Critical level statistics for weakly disordered graphene

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Abstract

In two dimensions chaotic level statistics with the Wigner spacing distribution $P(S)$ is expected for massless fermions in the Dirac region. The obtained $P(S)$ for weakly disordered finite graphene samples with zigzag edges turns out, however, to be neither chaotic (Wigner) nor localized (Poisson). It is similar to the intermediate statistics at the critical point of the Anderson metal-insulator transition. The quantum transport of finite graphene for weak disorder, with critical level statistics can occur via edge states as in topological insulators, and for strong disorder, graphene behaves as an ordinary Anderson insulator with Poisson statistics.

Keywords: Anderson localization, critical level statistics, graphene, Dirac region

(Some figures may appear in colour only in the online journal)
\[ H = \sum_i \varepsilon_i c_i^\dagger c_i - \sum_{i,j>\neq} \gamma_{i,j} (c_i^\dagger c_j + c_j^\dagger c_i). \] (1)

\( c_i^\dagger (c_i^\dagger) \) annihilates (creates) an electron at the A or B site \( i \) of the honeycomb lattice, the diagonal disorder \( \varepsilon_i \) is constant in the range \([-\frac{W}{2}, \frac{W}{2}]\), \( W \) is the disorder strength and \( \langle i, j \rangle \) denotes nearest neighbours with hopping matrix elements \( \gamma_{i,j} = 1 \). For \( W = 0 \) (no disorder) the band structure displays two non-equivalent valleys which act as pseudospin states and are related by time reversal [5, 6]. In the Dirac region at long length scales, equation (1) can be replaced by the continuous Dirac equation [6]. The short-range diagonal disorder is chosen via random \( \varepsilon_i \) which causes intervalley scattering mixing the two valleys and leads to localization. The decoupling of valleys occurs by breaking time-reversal symmetry, e.g. for a smooth long-range disordered potential, which involves scattering within a single valley only and gives weak antilocalization familiar from spin–orbit coupling [18]. The chosen diagonal disorder of strength \( W \) also destroys A, B sublattice symmetry.

We have cut the honeycomb lattice into various shapes, circular, stadium, square, etc and considered the corresponding tight-binding Hamiltonians (in the low \( E \) region). In our computations the brick-wall lattice is mostly used, which has exactly the same Hilbert space structure as the honeycomb. The brick-wall lattice differs from the honeycomb only in the included sites at the boundaries, which arise from fitting the different shapes into it. We find no significant difference between the brickwall and the honeycomb lattice for the sizes considered and this difference further diminishes as the size increases.

The eigenvalues of equation (1) are obtained in the Dirac region via Lanczos numerical diagonalization, by building a statistical ensemble of random \( H \) matrices for every \( W \). For \( W = 0 \) (no disorder) and peculiar shape boundaries quantum chaos is expected for stadium flakes and integrability is expected for circular flakes. In addition, for the graphene (bulk) the A, B sublattice symmetry guarantees the presence of \( \pi \) edge states which belong to one type of sublattice (A or B). They arise [8, 9] from quantum interference of an incoming wave from one bond which splits into two in the tight-binding equations. Their amplitude is nonzero only for \( m = 0 \); \( m \) counts the sites far from the boundary, and since they are localized in the boundary, are one-dimensional with fractal dimension 1. The edge states are reflected in the Hilbert space structure by the lattice topology and are protected against disorder. In the presence of weak disorder (nonzero \( W \)) they spread almost uniformly in the Dirac region [10] and diffuse into the bulk with their fractal dimension becoming greater than one. The fractal dimension of totally diffusing (chaotic) states is two. In graphene for finite \( W \) the massless degrees of freedom close to the edges are remnants of the sublattice symmetry which is broken by the diagonal disorder of equation (1).

In figure 2 the averaged density of states \( \rho(E) \) for various values of the disorder \( W \) is shown. In the absence of disorder (\( W = 0 \)) the \( zz \) edges contribute only to zero energy. For nonzero disorder \( W \) they spread almost uniformly in the Dirac region and diffuse into the bulk with their fractal dimension becoming greater than one. In a log–log plot we find constant \( N(E)/E \) vs \( E \) which implies constant \( \rho(E) \) for very low \( E \) for slightly higher \( E \) the \( \rho(E) \) decreases for \( W < W_c \) (due to a minigap) and it increases for \( W > W_c \) (no minigaps). For

![Figure 1](image1.png)

**Figure 1.** The energy levels \( E \) versus the strength of disorder \( W \) for a quarter-circle graphene flake of 9691 sites. For \( W < W_c \) the level statistics is critical and for \( W > W_c \) it is localized (Poisson). The levels were unfolded by removing variations of the density of states \( \rho(E) \) averaged over 5000 realizations of disorder. In this case \( W_c \approx 2.3 \).

![Figure 2](image2.png)

**Figure 2.** The averaged density of states \( \rho(E) \) for circular graphene flakes with disorder \( W \) obtained from more than one million eigenvalues of equation (1). For \( W = 1, 2 \) the edge states lie close to \( E = 0 \) where \( \rho(E) \) is nonzero and almost constant. For strong disorder (\( W = 5 \)) their proportion becomes vanishingly small, while in the opposite limit of pure (\( W = 0 \) ) graphene, \( \rho(E) = \frac{1}{2\pi} |E| \) (continuous line) is linear. Inset: the averaged integrated density of states for weaker disorder \( W = 0.01, 0.1 \). The \( N(E) = \int_0^\infty \rho(E) dE \) (the \( E = 0 \) states are not included) shows minigaps due to low \( \rho(E) \) values, while for higher \( W \) the structure disappears.
strong disorder \((W = 5)\) the states fill up the gaps and make \(\rho(E)\) non-zero and constant in the Dirac region.

We have examined in detail the perimeter of the considered flakes and identified each type of lattice edge and its contribution to \(\rho(E)\). We find mostly armchair and zz edges (the dangling bonds are rare), with the most frequent edges being zz [10, 11]. The ratio of zz-to-armchair edges for circular flakes is about \(\sim 3.8\) and it varies linearly with the averaged flake radius \(R\) (the curve for the zz edges is also linear but showed more oscillations). The ratio of zz edges over the total number of sites tends to zero inversely proportional to \(R\), since their number is \(\sim R\) and the total number of sites is proportional to the area of the flake \(\sim R^2\). The density of states at zero energy \(\rho(0)\) reaches a maximum before it vanishes as \(1/R\) for large \(R\).

Let us now discuss the eigenvalues of equation (1). We examined the level statistics of the unfolded energy spectra via the nearest spacing distribution \(P(S)\) which can distinguish between chaotic (Wigner) and localized (Poisson) distributions [12]. In figure 3 the obtained \(P(S)\) for the first two positive levels \((S = E_2 - E_1)\) is shown for the critical region of \(W < W_c\). The \(P(S)\) is independent of the size and fits into a curve which has mixed chaotic and localized character. It is chaotic for small spacing \(S\) and localized for large \(S\) [16], is described by \(P(S) = 4S\exp(-2S)\) and belongs to the semi-Poisson family [19]. The critical \(P(S)\) interpolates between chaotic and localized limits: \(P(S) \sim S^\beta\) for \(S \rightarrow 0\) and \(P(S) \sim \exp(-(1 + \beta)S)\) for \(S \rightarrow \infty\). The universality class index \(\beta = 1\) for broken time-reversal symmetry via added magnetic field becomes \(\beta = 2\) [12], and for broken spin rotation via spin-orbit coupling it is \(\beta = 4\) [18], according to the scaling theory of Anderson localization [20].

For pure graphene \((W = 0)\) Poisson (integrable) level statistics exists in the Dirac region where \(\rho(E) \sim E\) and the integrated density of states \(N(E) \sim E^2\), with \(E \sim \sqrt{k_x^2 + k_y^2}\). The unfolded energy levels \(E^2 \sim k_x^2 + k_y^2\) replace the \(E\) and the statistics becomes that of \(E_{nm} = \alpha n^2 + m^2\), \(n, m = 1, 2, \ldots\), with \(\alpha\) an irrational number fixed by the adopted sample. For a square sample \(\alpha \sim 1\) and the statistics is obviously Poisson (integrable). For disordered graphene with zz edges and \(W < W_c\) (figure 1) the critical \(P(S)\) replaces the Poisson statistics; for small spacings \(S\) it is Wigner-like and for large \(S\) it is Poisson-like. In other words, the obtained critical distribution interpolates between chaotic and localized limits. This was previously found in 3D critical disordered systems, in pseudo-integrable billiards, etc [19]. In graphene localization is easier (see figure 4 where the approach to Poisson is fast for strong disorder) than in other 2D disordered systems, e.g. square or triangular, due to the smaller coordination number \((3)\) of the honeycomb lattice. The flow of \(P(S)\) towards a Poisson distribution as the system size increases is also faster for graphene than for the square lattice. On the other hand, the chirality of electrons in the Dirac region of graphene favours de-localization. These two contradictory factors are combined in the hybrid critical distribution \(P(S)\) found. The effect of the edges vanishes by taking periodic boundary conditions and this is the reason why the critical regime was not found in previous numerical studies [21, 22]. For strong disorder the Dirac region vanishes altogether and Poisson statistics is obtained for localized states similarly to zero disorder. The critical phase found in figure 1 vanishes for infinite size and/or strong disorder.

Our work was partially motivated by the fabrication of graphene quantum dots for diameters ranging from 40 nm to 100 nm [15]. The experimental level statistics for small flakes is increasingly non-Poisson while the very small flakes, of a few nm width, remained always conductive. The obtained critical level statistics for weak disorder \(W < W_c\) is due to the edge states which do not appear in other 2D disordered systems. The edge states survive for weak disorder; they are simply shifted to the small \(\sim R\) and the total number of sites is proportional to the area of the flake \(\sim R^2\). The density of states at zero energy \(\rho(0)\) reaches a maximum before it vanishes as \(1/R\) for large \(R\).

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In summary, we report a critical phase for $W < W_c$ in weakly disordered graphene flakes with short-ranged disorder. The obtained level statistics for $W < W_c$ is not chaotic, as in 2D disordered systems where the states overlap giving rise to level repulsion, but it is intermediate between the chaotic and the integrable, similar to that at the critical point of the Anderson metal-insulator transition. Our results show that conduction in weakly disordered graphene is determined by the topology of the perimeter and the presence of edge states. The sharp transition found at $W_c$ (figure 1) distinguishes between a critical phase for $W < W_c$ where graphene can conduct via its edges and a localized phase for $W > W_c$ which is usually expected in disordered 2D.

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