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Strain-induced transitions to quantum chaos in graphene

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DIRAC FERMIONS IN STRAINED GRAPHENE

SYMMETRIES OF THE HAMILTONIAN

The effective Hamiltonian for low-energy excitations reads

$$\mathcal{H}_{\rm eff} = v_F\tau_0\boldsymbol{\sigma}\cdot(\boldsymbol{p}+e\mathbf{A}) - v_F\tau_z\boldsymbol{\sigma}\cdot\tilde{\boldsymbol{A}},$$

and is invariant, in the absence of gauge fields $\mathbf{A}=\tilde{\boldsymbol{A}}=0$ with respect to standard time reversal and two *special time reversals*:

$$\mathcal{T}_k = \sigma_y\otimes\tau_k\mathcal{C}, \qquad k=0,1,2,$$

where $\mathcal{C}$ denotes complex conjugation. We notice that $\mathcal{T}_y^2=1$ and thus $\mathcal{T}_y$ represents the true time reversal coupling the two valleys; whereas $\mathcal{T}_0^2=\mathcal{T}_x^2=-1$ leading to the Kramer's degeneracy of the two valleys and to the additional Kramer's degeneracy in each valley.

1. WEAK INTERVALLEY SCATTERING

The system consists of two independent subsystems (one for each valley). Each subsystem lacks TRS. Because the Kramer's degeneracy 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 become irrelevant. For **B**=0, we have 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

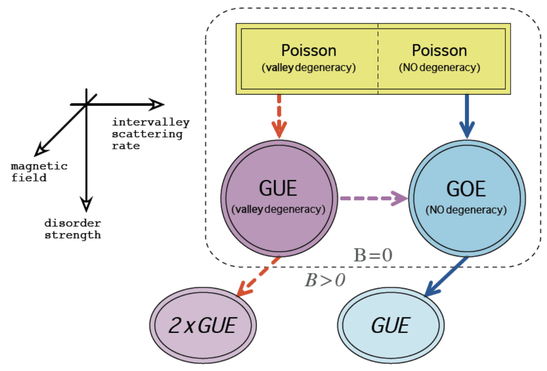

FIG. 1: Transitions between symmetry classes and random matrix ensembles relevant for *closed* nanosystems in graphene characterized by the disorder strength, the intervalley scattering rate, and (optionally) placed in the weak magnetic field B. Solid arrows in the right part indicate transitions already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

*[Previous work: AR, PRB **85**, 245424 (2012)]*

The model

Geometric deformations in the tight-binding model on a honeycomb lattice

The lattice Hamiltonian for disordered graphene in weak magnetic field reads

$$\mathcal{H}_{\rm TB} = -t_0\sum_{\langle ij\rangle}\left(1-\beta\frac{\delta d_{ij}}{d_0}\right) \times\left[\exp\left(i\frac{2\pi}{\Phi_0}\int_i^j\mathbf{A}\cdot d\mathbf{l}\right)|i\rangle\langle j| + \text{h.c.}\right]$$

where $\delta d_{ij}/d_0$ is relative change in the bond length and β=2 is the electron-phonon coupling.

$H_{\rm TB}$ was diagonalized numerically for the two distinct types of geometric deformations.

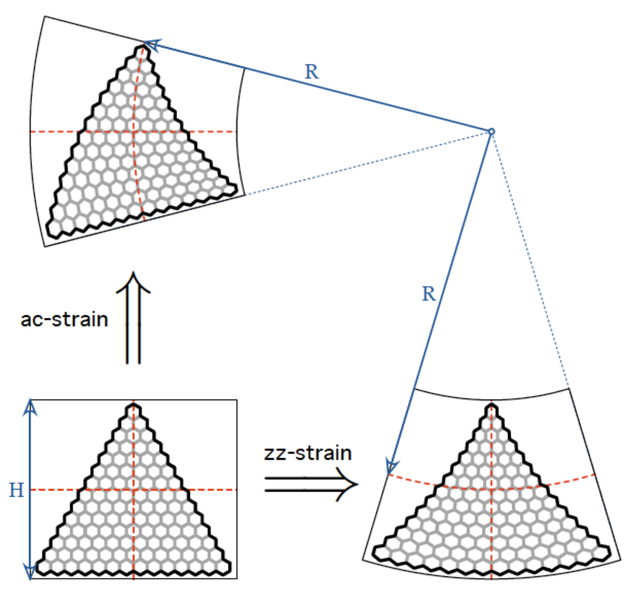

FIG. 1: Systems studied numerically in the paper. Bottom left: Triangular graphene nanoflake with zigzag edges characterized by the height H. Remaining plots: The same system bent in-plain employing the strain geometry proposed by Guinea *et al.* [15] (top left) in the variant breaking all geometric symmetries (*ac-strain*), and (bottom right) in the variant preserving the mirror symmetry (*zz-strain*). The radii of arcs limiting the flake area are $R\pm H/\sqrt{3}$ for ac-strain or $R\pm H/2$ for zz-strain. The ratio $H/R=2$ in both cases.

Numerical results

Random matrices and spectra of strained nanosystems

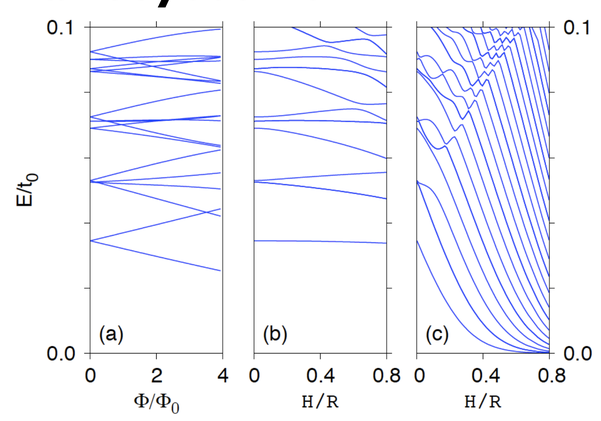

FIG. 3: Evolution of energy levels for a triangular nanoflake containing $N_{\rm C}=32758$ carbon atoms with varying magnetic field (a), ac-strain (b), and zz-strain (c).

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 strained graphene flakes is rationalized using additive random-matrix models as the above. 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.) Additionally, *all* geometric symmetries must be broken by the deformation. In case if a single mirror symmetry is left, spectral fluctuations following GOE rather than GUE are expected.

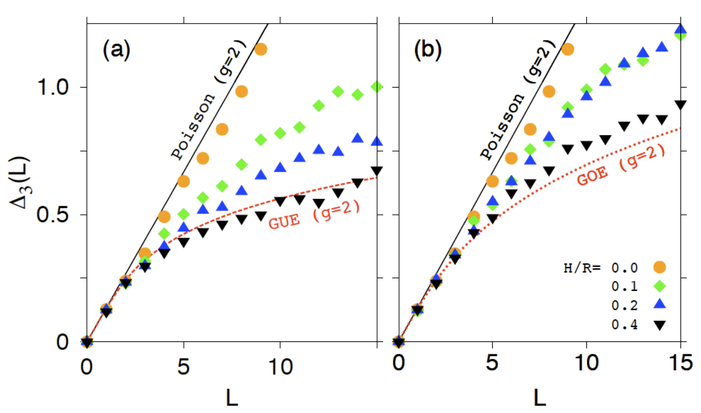

FIG. 7: Spectral rigidity $\Delta_3(L)$ for the same system as in Figs. 3–6 in the presence of ac-strain (a) or zz-strain (b). Datapoints show the results obtained numerically for different values of the strain parameter H/R (specified for each dataset). Lines are the theoretical expectations for the relevant ensembles of random matrices.

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