Evora08

General relativity and graphene

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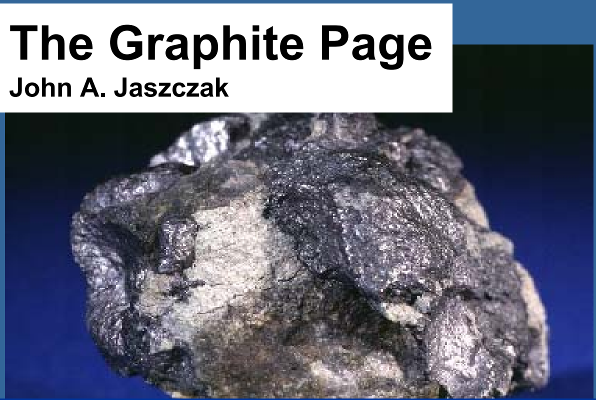
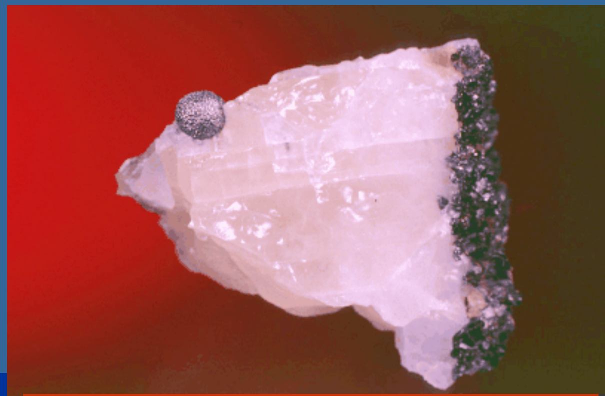
A brief history of graphene

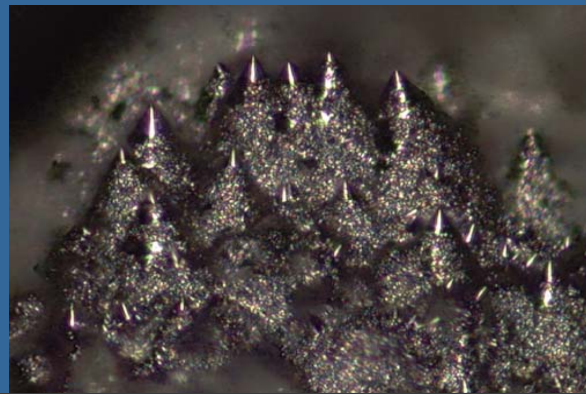
In the beginning it was graphite…



Graphite (5 cm across) from the famous Plumbago mine, Seathwaite, England.



3 mm graphite sphere etched from calcite, with associated schist.



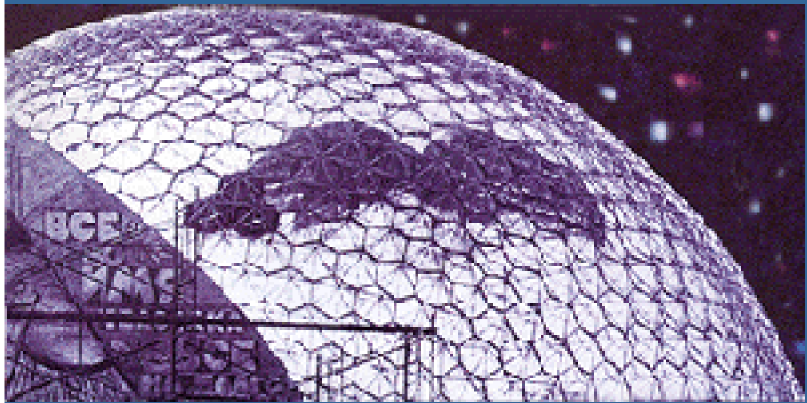
Graphite cones 50 microns long on the surface of a spheroidal graphite aggregate

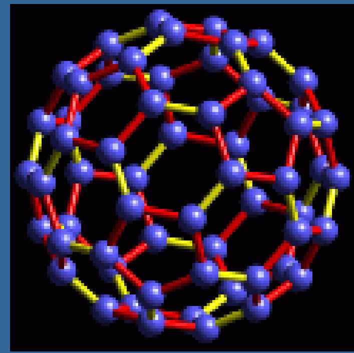
Graphite classical applications based on its amazing electronic properties.

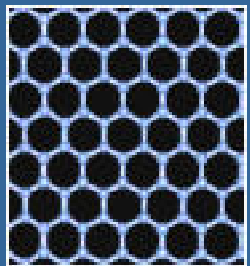
Conductivity:	
Electrical Resistivity (ohm.m) perpendicular to c-axis parallel to c-axis natural	 9.8x10^-6 4.1x10^-5 1.2x10^-6
Thermal (Watts/meter.kelvin at 273K) perpendicular to c-axis parallel to c-axis natural	 250 80 160
Optical:	
Bireflectance and reflection pleochroism	o-vibration: higer reflectance and yellow or brownish tint e-vibration: bluish-grey tint

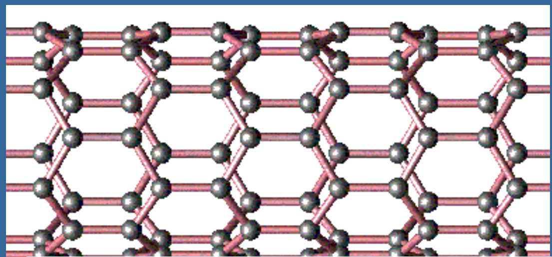
Mechanical:	
Bulk Modulus (single xtl)	34 GPa
Bulk Modulus (polycrystal)	7.3-10.7 GPa (non-irradiated, uncoated) 2.5-7.3 GPa (non-irradiated, coated) 14.0-16.9 GPa(irradiated, uncoated) 7.8-8.4 GPa (irradiated, coated)
Magnetic:	
Magnetic Susceptibility (pyrolitic) (pyrolitic) (rod)	strongly diamagnetic -450x10^-6 perpendicular to c-axis -85x10^-6 parallel to c-axis -160x10^-6

First revolution: fullerenes ('80)

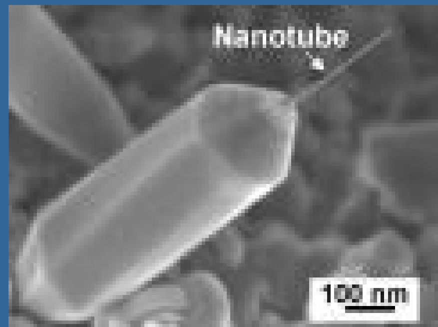




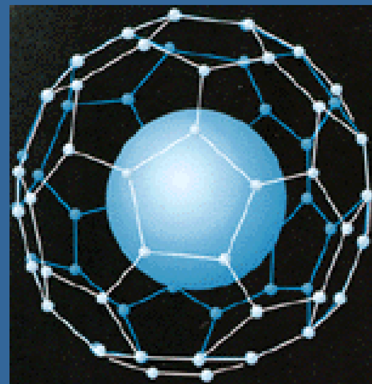




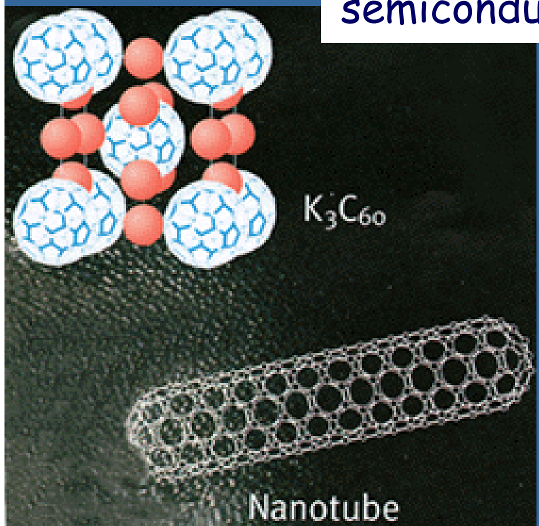
semiconductor or insulator



STM



Medical applications



Superconductor

Nanotecnology born. The big technological promise was in the nanotubes.

Graphene existed before. It was curved and compact.

Second revolution: graphene (05)

What is graphene?

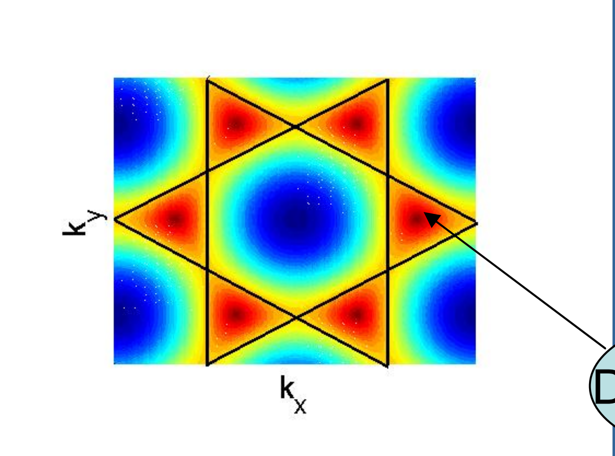
A two dimensional atomic crystal of carbon

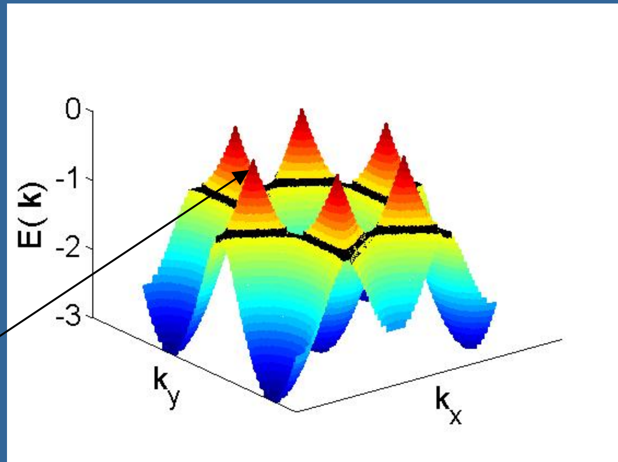
Why is it so special?

- It exists
- And its electrons conduct –strangely-
- It connects beautifully different branches of physics
- As with HTS we had to study hard again

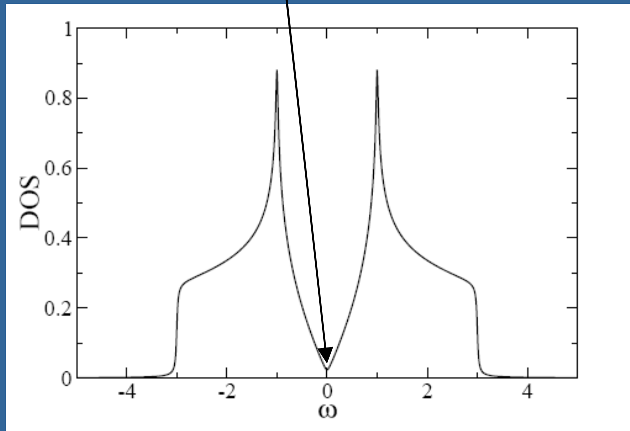
Electronic properties

$$\varepsilon^0(\mathbf{k}) = \pm t\sqrt{1 + 4\cos^2\frac{\sqrt{3}}{2}ak_x + 4\cos\frac{\sqrt{3}}{2}ak_x\cos\frac{3}{2}ak_y}\ ,$$





Dirac points

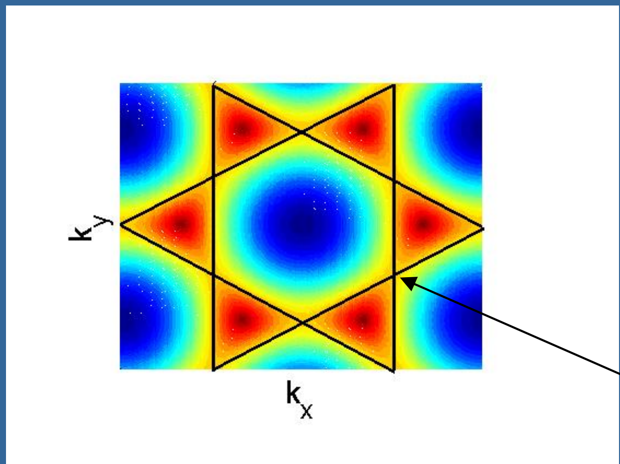


Dirac points topologically protected if some symmetries are preserved by interactions and disorder.

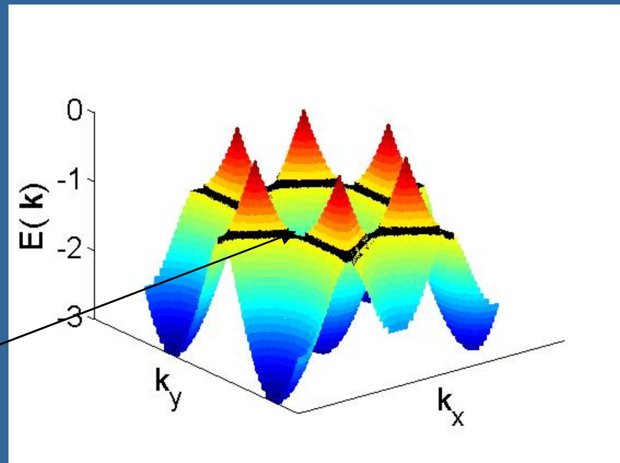
J. Mañes, F. Guinea, MAHV, PR B **75,** 155424 (07).

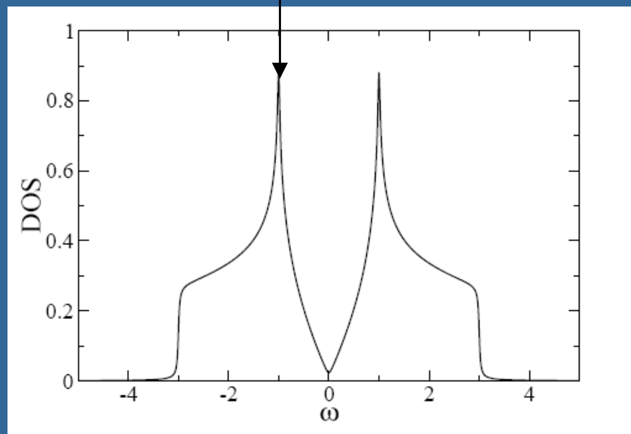
Other interesting points of the dispersion relation

$$\varepsilon^0(\mathbf{k}) = \pm t\sqrt{1 + 4\cos^2\frac{\sqrt{3}}{2}ak_x + 4\cos\frac{\sqrt{3}}{2}ak_x\cos\frac{3}{2}ak_y}\ ,$$



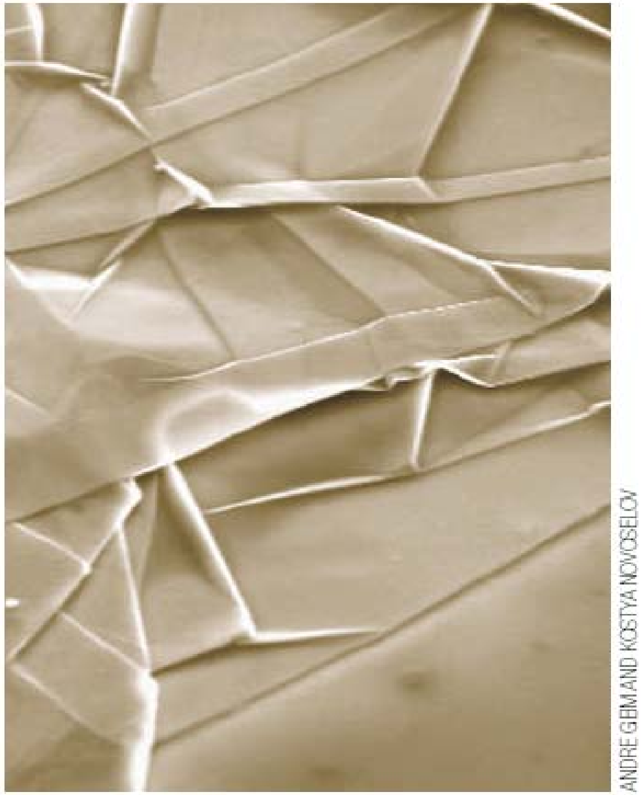
VHs





See poster by A. Cortijo, B. Valenzuela and MAHV

Structural properties



Graphene thrown on a silicon wafer like a veil of silk on a surface. More intriguing science seems to be hiding within the weave of this carbon sheet.

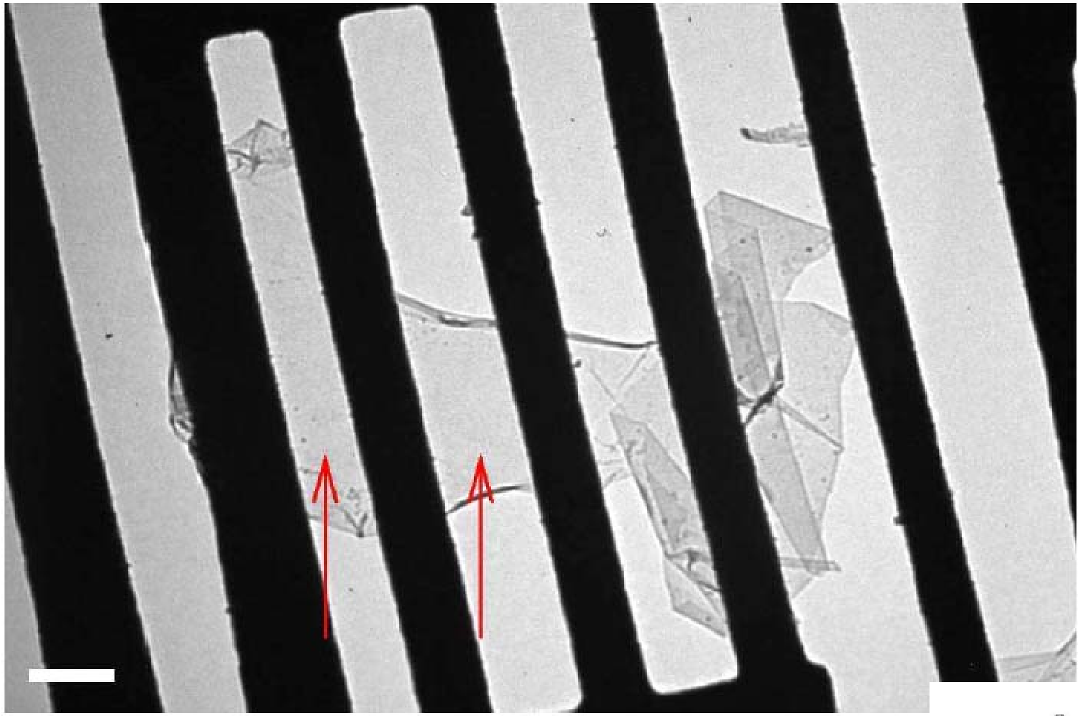
Nature Mat. **6** (2007)

Puzzling:

- A 2D crystal is exotic enough.
  Mechanical: very high Young moduls (TPa).
- Some TEM experiment show defects forming and disappearing (membrane?)
- It has a rippled structure. 2D curvature can only be provided by topological defects.

The most misterious aspect of graphene

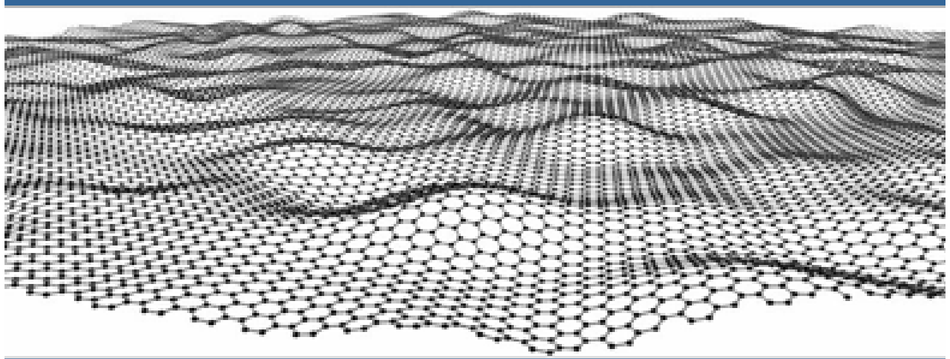
Ripples on graphene

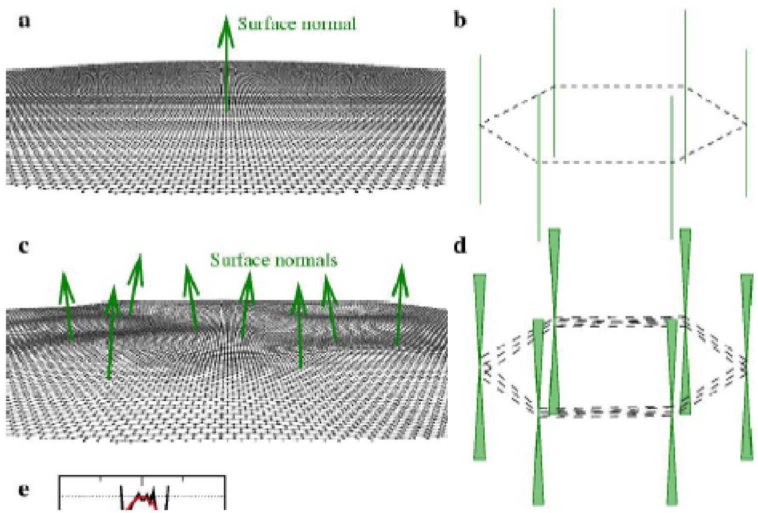


Freely suspended graphene membrane is partially crumpled

J. C. Meyer et al, Nature 446, 60 (2007)

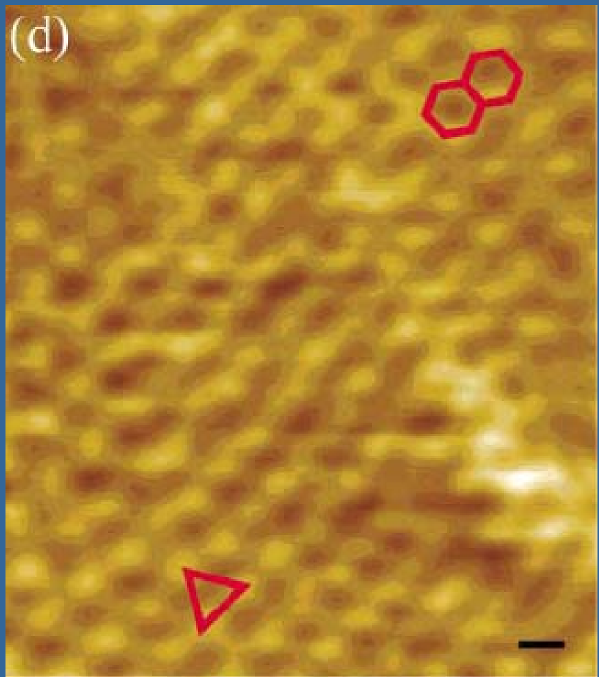
TEM
Ripples of height 0.5 nm and 5nm of lateral size adjust best the data



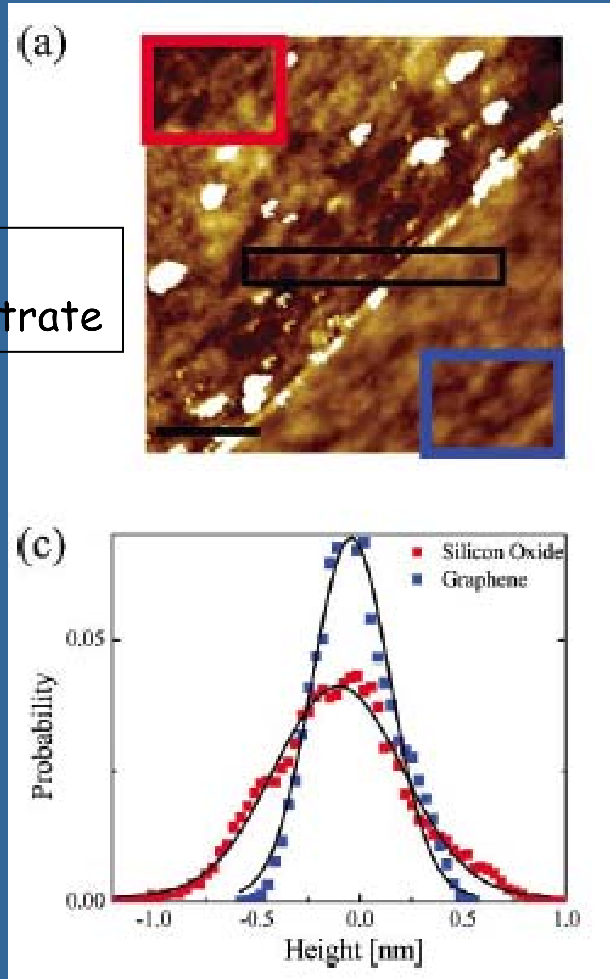


STM

Atomic Structure of Graphene on SiO_2



Boundary
graphene-substrate



Masa Ishigami et al,
Nanoletters 7, 1643 (07)

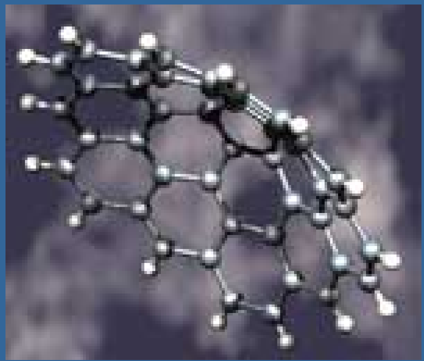
The structure of graphene seems
to follow the morphology of the substrate.

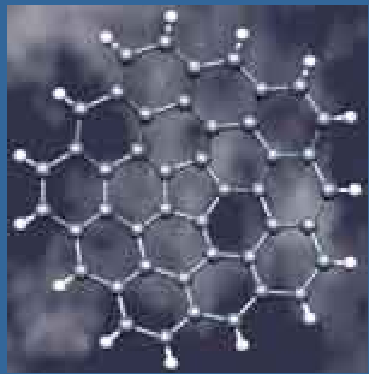
Physical origin of the curvature

- Elastic fluctuations (very unlikely).
- Interaction with the substrate –observed, but ripples are also observed in suspended samples-.
- Topological defects. Present in previous graphene-like structures (nanotubes, fullerenes and damaged graphite).

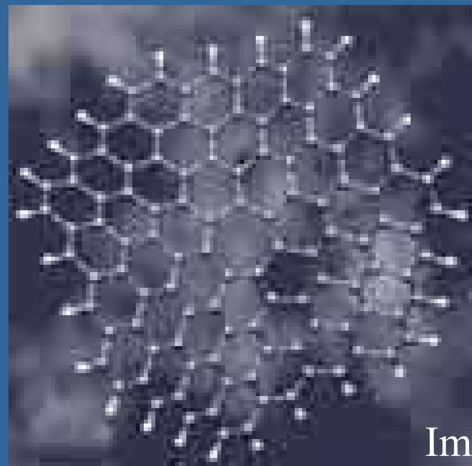
We will take curvature as a matter of fact and study its physical consequences.

Topological disorder in graphene



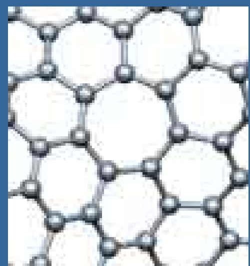


Topological defects are formed by replacing a hexagon by a n-sided polygon



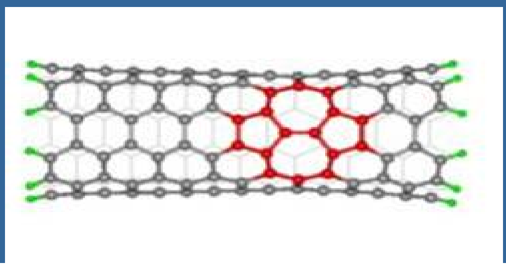
Images: C. Ewels

Pentagon: induces positive curvature



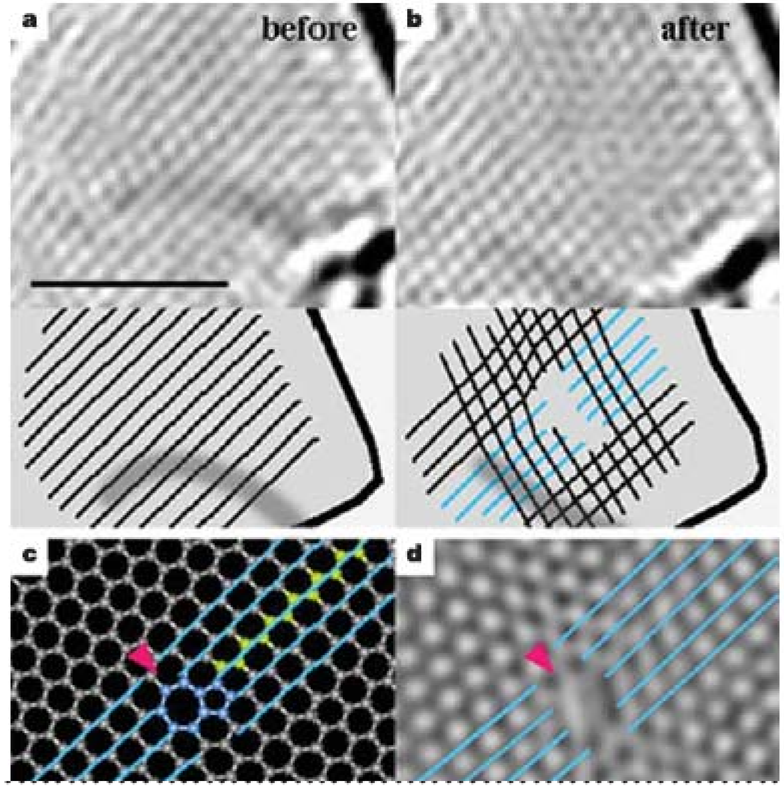
Heptagon: induces negative curvature

The combination of a pentagon and an heptagon at short distances can be seen as a dislocation of the lattice.



The most common defects in nanotubes are made by pentagons, heptagons, and pairs of them (Stone-Wales defects)

Observation of topological defects in graphene



Direct evidence for atomic defects in graphene layers

Ayako Hashimoto[1], Kazu Suenaga[1], Alexandre Gloter[1,2], Koki Urita[1,3] & Sumio Iijima[1]

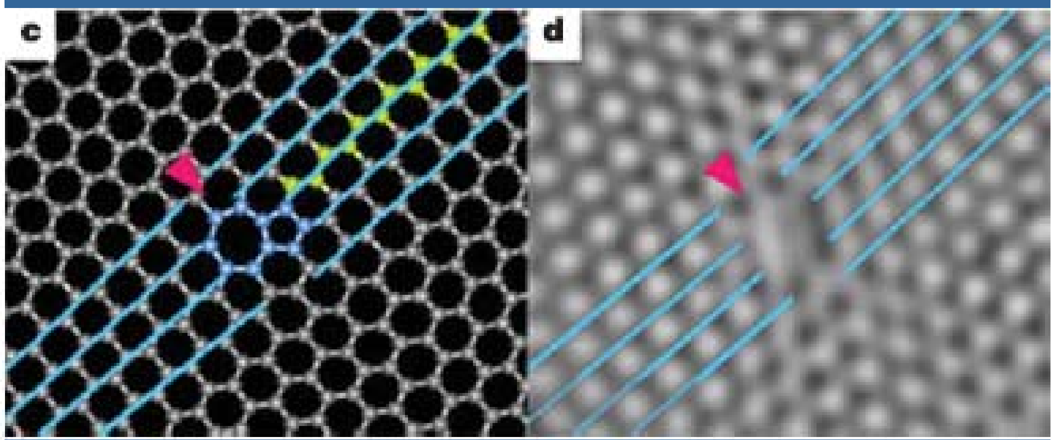
Nature 430 (2004)

model of the pentagon–heptagon pair in the graphitic network. **d**, A simulated HR-TEM image shows a good comparison with the HR-TEM image shown in **b**. Scale bar, 2 nm.

In situ of defect formation in single graphene layers by high-resolution TEM.

Defects must be present in all graphene samples and have a strong influence on the electronic properties

Vacancies
Ad-atoms
Edges
Topological defects



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Vol. xx, No. x
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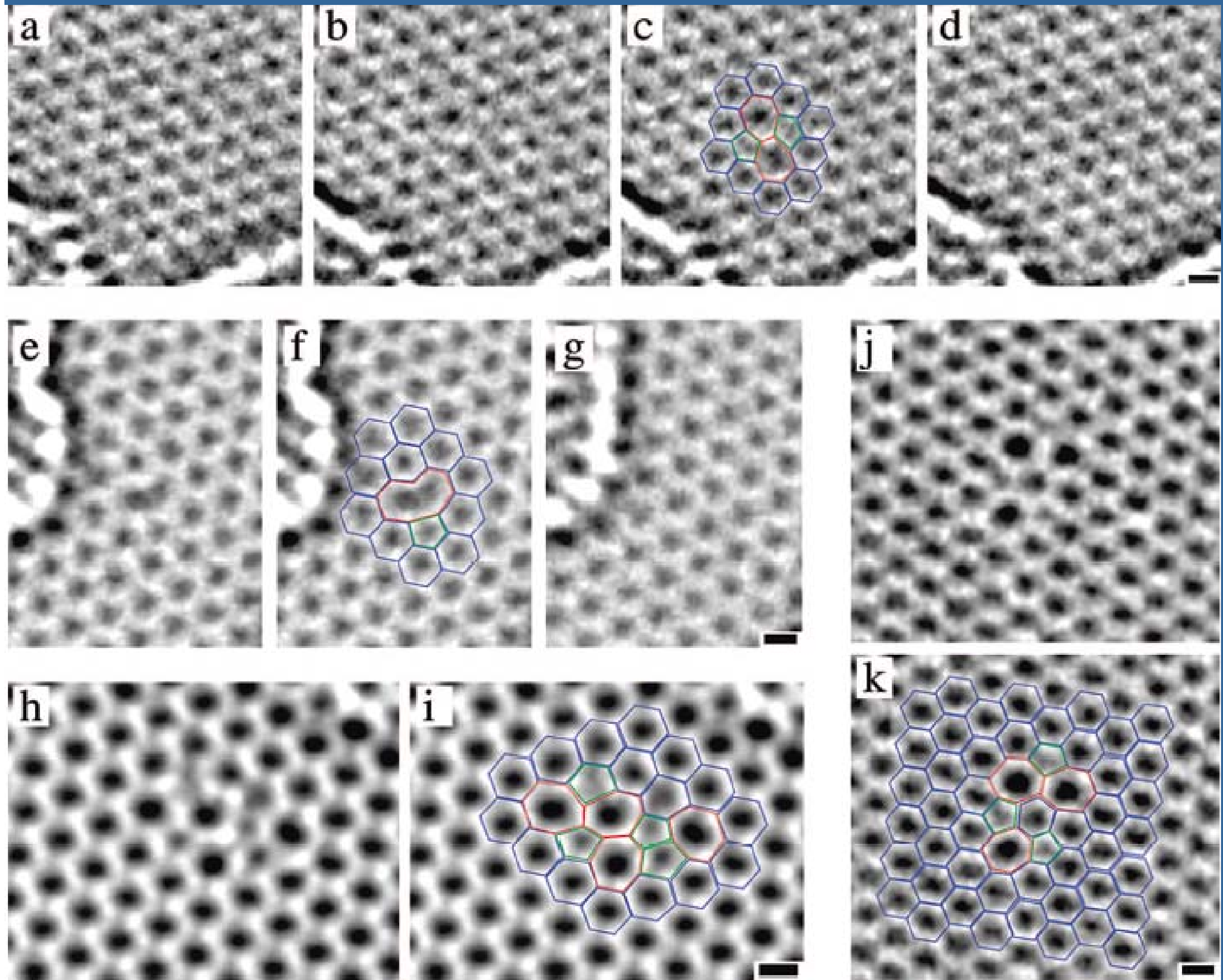
Direct Imaging of Lattice Atoms and Topological Defects in Graphene Membranes

Jannik C. Meyer,[†] C. Kisielowski,[‡] R. Erni,[‡] Marta D. Rossell,[‡] M. F. Crommie,[†] and A. Zettl*,[†]

Received May 14, 2008

TEM

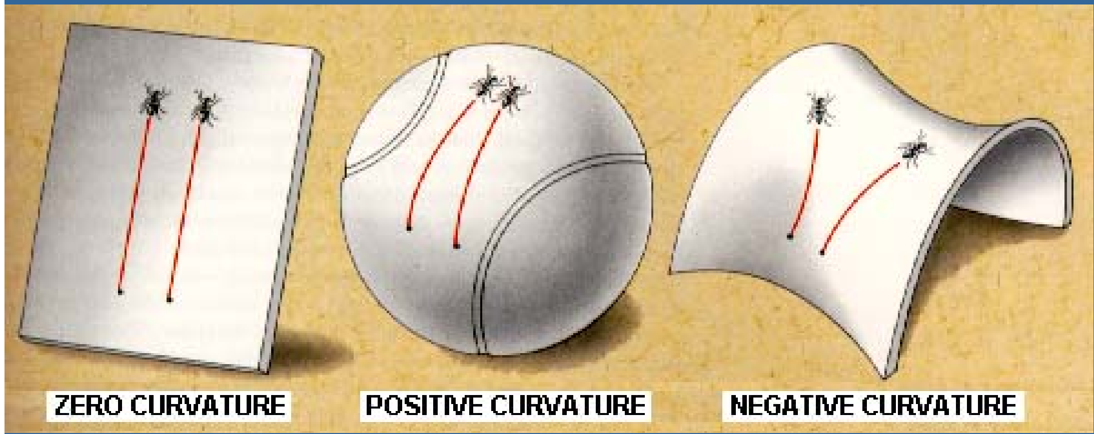


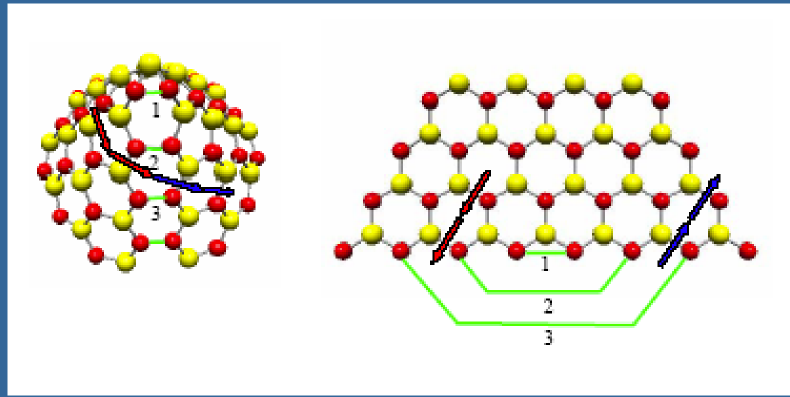
- SW unstable: they anneal to the perfect lattice in ~4 s (c,d).
- Pentagon-heptagon defects are found to last ~ 8s (i,k).
- No strain in the samples.

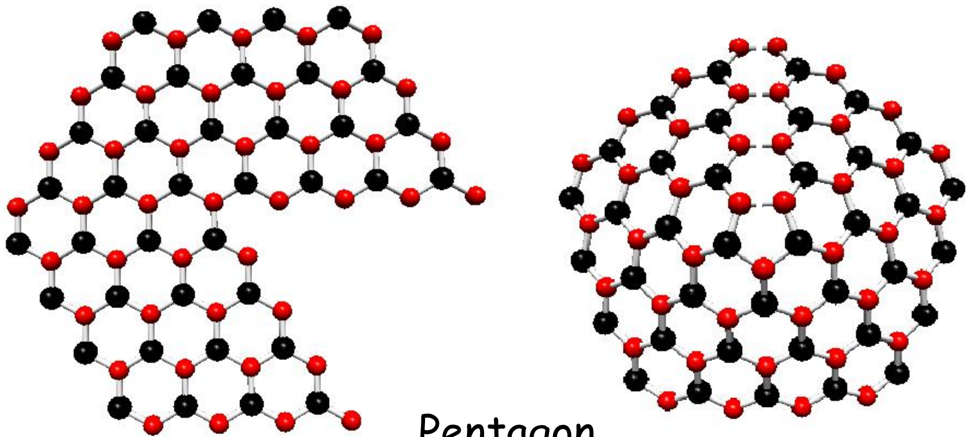
Flat samples behave very different from CNT or fullerenes.

???

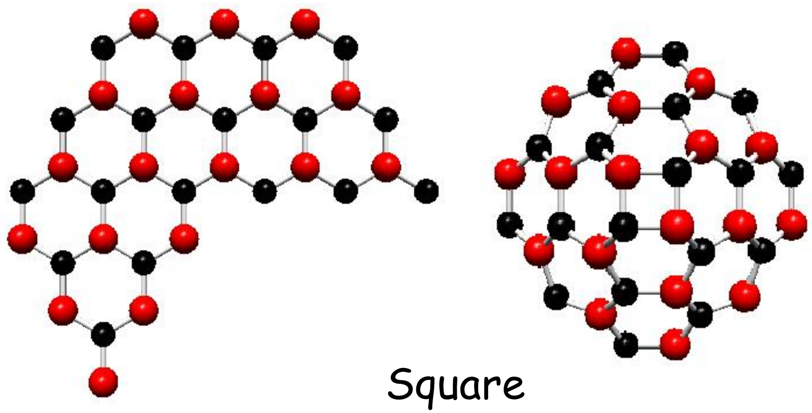
Formation of topological defects







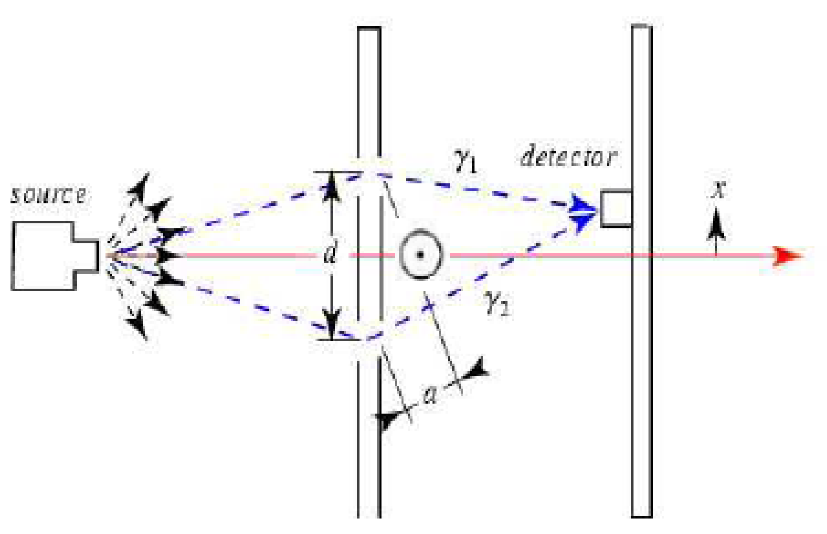
Pentagon



Square

Odd-membered rings frustrate the sublattice structure

The model for a single disclination



The Bohm-Aharonov effect

J. González, F. Guinea, and M. A. H. V., Phys. Rev. Lett. 69, 172 (1992)

$$\Psi_1 = \Psi_1^0 e^{-iS_1/h} \quad , \quad \Psi_2 = \Psi_2^0 e^{-iS_2/h}$$

$$(S_1 - S_2) = \frac{e}{c} \oint A.dx = \frac{e}{hc} \phi_0$$

A gauge potential induces a phase in the electron wave function

An electron circling a gauge string acquires a phase proportional to the magnetic flux.

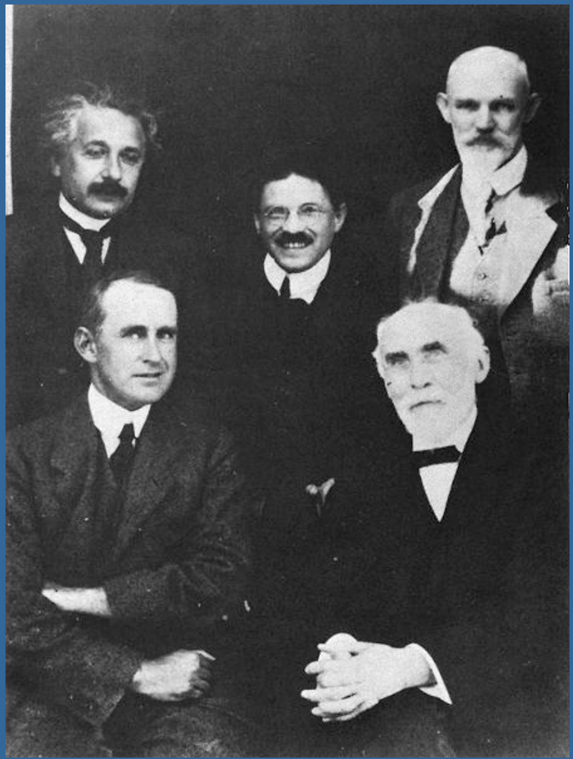
Invert the argument: mimic the effect of the phase by a fictitious gauge field

$$H = \vec{\sigma}.(\vec{p} + ie\vec{A})$$

With this we only take care of the "holonomy"

Dirac in curved space

We can include curvature effects by coupling the Dirac equation to a curved space



$$\gamma^a e_a^\mu \left(\partial_\mu - \Omega_\mu(x)\right)\psi = E\Psi$$

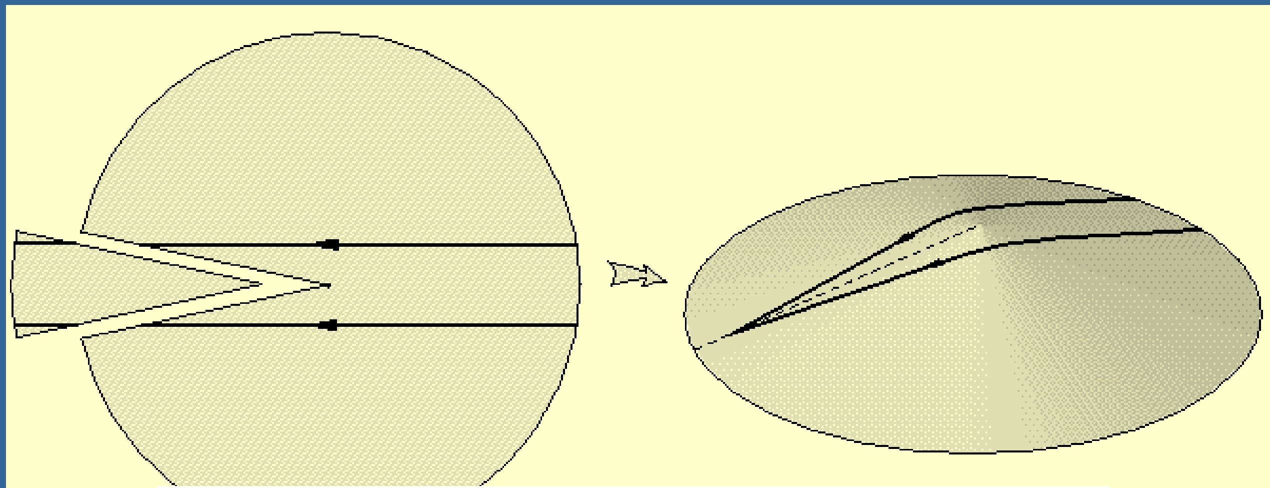
Need a metric and a "tetrad".

$$e_\mu^a e_\nu^b \eta_{ab} = g_{\mu\nu}$$

Generate r-dependent Dirac matrices and an effective gauge field.

$$\Omega_\mu = \frac{1}{4}\gamma^a \gamma^b e^\nu{}_{a;\mu} e_{b\nu}$$

The metric for topological defects: Cosmic strings

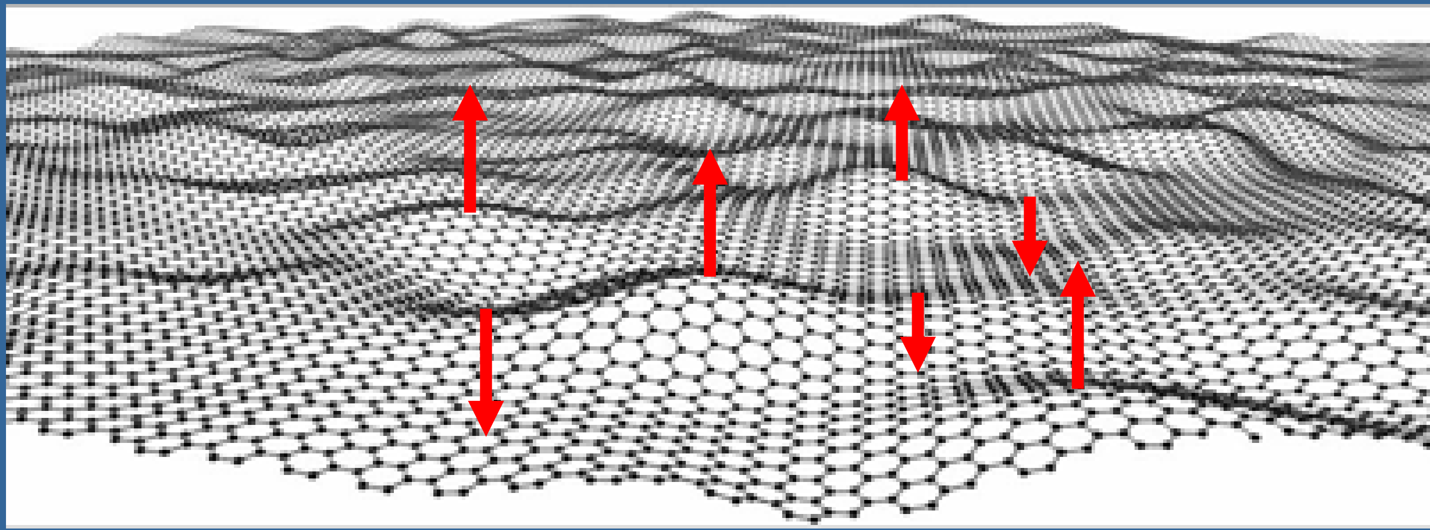


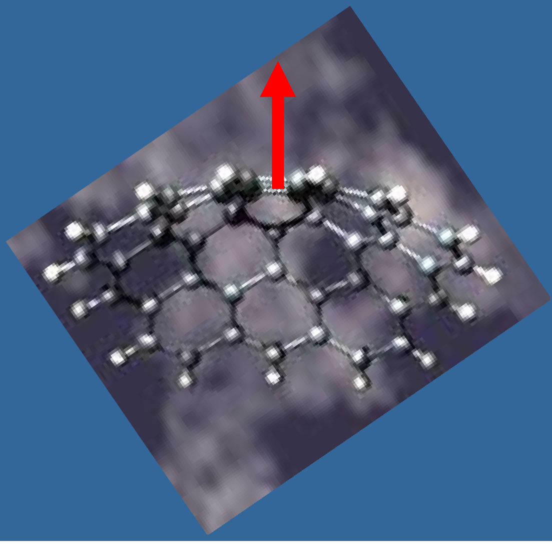
Conical spacetime around a cosmic string.

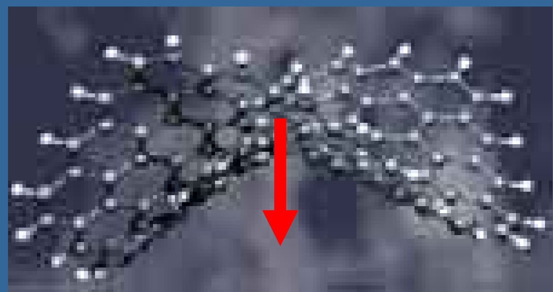
$$ds^2 = dt^2 - dz^2 - dr^2 - b^2\, r^2\, d\theta^2$$

With dt=dz=0 describes a cone. Not a big deal.

Multiple defects

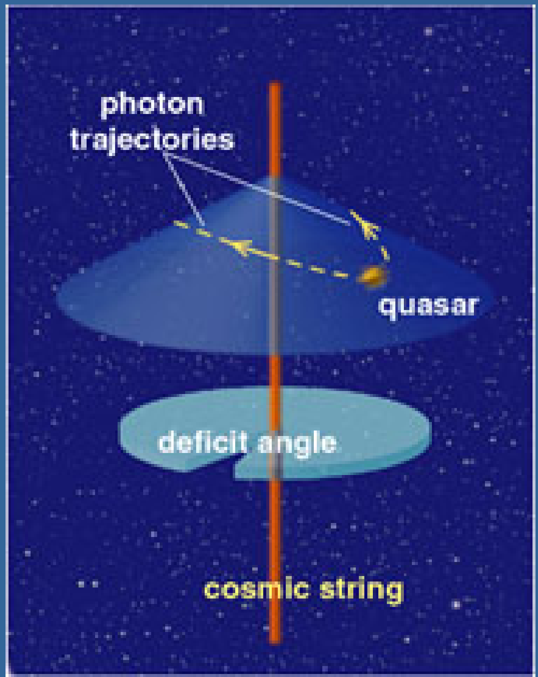






Generalization

A. Cortijo and MAHV,
EPL (07), Nucl. Phys. **B** (07).



Cosmic strings induce conical defects in the universe. The motion of a spinor field in the resulting curved space is known in general relativity.

Generalize the geometry of a single string by including negative deficit angles (heptagons). Does not make sense in cosmology but it allows to model graphene with an arbitrary number of heptagons and pentagons.

$$ds^2 = -dt^2 + e^{-2\Lambda(x,y)}(dx^2 + dy^2)$$

$$\Lambda(\mathbf{r}) = \sum_{i=1}^{N} 4\mu_i \log(r_i) \ , \quad r_i = \left[(x-a_i)^2 + (y-b_i)^2\right]^{1/2}$$

The metric of N cosmic strings located at $(a, b)_i$ with deficit (excess) angles μ_i.

Cosmology versus condensed matter

- G. E. Volovik: "The universe in a helium droplet", **Clarendon press, Oxford 2000.**
- Bäuerle, C., *et al*. Laboratory simulation of cosmic string formation in the early universe using superfluid ^{3}He. *Nature* **382**:332-334 (1996).
- Bowick, M., et al. The cosmological Kibble mechanism in the laboratory: String formation in liquid crystals. *Science* **236**:943-945 (1994).

We play the inverse game: use cosmology to model graphene

Effects of the curvature

The curved gamma matrices: $\gamma^{\mu}(r) = \gamma^{a} e_{a}^{\mu}(r)$

- Can be seen as a position-dependent Fermi velocity

The spin connection

- It can be seen as an effective gauge field with a matrix structure. Geometrical: σ_3.
- It has opposite signs at the two Fermi points (unlike a real magnetic field).

Extra gauge fields:

In the case of topological defects (pentagons, heptagons) other gauge fields arise due to topology and lattice effects.

Computation of observables

Equation for the Dirac **propagator** in curved space.

$$i\gamma^{\mu}(\mathbf{r})(\partial_{\mu}-\Omega_{\mu})G(x,x')=\frac{1}{\sqrt{-g}}\delta^{3}(x-x')$$

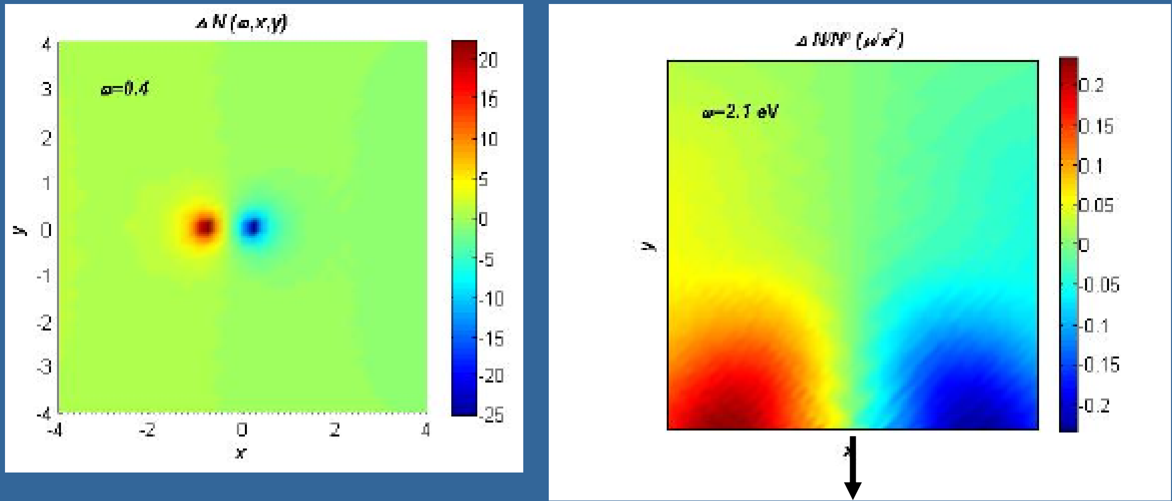
Curved gamma matrices

Gauge field.
It has a matrix structure

Covariant delta function

Expand around flat space and rewrite at first order as flat in an effective potential

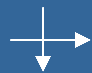
Several defects at fixed positions

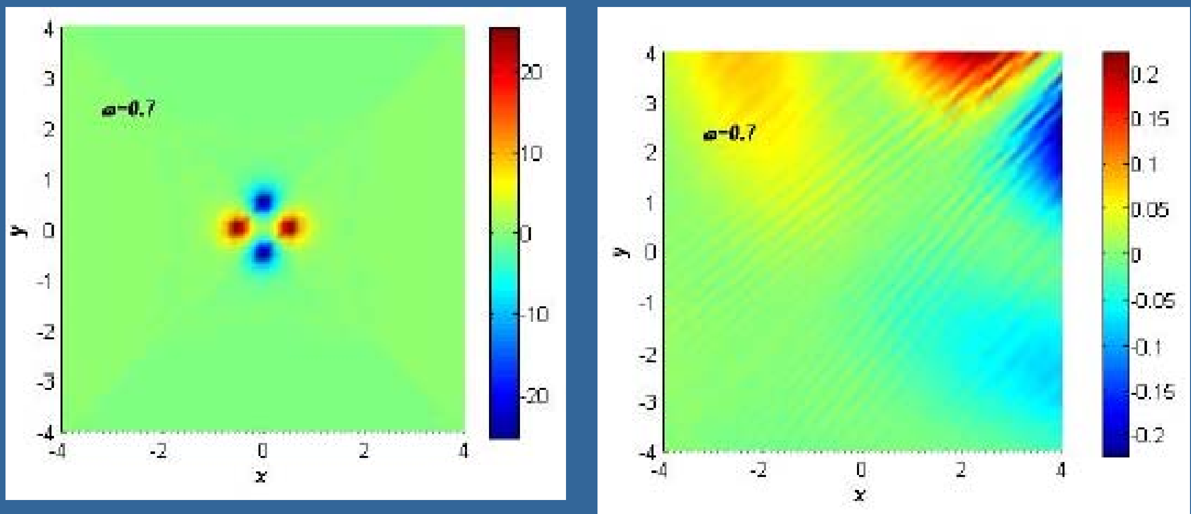


Local density of states around a hept-pent pair

Pentagons (heptagons) attract (repel) charge.

Pentagon-heptagon pairs act as dipoles.





Local density of states around a Stone-Wales defect

Averaging over disorder

A. Cortijo and M.A.H V , arxiv 0709.2698 .

Topological defects induce long range correlated disorder. The effective potential:

$$V = \underbrace{i\eta\Lambda(r)\bar{\psi}\gamma^i\partial_i\psi}_{V_1} \underbrace{-i\tfrac{\eta}{2}(\partial_i\Lambda(r))\bar{\psi}\gamma^i\psi}_{V_2}$$

from the curved gamma matrices

from the spin connection

It can be argued that V has the following variance:

$$\langle V_i(q)V_j(-q)\rangle = \delta_{ij}\frac{n}{q^2}$$

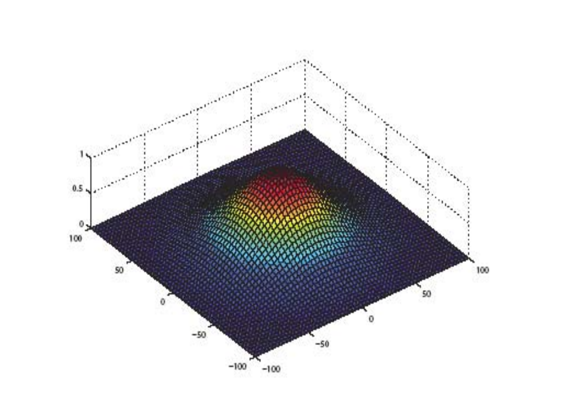
n=density of disorder

$$\sigma(\omega=0) = \frac{8e^2}{h}\left(\frac{4}{3\pi g}\right)$$

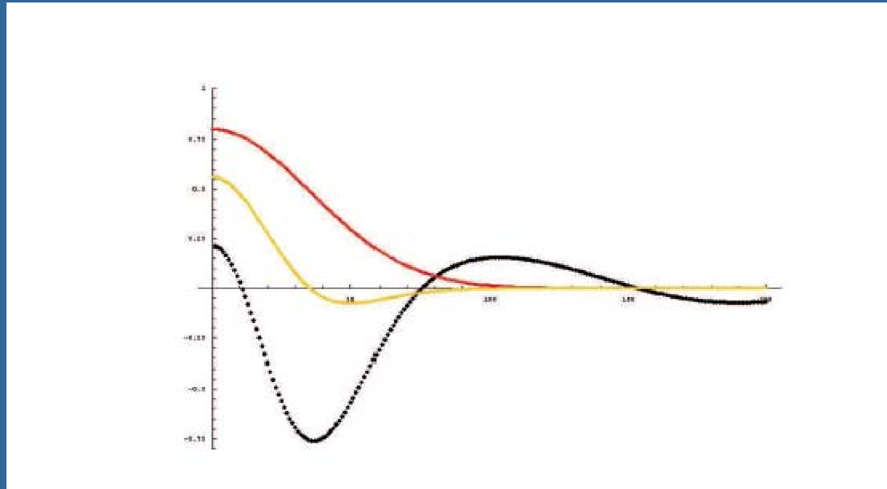
Modeling smooth ripples

F. de Juan, A. Cortijo, MAHV
PRB76, 165409 (2007).

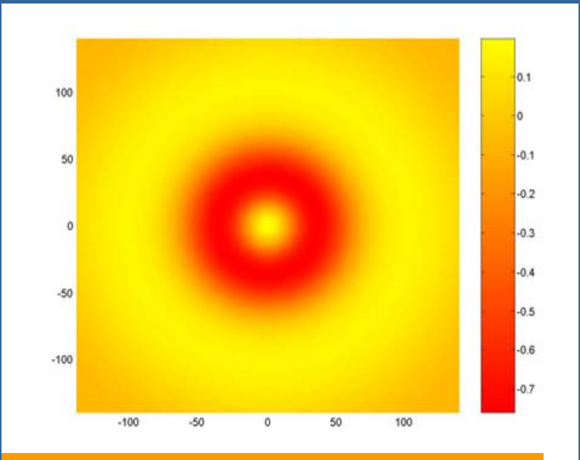
Coming from substrate



$$z(r) = A\exp\left(-\mathrm{r}^2/b^2\right)$$



LDOS vs. curvature and shape



Correction to the LDOS

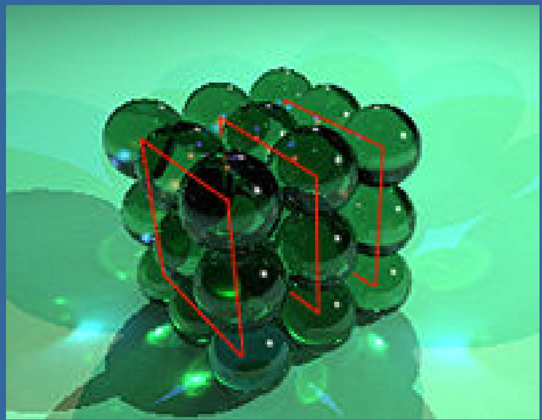
The correction to the LDOS follows the curvature of the bump and has a maximum at the inflection point

$$v_r(r) = \frac{1}{\sqrt{1 + z'(r)^2}}$$

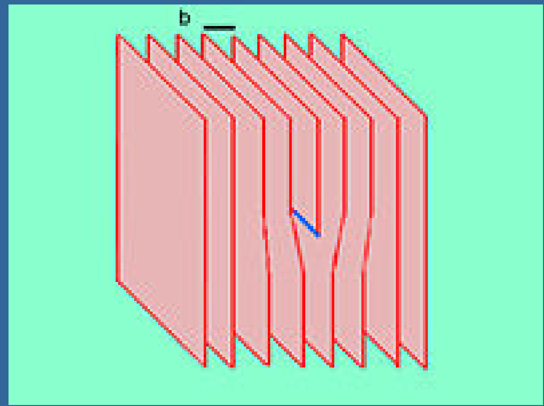
Dislocations in crystals

Characterized by the Burgers vector **b**

3D

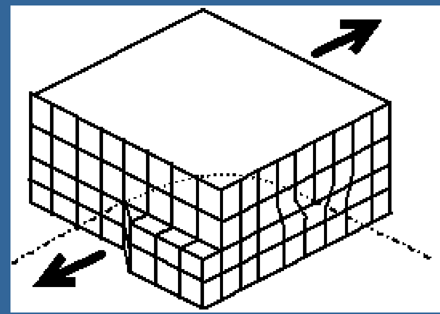


Crystal structure



Edge dislocation

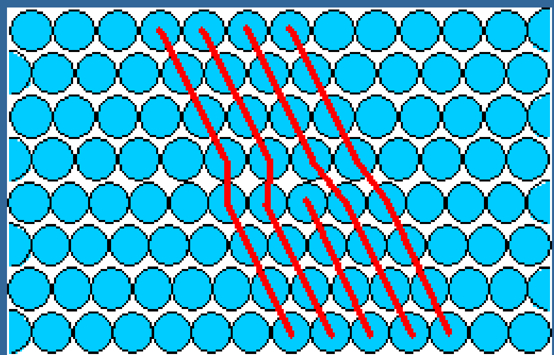
$\vec{b} \perp \vec{t}$

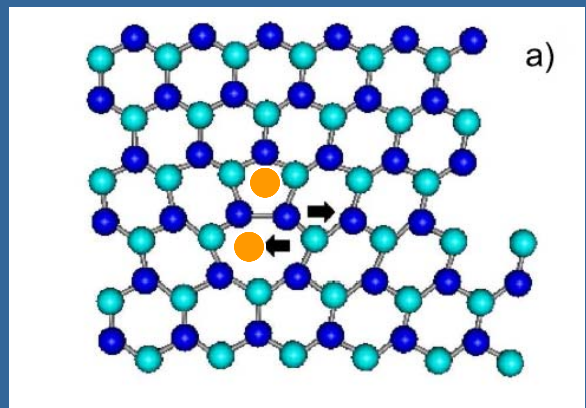


Screw dislocation

$\vec{b} \parallel \vec{t}$

2D





Geometrical description?

Gauge theory of linear defecs in solids: metric approach to elasticity

M.O. Katanaev and I.V. Volovich, Ann. Phys. (N.Y.) 216 (1992) 1

V.A. Osipov, Phys. Lett. A 175 (1993) 65; Physica A 175 (1991) 369

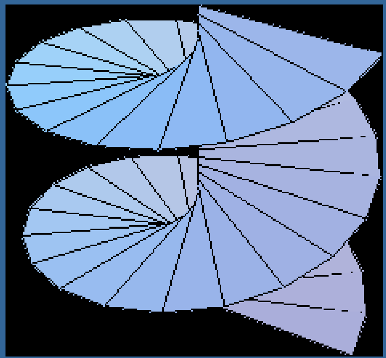
C. Furtado, F. Moraes, Physics Letters A 188 (1994) 394.

Elastic deformations	${R_{\mu\nu}}^{ij} = 0$	${T_{\mu\nu}}^{i} = 0$
Dislocations	${R_{\mu\nu}}^{ij} = 0$	${T_{\mu\nu}}^{i} \neq 0$
Disclinations	${R_{\mu\nu}}^{ij} \neq 0$	${T_{\mu\nu}}^{i} = 0$
Dislocations and disclinations	${R_{\mu\nu}}^{ij} \neq 0$	${T_{\mu\nu}}^{i} \neq 0$

H. Kleinert, Gauge fields in condensed matter, vol 2.

Dislocations can be described in the covariant formalism by adding torsion to the spacetime connection.

Torsion in differential geometry

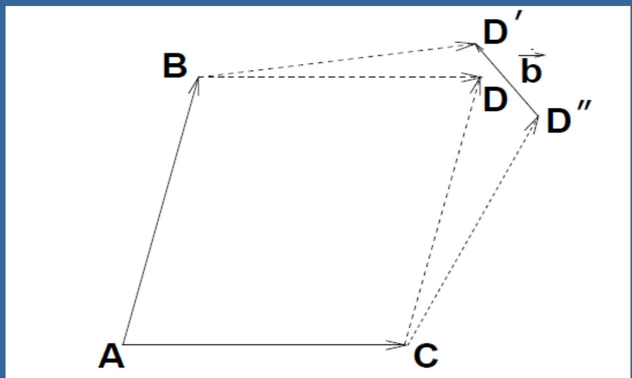


Basic buildings of geometry in manifolds:
Metric tensor
Covariant derivative (connection)

$$D_\mu v^\nu = (\partial_\mu + \Gamma^{\ \nu}_{\mu\rho}) v^\rho$$

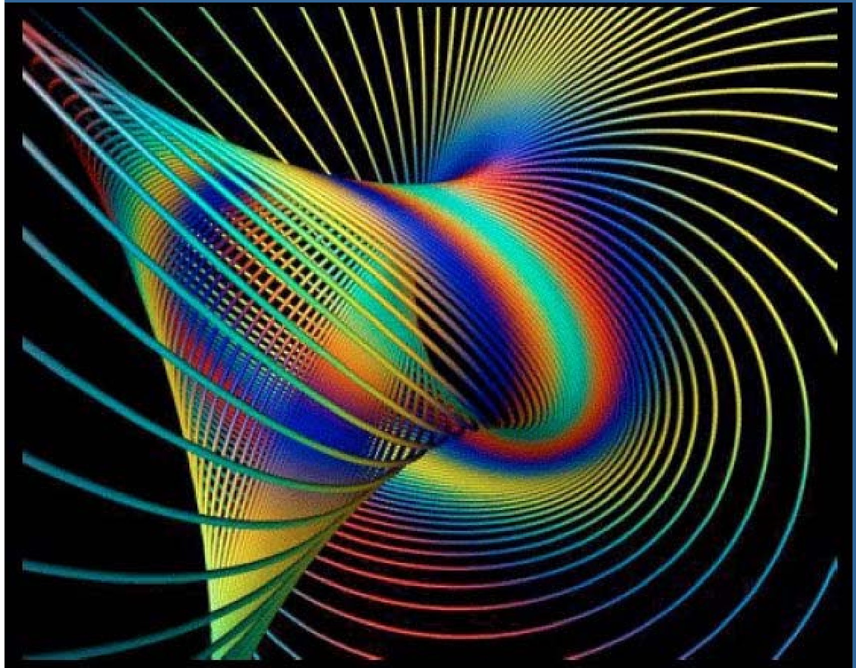
$$\Gamma^{\ \rho}_{\mu\nu} = \left\{ {\rho \atop \mu\nu} \right\} + T^{\ \rho}_{\mu\nu}$$

The derivative of a vector implies evaluating it at two different points.
The vector has to be parallel transported along infinitesimal path **dx**.



In spaces with torsion infinitesimal parallelograms do not close. Autoparallel and geodesics are not the same.

Torsion in General relativity



Torsion Field: Einstein's Metric Torsion Tensor allows a spin-field to twist spacetime.

Einstein-Cartan relativity

E. Cartan

$$G^{ij} = R^{ij} - \frac{1}{2}g^{ij}R^k_k \;\; = \kappa\Sigma^{ij},$$ [1]

The energy-momentum tensor of a spinor field is antisymmetric

$$\Sigma^{ij} = -\frac{\hbar c}{2}[(\nabla^i\bar{\Psi})\gamma^j\Psi - \bar{\Psi}\gamma^j\nabla^i\Psi],$$

and can not be included in [1]

Include a general connection with antisymmetric part (torsion).
Curvature couples to mass and torsion to spin.

Dirac fermions in curved space with torsion

$$L = \overline{\Psi}\gamma^{\mu}\left(\partial_{\mu} - \Omega_{\mu}(x))\Psi\right) + ig_{v}\overline{\Psi}\gamma^{\mu}T_{\mu}\Psi + g_{A}\overline{\Psi}\gamma_{5}\gamma^{\mu}S_{\mu}\Psi$$

$$\Omega_{\mu} = \frac{1}{4}\gamma^{a}\gamma^{b}e^{\nu}{}_{a;\mu}e_{b\nu}$$

$$T_{\rho} = g^{\nu}_{\mu}S^{\mu}{}_{\nu\rho} \quad , \quad \mathrm{S}_{\sigma} = \varepsilon_{\mu\nu\rho\sigma}S^{\mu\nu\rho}$$

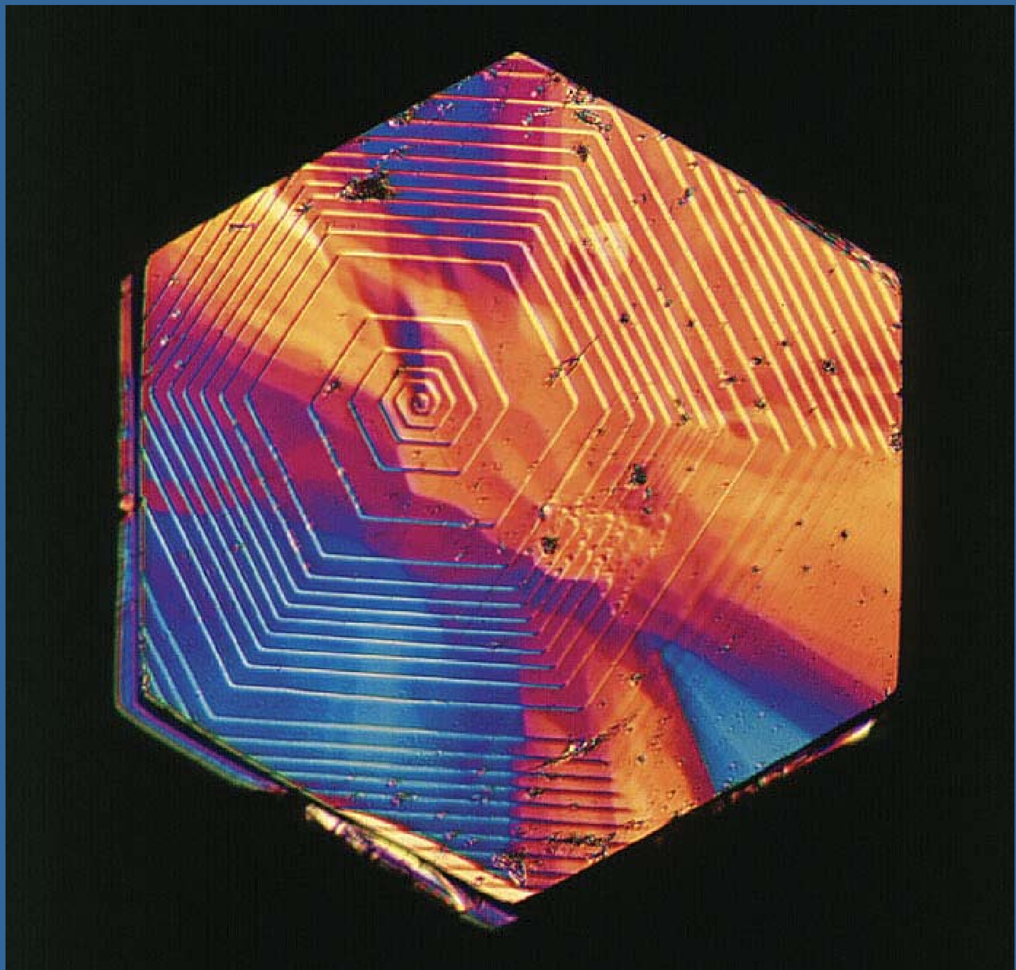
The trace part of the torsion is associated to edge dislocations –change in volume element - and couples as a usual vector gauge field.

The axial part associated to screw dislocations induces an axial coupling that affects the Berry phase of the fermions.

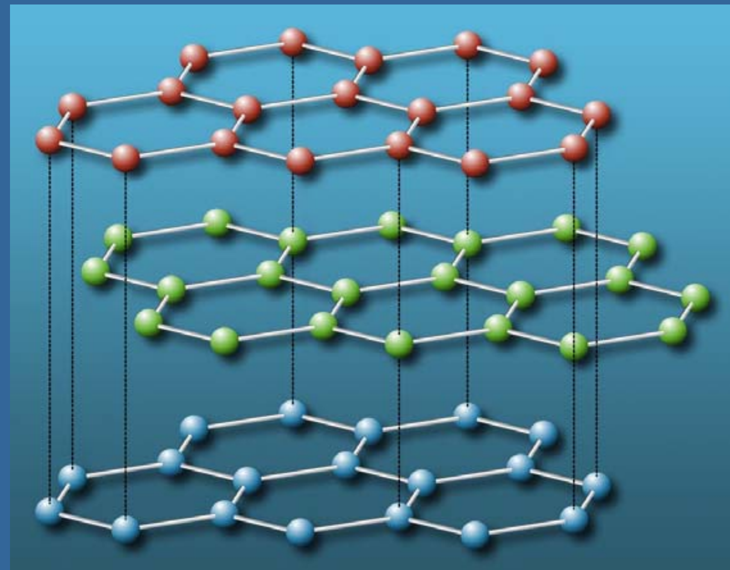
In a 2D surface (graphene) only edge dislocations can exist and their (non-minimal) coupling to the electronics degrees of freedom generates –yet another- standard vector gauge field.

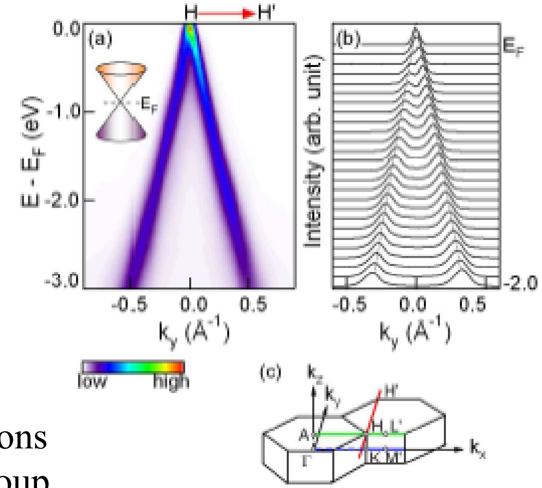
F. de Juan, A. Cortijo, MAHV, work in progress.

Other systems: 3D graphite



1.2 mm graphite crystal with spiral growth steps; etched from calcite.
Nomarski differential interference contrast imaging.
Valentine deposit, Harrisville, NY
John A. Jaszczak collection 1744a and photo 91-17.





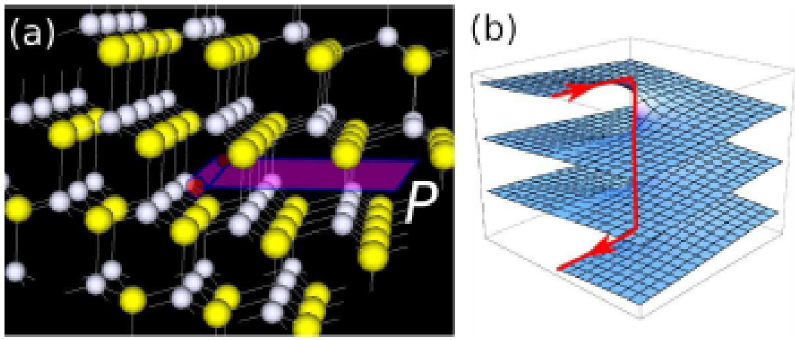
Dirac fermions
Lanzar's group
Nature Phys. 2, 595 (06).

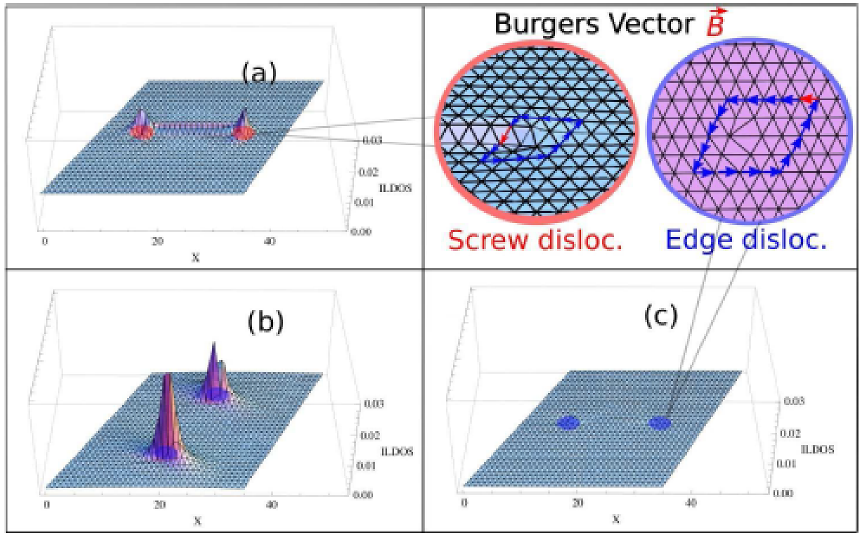
Similar models. Future.

Helical Metal Inside a Topological Band Insulator

arXiv:0810.5121

Ying Ran[1,2], Yi Zhang[1], and Ashvin Vishwanath[1,2]





304 Brazilian Journal of Physics, vol. 30, no. 2, June, 2000

Condensed Matter Physics as a Laboratory for Gravitation and Cosmology

Fernando Moraes

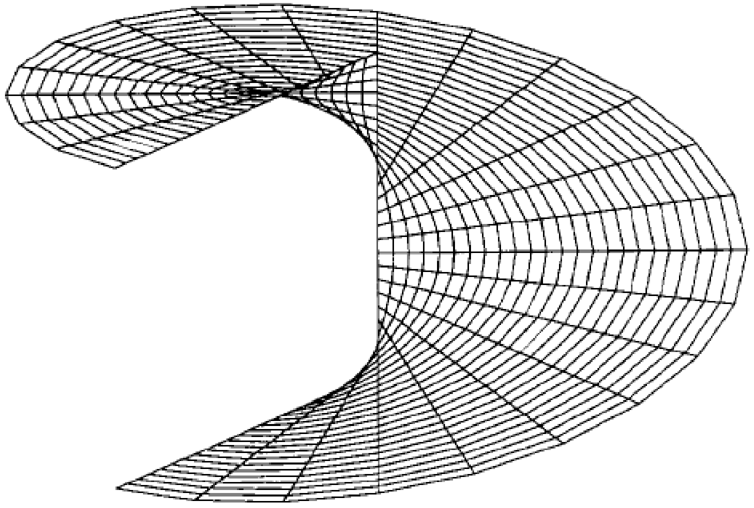


Figure 1. Screw Dislocation

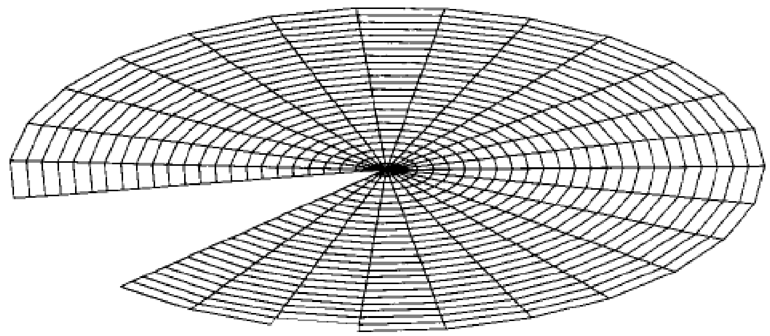


Figure 2. Disclination

Correction to the anomalous magnetic moment of electrons due to the defects.

Summary

- Ripples occur naturally in graphene
  either smooth (substrate) or induced by topological defects.

- Curved portions induce an effective gauge field
  and a space-dependent Fermi velocity.

- The LDOS oscillates within regions of the ripple's size. The correlations of morphology and electronics can be observed with local probes (STM) or ARPES.

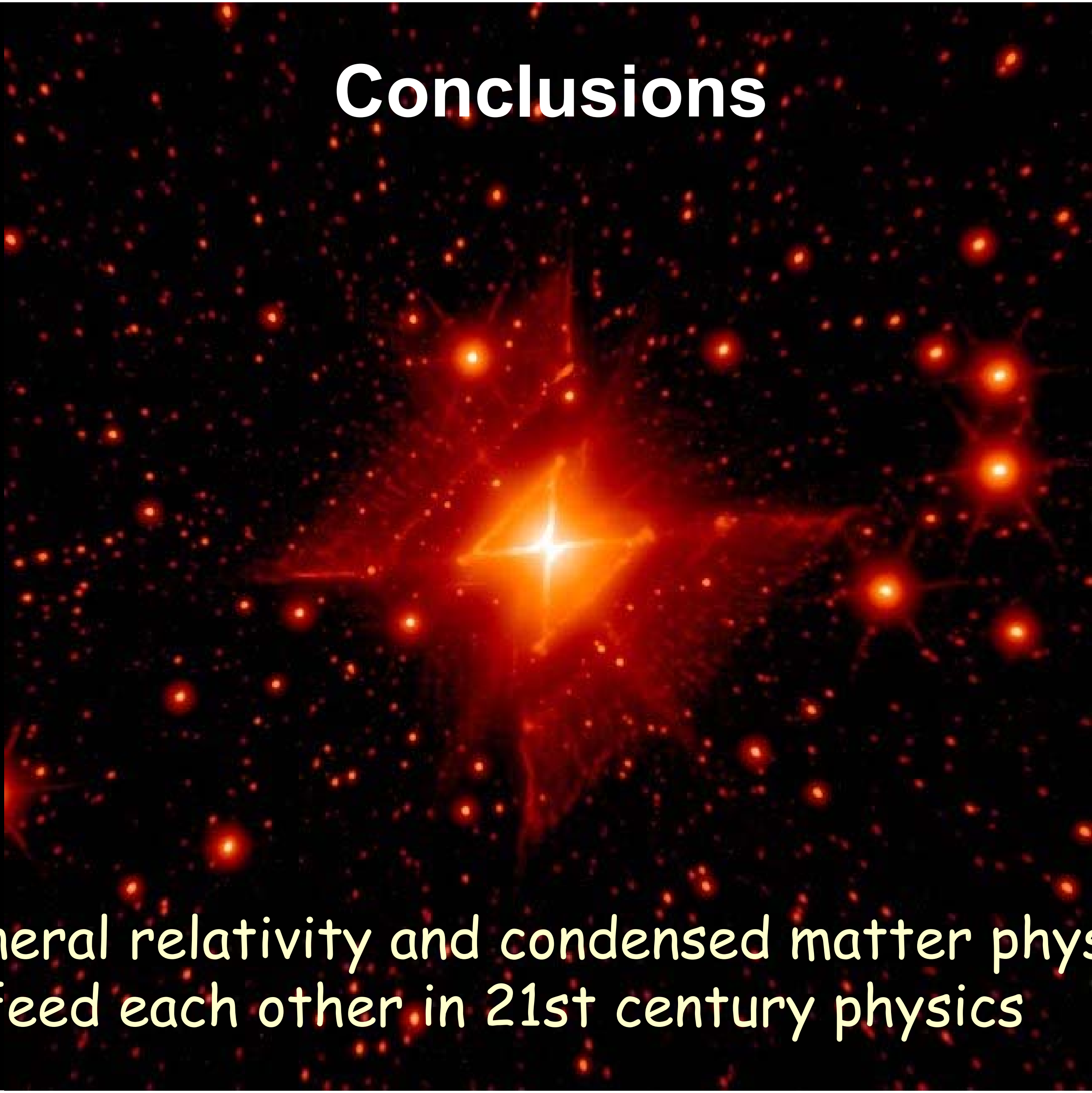
- The minimal conductivity induced by topological defects depends inversely on the density of disorder

- **Dislocations induce an pseudovector coupling that breaks T symmetry and can have a strong influence on the physical properties (Klein paradox, weak localization). In progress.**

Open problems

- The metric approach implies a concept of “spinors living in an external surface” which is not exactly how the model is obtained from tight-binding.
- (More technical): the equivalent to “weak field expansion” or how to define a perturbative paramenter in the topological case.
- Can we derive the geometrical factors from tight binding in “curved lattices”? (work in progress)
- If going to discrete curved lattice there are no-go theorems to put chiral fermions (lattice gauge theories).

Conclusions



General relativity and condensed matter physics feed each other in 21st century physics