

Beautiful Graphene, Photonic Crystals, Schrödinger and Dirac Billiards and Their Spectral Properties



TECHNISCHE
UNIVERSITÄT
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Cocoyoc 2012

- Something about graphene and microwave billiards
- Dirac spectrum in a photonic crystal
 - Experimental setup
 - Transmission and reflection spectra
- Photonic crystal in a box: Dirac billiards
 - Measured spectra
 - Density of states
 - Spectral properties
- Outlook

Supported by DFG within SFB 634

S. Bittner, B. Dietz, J. Isensee, T. Klaus, M. Miski-Oglu, A. R., C. Ripp

N. Pietralla, L. von Smekal, J. Wambach



Nobel Prize in Physics 2010



Photo: Sergeom, Wikimedia Commons

Andre Geim



Photo: University of Manchester, UK

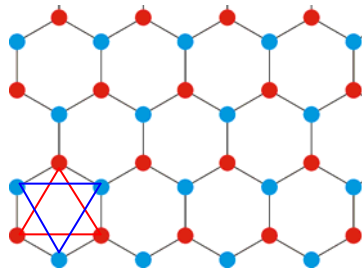
Konstantin
Novoselov

The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov *"for groundbreaking experiments regarding the two-dimensional material graphene"*

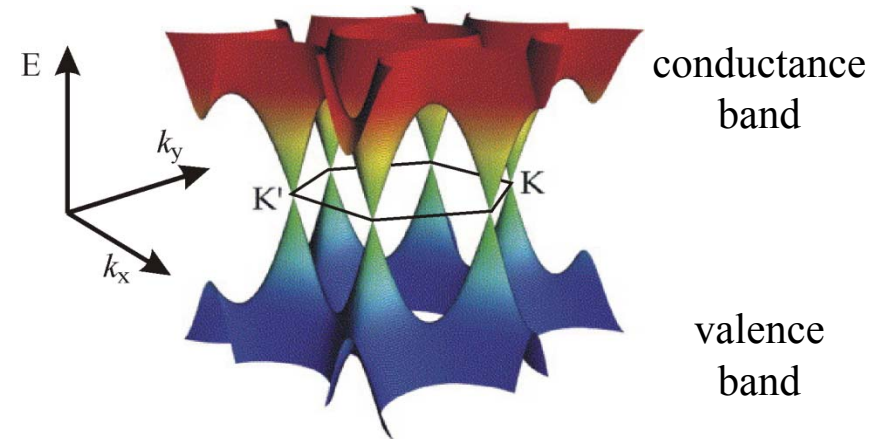
Graphene

- “What makes graphene so attractive for research is that the spectrum closely resembles the Dirac spectrum for **massless fermions**.”

M. Katsnelson, Materials Today, 2007

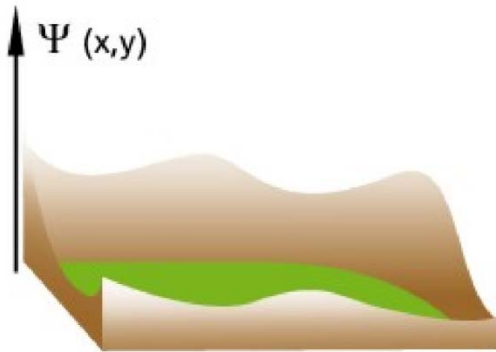


- Two triangular sublattices of carbon atoms
- Near each corner of the first hexagonal Brillouin zone the electron energy E has a conical dependence on the quasimomentum
- $E = \hbar v_F k$ but low $v_F \approx c/300$
- Experimental realization of graphene in analog experiments of microwave photonic crystals

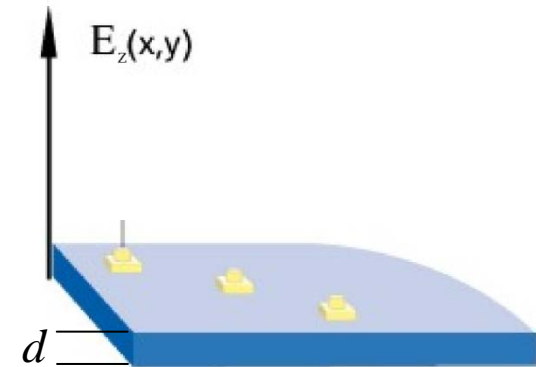


Quantum Billiards and Microwave Billiards

Quantum billiard



Microwave billiard



Analogy for $\lambda > 2d$

$$\left(\frac{\hbar}{2m} \Delta + E \right) \Psi = 0, \quad \Psi|_{\partial\Omega} = 0 \quad \longleftrightarrow \quad (\Delta + k^2) E_z = 0, \quad E_z|_{\partial\Omega} = 0$$

eigenvalue E

\leftrightarrow

wave number

$$k = \frac{2\pi f}{c}$$

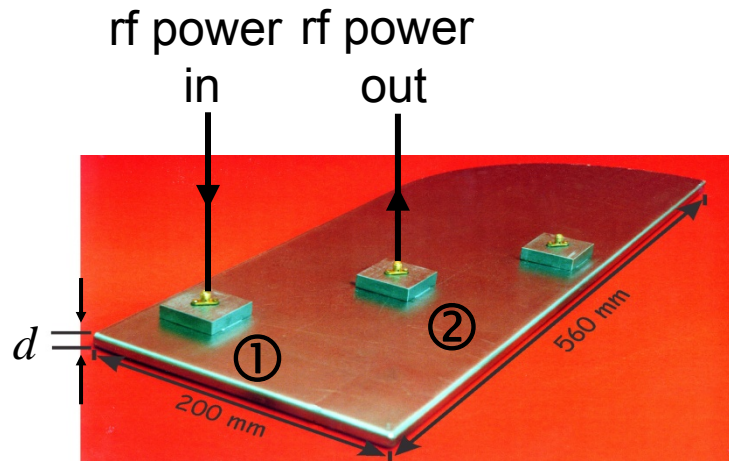
eigenfunction Ψ

\leftrightarrow

electric field strength E_z

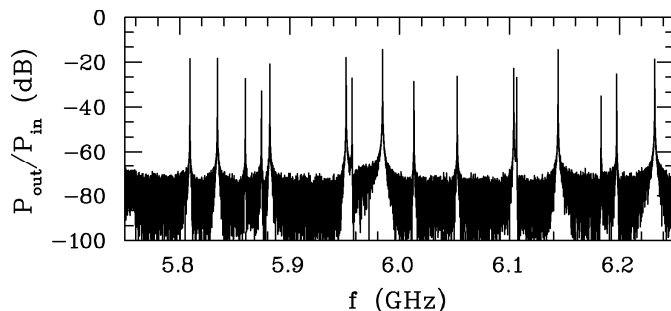
Measurement Principle

- Measurement of scattering matrix element S_{21}



$$\frac{P_{out,2}}{P_{in,1}} = |S_{21}|^2$$

Resonance spectrum



Resonance density

$$\rho(f) = \sum_v \delta(f - f_v)$$

$$\rho(f) = \rho_{Weyl}(f) + \rho_{fluc}(f)$$

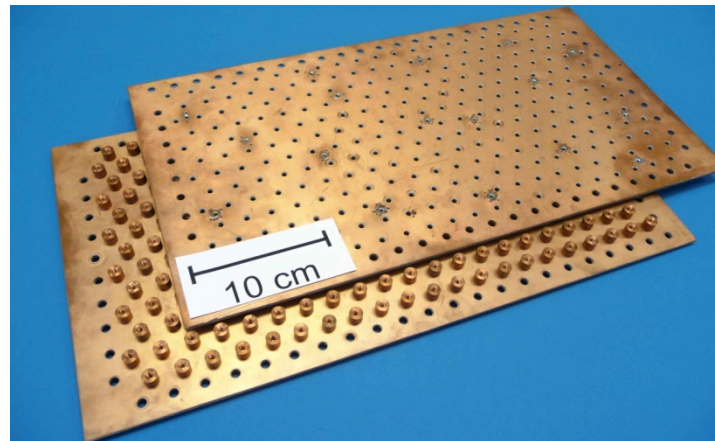
FT
→

Length spectrum
(Gutzwiller)

$$\tilde{\rho}(l)$$

Open Flat Microwave Billiard: Photonic Crystal

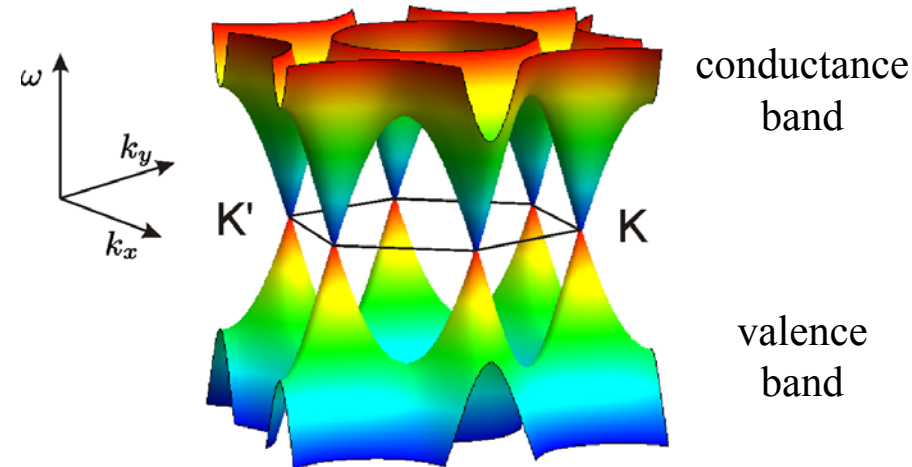
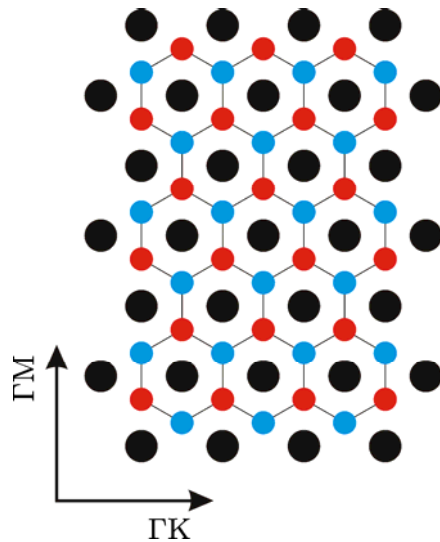
- A photonic crystal is a structure, whose electromagnetic properties vary periodically in space, e.g. an array of metallic cylinders
→ open microwave resonator



- Flat “crystal” (resonator) → E-field is perpendicular to the plates (TM_0 mode)
- Propagating modes are solutions of the scalar Helmholtz equation
→ Schrödinger equation for a quantum multiple-scattering problem
→ Numerical solution yields the band structure

Calculated Photonic Band Structure

- Dispersion relation $\omega(\vec{k})$ of a photonic crystal exhibits a band structure analogous to the electronic band structure in a solid

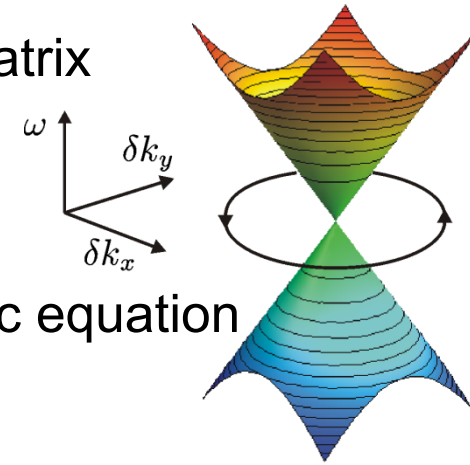


- The triangular photonic crystal possesses a conical dispersion relation
→ Dirac spectrum with a Dirac point where bands touch each other
- The voids form a honeycomb lattice like atoms in graphene

Effective Hamiltonian around the Dirac Point

- Close to Dirac point the effective Hamiltonian is a 2x2 matrix

$$\hat{H}_{\text{eff}} = \omega_D \mathbb{1} + v_D (\delta k_x \hat{\sigma}_x + \delta k_y \hat{\sigma}_y)$$

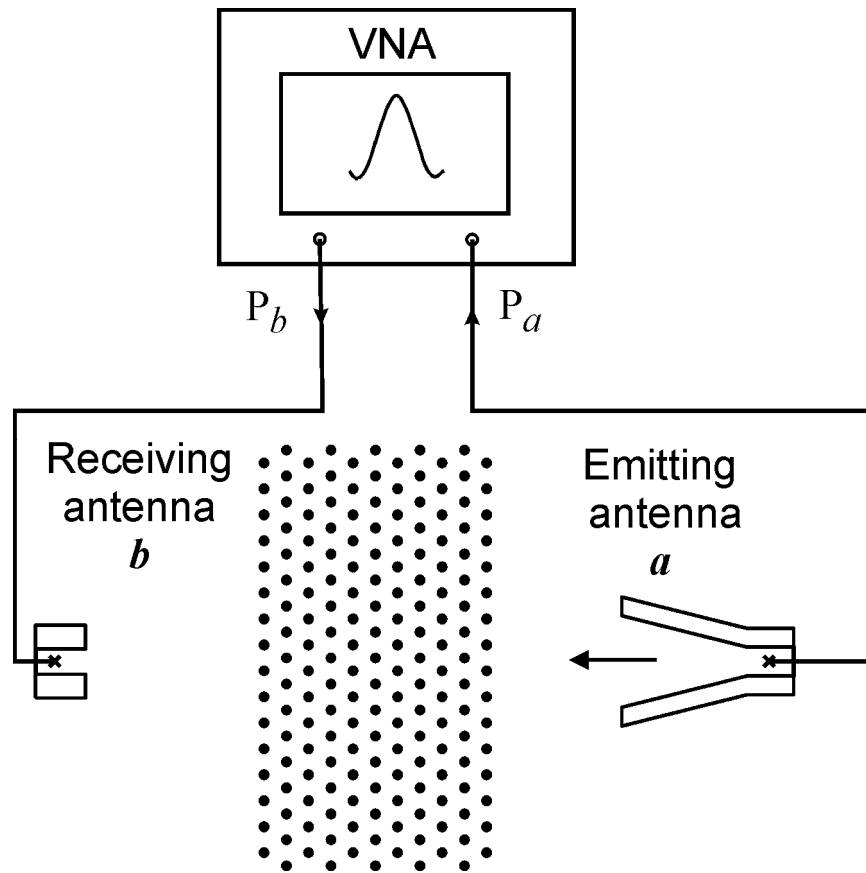


- Substitution $\delta k_x \rightarrow -i\partial_x$ and $\delta k_y \rightarrow -i\partial_y$ leads to the Dirac equation

$$\begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = i \frac{\omega - \omega_D}{v_D} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

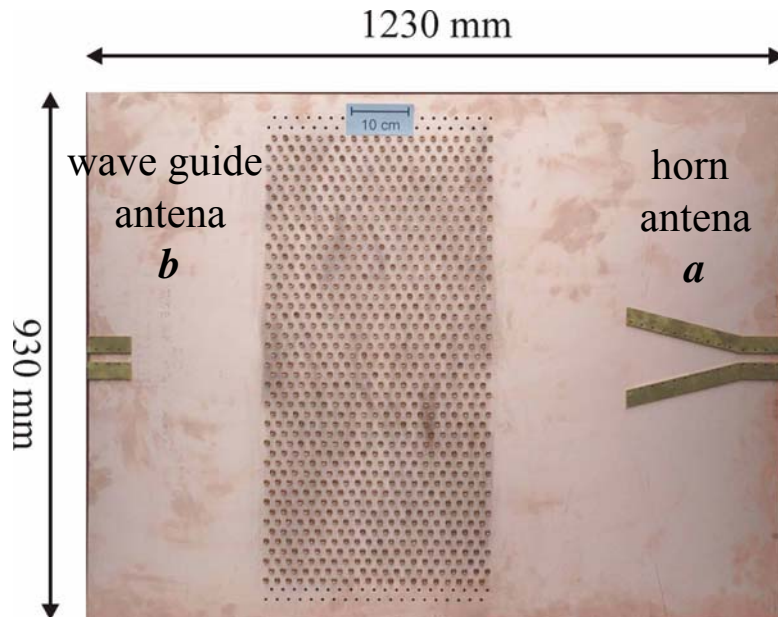
- Experimental observation of a Dirac spectrum in open photonic crystal (S. Bittner *et al.*, PRB **82**, 014301 (2010))
- Scattering experiment

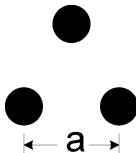
Scattering Experiment



- Horn antenna emits approximately plane waves
- VNA measures the modulus of the scattering matrix given by
$$|S_{ba}|^2 = \frac{P_b}{P_a}$$
- Transmission: $|S_{ab}|^2, |S_{ba}|^2$
- Reflection: $|S_{aa}|^2, |S_{bb}|^2$

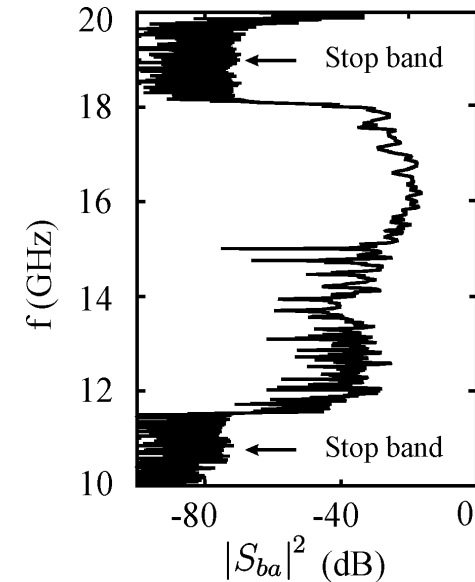
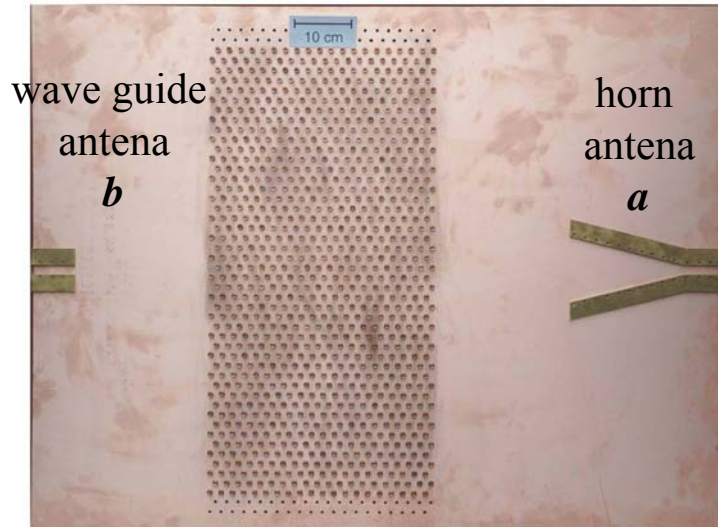
Experimental Realization of 2D Photonic Crystal



- # cylinders: $23 \times 38 = 874$
- Cylinder radius: $R = 5 \text{ mm}$
- Lattice constant: $a = 20 \text{ mm}$ 
- Crystal size: $400 \times 900 \times 8 \text{ mm}$
- Frequency: $f_{\text{max}} = 19 \text{ GHz}$

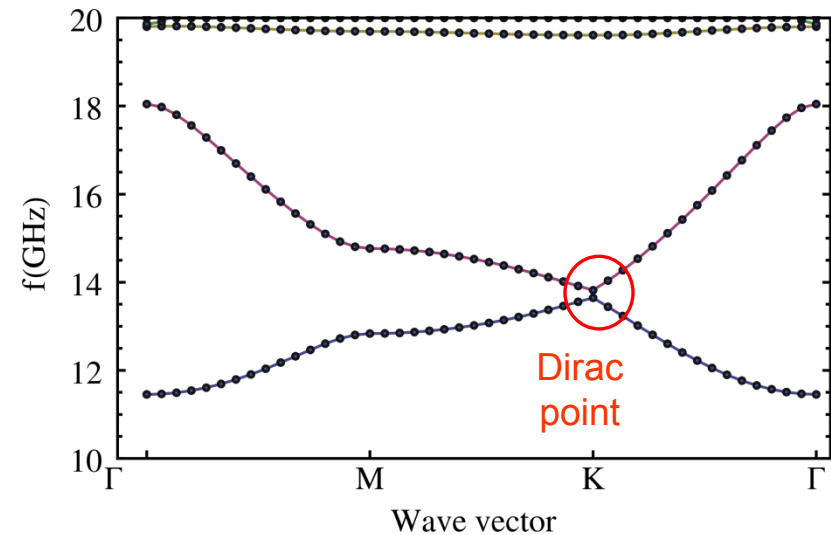
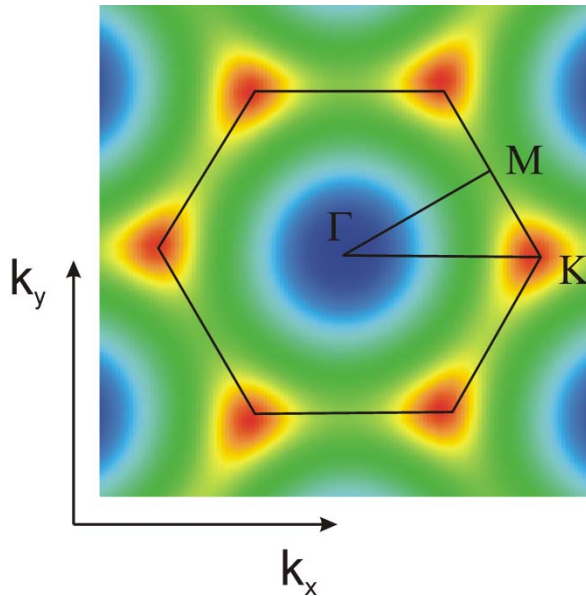
- First step: experimental observation of the band structure

Transmission through the Photonic Crystal



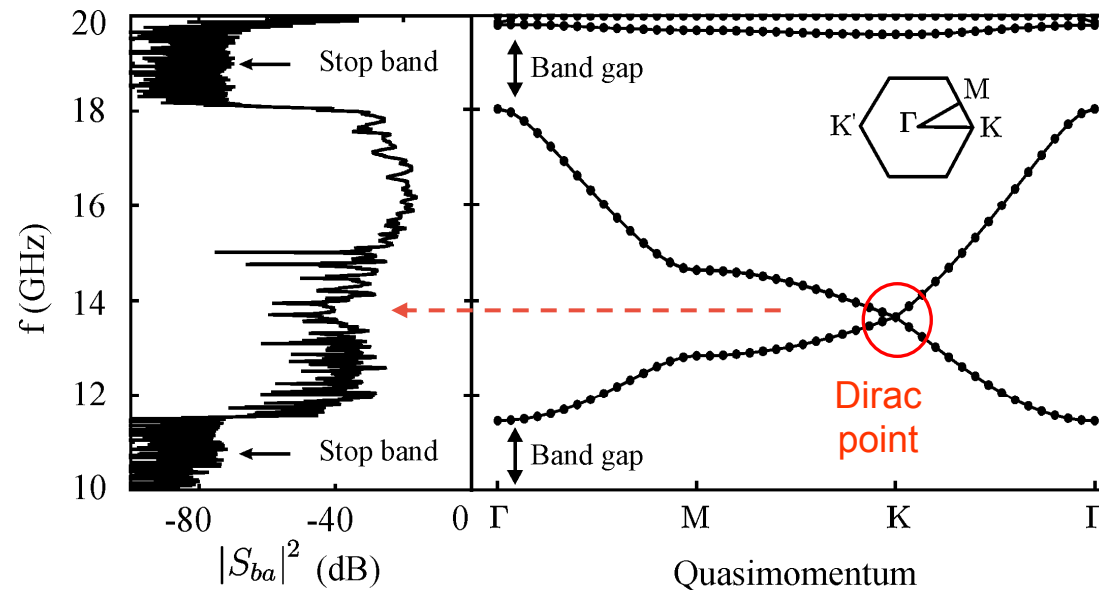
- Transmission spectrum possesses two stop bands
- Comparison with calculated band structure

Projected Band Diagram



- The density plot of the 1st frequency band
- The projected band diagram along the irreducible Brillouin zone Γ M K
- The 1st and 2nd frequency bands touch each other at the corners of the Brillouine zone \rightarrow **Dirac Point**

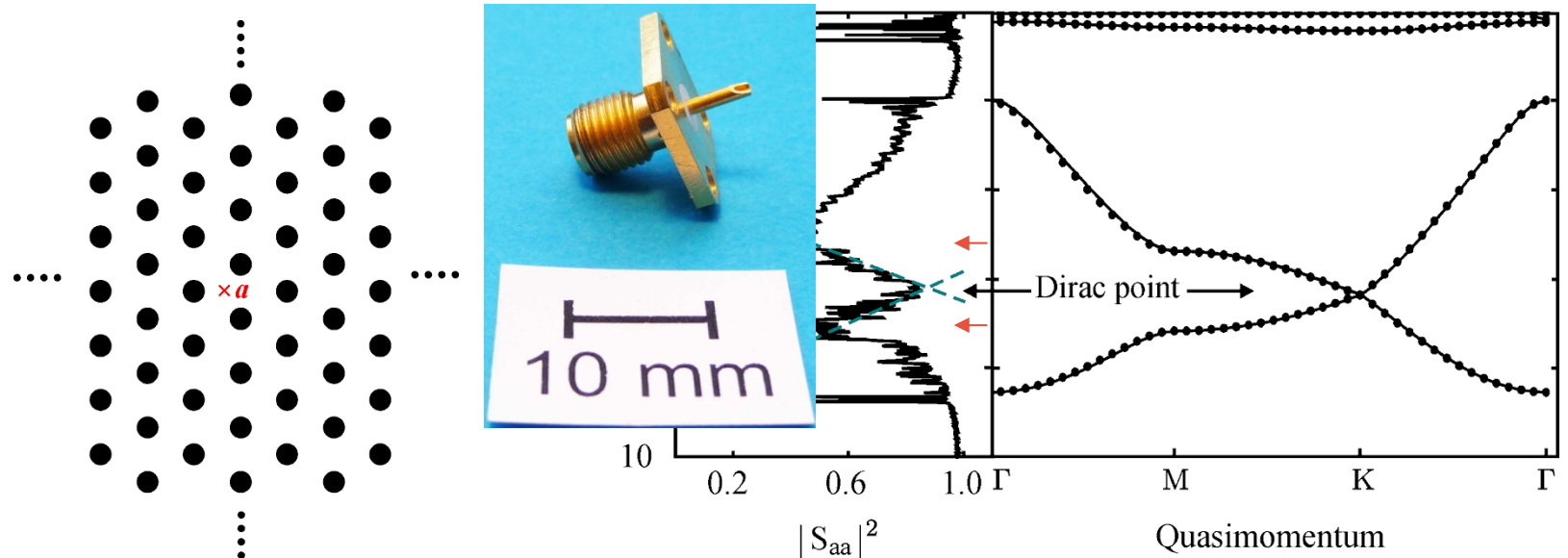
Transmission through the Photonic Crystal



- The positions of measured stop bands coincide with the calculated ones
→ lattice parameters chosen correctly
- Dirac point is not sufficiently pronounced in the transmission spectra
→ single antenna reflection measurement

Single Antenna Reflection Spectrum

- Measurement with a wire antenna a put through a drilling in the top plate
→ point like field probe



- Characteristic cusp structure around the Dirac frequency
- Van Hove singularities at the band saddle point $|\vec{\nabla}_k \omega(\vec{k})| = 0$
- Next: analysis of the measured spectrum

Local Density of States and Reflection Spectrum

- The scattering matrix formalism relates the reflection spectra to the local density of states (LDOS)

$$1 - |S_{aa}(f)|^2 \propto L(\vec{r}_a, f)$$

- LDOS

$$L(\vec{r}, f) \propto \int_{BZ} |\psi(\vec{k}, \vec{r})|^2 \frac{1}{2\pi} \delta(f - f(\vec{k})) d^2k$$

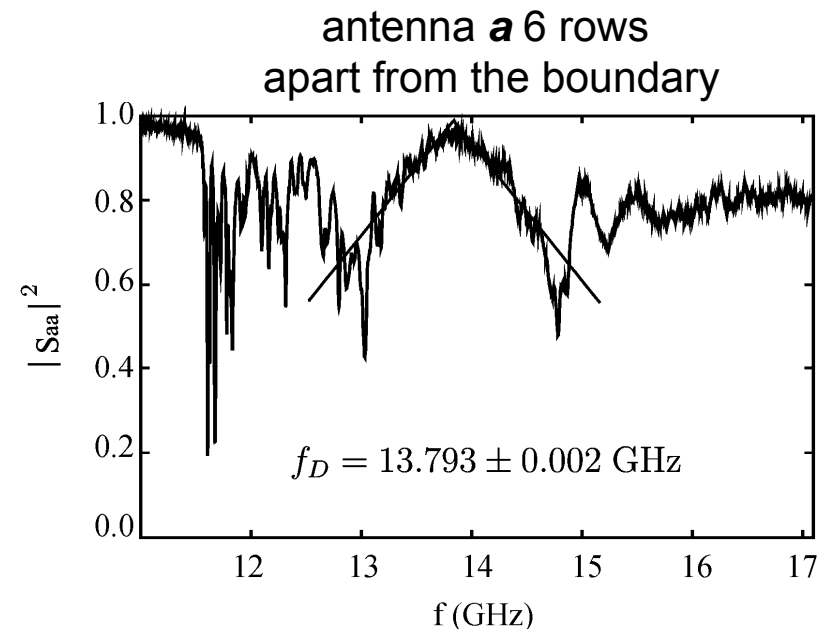
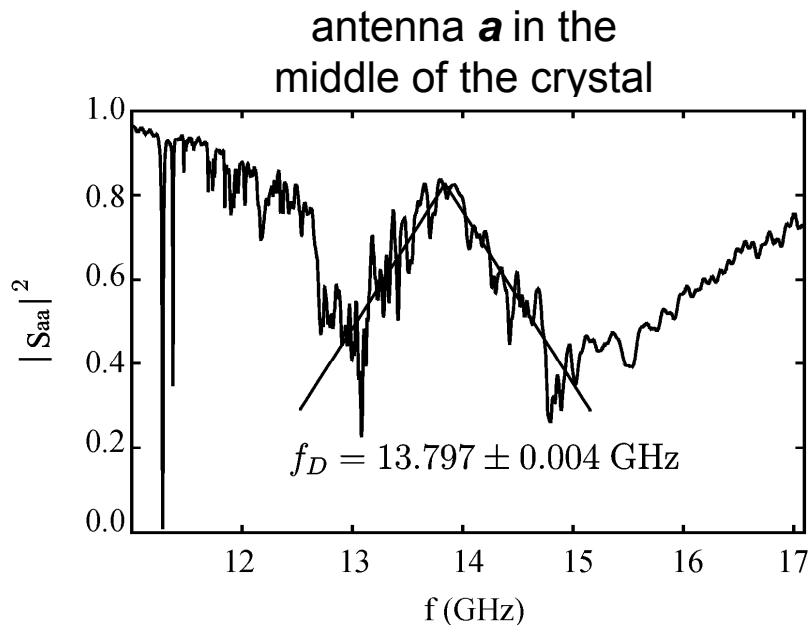
- LDOS around the Dirac point (Wallace, 1947)

$$L(\vec{r}_a, f) \sim \frac{\langle |\psi(\vec{r}_a)|^2 \rangle}{v_D^2} |f - f_D|$$

- Three parameter fit formula $|S_{aa}(f)|^2 = \underset{\substack{\uparrow \\ \text{fit}}}{D} - \underset{\substack{\uparrow \\ \text{parameters}}}{C} |f - \underset{\substack{\uparrow \\ \text{parameters}}}{f_D}|$

Reflection Spectra

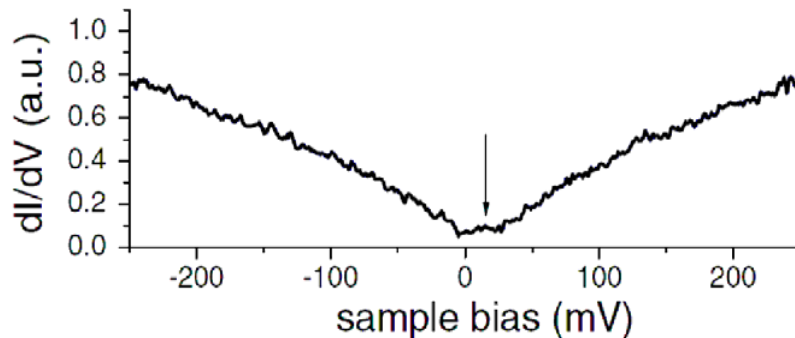
- Description of experimental reflection spectra $|S_{aa}(f)|^2 = D - C|f - f_D|$



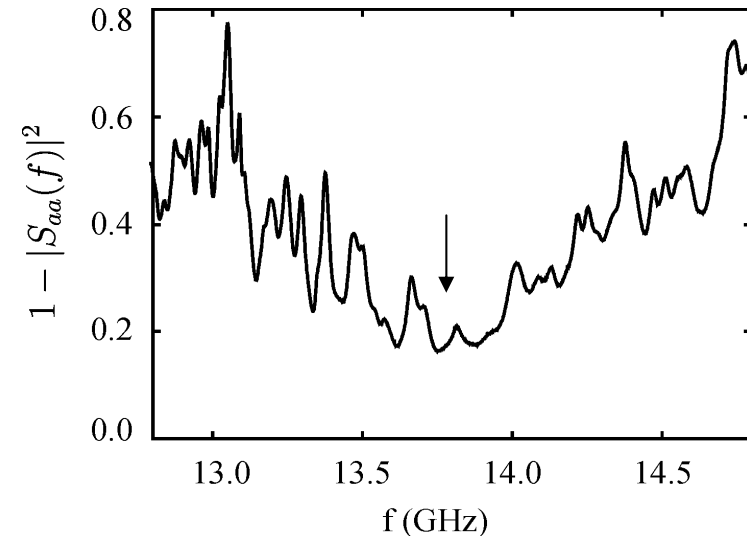
- Experimental Dirac frequencies agree with calculated one, $f_D = 13.81$ GHz, within the standard error of the fit
- Oscillations around the mean intensity → origin?

Comparison with STM Measurements

graphene flake, Li *et al.* (2009)



photonic crystal



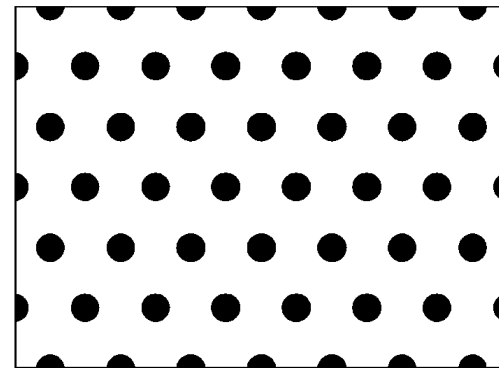
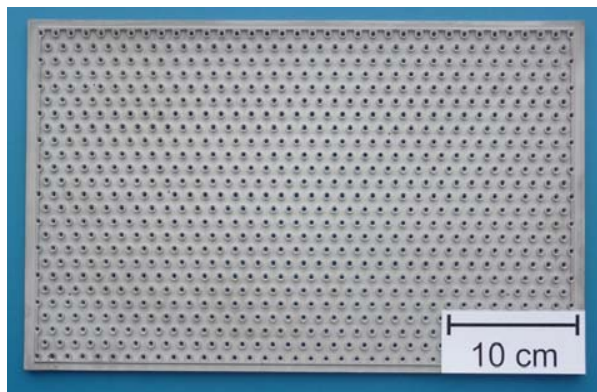
- Tunneling conductance is proportional to LDOS
- Similarity with measured reflection spectrum of the photonic crystal
- Oscillations in STM are not as pronounced due to the large sample size
- Finestructure in the photonic crystal shows fluctuations (RMT)

Summary I

- Connection between reflection spectra and LDOS is established
- Cusp structure in the reflection spectra is identified with the Dirac point
- Photonic crystal simulates one particle properties of graphene
- Results are published in Phys. Rev. B **82** 014301 (2010)
- Measured also transmission near the Dirac Point
- Dirac billiards

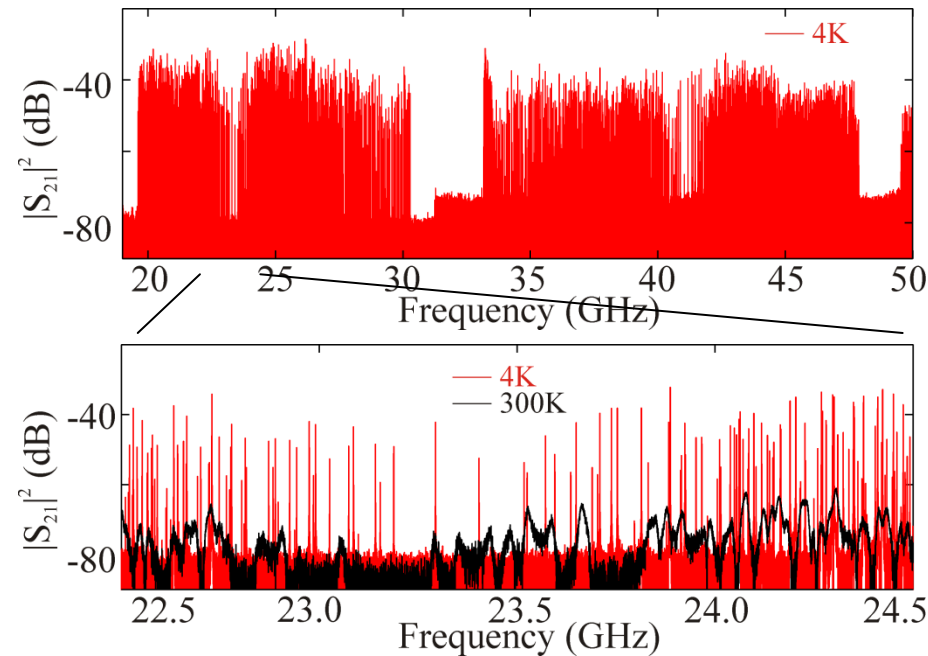
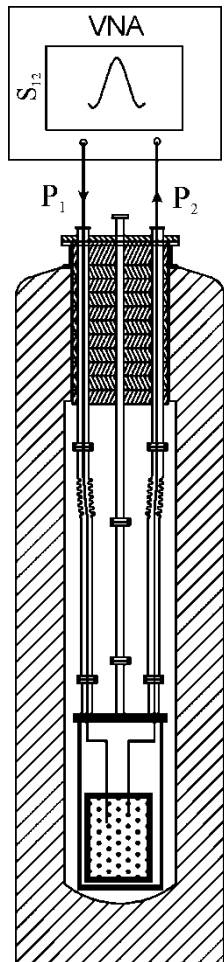
Dirac Billiard

- Photonic crystal → box: bounded area = billiard



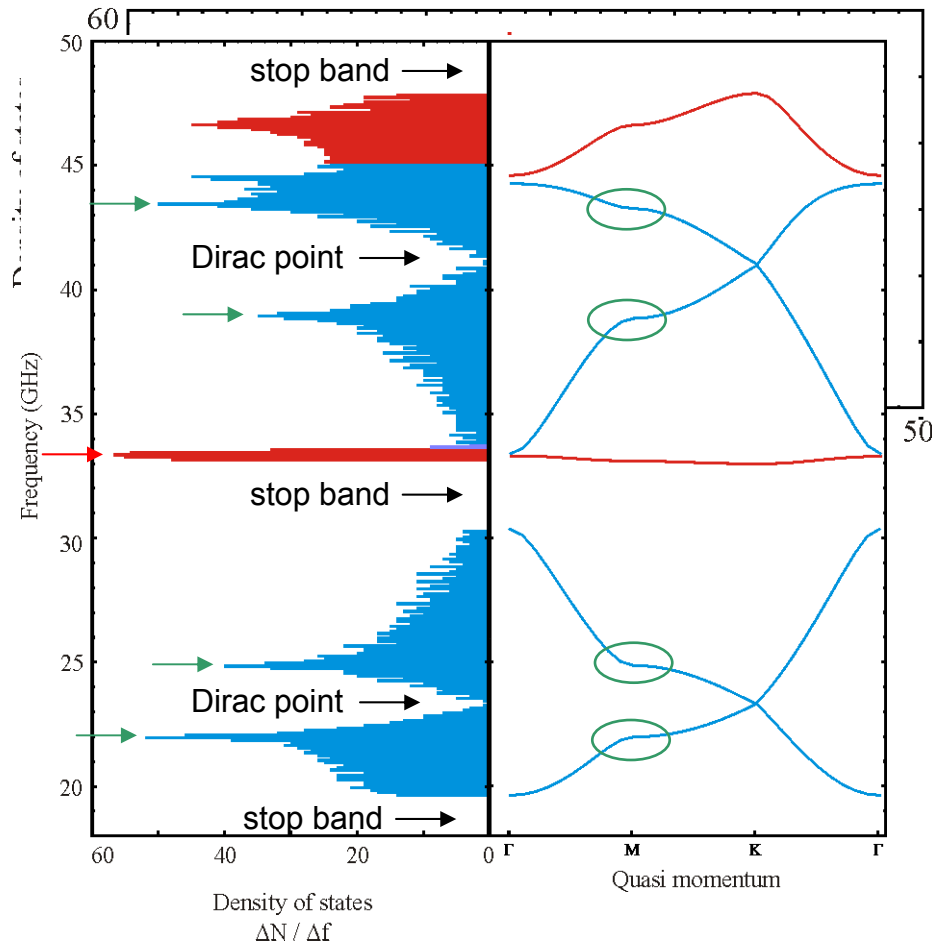
- 888 cylinders (scatterers) milled out of a brass plate
- Height $d = 3 \text{ mm} \rightarrow f_{max}^{2D} = 50 \text{ GHz}$ for 2D system
- Lead plated → superconducting below 7.2 K → high Q value
- Boundary does not violate the translation symmetry → no edge states
- Relativistic massless spin-one half particles in a billiard (Berry and Mondragon, 1987)

Transmission Spectrum at 4 K



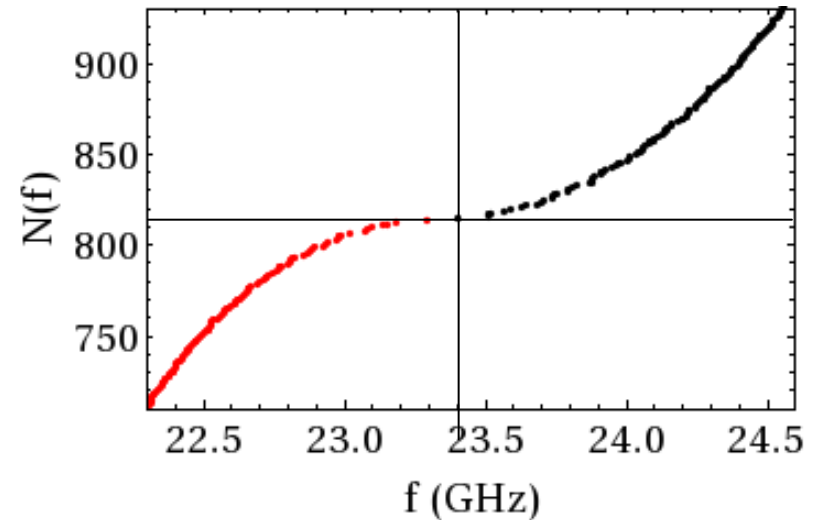
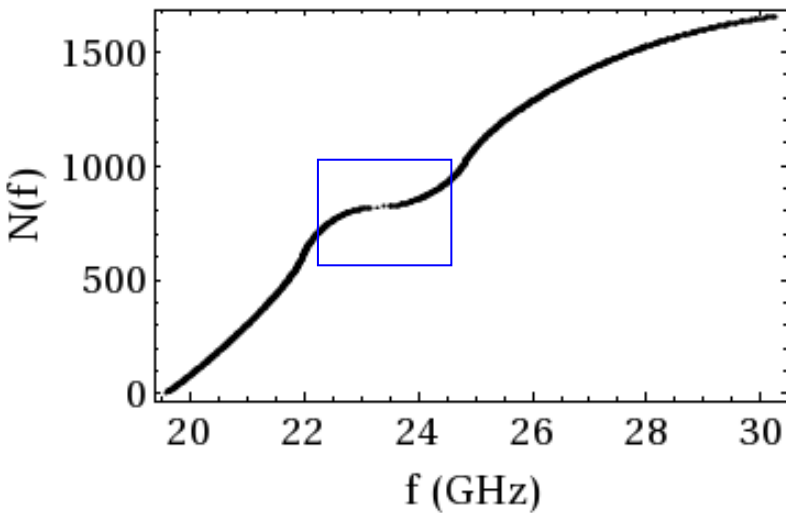
- Pronounced stop bands
- Quality factors $> 5 \cdot 10^5$
- $\langle \Gamma \rangle / \langle D \rangle = 10^{-3} \rightarrow$ complete spectrum
- Altogether 5000 resonances observed

Density of States of the Measured Spectrum and the Band Structure



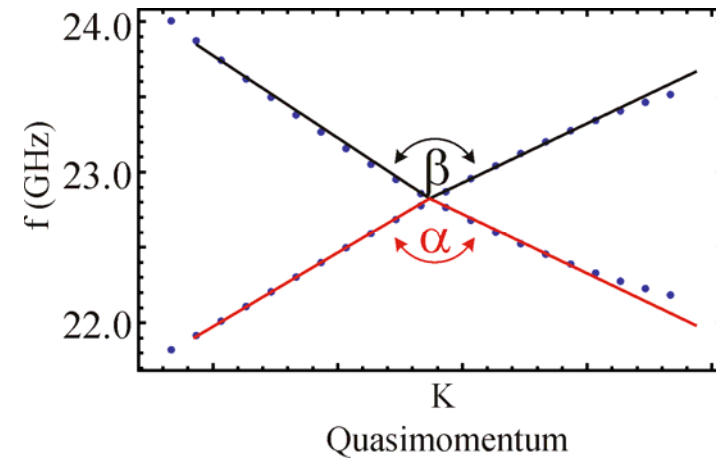
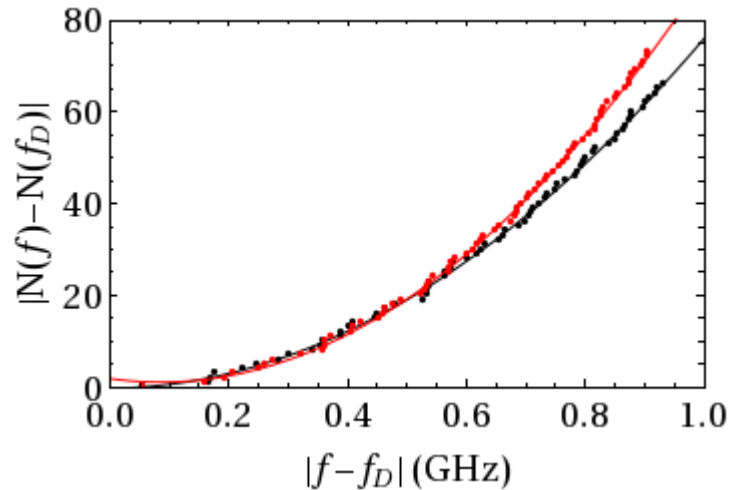
- Positions of stop bands are in agreement with calculation
- DOS related to slope of a band
- Dips correspond to Dirac points
- High DOS at **van Hove singularities** → ESQPT?
- **Flat band** has very high DOS
- Qualitatively in good agreement with prediction for graphene
(Castro Neto *et al.*, RMP **81**,109 (2009))


Integrated Density of States: 1st and 2nd Bands



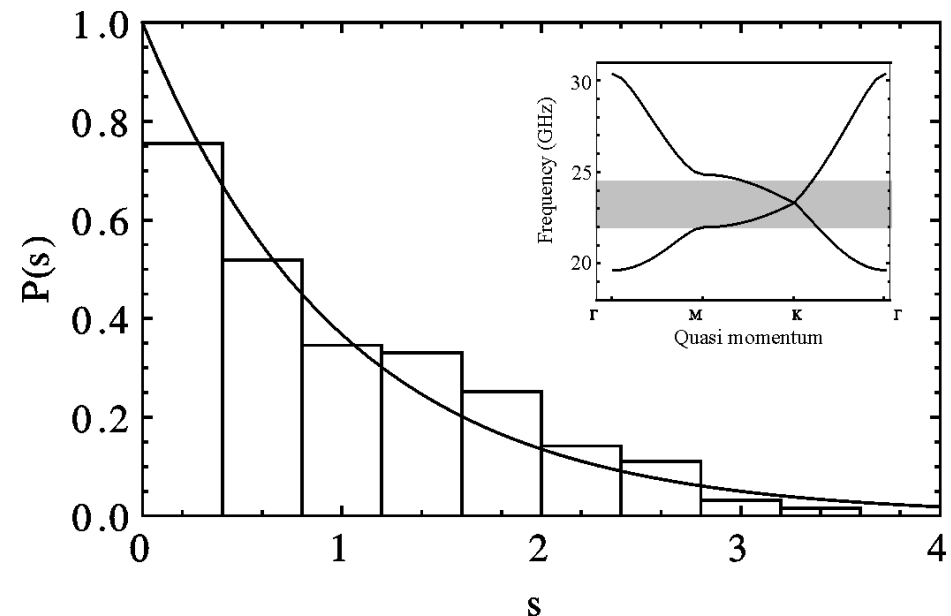
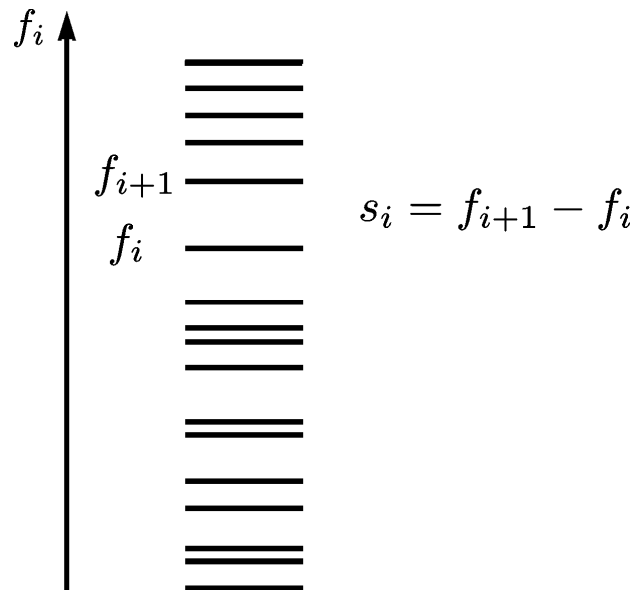
- Does not follow Weyl law for 2D resonators ($N_{Weyl}(f) = \frac{4\pi A}{c^2} f^2$)
- Small slope at the Dirac frequency \rightarrow DOS nearly zero
- Nearly symmetric with respect to the Dirac frequency
- Two parabolic branches

Integrated DOS near Dirac Point



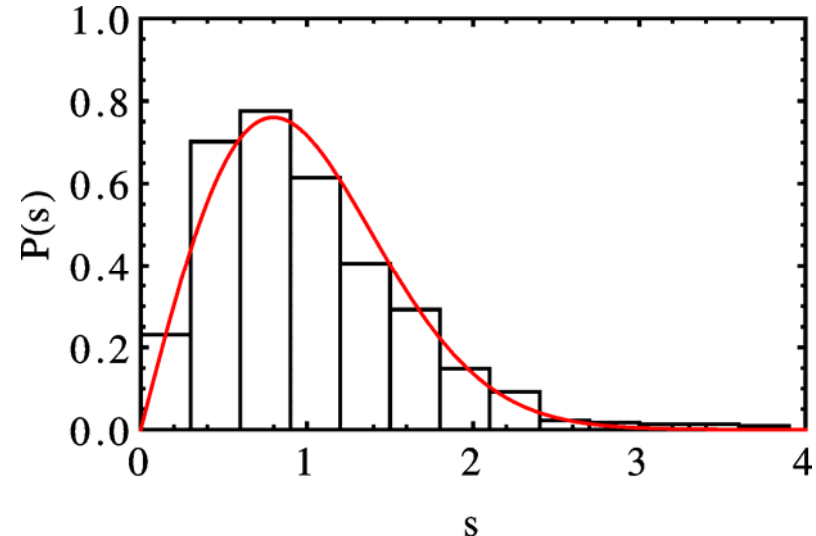
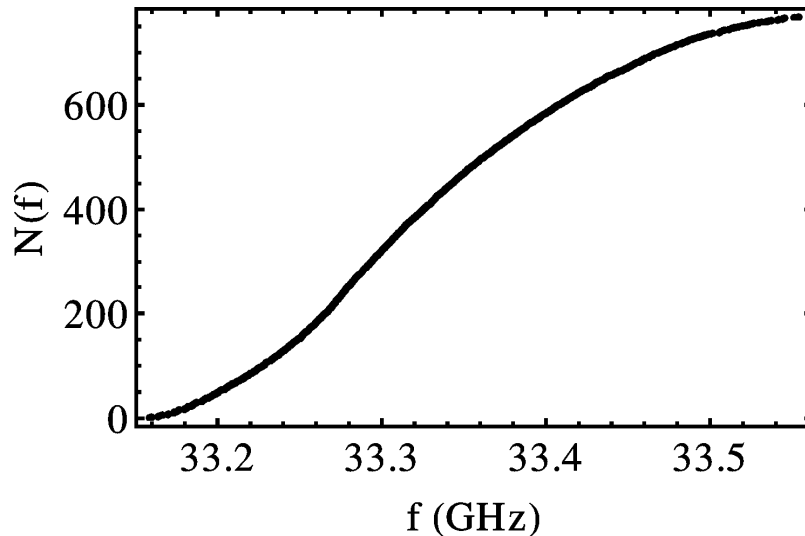
- Weyl law for Dirac billiard $N(k) = \frac{A}{2\pi}k^2 + \frac{U_{zz}}{\pi}k + C$ (J. Wurm *et al.*, PRB **84**, 075468 (2011))
 - U_{zz} is length of zigzag edges 
 - $k = 2\pi \frac{|f - f_D|}{v_D}$
 - group velocity v_D is a free parameter
- Same area A for two branches, but different group velocities $\rightarrow \alpha \neq \beta$
 \rightarrow electron-hole asymmetry like in graphene

Spectral Properties of a Rectangular Dirac Billiard: Nearest Neighbour Spacing Distribution



- 159 levels around Dirac point
- Rescaled resonance frequencies such that $\langle s_i \rangle = 1$
- Poisson statistics
- Similar behavior at second Dirac point

NND: 3rd Band



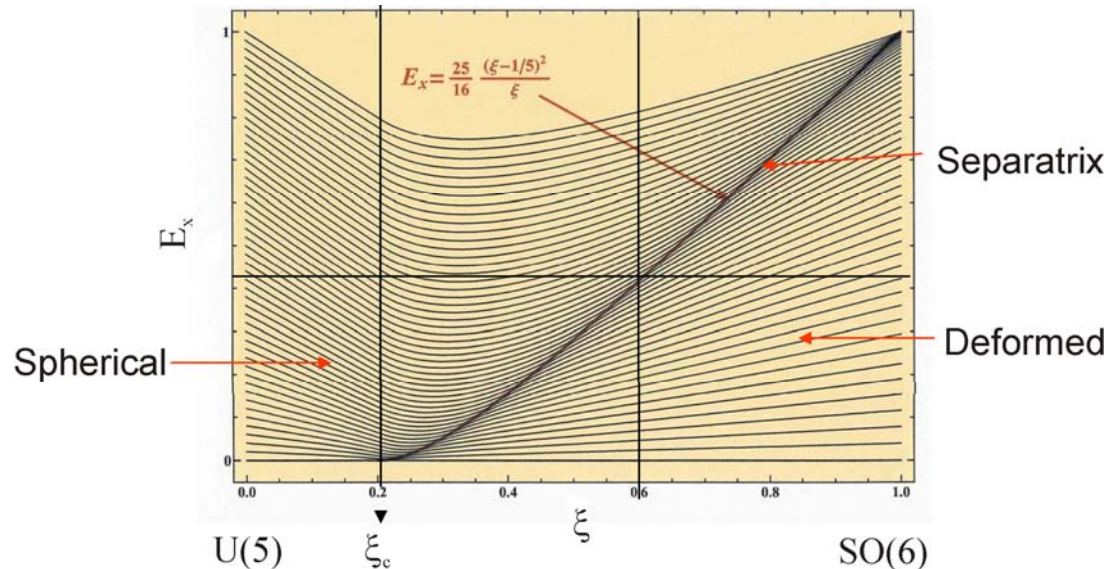
- Very dense spectrum $\langle \Gamma \rangle / \langle D \rangle \approx 10^{-1}$
- Unfolding with a polynomial of 8th order
- Missing levels?
- Seems to agree with GOE

Summary II

- Photonic crystal simulates one particle properties of graphene
- Observation of edge states in the Dirac billiard (not shown)
- Realisation of superconducting microwave Dirac billiard i.e. photonic crystal in a metallic box serves as a model for a relativistic quantum billiard
- Experimental DOS agrees with calculated photonic band structure
- Fluctuation properties of the spectrum were investigated
- Open problems:
 - (i) Length spectrum of periodic orbits
 - (ii) Do we see an excited state quantum phase transition?

Excited State Quantum Phase Transitions

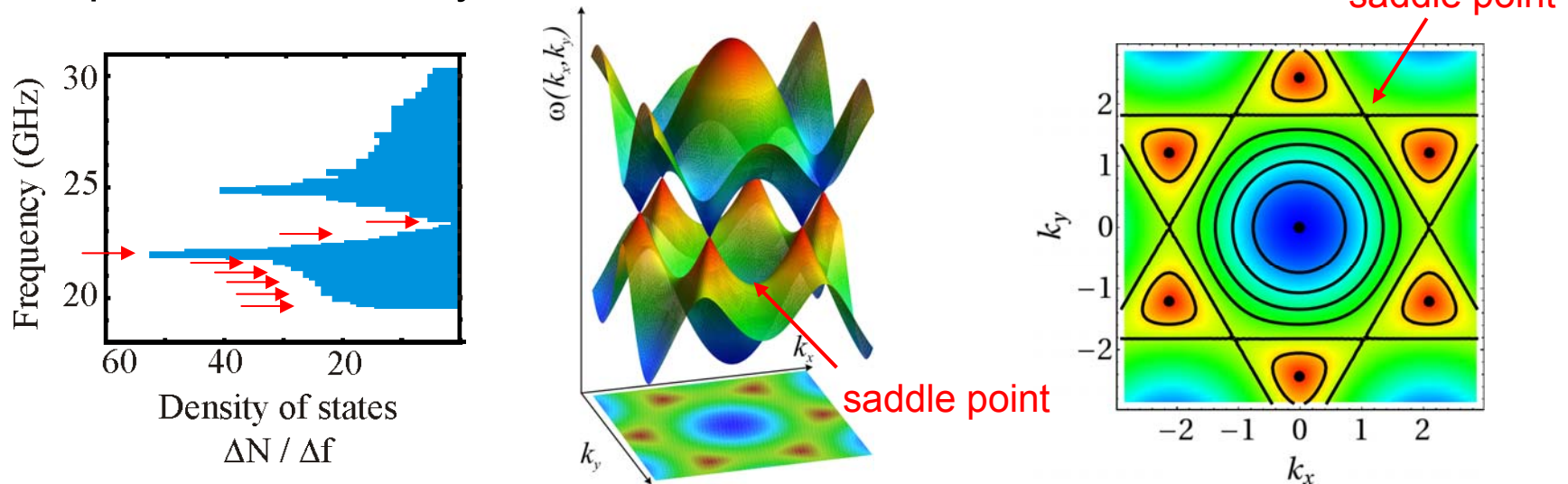
- Francesco Iachello at the “6th International Workshop in Shape-Phase Transitions and Critical-Point Phenomena in Nuclei” Darmstadt 2012



- Control parameter ξ
- At the separatrix the density of states diverges (Caprio, Cejnar, Iachello, 2008)

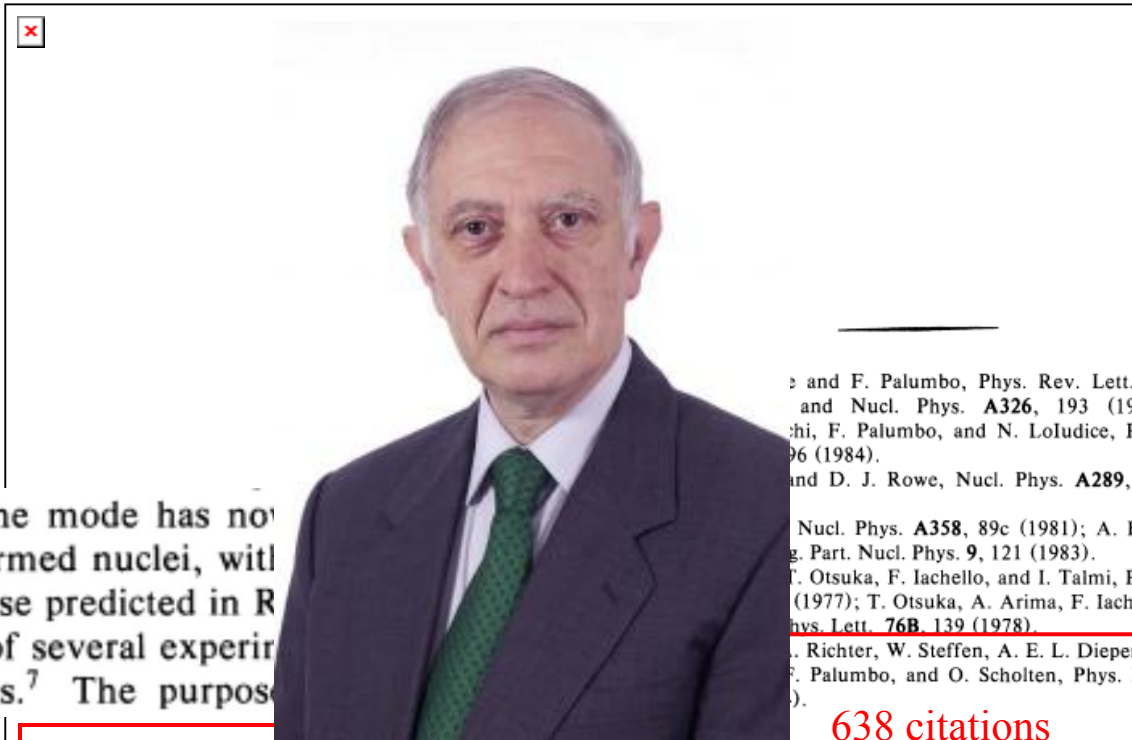
Excited State Quantum Phase Transition in Dirac Billiard

- Experimental density of states in the Dirac billiard



- Van Hove singularities at saddle point: density of states diverges at $k=M$
- Possible control parameters
 - chemical potential
 - sublattice dependent potential
 - ...

Personal Remarks



.... The mode has no several deformed nuclei, with closer to those predicted in R the subject of several experim investigations.⁷ The purpos

and F. Palumbo, Phys. Rev. Lett. **41**,
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638 citations

All the best and many more fruitful years together!

This work has clearly very much been stimulated by Franco Iachello. We thank him and Wolfgang Knüpfer and Bernard Metsch for several discussions,