Electronic properties of curved graphene sheets

Alberto Cortijo, María A. H. Vozmediano
Universidad Carlos III de Madrid-ICMM

Outline
2. Topological defects.
3. A cosmological model.
4. Effect on the density of states.
5. Summary and future.
Observation of topological defects in graphene

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

Vacancies
Ad-atoms
Edges
Topological defects

Direct evidence for atomic defects in graphene layers

Ayako Hashimoto¹, Kazu Suenaga¹, Alexandre Gioter¹,², Koki Urita¹,³ & Sumio Iijima¹

In situ of defect formation in single graphene layers by high-resolution TEM.
Observation of cones of various deficit angles

Graphitic cones and the nucleation of curved carbon surfaces


Transmission electron micrograph of the microstructures in the sample. Scale bar 200nm

Figure 3 a. Statistical distribution of the measured cone angles among the microstructures; b, averaged distribution centred at the seven possible disclinations. The open circles and dotted line represent the calculated Boltzmann distribution of microstructures for a temperature of 2,000°C and a pentagon energy of formation of 0.75 eV (ref. 19).
The cone morphologies, which are extremely rare in the mineral and material kingdom, can dominate the graphite surfaces.
Observation of a single pentagon in graphene

Single pentagon in a hexagonal carbon lattice revealed by scanning tunneling microscopy. B. An, S. Fukuyama, et. al.
Stone-Wales defect

- A 90 degrees local bond rotation in a graphitic network leads to the formation of two heptagons and two pentagons
- Static (dynamic) activation barrier for formation 8-12 (3.6) eV in SWCNs
In the pentagon road model pentagons are formed in seed structures in order to eliminate high-energy dangling bonds, and as an annealing mechanism to reduce the overall energy of the structure.

P. M. Ajayan et al., Phys. Rev. Lett. 81 (98) 1437

The second mechanism of the radiation defect annealing is the mending of vacancies through dangling bond saturation and by forming non-hexagonal rings and Stone-Wales defects.
Formation of topological defects

Fig. 1. (a) Formation of a $\pi/3$ wedge disclination and (b) a $-\pi/3$ wedge disclination. (a) Geodesic polygon around a $\pi/3$ disclination, and (b) that around a $-\pi/3$ disclination are also shown with bold lines. The points marked with A's and B's should be merged in each figure, so that the bold lines are closed.

Odd-membered rings frustrate the lattice.
The model for a single disclination

J. González, F. Guinea, and M. A. H. V.,

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

\[ (S_1 - S_2) = \frac{e}{c} \int A.dx = \frac{e}{hc} \phi_0 \]

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 reasonment: mimic the effect of the phase by a fictitious gauge field

\[ H = \vec{\sigma}.(\vec{p} + ie\vec{A}) \]
Substitution of an hexagon by an odd membered ring exchanges the amplitudes of the sublattices AB of graphene.

But it also exchanges the two Fermi points.

\[ \Psi_+ = \sum_{i \in \alpha} e^{i \mathbf{k} \cdot \mathbf{r}_i} a_i^+ |O\rangle \]

\[ \Psi_- = \sum_{i \in \alpha} e^{i \mathbf{k} \cdot \mathbf{r}_i} a_i^+ |O\rangle \]

\[ \mathcal{H}_\pm = \begin{pmatrix} 0 & \gamma \sum_j e^{i \mathbf{k} \cdot \mathbf{u}_j} \\ \gamma \sum_j e^{i \mathbf{k} \cdot \mathbf{v}_j} & 0 \end{pmatrix} \]

\[ \lim_{a \to 0} \mathcal{H}_+ / a = -\frac{3}{2} \gamma \sigma^T \cdot \delta k \bigg|_{k = (4\pi/3\sqrt{3})e_x} \]

\[ \lim_{a \to 0} \mathcal{H}_- / a = \frac{3}{2} \gamma \sigma^T \cdot \delta k \bigg|_{k = -(4\pi/3\sqrt{3})e_x} \]

Use a non-abelian gauge field

\[ \vec{A} = \vec{A}_\alpha T^\alpha \]

For a pentagon

\[ T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]
Different types of disorder

Disorder can be included in the system by coupling the electrons to random gauge fields.

- Theory of localization in two dimensions \( P. \, Lee, \, Ramakrishnan, \, RMP'85 \)
- Integer quantum Hall effect transitions \( Ludwig, M. \, Fisher, Shankar, Grinstein, \, PRB'94 \)
- Disorder effects in d-wave superconductors \( Tsvelik, Wenger \)

\[
H_{\text{dis}} = v_T \int d^2x \overline{\Psi}(x) \Gamma \cdot \mathbf{A} \Psi(x)
\]

Types of disorder: represented by the different possible gamma matrices.

\( \gamma_0 \) Random chemical potential
\( \gamma_{1,2} \) Random gauge potential
\( I \) Random mass

\( \gamma_5 \) Topological disorder \( \rightarrow \) New, associated to the graphite system.

The problem of including disorder and interactions is that CFT techniques can not be used.
**Topological disorder**. Substitute some hexagons by pentagons and heptagons.

Conical singularities: curve the lattice and exchange the A, B spinors.

**Model**: introduce a non-abelian gauge field which rotates the spinors in flavor space.

\[
\left( \begin{array}{c} \psi_A \\ \psi_B \end{array} \right) \quad \text{Isospin doublet} \quad A \equiv A^{(a)} \tau^{(a)} ; \quad \tau : \text{Pauli matrices}
\]

\[
A_\varphi = \frac{\varphi}{2\pi} \tau^{(2)} ; \quad \varphi = \frac{\pi}{2} ; \quad e^{i \oint A} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}
\]

GGV, Phys. Rev. B63, 13442 (01)

The combination of a pentagon and an heptagon at short distances can be seen as a dislocation vortex-antivortex pair.

Pentagon: disclination of the lattice.

Lattice distortion that rotates the lattice axis parametrized by the angle \( \theta(r) \). It induces a gauge field:

\[
A(r) = 3 \nabla \theta(r) \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} .
\]

Random distribution of topological defects described by a (non-abelian) random gauge field.

\[ \langle A(r), A(r') \rangle = \Delta \delta^2 (r - r') ; \]

\[ \Delta \text{ gives rise to a marginal perturbation which modifies the dimension of the fermion fields and enhances the density of states.} \]

**Short-range interactions enhanced.**
Inclusion of disorder in RG

Disorder can be included in the RG scheme by coupling the electrons to random gauge fields.

\[ H_{\text{dis}} = v_f \int d^2 x \overline{\Psi}(x) \Gamma \cdot \vec{A} \Psi(x) \]

\[ \langle A_\mu(x), A_\nu(y) \rangle = \Delta \delta^2(x-y) \delta_{\mu\nu} \]

\( A \)'s are random in space and constant in time

\[ \langle A(x) \rangle = 0 \]

Add new propagators and vertices to the model and repeat the RG analysis.

New diagrams at one loop

Affect the renormalization of the Fermi velocity, hence of \( g \).

Renormalize the disorder couplings.

[Diagrams showing new diagrams]

Electron propagator

Disorder line averaged

Photon propagator

T. Stauber, F. Guinea and MAHV, Phys. Rev. B 71, R041406 (05)
Phase diagrams

RG flow equations can be encoded into a single parameter $v_F$

$$\frac{d}{dl} v_F^{\text{eff}} = \frac{1}{16\pi} \left[ \frac{e^2}{v_F^{\text{eff}}} - \frac{\Delta}{2} \left( \frac{v_F^{\text{eff}}}{v_F^{\text{eff}}} \right)^2 \right]$$

Random chemical potential
$$\Gamma = \gamma^0 \rightarrow \nu_\mu = \nu_1 \text{ (const)}$$

Random vector field
$$\Gamma = \gamma \rightarrow \nu_A = \nu_F$$

Topological disorder (or random mass)
$$\Gamma = \gamma^5, \Gamma \rightarrow \nu_m = \nu_F^2 / \nu_3$$

Unstable fixed line
Divides the phase space in a strong and a weak coupling regime.

Line of fixed points

New, non-trivial interacting phases
Topological Disorder

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
Continuum model for the spherical fullerenes

Promediate the curvature induced by the (12) pentagons and write the Dirac equation on the surface of a sphere.

To account for the fictitious magnetic field traversing each pentagon put a magnetic monopole at the center of the sphere with the appropriate charge.

$$i\sigma^a\epsilon^\mu \left( \nabla_\mu - iA_\mu \right)\Psi_n = \epsilon_n \Psi_n \quad , \quad a, \mu = 1, 2$$

Spectrum

$$\epsilon_J = \frac{\hbar v_F}{R} \sqrt{J(J+1) - l(l+1)} \quad J \geq l$$

Solving the problem in the original icosahedron much more difficult. Want to model flat graphene with an equal number of pentagons and heptagons.
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.

Gravitational lensing: massive objects reveal themselves by bending the trajectories of photons.

Capodimonte Sternberg Lens Candidate N.1
Cosmology versus condensed matter


We play the inverse game: use cosmology to model graphene
The model

The metric of $N$ cosmic strings located at $(a_i, b_i)$ with deficit (excess) angles $\mu_i$.

$\Lambda(r) = \sum_{i=1}^{N} 4\mu_i \log(r_i)$,

$r_i = \left[ (x - a_i)^2 + (y - b_i)^2 \right]^{1/2}$

The local density of states

$N(\omega, r) = \text{Im} \text{Tr} S_F(\omega, r)$

The result:

$\delta N(\omega, r) = \frac{\mu}{2\pi^3 v_F^2} 2\omega \sum_{i=1}^{N} \int \frac{dk}{k} \frac{J_0(\omega r_i)}{k^2} (4\omega^2 - k^2) F(\omega, k)$

$F(\omega, r) = \begin{cases} 
-\text{atanh} \left( \frac{\sqrt{k^2 - 4\omega^2}}{\sqrt{k^2 - 4\omega^2}} \right), & 4\omega^2 < k^2 \\
\text{atan} \left( \frac{\sqrt{4\omega^2 - k^2}}{\sqrt{4\omega^2 - k^2}} \right), & 4\omega^2 > k^2
\end{cases}$
A single disclination

Even-membered rings

The total DOS at the Fermi level is finite and proportional to the defect angle for even membered rings.

Odd-membered rings break e-h symmetry. DOS(E_f) remains zero.

Odd-membered rings

The zero energy states are peaked at the site of the defect but extend over the whole space. The system should be metallic.

Electronic density around an even-membered ring

The Fermi velocity is smaller than the free: competition with Coulomb interactions.
Several defects at fixed positions

Pentagons (heptagons) attract (repell) charge.

Pentagon-heptagon pairs act as dipoles.

Local density of states around a hept-pent pair

Local density of states around a Stone-Wales defect
Evolution with the energy
Averaging over disorder

\[ S = \int d\vec{r} dt \bar{\Psi} iv_F (\gamma^\mu \partial_\mu) \Psi - \int d\vec{r} dt \bar{\Psi} iv_F (\Lambda(r) \nabla + \frac{1}{2} \gamma \nabla \Lambda(r)) \Psi \]

\[ < \Lambda(q) \Lambda(q') > = \frac{g}{q^2} \delta(q + q') \]

\[ < \nabla^i \Lambda(q) \nabla^j \Lambda(q') > = g \delta^{ij} \delta(q + q') \]

- unscreened singular interaction
- four-Fermi effective interaction
For small $\omega$, $\text{Im} \Sigma$ behaves as $\sim 1/\omega$.

For large $\omega$, the electron-electron interaction dominates, but is modified by the effective local interaction:

$$\text{Im} \Sigma \sim \left( \frac{e^4}{\varepsilon_0^2 v_F^2} - \frac{g}{4\pi} \right) \omega$$
Conclusions and future

• Topological defects occur naturally in graphite and graphene.

• They induce long range interactions in the graphene system.

• Single conical defects enhance the metallicity of the system.

• A set of defects give rise to characteristic energy-dependent inhomogeneities in the local density of states that can be observed with STM and can help to characterize the samples.

• Localization (or not) of the states around the defects.

• Influence on ferromagnetism: interplay of DOS and Fermi velocity renormalization. RKKY with a disordered medium.

• Universal properties of a random distribution of defects.
A living curiosity:

Cell Division Program
Sergei Fedorov (Moscow) and Michael Pyshnov (Toronto)

Surface of the epithelium of the villus.

FIG. 4. Rules of cell division. (a) Division in the hexagonal row between pentagons. Emergence of the new division wave (dashed lines), when two division waves (thin solid approach the same pentagon from adjacent cells (c) and from non-adjacent cells (e). (b), The corresponding areas after division; sister cells are connected with dots. Note that three cells have divided twice and correspondingly in (f) two cell generations are connected with dots.

Michael Pyshnov