On the critical level curvature distribution

S N Evangelou

Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, D-01187 Dresden, Germany
E-mail: sevagel@cc.uoi.gr

New Journal of Physics 6 (2004) 200
Received 26 July 2004
Published 14 December 2004
Online at http://www.njp.org/
doi:10.1088/1367-2630/6/1/200

Abstract. The parametric motion of energy levels for non-interacting electrons at the Anderson localization critical point is studied by computing the energy level curvatures for a quasi-periodic ring with twisted boundary conditions. We find a critical distribution which has the universal random matrix theory form \( \bar{P}(K) \sim |K|^{-3} \) for large level curvatures \(|K|\) corresponding to quantum diffusion, although overall it is close to approximate log-normal statistics corresponding to localization. The obtained hybrid distribution resembles the critical distribution of the disordered Anderson model and makes a connection to recent experimental data.

The Landauer–Buttiker (LB) scattering approach [1] is nowadays almost exclusively used for computing the conductance \( g \) for many materials in nanoscience. This very appealing formalism, although not extremely rigorous, is particularly suitable for small systems, something which became obvious following the discovery of conductance steps in ballistic point contacts more than a decade ago [2]. In such a scattering approach one gets the non-equilibrium transport for any sufficiently realistic system if it is connected to two ideal leads. The conductance is simply the transmission probability through the sample scatterer which can be evaluated (e.g. via Green’s function techniques) at any energy monitored by gates. Although \( g \) is, strictly speaking, a property of open systems, it can be also probed for a closed system from the eigensolutions of the stationary Schrödinger’s equation. This is done via Thouless’s intuitive definition of conductance which involves a measure of the sensitivity of eigenvalues to twisted boundary conditions (BC) [3]. In the latter approach, the conductance is related to the so-called level-curvatures and is usually expressed by the ratio of the geometric mean of the absolute curvature at zero twist over the local mean level-spacing. The scattering approach for open systems and the eigenvalue shift approach for closed systems are two established definitions of conductance, which compare rather favourably with each other for electrons in disordered systems (see [4]).

1 Permanent address: Physics Department, University of Ioannina, Ioannina 45110, Greece.
The search for universal features in the statistics of stationary electronic levels and their motion as a function of some parameter is a large area of study with obvious consequences for quantum transport. For example, avoided level-crossings which characterize the spectrum of a chaotic system under a perturbation (e.g. application of external fields) evolve with universal random matrix theory (RMT) laws [5]. For avoided level-crossings, the very small level-spacings correspond to large absolute level curvatures so that the tail of the level-curvature distribution \( \bar{P}(K) \) is intimately related to the small part of the level-spacing distribution. Therefore, in the absence of symmetry-breaking mechanisms the linear part of the Wigner distribution for small level spacings implies large level curvatures having a decreasing asymptotic behaviour \( \bar{P}(K) \sim 1/|K|^{2+\beta} \), with \( \beta = 1 \) [6]–[8]. This has been confirmed experimentally for level-curvature distributions of acoustic resonance spectra from quartz blocks [9].

We focus on the critical distribution of level curvatures by obtaining the response of a quasi-periodic complex system’s energy spectrum to different BC [10], within Thouless’s approach to quantum transport. For this purpose a phase factor \( \exp(i\phi) \) is imposed on the hopping probability connecting the first and the last sites of a ring and the resulting parametric dependence of the energy levels to changes in \( \phi \) is obtained. This allows us to explore the nature of the corresponding eigenstates from extended to localized, since extended states simply feel any changes in BC having large curvatures while localized states are insensitive to BC having curvatures which approach zero. Nevertheless, the studied quasi-periodic Harper model is interesting only at the metal–insulator transition point, since it satisfies duality between the extended (quasi-ballistic) and the localized (non-random) regimes [11]. One might wonder what the level-curvature distribution might be at the metal–insulator transition for such a quasi-periodic system which has Cantor set-like fractal electronic structure and a semi-Poisson hybrid distribution of level-spacings [10].

Deviations around the maximum peak between level curvatures obtained in experiment [9] and RMT were attributed to the presence of hidden symmetries [12, 13]. In our study, the critical distribution of level curvatures is obtained in a convenient one-dimensional setting which allows to discuss both the three-dimensional disordered system and questions of universality in general. Our finding is a scale-invariant \( \bar{P}(K) \) which resembles the distribution obtained for the normalized level-curvatures in 3D critical disordered systems [14, 15], having both a diffusive tail and overall localized behaviour [4]. For a finite system, the transition from extended to localized states involves broadening of the distribution \( \bar{P}(K) \) and lowering its maximum peak as the curvatures move to lower values by increasing disorder. Our study, on one hand, is in agreement with the semi-Poisson level-spacing distribution for the same system [10]. On the other hand, the coexistence of the localized almost log-normal broad form with the diffusive tail might be the reason for the lowering of the maximum peak observed in the experiment [9].

We have studied the distribution function of level curvatures, defined as

\[
K_\alpha = \left. \frac{d^2 \epsilon_\alpha}{d\phi^2} \right|_{\phi=0},
\]

\(2\) Fyodorov and Sommers [8] showed analytically the linear relation between the mean conductance and the mean absolute value of the curvature in the diffusive regime.

3 The duality is a well-known property of the Harper model since it was introduced by Aubry and Andre [11].

4 Canali et al [14] generalized RMT to the critical regime in the absence of symmetry breaking fields (\( \beta = 1 \)) where \( \bar{P}(K) \sim (1 + K^{\mu})^{-3/\mu} \), \( \mu = 2 \) for RMT and \( \mu \approx 1.6 \) for the 3D critical disordered system.
for the energy levels $\varepsilon_\alpha$ of a quasi-periodic ring in the presence of phase $\exp(i\phi)$, obtained from the critical tight-binding model Hamiltonian [10]

$$H = \sum_n V_n c_n^\dagger c_n - \sum_{\langle nm \rangle} (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) - (\exp(i\phi)c_1^\dagger c_L + \exp(-i\phi)c_L^\dagger c_1).$$

The sum is taken over all sites $n = 1, \ldots, L$, $c_n$ ($c_n^\dagger$) is the annihilation (creation) operator on site $n$, $\langle nm \rangle$ denote nearest neighbours of the open finite chain and the potential $V_n = 2\cos(2\pi\sigma n)$ is chosen at criticality with $\sigma$ the golden mean irrational. The third term in equation (2) which includes the phase $\exp(i\phi)$ connects the two ends of the chain forming a ring ($\phi = 0$ corresponds to periodic BC). The eigenvalues $\varepsilon_\alpha$ have corresponding eigenvectors $|\alpha\rangle = \sum_{x=1,L} \psi_\alpha(x)|x\rangle$ with amplitudes $\psi_\alpha(x) = \langle x|\alpha\rangle$ for a finite chain of size $L = F_i$ with $\sigma = F_{i-1}/F_i$, the ratio of two successive Fibonacci numbers $F_{i-1}$ and $F_i$. The imposed general boundary condition to the wave function $\psi(x + L) = e^{i\phi}\psi(x)$ is equivalent to piercing the ring by the Aharonov–Bohm magnetic flux $\Phi$ via $\phi = 2\pi\Phi/\Phi_0$, with $\Phi_0 = \hbar/e$ the flux quantum.

The curvatures $K_\alpha$ are properties of the energy levels in the limit of zero flux so that perturbation theory can be applied [4]. Using the small-$\phi$ expansion $\exp(\pm i\phi) = 1 \pm i\phi - \phi^2/2 + \cdots$ the relevant terms up to second order are: the unit term for periodic BC, the first term $\langle \alpha|V|\alpha\rangle = -\phi^2 \langle \alpha|1\rangle \langle 1|\alpha\rangle$ and the second term $\langle \alpha|V|\beta\rangle = i\phi(\langle \alpha|1\rangle \langle 1|\beta\rangle - \langle \alpha|L\rangle \langle 1|\beta\rangle)$. The level curvature for the eigenvalues $\varepsilon_\alpha$ becomes

$$K_\alpha = 2\psi_\alpha(L)\psi_\alpha(1) + 2 \sum_{\beta \neq \alpha} \frac{(\psi_\beta(L)\psi_\alpha(1) - \psi_\beta(1)\psi_\alpha(L))^2}{\varepsilon_\beta - \varepsilon_\alpha},$$

$\alpha = 1, 2, \ldots, L$, in terms of the eigenvalues $\varepsilon_\alpha$ and eigenvector amplitudes $\psi_\alpha$ of the unperturbed ring ($\phi = 0$). The level curvatures $K_\alpha$ which give quantum transport properties are more difficult to obtain than level spacings since one also needs the eigenvectors of the Hamiltonian. The formula of equation (3) is exact as long as $\varepsilon_\beta \neq \varepsilon_\alpha$, since higher orders vanish at $\phi = 0$. Moreover, it is also both conceptually and numerically meaningful since the wave function amplitudes at the two ends of the chain $\psi_\alpha(1)$, $\psi_\alpha(L)$ are expected to play a role for transport, while linear algebra relates the first term in equation (3) to the error in the eigenvalue determination from truncating an infinite tridiagonal matrix [16].

To use (3) we only need the eigensolutions of the periodic BC problem, that is the solutions of the Hamiltonian of (2) with $\phi = 0$. The studied problem simplifies further by the presence of the parity symmetric potential $\cos(x) = \cos(-x)$ which allows us to find symmetric and antisymmetric solutions separately, dealing with two tridiagonal matrices instead of the full matrix in the presence of BC [17]. This dramatic reduction in storage requirements is achieved if the one-electron basis is rearranged to run within $-s$, $-s + 1, \ldots, s - 1, s$ also by distinguishing between even and odd size $L$. For example, for odd $L = 2s + 1$ the problem is reduced to a tridiagonal matrix of size $s + 1$ for the symmetric states which has the potential values $V_0$, $V_1$, $\ldots$, $V_{s-1}$, $V_s + 1$, for the diagonal matrix elements, unity elements lying next to the diagonal, except in the first (second) row second(first) column where the value is $\sqrt{2}$, and each eigenvector amplitude $(\chi(0), \chi(1), \ldots, \chi(s))$ is related to the original via the symmetric rule $\psi(0) = \chi(0)$, $\psi(-s) = \psi(s) = \chi(s)/\sqrt{2}$. The second tridiagonal matrix for the antisymmetric states is of size $s$ with matrix elements $V_1$, $\ldots$, $V_{s-1}$, $V_s$ on the diagonal and unity next to diagonal with corresponding eigenvector amplitudes $(\chi(1), \ldots, \chi(s))$ related to the original via
The computed critical distribution for the logarithm of level curvatures $P(\ln |K|)$ and various sizes $L$ is shown to be almost scale-invariant. The histograms for each size are obtained from the diagonalization of equation (2) employing the formula for the level curvatures of equations (4) and (5). The continuous line is a Gaussian fit of the data.

Antisymmetry $\psi(0) = 0$, $\psi(-s) = -\psi(s) = -\chi(s)/\sqrt{2}$. By replacing $\psi$ with $\chi$, equation (3) splits into a symmetric part labelled by $\alpha = 1, 2, \ldots, s+1$

$$K_\alpha = (\chi_\alpha(s))^2 + 2 \sum_{\beta=s+1}^{2s+1} \frac{(\chi_\beta(s)\chi_\alpha(s))^2}{\epsilon_\beta - \epsilon_\alpha},$$

and an antisymmetric part for $\alpha = s+2, s+3, \ldots, 2s+1$

$$K_\alpha = -(\chi_\alpha(s))^2 + 2 \sum_{\beta=1}^{s+1} \frac{(\chi_\beta(s)\chi_\alpha(s))^2}{\epsilon_\beta - \epsilon_\alpha}.$$

In equations (4) and (5) the $s$th last element of each eigenvector can be computed iteratively with no need to increase the storage requirements beyond that of a tridiagonal matrix. Moreover, the corresponding sums over $\beta$ run over opposite kinds of symmetric and antisymmetric states, respectively, being precisely zero for species of the same symmetry. A similar formula for even $L$ is easily obtained.

A ballistic ring has $K_\alpha = (8\pi^2/L^2) \cos(2\pi\alpha/L)$ which give square-root singularities for $\tilde{P}(K)$. These disappear for the critical ring studied, where the curvature distribution $\tilde{P}(K)$ is much more complex; so it turns out more convenient to consider the logarithmic distribution $P(\ln |K|) = |K| \tilde{P}(K)$, instead. The computed critical distribution presented in figure 1 for various sizes $L$ is shown to be scale-invariant, overall approximated by a logarithmic normal form. In figure 2 we present a log–log plot of $P(\ln |K|)$ which demonstrates the diffusive universal tail $\tilde{P}(K) \sim |K|^{-3}$ for large-$|K|$. For small-$|K|$, we approximately find $P(\ln |K|) \sim |K|^2$. 

Figure 1. The computed critical distribution for the logarithm of level curvatures $P(\ln |K|)$ and various sizes $L$ is shown to be almost scale-invariant. The histograms for each size are obtained from the diagonalization of equation (2) employing the formula for the level curvatures of equations (4) and (5). The continuous line is a Gaussian fit of the data.
Figure 2. Log–log plot of the critical level curvature distribution for various sizes $L$ as in figure 1. Apart from the less accurate points in the left corner we see a slower behaviour for small-$|K|$ by plotting the equivalent of $\bar{P}(K) \sim |K|$, while for large-$|K|$ the diffusive asymptotic tail becomes $\bar{P}(K) \sim |K|^{-3}$. Note that the large-$|K|$ form arises from the law $P(\ln |K|) \sim |K|^{-2}$ shown in the right-hand side of this figure.

Unfortunately, rapid loss of accuracy for the too small curvatures does not permit to extract reliable exponents from fits of $\bar{P}(K)$ to the form suggested in [14]. However, the overall behaviour of the critical distribution shown in figure 3 looks similar to the obtained critical distribution for the 3D Anderson model [14, 15].

The level curvatures in disordered or chaotic systems exploit a sort of ‘dynamics’ of the quantum stationary spectra as a function of flux which might be thought of as ‘time’. The conductance is then obtained from the level curvatures in terms of eigenvalues and eigenvectors of the tight-binding system with periodic BC. In our case, the computational effort is minimized because the parity symmetry of the potential reduces our problem to two simple tridiagonal matrices for the determination of symmetric and antisymmetric states. The required last element of each eigenvector can also be computed efficiently with no increase of storage so that the size $L$ of the matrices can easily exceed $10^5$. We remind the reader that for diffusive disordered systems the computed averaged LB conductance $\langle g \rangle$ was shown [4, 8] to be related to the mean absolute curvature via $\langle g \rangle = \pi \langle |K| \rangle / \Delta$, where $\Delta$ is the local mean-level spacing. For localized disordered systems, the curvatures diminish and both distributions approach a log-normal form with $\langle \ln g \rangle = \pi \langle \ln(|K|) \rangle$. Our study of the unnormalized level curvatures for the quasi-periodic system enabled us to obtain the critical $\bar{P}(K)$ for very large system sizes. The curvatures become very small for such large systems which set limits to the accuracy of the distribution. Our results are similar to those obtained for 3D critical disordered systems. Moreover, such computations might suggest that the lowering of the maximum peak observed in experiment [9] could be thought off as due to an approach towards the critical region. Although the critical distribution shown in figure 3 still displays a diffusive tail of the log-normal form, it is much broader having less height than the pure diffusive RMT case.
Figure 3. Another demonstration of the critical level curvature distribution for two sizes \( L = 17711 \) and 28 657 which resembles the distribution for a 3D disordered system [14, 15]. The distributions for the quasi-periodic and the disordered system are rather similar although in the disordered case the curvatures are normalized divided by the local mean level-spacing \( \Delta \).

The obtained results for non-interacting fermions in a quasi-periodic ring complement and confirm previous studies at the metal–insulator transition of disordered systems [18, 19].\(^5\)\(^6\) The distribution \( \tilde{P}(K) \) for the ensemble of critical states at the transition (there is no ensemble over disorder) is scale-invariant like the corresponding level-spacing distribution which is known to depend sensitively on BC [10]. After averaging over BC, the critical distribution of the level-spacings can be described by the semi-Poisson curve which combines both extended and localized behaviour. Similarly, the obtained \( \tilde{P}(K) \) exhibits a hybrid character like what is obtained for critical 3D disordered systems. In closing, it is remarkable that such a simple one-dimensional non-random model can capture most features displayed at the Anderson metal–insulator transition of realistic disordered systems.

References

[1] Landauer R 1970 Phil. Mag. 21 863
Buttiker M, Imry Y, Landauer R and Pinhas S 1985 Phys. Rev. 31 6207
Buttiker M 1988 Phys. Rev. B 38 9375
[2] Imry Y 1997 Introduction to Mesoscopic Physics (Oxford: Oxford University Press)
[3] Edwards J T and Thouless D J 1972 J. Phys. C: Solid State Phys. 5 807
Thouless D J 1974 Phys. Rep. 13 93
[4] Braun D, Hofstetter E, Montambaux G and MacKinnon A 1997 Phys. Rev. B 55 7557
[5] Guhr, T Müller-Groeling A and Weidenmüller H 1998 Phys. Rep. 229 189

\(^5\) Zyczkowski et al [18] were the first to address numerically the statistics of level curvatures at criticality.

\(^6\) Titov et al [19] provided an analytical derivation of the log-normal distribution in the localized regime of a 1D disordered system.
[6] Zakrzewski J and Delande D 1993 Phys Rev. E 47 1650
[7] von Oppen F 1995 Phys Rev. E 51 2647
[8] Fyodorov Y V and Sommers H-J 1995 Phys Rev. E 51 R2719
[9] Bertelsen P, Ellegaard C, Guhr T, Oxborrow M and Schaad K 1999 Phys. Rev. Lett. 83 2171
[10] Evangelou S N and Pichard J-L 2000 Phys. Rev. Lett. 84 1643
[11] Aubry S and Andre G 1980 Ann. Israel Phys. Soc. 3 133
[12] Ergün G and Fyodorov Y V 2003 Phys. Rev. E 68 046124
[13] Hussein M S, Malta C P, Pato M P and Tufaile A P B 2002 Phys. Rev. E 65 057203
[14] Canali C M, Basu C, Stephan W and Kravtsov V E 1996 Phys. Rev. B 54 3
[15] Zharekeshev I Kh and Kramer B 1999 Physica A 266 450
[16] Fox A 1964 Introduction to Numerical Linear Algebra (Oxford: Clarendon)
[17] Thouless D J 1983 Phys. Rev. B 28 4272
[18] Zyczkowski K, Molinari L and Israilev F M 1994 J. Phys. I 4 1469
[19] Titov M, Braun D and Fyodorov Y V 1997 J. Phys. A: Math. Gen. 30 L339