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Critical level-spacing distribution for general boundary conditions

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Abstract

It is believed that the semi-Poisson function $P(S) = 4S\exp(-2S)$ describes the normalized distribution of the nearest level-spacings S for critical energy levels at the Anderson metal–insulator transition from quantum chaos to integrability, after an average over four obvious boundary conditions (BC) is taken (Braun *et al* 1998 *Phys. Rev. Lett.* **81** 1062). In order to check whether the semi-Poisson is the correct universal distribution at criticality we numerically compute it by integrating over all possible boundary conditions. We find that although $P(S)$ describes very well the main part of the obtained critical distribution small differences exist particularly in the large-S tail. The simpler crossover between the integrable ballistic and localized limits is shown to be universally characterized by a Gaussian-like $P(S)$ distribution instead.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Chaos in quantum systems is known to appear in the level statistics of the spectral fluctuations for stationary energy levels obtained from Hamiltonians defined in appropriate Hilbert spaces [2]. In the quantum chaotic regime the loss of most symmetries is manifested via the appearance of level-repulsion between nearest-neighbour energy levels which implies a highly correlated spectrum [3]. Integrable systems display, instead, uncorrelated spectra with random levels which allow spectral degeneracies as unambiguous signatures of high symmetry. The solution of Schrödinger equation for billiards having zero potential inside and infinite outside a bounded domain manifests integrable or chaotic quantum behaviour depending on the shape of the domain boundary. This quantum crossover corresponds to the classical transition from

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integrability to chaos in billiards [4]. Wave chaotic behaviour has recently been observed experimentally for optical billiards [5].

Disorder in quantum systems, e.g. a random potential for electrons in a lattice, is known to cause an Anderson metal–insulator transition from extended to localized wavefunctions [6]. This is a true quantum phase transition from chaos to integrability with the extended wavefunctions of weakly disordered metals corresponding to quantum chaos and the localized wavefunctions of strongly disordered insulators to integrability. By adding weak disorder to a perfect system a ballistic to chaotic quantum crossover also occurs, similar to quantum billiards. Only for stronger disorder one can obtain the metal–insulator transition from diffusive extended to integrable localized states. One dimension is exceptional in this respect since no intermediate quantum chaotic behaviour can be seen with a crosover straight from ballistic to localized behaviour.

The critical region at the metal–insulator transition between diffusion and localization has also been explored for level statistics in terms of the nearest neighbour level-spacing distribution $P(S)$ [7, 8]. The disordered problem has certain advantages, such as the existence of many energy levels at the transition and a statistical ensemble over disorder which complements the usual energy ensemble. The corresponding critical $P(S)$ turns out to be a scale-invariant hybrid of chaotic Wigner-like linear small S and an integrable Poisson-like exponential for large S. The main surprise, however, in these studies was the generic sensitivity of the obtained critical level statistics to boundary conditions (BC) [1]. This is now well understood since it simply reflects the nature of critical wavefunctions, which are in between extended and localized, described by scale-invariant fractal distributions. Their filamented structure, closer to one-dimensional, brings little overlap at the boundaries so it is accompanied by extreme sensitivity in boundary conditions. This is the reason for the corresponding generic dependence of critical level statistics to BC. In this paper we generalize the argument of [1] by including many possible BC via the introduction of all Aharonov–Bohm fluxes and perform an integration over them.

Our aim is to compare the obtained level-spacing distribution at the metal–insulator transition with the simple semi-Poisson form $P(S) = 4S\exp(-2S)$ [9][2]. Although a similar hybrid distribution describes, at least partially, the level-spacings in various metal–insulator transitions in disordered systems including a system with spin–orbit coupling [10], the precise semi-Poisson form often fails to describe criticality and is not widely accepted as the universal critical distribution. We ask the question of whether a semi-Poisson might be the appropriate critical distribution to describe averages over all possible BC. For this purpose we set up and diagonalize Hamiltonians with disorder defined for cubic lattice clusters in three dimensions (3D) with many possible BC and integrate over all of them. We shall also consider the simpler quantum crossover from the ballistic to localized phase in 1D disordered systems. In this case we obtain a universal Gaussian-like distribution at the crossover where the scaling parameter of the localization length ξ over size L is fixed to unity.

Quantum chaotic systems are well described by random matrix ensembles via random matrix theory (RMT) [2–4]. The level-spacing distribution for small S involves the level-repulsion condition $P(S) \propto S^{\beta}$, where the so-called universality class index $\beta = 1, 2, 4$ is determined from the remaining fundamental symmetries of quantum chaotic systems. In the presence of time-reversal invariance one obtains the orthogonal universality class with $\beta = 1$. An applied magnetic field which breaks the time-reversal invariance leads to a unitary universality class with $\beta = 2$ while spin–orbit coupling with time reversal to a symplectic

[2] In [9] Bogomolny *et al* proposed the semi-Poisson $P(S)$ for certain pseudointegrable billiards and pointed out its similarity to the Anderson model at the transition point.

universality class with $\beta = 4$. The critical $P(S)$ is also not independent of the remaining symmetries of a chaotic system either so that appropriate expressions for the corresponding critical $P(S)$ in different universality classes can be found [10]. In the rest of the paper we shall rely on numerical tools in order to explore level statistics at criticality. Our aim is to answer the previously posed question of whether the semi-Poisson distribution appears after averaging over all possible BC.

2. Calculations

We obtain spectra and their fluctuations in cubic 3D lattices with disorder. We have used standard diagonalization algorithms to compute eigenvalues for complex Hermitian sparse random matrices of size L^3 which include flux. Many possible BC are considered by adding fluxes in all directions. More details of the numerical BC integration method can be found in [11] where it was used for Hubbard models to describe interacting electrons. In the quantum coherent chaotic metallic regime the results for the eigenvalue level-spacing distribution $P(S)$ are described by the Wigner surmise [3]. In the insulating integrable regime quantum coherence is lost since the localized states do not communicate with each other located in random positions, so that one obtains the random Poisson distribution. At criticality after integration over all BC we obtain a critical $P(S)$ which is closely described by semi-Poisson. However, we also find rather small deviations, particularly in the large-S tail of the distribution.

We consider a tight-binding model with site randomness defined on a $L \times L \times L$ finite lattice described by the Hamiltonian with potential energy and kinetic energy terms

$$H = \sum_n V_n c_n^\dagger c_m - \sum_{\langle nm \rangle} \left(c_n^\dagger c_m + c_m^\dagger c_n \right). \tag{1}$$

The sum is taken over all lattice sites n and all bonds $\langle nm \rangle$ where n, m denote nearest neighbour lattice sites, c_n is an annihilation operator of an electron on site n, $c_n^\dagger$ is a corresponding creation operator of an electron and V_n is the random site potential, a real independent random variable satisfying a box distribution $P(V_n) = \frac{1}{W}$, for $-\frac{W}{2} \leqslant V_n \leqslant \frac{W}{2}$ of zero mean and width W which measures the strength of disorder. We impose the generalized periodic boundary conditions on the wavefunctions $\psi(x, y, z)$ in all directions

$$\begin{aligned} \psi(x + L, y, z) &= \mathrm{e}^{\mathrm{i}\alpha_x} \psi(x, y, z) \\ \psi(x, y + L, z) &= \mathrm{e}^{\mathrm{i}\alpha_y} \psi(x, y, z) \\ \psi(x, y, z + L) &= \mathrm{e}^{\mathrm{i}\alpha_z} \psi(x, y, z), \end{aligned} \tag{2}$$

which is equivalent to applying Aharonov–Bohm magnetic flux $\vec{\alpha}$ with components $(\alpha_x, \alpha_y, \alpha_z)$ varying in $[0, 2\pi)$.

For the zero disorder $W = 0$ ballistic limit equation (1) has eigenvalues $\epsilon_{j_x, j_y, j_z}(k_x, k_y, k_z) = -2(\cos k_x + \cos k_y + \cos k_z)$ and plane wave eigenstates $\psi_{j_x, j_y, j_z}(x, y, z) = L^{-3/2} \exp(-\mathrm{i}(k_x x + k_y y + k_z z))$, with the positions of the $\vec{k}$-vectors determined by the BC of equation (2) via

$$\begin{aligned} k_x &= \frac{\alpha_x + 2\pi j_x}{L}, \qquad j_x = 0, \ldots, L - 1 \\ k_y &= \frac{\alpha_y + 2\pi j_y}{L}, \qquad j_y = 0, \ldots, L - 1 \\ k_z &= \frac{\alpha_z + 2\pi j_z}{L}, \qquad j_z = 0, \ldots, L - 1. \end{aligned} \tag{3}$$

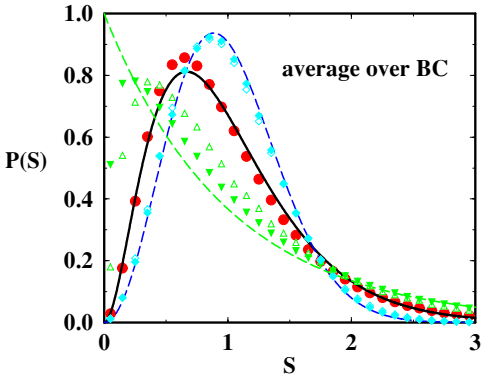

Figure 1. Metal–insulator transition. The level-spacing distribution function $P(S)$ is shown in 3D disordered systems for the integrable, critical and chaotic regimes for ten random configurations of linear size $L = 4, 10$ by integrating over 1000 possible boundary conditions, including periodic and antiperiodic, corresponding to 1000 points in $\vec{k}$-space making up a total number of a few million eigenvalues. As the system size increases the data for the metallic regime with $W = 10$ and the insulating regime with $W = 30$ approach the dashed lines on the right and left of the figure, which are the Wigner surmise $P(S) = (\pi/2)S\exp(-(\pi/4)S^2)$ and the Poisson law $P(S) = \exp(-S)$, respectively. The filled dots of the computed scale-invariant distribution at critical disorder strength $W_c = 16.4$ are compared with the semi-Poisson distribution $P(S) = 4S\exp(-2S)$ denoted by the solid line.

For a given set of BC the allowed values of k_x, k_y, k_z form a rigid grid of $L \times L \times L$ points in the Brillouin zone. By varying the $\alpha_{x,y,z}$ within $[0, 2\pi)$ each k-point in the Brillouin zone shifts to cover its own box so that the boxes of all points partition exactly the Brillouin zone [11]. When $\alpha_{x,y,z} = 0$ or π the added flux is equivalent to periodic, antiperiodic BC in the appropriate x, y, z direction, respectively. For critical disorder $W_c = 16.4$ [7, 8] equation (1) has eigenvalues ϵ_{j_x,j_y,j_z} and fractal eigenstates $\psi_{j_x,j_y,j_z}(x, y, z)$. For any disorder W and size L the eigenvalues are obtained by numerical diagonalization.

To characterize spectral fluctuations we compute the nearest level-spacing $P(S)$ distribution function. First, we make the local mean level-spacing $\Delta(E) \propto 1/\rho(E)$ constant equal to one where ρ is the mean density of states, by 'unfolding' the spectrum via local rescaling of the energy. For this purpose one needs the local average level-spacing $\Delta(E)$ which can be obtained over many levels around E. Alternatively, the ith 'unfolded' energy level $\mathcal{E}_i = \mathcal{N}_{\rm av}(E_i)$ can be obtained from the averaged integrated spectral density $\mathcal{N}_{\rm av}(E)$, leading to average nearest level-spacing $\langle S\rangle = \langle \mathcal{E}_i - \mathcal{E}_{i-1}\rangle = 1$. In the studied energy regime around the band centre the results did not change much with or without a proper unfolding since the mean density of states is almost constant [7].

2.1. Metal to insulator transition

In figure 1 we present the obtained level-spacing distribution $P(S)$ in 3D for various sizes L with disorder W by integrating over 1000 boundary conditions (BC). We have used the majority (about a third of the total) of energy levels centred around the band centre ignoring only those at band tails. For a given finite size L the results of disorder strength W corresponding to localization length ξ lie in-between the Wigner surmise ($L \to \infty$ asymptotic for extended states) and the Poisson distribution ($L \to \infty$ asymptotic for localized states) [7]. Only for large enough $L \gg \xi$ the data eventually approach the Poisson curve which for $W > W_c$ indicates only localized states in 3D. For $W < W_c$ the data lie close to Wigner surmise which

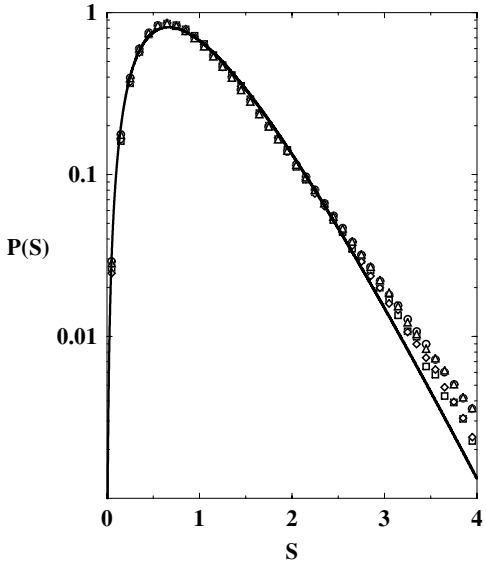

Figure 2. A linear-log plot of the critical $P(S)$ shown in figure 1 where prominent deviations from the semi-Poisson can be seen in the large-E tail.

is also quickly approached for large size. Our results of figure 1 below the critical point ($W = 10 < W_c$) demonstrate a $P(S)$ which approaches Wigner and above the critical point ($W = 30 > W_c$) a $P(S)$ which approaches Poisson, respectively. At $W = W_c$ the obtained scale-invariant critical $P(S)$ averaged over BC has Wigner-like small spacing behaviour and Poisson-like large spacing behaviour. It is roughly described by the semi-Poisson curve [1] although some differences become obvious, particularly in the tail of the distribution as seen in the semi-log plot of figure 2. These deviations also seem to violate the scale invariance of the critical curve, since they slightly increase by increasing L. However, in this part of the distribution $P(S)$ is very low and it is much more likely that the numerical accuracy of the data is lost.

2.2. Ballistic to localization crossover

We have also examined the simpler ballistic to localization crossover. It occurs in 1D disordered systems between two integrable limits, one purely quantum where the kinetic energy term of H in equation (1) dominates and the other classical characterized the fluctuating random potential energy term of equation (1). In the ballistic regime one asymptotically reaches a simple δ-function $P(S)$ while in the localized regime the Poisson distribution. Our results taken at the band centre $E \approx 0$ are displayed in figure 3. Since the localization length is easily computed with the anomalous perturbational result $\xi \approx 105.24W^{-2}$ at $E = 0$ [12, 13],[3] different from usual perturbation $\xi \approx 96W^{-2}\sqrt{1-(E/2)^2}$ valid at most energies E. We vary W for many random configurations which changes ξ by considering appropriate sizes L to keep the scaling ratio ξ/L fixed. In the ballistic limit we find that a delta function $P(S)$ is approached for $\xi/L \gg 1$ while in the localized limit Poisson is reached for $\xi/L \ll 1$. For $\xi/L = 1/5$ we obtain a $P(S)$ closer to Poisson shown in figure 3(b). In figure 3(a) we

[3] In [13] Schomerus and Titov showed a few per cent deviations from single parameter scaling at special energies, e.g. at $E = 0$.

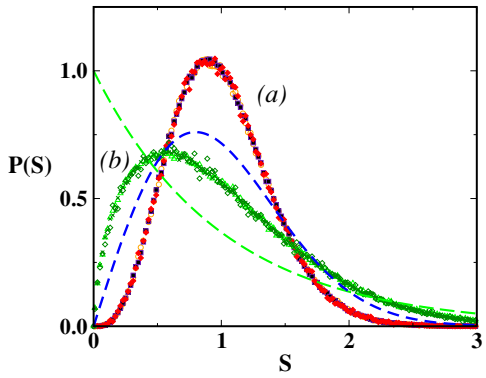

Figure 3. Ballistic to localized crossover. The level-spacing distribution function $P(S)$ in 1D disordered systems is shown to depend on the scaling parameter ξ/L, where ξ is the localization length and L the size. (a) In the crossover regime between ballistic and localized states having fixed $\xi/L = 1$ from diagonalization of 100 000, 500 000 and 100 0000 random matrixes of size $L = 500, 1000, 5000$ for energies close to $E = 0$ with appropriate disorder values W. (b) In the localized regime having $\xi/L = 1/5$ from diagonalization of 500 000 random matrices of $L = 500, 1000, 5000$. In the ballistic regime $\xi/L > 1$ the $P(S)$ (not shown) rapidly approaches a delta function centred around the mean $S = 1$.

display the obtained crossover distribution at the fixed ratio $\xi/L = 1$ for various ξ (varying W) and L. We observe that the scale-invariant crossover distribution is similar to a simple Gaussian. Of course differences exist, such as the requirement of positive S which does not allow the existence of Gaussian tails moving on the left-hand side. We emphasize that the computed $P(S)$ measures fluctuations over the disorder ensemble precisely at the band centre, rather than fluctuations in the energy domain studied in billiards.

3. Discussion

We have presented numerical results for the level-spacing distribution $P(S)$ of non-interacting electrons in the presence of potential energy fluctuations at the Anderson metal–insulator transition. The critical behaviour characterized by multifractal eigenstates leads to a generic sensitivity to BC [1]. In the present work imposed Aharonov–Bohm fluxes are equivalent to considering many BC. For example, a continuous set of BC in 1D leads to the equivalent problem of studying the non-overlapping mini-band widths [14]. The AB-flux controlled crossover from orthogonal to unitary studied in [15] has also revealed sensitivity to the imposed AB fluxes. Although such sampling over the Brillouin zone via the Aharonov–Bohm fluxes breaks time-reversal invariance changing the universality class from orthogonal to unitary, the obtained results remain valid for the orthogonal case. This means that averaging over BC restores time-reversal symmetry, in other words there exists a basis where the averaged Hamiltonian is real.

In summary, the $P(S)$ distribution for disordered systems is computed to test the semi-Poisson form at criticality. The obtained results complement previous studies for understanding the metal–insulator transition. Our main finding is that the corresponding critical statistics is reasonably well described by the semi-Poisson function after an average over many BC is taken. Small but rather persistent deviations occur mostly in the difficult to reach large-S tail, possibly due to numerical artefacts arising from limited accuracy. The spectral fluctuations studied here could help us to understand various properties of

current-currying states in mesoscopic systems and might also suggest a critical RMT. A disordered system is seen to progress from ballistic extended (periodic integrable) to diffusive (chaotic) and finally to localized (random integrable) regimes. The ballistic regime is dominated by quantum correlations and the localized regime by random potential energy fluctuations, respectively. The intermediate quantum chaotic regime is reached either by shape peculiarities in billiards or for moderate disordered potential in solids. We add the remark that the Gaussian-like $P(S)$ observed for the addition spectra of the conductance peaks in Coulomb blockade [16], if it could be interpreted within a non-interacting electron framework, would suggest an analogy to the obtained crossover between two integrable regimes with and without disorder.

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