to occur near the mobility edge in other disordered systems. Results on critical two-dimensional systems in the presence of spin-orbit scattering will appear in a forthcoming publication.

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