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Random matrices and quantum chaos in graphene nanoflakes

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DIRAC FERMIONS IN WEAKLY-DISORDERED GRAPHENE

SYMMETRIES OF THE HAMILTONIAN

The effective Hamiltonian for low-energy excitations reads

$$\mathcal{H}_{\rm Dirac} = v_F(p_x+eA_x)\,\sigma_x\otimes\tau_z + v_F(p_y+eA_y)\,\sigma_y\otimes\tau_0 + M(x,y)\,\sigma_z\otimes\tau_0 + U(x,y)\,\sigma_0\otimes\tau_0,$$

and is symmetric (at **B**=0) with respect to standard time reversal and two *special time reversals*:

$$\mathcal{T} = (\sigma_0\otimes\tau_x)\mathcal{C},$$
$$\mathcal{T}_{\rm sl} = -i(\sigma_y\otimes\tau_0)\mathcal{C}, \quad \mathcal{T}_v = -i(\sigma_0\otimes\tau_y)\mathcal{C},$$

where $\mathcal{C}$ denotes complex conjugation. The mass term $M(x,y)\sigma_z\otimes\tau_0$ breaks *symplectic symmetry* leading to the two possible scenarios listed below.

1. WEAK INTERVALLEY SCATTERING

$\mathcal{T}_v$ commutes with $\mathcal{H}_{\rm Dirac}$ so the system consists of two independent subsystems (one for each valley). Each subsystem lacks TRS as $\mathcal{T}$ commutes only with full $\mathcal{H}_{\rm Dirac}$. Because the Kramer's degeneracy ($\mathcal{T}_v^2 = -I$) the Hamiltonian of a chaotic system consists of two degenerate blocks (one per each valley), each of which may be modeled by a random matrix belonging to the *Gaussian Unitary Ensemble* (GUE).

2. STRONG INTERVALLEY SCATTERING

For irregular and abrupt system edges (or a potential abruptly varying on the scale of atomic separation) the two sublattices are nonequivalent, so both special time-reversal symmetries $\mathcal{T}_{\rm sl}$ and $\mathcal{T}_v$ become irrelevant. For **B**=0, $\mathcal{T}$ commutes with $\mathcal{H}_{\rm Dirac}$ leading to the orthogonal symmetry class and statistical properties following from the *Gaussian Orthogonal Ensemble* (GOE) of random matrices. When increasing |**B**|, transition GOE-GUE appears.

Introduction

Transitions between symmetry classes

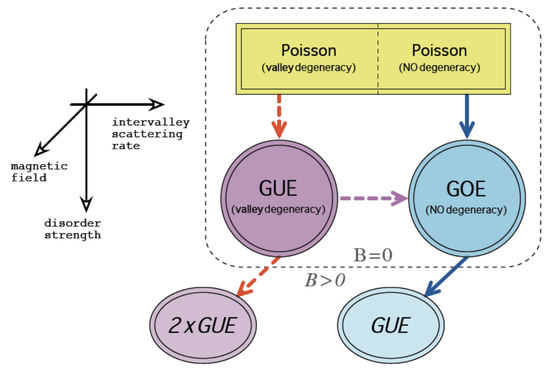

FIG. 1: Transitions between symmetry classes and random matrix ensembles relevant for *closed* nanosystems in graphene characterized by the disorder strength, the intervalley scattering rate, and (optionally) placed in the weak magnetic field B. Solid arrows in the right part indicate transitions already reported in the literature; dashed arrows in the central part indicate remaining transitions.

The model

Potential disorder in the tight-binding model on a honeycomb lattice

The lattice Hamiltonian for disordered graphene in weak magnetic field reads

$$\mathcal{H}_{\rm TBA} = \sum_{\langle ij\rangle}\left[\,t_{ij}(\mathbf{A})|i\rangle\langle j| + \text{h.c.}\,\right] + \sum_i\left[\,M_V(\mathbf{r}_i) + U_{\rm gate}(\mathbf{r}_i) + U_{\rm imp}(\mathbf{r}_i)\,\right]|i\rangle\langle i|.$$

where

$$U_{\rm imp}(\mathbf{r}) = \sum_{n=1}^{N_{\rm imp}} U_n \exp\left(-\frac{|\mathbf{r}-\mathbf{R}_n|^2}{2\xi^2}\right).$$

$H_{\rm TBA}$ was diagonalized numerically for each quasirandom realization of the impurity potential.

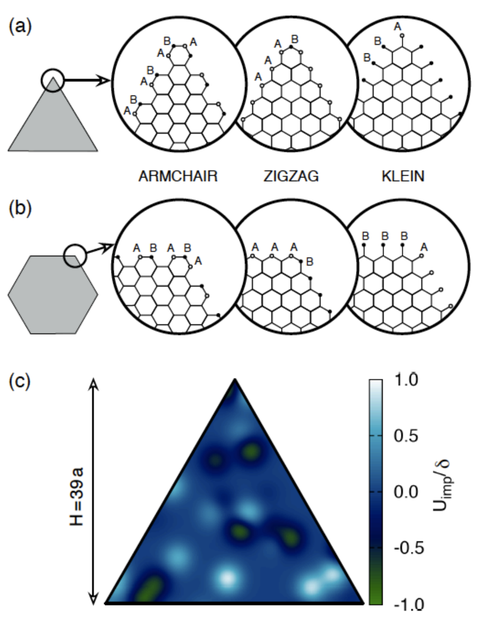

FIG. 2: Systems studied numerically in the paper. (a), (b) Triangular and hexagonal nanoflakes with armchair, zigzag and Klein edges. (c) Typical impurity potential landscape $U_{\rm imp}(\mathbf{r})$ for a triangular flake with armchair edges and 2106 carbon atoms. The triangle height is $H = 39\,a \simeq 10\,$nm, the impurity concentration and the disorder correlation length are $N_{\rm imp}/N_{\rm tot} = 0.01$ and $\xi = \sqrt{3}\,a$, respectively.

Numerical results

Random matrices and spectral statistics of disordered systems

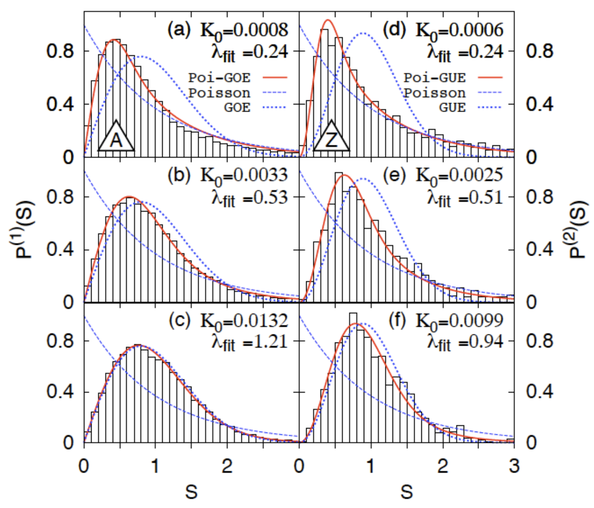

FIG. 5: Level-spacing distributions $P^{(1,2)}(S)$ for triangular nanoflakes with armchair (a)–(c) and zigzag (d)–(f) edges.

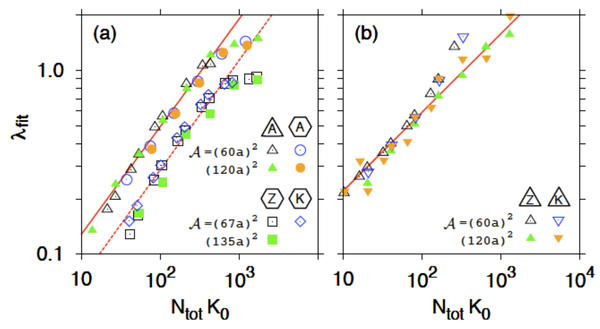

FIG. 6: Least-squares fitted parameters $\lambda_{\rm fit}$ for (a) transition Poisson-GOE and (b) transition Poisson-GUE [see Eqs.

When generic integrable system undergoes the transition to quantum chaos, its spectral properties may be reproduced by the random Hamiltonian

$$H(\lambda) = \frac{H^0 + \lambda V}{\sqrt{1+\lambda^2}},$$

where H^0 is is diagonal random matrix, which elements follow a Gaussian distribution with zero mean and the unit variance, whereas V is a member of GOE or GUE. (For $\mathcal{N}$=2, the level-spacings distribution can be found analytically for any λ.)

The transition to quantum chaos in disordered graphene flakes is rationalized using additive random-matrix models as the above. The functional relation between the best-fitted model parameter $\lambda_{\rm fit}$ and the disorder strength has a form of a power law. The unitary symmetry class is observed in spectral statistics, providing almost all terminal atoms belong to one sublattice. This is satisfied for equilateral triangles with zigzag or Klein boundaries, which also show an approximate valley degeneracy of each energy level. The degeneracy is lifted at weak magnetic fields.

For a fixed disorder strength in the chaotic range and increasing the number of edge vacancies we have observed the transition to GOE distribution.

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