Distribution of level curvatures for the Anderson model at the localization-delocalization transition

C. M. Canali, Chaithali Basu, W. Stephan and V. E. Kravtsov

1 International Centre for Theoretical Physics, 34100 Trieste, Italy
2 Dipartimento di Fisica, Università "La Sapienza", Roma
3 Landau Institute for Theoretical Physics, Moscow, Russia

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We compute the distribution function of single-level curvatures, \( P(k) \), for a tight binding model with site disorder, on a cubic lattice. In metals \( P(k) \) is very close to the predictions of the random-matrix theory (RMT), in insulators \( P(k) \) has a logarithmically-normal form. At the Anderson localization-delocalization transition \( P(k) \) fits very well the proposed novel distribution \( P(k) \propto (1 + k^2)^{-\mu} \) with \( \mu \approx 1.58 \), which approaches the RMT result for large \( k \) and is non-analytical at small \( k \). We ascribe such a non-analyticity to the spatial multifractality of the critical wave functions.

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An important consequence of the one-parameter scaling theory of the Anderson transition is the existence of three universality classes for the energy level statistics of disordered systems. In the metallic regime they are described by the strongly correlated Wigner-Dyson (WD) distribution, while in the insulating regime they follow an uncorrelated Poissonian law. This difference has its fundamental origin in the underlying nature of the corresponding eigenstates, being extended and strongly overlapping in the first case but localized in the second.

The properties of the third universal statistics, describing the spectral correlations at the critical point, have been only recently the subject of intense investigation, both analytical and numerical. Using the results of numerical simulations, Shklovskii et al. suggested that the spacing distribution function \( P(s) \) has the WD form \( P(s) \sim s \) for small \( s \) and the Poissonic tail \( P(s) \sim e^{-s} \) for large \( s \). Further analytical investigations showed that the two-level correlation function \( R(s) \) in the critical region has a novel power-law asymptotic decay \( R(s) = -e^{s^{2-\gamma}} \) with a nontrivial exponent \( \gamma = 1 - 1/\nu d \). Here \( \nu \) is the critical exponent of the correlation/localization length \( \xi \), which depends on the dimensionality \( d \). Thus the two-level correlation function in the critical region resembles qualitatively the WD function which applies to the metallic phase. On the other hand, the level number variance \( \Sigma_2(N) = \langle \delta N \rangle^2 \) in an energy strip of width \( N \Delta \), \((\Delta \text{ is the mean level spacing})\), still contains a dominant Poissonic term, linear in \( N \), which is typical for insulators.

It can be shown that the Poissonic term in \( \Sigma_2(N) \) is only possible if a normalization sum rule on \( R(s) \) is violated in the thermodynamic limit (TL) \( L \to \infty \), \((L \text{ is the system size})\) which signals a qualitative change in the statistics of wave functions \( \Psi(\mathbf{r}) \). An analogous situation occurs in certain random matrix ensembles with broken unitary symmetry, that turn out to describe the critical statistics \( \Sigma_2(N) \) and \( P(s) \) very well.

Since the Poisson statistics describe localized states, it was put forward that the cause of the linear term in \( \Sigma_2(N) \) is the existence near the Anderson transition of pre-localized states, for which sharp peaks in \( |\Psi(\mathbf{r})|^2 \) contribute significantly to the normalization integral. In fact the existence of the pre-localized states - even in good metals - had been already conjectured in Ref. [10] for the interpretation of a slow current relaxation in disordered conductors [11]. Recently this conjecture has been confirmed in a more direct way using the supersymmetric sigma-model. Furthermore, the multifractal structure of wave functions \( \Psi(\mathbf{r}) \), expected at the Anderson transition, [12] can be represented as a superposition of peaks in \( |\Psi(\mathbf{r})|^2 \) corresponding to pre-localized states with a certain distribution of amplitudes and exponents for their power-law spatial decay.

A statistical property that may shed some light on the problem of pre-localized states is the distribution of curvatures of the single energy-levels. The level curvature measures the sensitivity of the energy spectrum to a change of the boundary conditions. For each single energy level \( \epsilon_n(\varphi) \), the curvature \( K_n \) is defined as

\[
K_n = \frac{1}{\Delta} \left. \frac{\partial^2 \epsilon_n(\varphi)}{\partial \varphi^2} \right|_{\varphi=0}
\]

The parameter \( \varphi \) enters in the definition of generalized boundary conditions in the \( z \) direction satisfied by the single-level wave functions, \( \Psi(x, y, z + L) = e^{i2\pi\varphi} \Psi(x, y, z) \). For a quasi-onedimensional sample, the parameter \( \varphi \) is equivalent to the phase generated by an Aharonov-Bohm flux \( \phi = \varphi \delta_0 \) that pierces a closed ring. The way in which an eigenvalue responds to a small twist of the boundary condition is obviously related to the nature of the corresponding wave function. Typically an eigenstate extended through the sample will feel any change in the boundary conditions and will have a large curvature, whereas a localized state, far from the edges, will be insensitive to the twist and its curvature will be close to zero. However we will see that this intuitive argument must be taken with caution.

In this paper we investigate numerically the curvature...
distribution of the 3d Anderson model. Similar calculations have been performed earlier by Zyczkowski et al., [5], who studied the distribution for all the three regimes of the disorder, and by Braun and Montambaux [6], who just looked at the metallic (diffusive) regime. The purpose of our work is to carry out an accurate scale analysis of the full curvature distribution right at the metal-insulator transition, which has not been done so far. We will first compute very accurately the curvature distribution for the metallic and insulating regime, and provide a physical interpretation of the numerical results in these two cases, based on the nature of their wave functions. We will then show that the critical distribution can be fitted extremely well by a functional expression similar to the RMT result that applies to metals, except for the presence of a new nontrivial exponent, which makes the distribution nonanalytical at $K = 0$. We will finally argue that such a behavior support the hypothesis of prelocalized states in the critical region.

We consider a tight binding model on a cubic lattice of volume $V = (L)^3$, where $L$ is the number of sites in any direction. The one-particle Hamiltonian is

$$H = \sum_i \epsilon_i c_i^\dagger c_i + t \sum_{\langle ij \rangle} (e^{i\theta_{ij}} c_i^\dagger c_j + e^{-i\theta_{ij}} c_j^\dagger c_i)$$

(2)

The site energies $\epsilon_i$ are randomly distributed with uniform probability between $-W/2$ and $+W/2$. The parameter $W$ controls the amount of disorder in the system. The phase shifts $\theta_{ij}$ in the hopping term are chosen in such a way that when a particle hops from $z$ to $z + L$ it picks up a total phase shift equal to $e^{2\pi i}$, coming from generalized boundary conditions in the $z$ direction. The Anderson transition is known to take place in such a system for $W_{c}/t \approx 16.5$ when $\varphi = 0$.

For each disorder configuration we can compute the zero-flux curvature of each single level. Since in the presence of the disorder the level velocity $v_n = \frac{\partial \epsilon_n}{\partial \varphi}|_{\varphi=0}$ is zero, the curvature can be calculated numerically in terms of the following finite difference

$$K_n(\varphi = 0) = 2 \frac{[\epsilon_n(\varphi) - \epsilon_n(0)]}{\varphi^2}$$

(3)

In order to get accurate approximations of the differentials with finite differences, particular care must be taken in the choice of the $\varphi$. We fitted the energy shift $[\epsilon_n(\pm\varphi) - \epsilon_n(0)]$ to a parabola $K_n\varphi^2$ and checked that the value found for $K_n$ is the same when we double $\varphi$. The optimal value of $\varphi$ ranges form $10^{-1}$ to $10^{-4}$ depending on disorder and system size, increasing with disorder. Our ensemble averages typically include several thousands disorder realizations, each one retaining half of the spectrum in an energy-window centered at $\epsilon = 0$.

We start with the metallic case where we know that classical RMT is applicable. Delande and Zakrewski [7] conjectured that the curvature distribution for complex systems described by RMT follows the expression

$$P_B(k) = C_B \frac{1}{(1 + k^2)^{1+\beta/2}}$$

(4)

with $\beta = 1, 2, 4$ for the orthogonal, unitary and symplectic ensemble respectively. The constant $C_B$ is fixed by normalization. The dimensionless curvature $k$ is given by $k = K/(K)$, where $(K)$ is the first moment of the distribution. It has been shown quite recently [8,9] that Eq. (4) is in fact exact for ensembles of large Gaussian matrices for all three symmetries.

![FIG. 1. Distribution of curvatures in the metallic regime $W/t = 5$, for different $L$, plotted with Eq. (4) for $\beta = 1$ as a comparison. In the inset $P(\log |k|) = |k|P(|k|)$ vs $\log |k|$.

In Fig. 1 we plot our results for the distribution of the rescaled curvatures $P(k)$ for several system sizes and $W = 5t < W_c$. It is seen that the RMT expression, Eq. (4) with $\beta = 1$, is remarkably accurate in the metallic regime for the whole range of $k$. It is universal, in the sense that, after rescaling $K$, $P(k)$ is scale invariant and disorder independent. Our results agree with Refs. [5,9] and settle the question of the $1/k^3$ dependence of $P(k)$ at large $k$, implying the divergence of the second moment. We emphasize that, for the 3d Anderson model in the metallic regime, $P(k)$ agrees very well with $P_B(k)$ of Eq. (4) also near $k = 0$, in contrast to the case of other quantum chaotic systems [3] that display nonuniversal features at small $k$, due to scarring of their wave functions. This point will be very useful in the interpretation of the critical $P(k)$ near $k = 0$.

An important property of $P_B(k)$ is the maximum at $k = 0$. Intuitively, on the basis of the above arguments, one would expect that in the metallic phase, where the eigenfunctions are extended, most of the curvatures should be large. In fact, as we show below, the maximum in $P(k)$ is related to the “ergodic” nature or lack of specific internal structure of the typical metallic eigenstate. Using second-order perturbation theory, the second derivative of the eigenvalues with respect to the parameter $\varphi$ due to a small perturbation is written as

$$\frac{\partial^2 \epsilon_n}{\partial \varphi^2} |_{\varphi=0} \propto \sum_{m \neq n} \left| \langle m | J_z | n \rangle \right|^2$$

(5)
where \( |m\rangle \) and \( \epsilon_m(0) \) are the eigenvectors and eigenvalues of \( H \) at zero flux, respectively. \( J_z \) is the current operator in the \( z \) direction. If we assume an ordered spectrum \( \epsilon_m - \epsilon_n = \Delta(m - n) \), then for each term of this sum relative to the eigenvalue \( \epsilon_{m,+} \), separated from \( \epsilon_n \) by an energy shift \( +\delta \epsilon_n = \epsilon_{m,+} - \epsilon_n \), there will be another term corresponding to \( \epsilon_{m,-} \) such that \( \epsilon_{m,-} - \epsilon_n = -\delta \epsilon_n \). Moreover the matrix elements of these two terms \( \langle m_+, | J_z | n \rangle \) and \( \langle m_-, | J_z | n \rangle \) must be equal if the corresponding unperturbed eigenstates are extended and structureless. Therefore we conclude that there is a cancellation in the sum of Eq. (5), causing the curvature to be zero. Of course the actual distribution is not simply \( \delta(k) \) because the spectrum is not fully ordered. Large values of the curvature \( |k| \sim 1/s \) are due to anomalously small spacings \( s = |\epsilon_m(0) - \epsilon_n(0)|/\Delta \ll 1 \) for \( m = n + 1 \) or \( m = n - 1 \), which occur with probability \( P(s) \sim s^\beta \). Thus for large \(|k|\) one obtains a power-law decay \( \mathcal{P}_\beta(k) \sim \int ds s^\beta \delta(k - 1/s) \sim |k|^{-(2 + \beta)} \) instead of zero, but the maximum of \( \mathcal{P}_\beta(k) \) remains at \( k = 0 \).

![FIG. 2. Distribution of curvatures \( \tilde{P}(\log |k|) \) vs \( \log |k| \) for the insulating regime \( W/t = 30 \) for different \( L \)'s. The dotted, dashed, etc. lines are gaussian fittings. The solid line is the RMT result for \( \beta = 1 \) in these coordinates.](image)

This simple argument allows us to interpret also the results for the other extreme case, namely the regime of strong disorder where localization is present. Indeed, from Eq. (8) we see that now the cancellation in the sum does not occur: two states \( |m_+\rangle \) and \( |m_-\rangle \), separated in energy from \( |n\rangle \) by \( \pm \delta \epsilon \) will have matrix elements that differ greatly from each other, since they are, in general, localized at different points. Therefore for a large but finite system size \( L \), the typical level curvature is small but non-zero. Thus \( \tilde{P}(k \to 0) = 0 \) for an insulator. We can guess the form of the distribution function in this case if we assume that the curvature \( k \) is related to the amplitude of the typical wave function at the edges, \( \log |k| \sim \log |\Psi| \), with \( |\Psi| \sim \exp(-L/L_o) \), where \( L_o \) is the radius of the localized wave function. If the distribution of \( 1/L_o \) is a Gaussian \( P(1/L_o) \propto e^{-(L_o/L_o)^2} \) centered around the inverse localization length \( \xi^{-1} \), we come immediately to the conclusion that the curvature distribution for an insulator must be log-normal, \( P(|k|) = C \exp[-A(\log |k|+B)^2] \), with \( A \sim 1/L^2 \) and \( B \sim L/\xi \). The numerical results of the simulations for the insulating regime are shown in Fig. 2, where we plot \( \tilde{P}(\log |k|) = |k| \mathcal{P}(|k|) \) vs. \( \log |k| \) for \( W = 30t > W_c \) and different system sizes. In these coordinates the distribution can be fitted rather well by gaussians, when the system size is large \( (L = 12) \), implying that \( \mathcal{P}(k) \) is log-normal, in agreement with what is found in Ref. [3]. The vanishing of \( \mathcal{P}(k) \) at \( k = 0 \) occurs very close to the origin and therefore is not easily resolved in a \( \mathcal{P}(k) \) vs \( k \) plot. However for smaller \( L \leq 8 \), \( \tilde{P}(\log |k|) \) clearly deviates from a gaussian distribution at small \( k \) and approaches the RMT function even for such a large disorder.

![FIG. 3. Distribution of curvatures \( P(|k|) \) vs \( |k| \) at the critical point \( (W_c/t = 16.5) \) for different \( L \)'s. In the inset \( \tilde{P}(\log |k|) \) vs \( \log |k| \) for \( L = 10, 12 \).](image)

We finally come to the central part of our work, the curvature distribution in the critical region. It was pointed out before that \( P(k) \) can be used to locate efficiently the Anderson transition point. Since according to the one-parameter scaling \( P(k) \) must be scale invariant at this point. However, there has been so far no detailed study of the full correlation function at the Anderson transition and its dependence on the sample size \( L \). The results for different system sizes at \( W_c/t = 16.5 \) are shown in Fig. 3 together with the RMT result \( \mathcal{P}_{\beta=1}(k) \) for comparison. One can see that the curvature distribution is close to Eq. (4) valid for metals. In particular, for large \( k \) the two curves are indistinguishable within our numerical precision. Thus even at the critical point the \( P(k) \) follows the \( |k|^{-3} \) rule, which corresponds to a spacing distribution \( P(s) \sim s \). On the other hand the curvature distribution \( P(k) \) at the critical point deviates slightly but significantly from \( \mathcal{P}_{\beta}(k) \) at small \( k \). Here the maximum at \( k = 0 \) moves above the metallic limit and apparently is size dependent. This seems to indicate that, in contrast to the prediction of one-parameter scaling, even at the transition point there is a finite length scale \( R \) such as for \( L << R \) the full distribution is indistinguishable from the RMT result, and for \( L >> R \) it saturates to a complete scale-invariant curve that differs...
from Eq. (4) at small $k < 1$. As shown in Fig. 4, where we plot the critical $P(k)$ for $L = 12$, this curve fits very well the distribution function

$$ F(k) = \frac{A}{[1 + k^\alpha]^{1/\beta}}, \quad (6) $$

where $A = \mu \Gamma(3/\mu)[\Gamma(1/\mu)\Gamma(2/\mu)]^{-1} > 1$ is determined by normalization. Once normalized, the distribution in Eq. (6) obeys the condition $\langle k \rangle = 1$ for all $\mu = 2 - \alpha$. Thus the full distribution $F(k)$ is determined uniquely by its value at $k = 0$, and with the known $P(k = 0)$ the fit of the whole curve is parameter free. This procedure yields $\alpha = 0.42 \pm 0.01$. For further evidence we have plotted, in the inset of Fig. 4, the derivative of $P(k)$ with respect to $k$, together with the derivative of $F(k)$. Equation (6) implies that $dP/dk \sim |k|^{1-\alpha}$ for small $|k|$.

However the exponents are different. This situation is analogous to what we find for the curvature distribution.

In conclusion, on the basis of numerical diagonalization of the tight-binding Anderson model we have suggested a novel level curvature distribution function $P(k)$ at the Anderson transition, which exhibits a non-analytical behavior for small $k$ and approaches the RMT result for large $k$. We relate this non-analyticity to the spatial multifractality of critical wave functions.

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