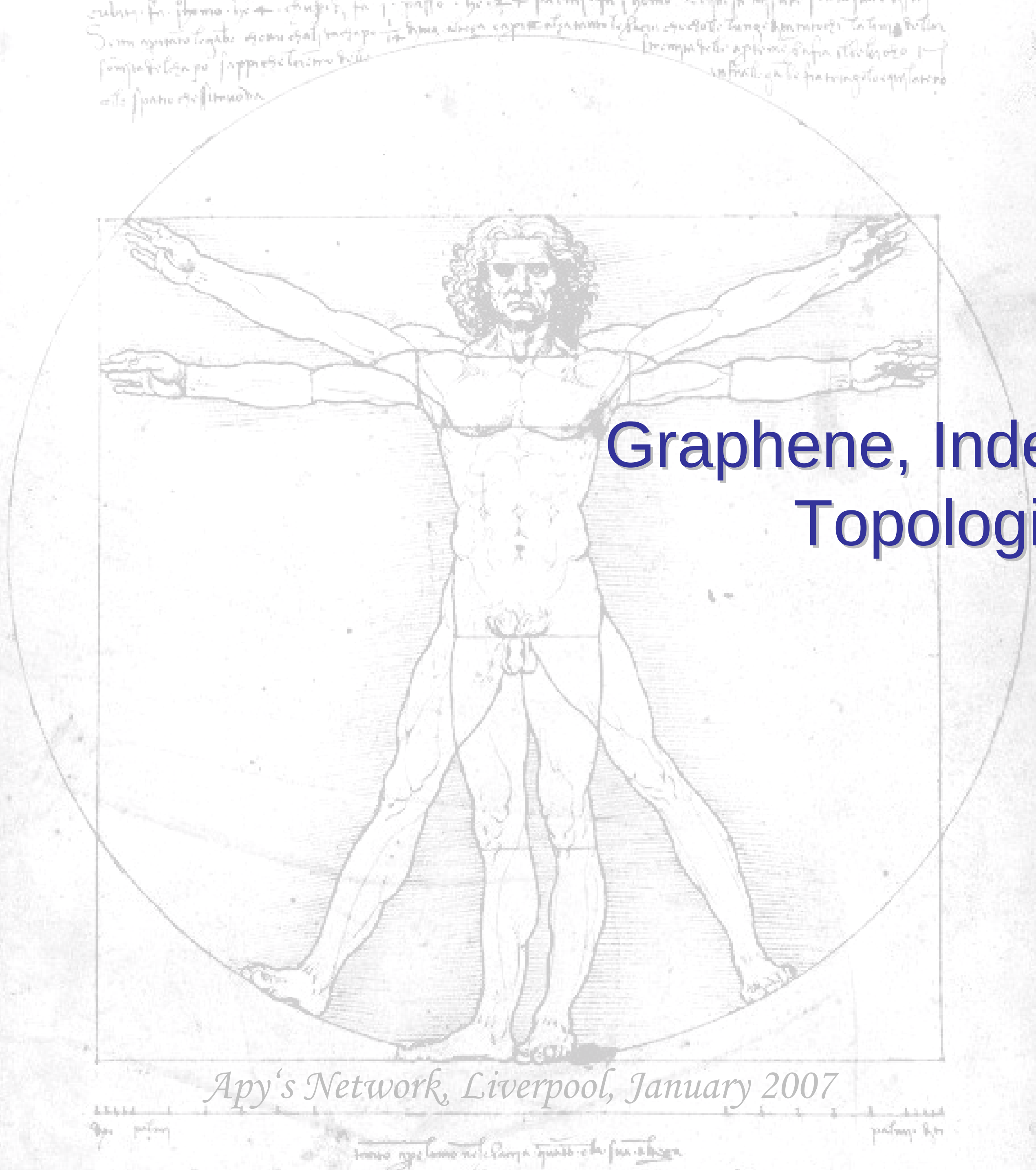

UNIVERSITY OF LEEDS

Graphene, Index Theorem and Topological Degeneracy

JKP

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cond-mat/0607394

Apy's Network, Liverpool, January 2007

THE ROYAL SOCIETY

Quantum Information, Physics and Topology

- **Encoding and manipulating QI** in small physical systems is pledged by **decoherence** and **control errors**.

- **Error correction** can be employed to resolve this problem by using a (huge) overhead of qubits and quantum gates.

- An alternative method is to employ **intrinsically error protected systems** such as **topological** ones => properties are described by integer numbers!

  protected by macroscopic properties: hard to destroy.

- E.g. you can employ system with **degenerate ground states**:

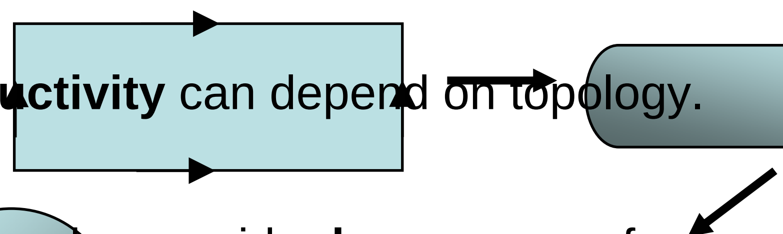
  - Make sure **degeneracy is protected by topological properties** (V)
  - Make sure degenerate states are **locally indistinguishable** (X)
  - Encode information in these **degenerate levels**

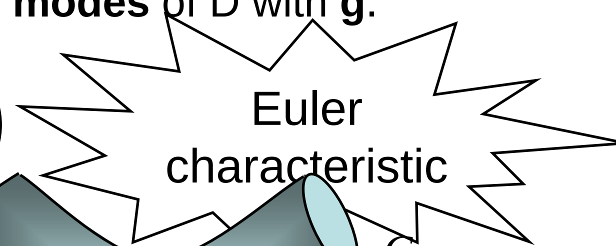
TOPOLOGICAL DEGENERACY

Overview

- **Graphene:** two dimensional layer of graphite –honeycomb lattice of C atoms
  - Fullerene: C60, C70
  - Nanotubes
- Conducting properties of these materials: zero energy modes.
- Can be used as miniaturized elements of circuits.

- **Index theorem** (Atiyah-Singer)
  - Smooth, orientable, compact, Riemannian manifolds, M, with genus, **g.**
  - Define elliptic operator **D** on M. Includes curvature and gauge fields.
  - The **index theorem** relates the **number of zero energy modes** of D with **g**.



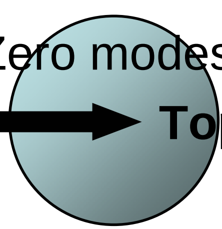


- **Conductivity** can depend on topology.

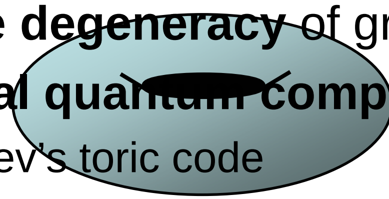
- Zero modes provide **degeneracy** of ground state: G zero modes → 2^G deg.

→ **Topological quantum computation**

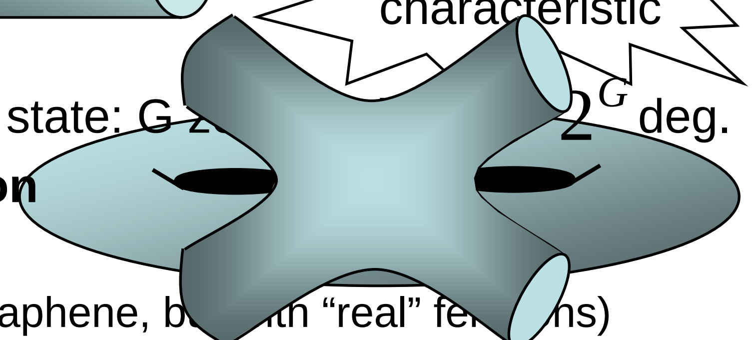
- Kitaev's toric code
- Honeycomb lattice (same as graphene, but with “real” fermions)



g=0



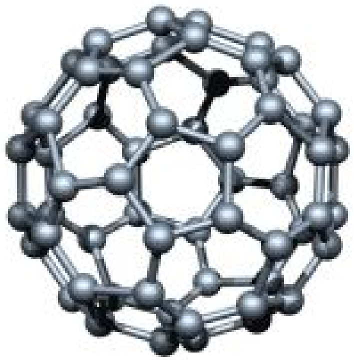
g=1

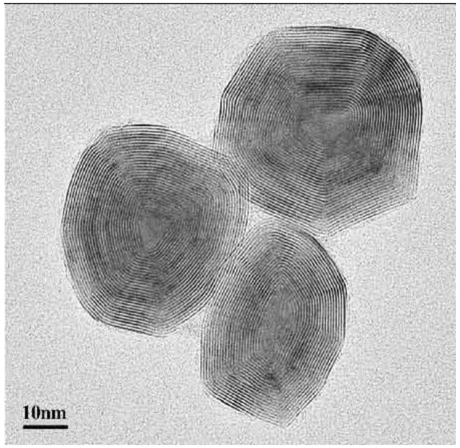


g=2

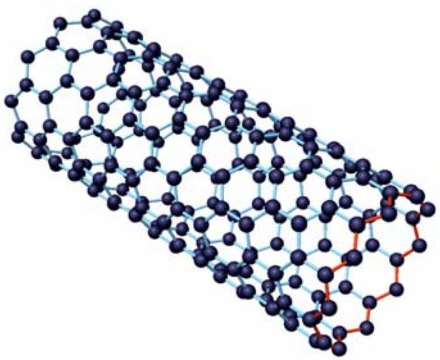
Different geometries of Graphene

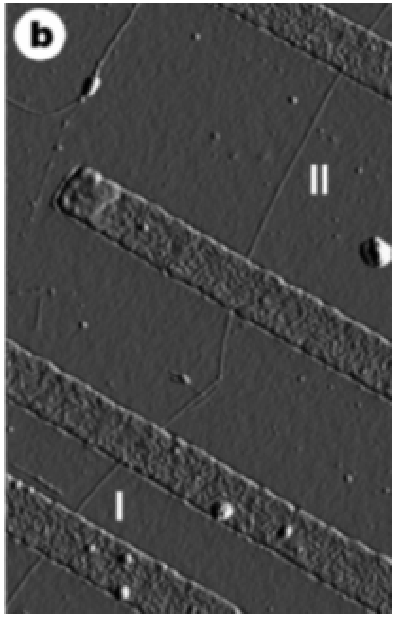
Fullerene (C60):

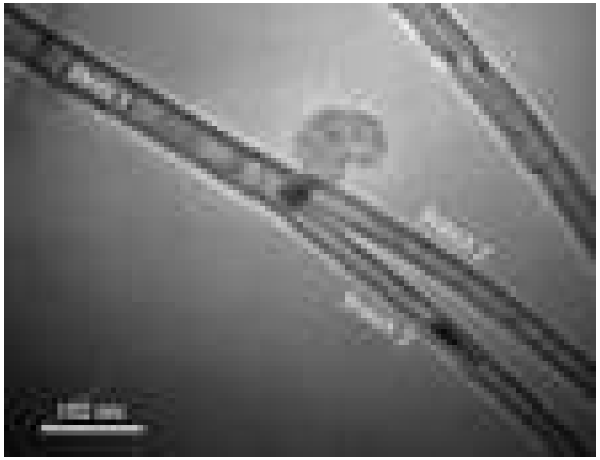




Nanotubes:

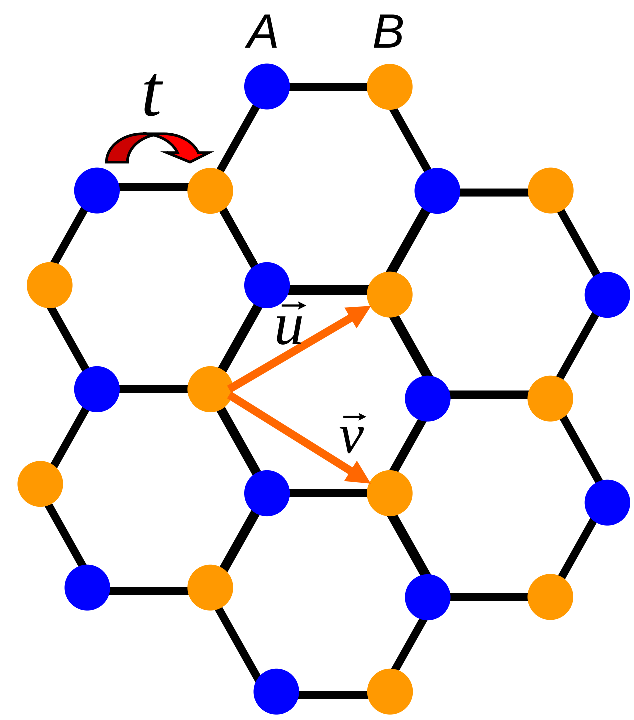






Graphene: structure

The Hamiltonian of graphene is given by



$$H = -t \sum_{<i,j>} a_i^+ a_j = -\frac{t}{2} \sum_{<i,j>} (a_i^+ b_j + b_i^+ a_j)$$

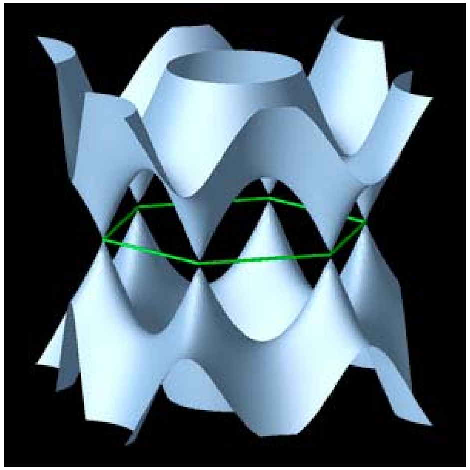
a_i fermionic modes

Fourier transformation:

$$H_{\vec{k}} = \begin{pmatrix} 0 & -t(1+e^{-i\vec{k}\cdot\vec{u}} + e^{-i\vec{k}\cdot\vec{v}}) \\ -t(1+e^{i\vec{k}\cdot\vec{u}} + e^{i\vec{k}\cdot\vec{v}}) & 0 \end{pmatrix}$$

$$E(\vec{k}) = \pm t\sqrt{3 + 2\cos\vec{k}\cdot\vec{u} + 2\cos\vec{k}\cdot\vec{v} + 2\cos\vec{k}\cdot(\vec{u}-\vec{v})}$$

E(kx,ky):



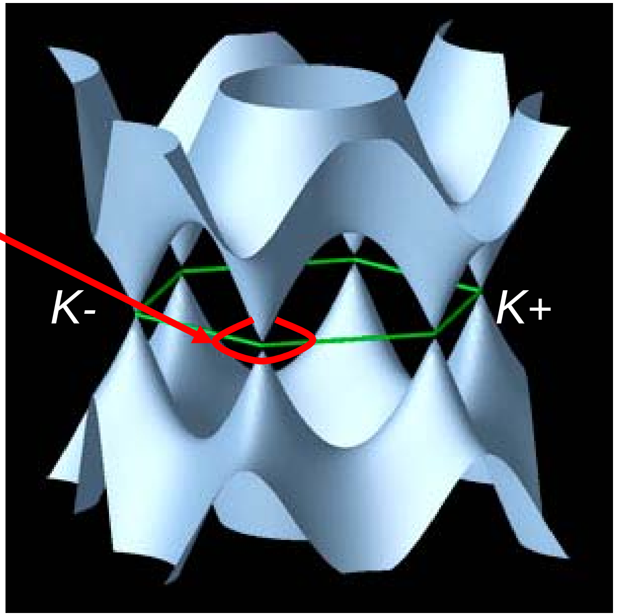
Fermi points: *E(k)=0*

Graphene: structure

$$E(\vec{k}) = \pm t\sqrt{3 + 2\cos\vec{k}\cdot\vec{u} + 2\cos\vec{k}\cdot\vec{v} + 2\cos\vec{k}\cdot(\vec{u}-\vec{v})}$$

Linearise energy $E(\vec{k})$ around a conical point,

$$\vec{k} = \vec{K} + \vec{p}$$



$$H_{\vec{p}} \approx \pm\frac{3t}{2}\begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix} = \pm\frac{3t}{2}\vec{\sigma}\cdot\vec{p}$$

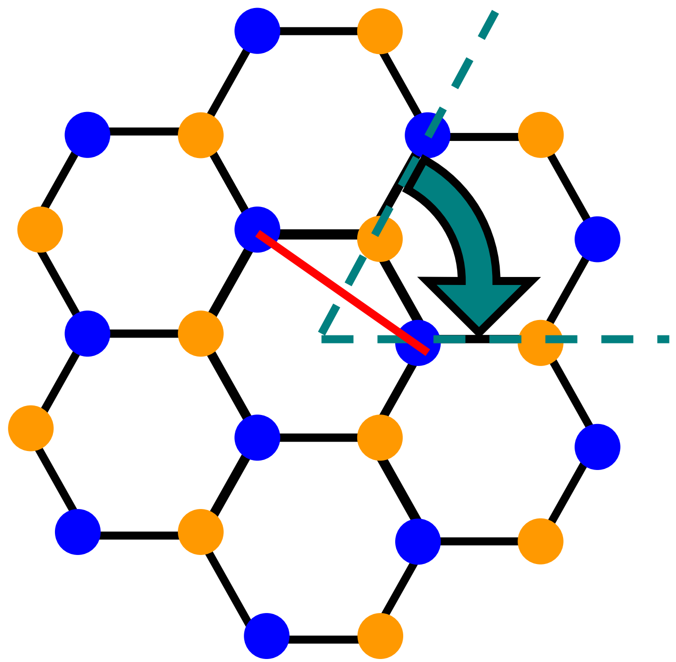
Relativistic Dirac equation at the tip of a pencil!

Two types of spinors: $\begin{pmatrix} |K_+, A\rangle \\ |K_+, B\rangle \end{pmatrix}, \quad \begin{pmatrix} |K_-, A\rangle \\ |K_-, B\rangle \end{pmatrix}$

$K_\pm$ are the Fermi points and A and B are the two triangular sub-lattices

Note: σ^z rotation maps to states with the same energy, but opposite momenta

Graphene: curvature



To introduce curvature:

cut $\pi / 3$ sector and reconnect sites.

This creates a single **pentagon** with no other deformations present.

Results in a **conical configuration**.

To preserve continuity of the spinor field when circulating the pentagon one can introduce two **additional fields**:

-Spin connection *Q*: $\oint Q_\mu dx^\mu = -\frac{\pi}{6}\sigma^z$ Mixes A and B components

-Non-abelian gauge field, *A*: $\oint A_\mu dx^\mu = -\frac{\pi}{2}\tau^y$ Mixes + and – spinors

Resulting 4x4 Dirac equation can be decoupled by simple rotation to a pair of 2x2 Dirac equations (k=1,2):

elliptic operator

$$\boxed{\frac{3t}{2}\sum_\mu \gamma^\mu (p_\mu - iQ_\mu - iA_\mu^k)}\psi^k = E\psi^k$$

$$\oint A_\mu^k dx^\mu = \pm\frac{\pi}{2}$$

Graphene: curvature

$$\frac{3t}{2}\sum_{a,\mu}\gamma^{\mu}(p_{\mu}-iQ_{\mu}-iA_{\mu}^{k})\psi^{k}=E\psi^{k}$$

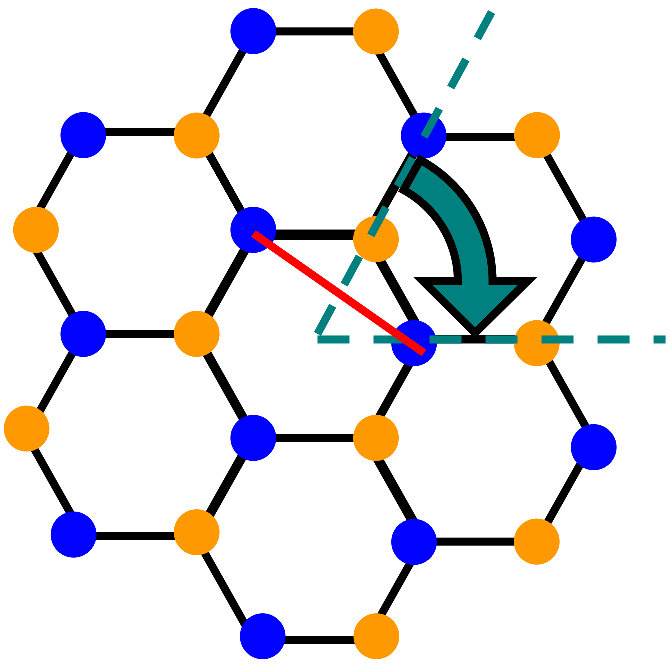
$$F_{\mu\nu}^{k}=\partial_{\mu}A_{\nu}^{k}-\partial_{\nu}A_{\mu}^{k}$$

$$\gamma^{\mu}=e_{a}^{\mu}\gamma^{a},\ g^{\mu\nu}=e_{a}^{\mu}e_{b}^{\nu}\eta^{ab}$$

$$\Gamma_{\mu\nu}^{\sigma}=\frac{1}{2}g^{\sigma\rho}(\partial_{\mu}g_{\nu\rho}+\partial_{\nu}g_{\mu\rho}-\partial_{\rho}g_{\mu\nu})$$

$$R^{\mu}{}_{\nu\rho\sigma}=\partial_{\sigma}\Gamma_{\nu\rho}^{\mu}-\partial_{\rho}\Gamma_{\nu\sigma}^{\mu}+\Gamma_{\nu\rho}^{\lambda}\Gamma_{\lambda\sigma}^{\mu}-\Gamma_{\nu\sigma}^{\lambda}\Gamma_{\lambda\rho}^{\mu}$$

$$R_{\mu\nu}=R^{\rho}{}_{\mu\nu\rho},\ R=g^{\mu\nu}R_{\mu\nu}$$



Continuous limit: Small energies => large wavelengths =>
insensitive to lattice spacing, conical singularity,…

Index Theorem

Consider operators, $P,\ P^+$ $\qquad V_+ \xrightarrow{P} V_-\,,\ V_- \xrightarrow{P^+} V_+$

$$\text{For } \lambda \neq 0,\quad P^+Pu = \lambda u \Rightarrow (PP^+)Pu = \lambda Pu$$

non-zero modes come in pairs

Define
(Dirac op.) $\not{D} = \begin{pmatrix} 0 & P^+ \\ P & 0 \end{pmatrix},\quad \not{D}^2 = \begin{pmatrix} P^+P & \\ 0 & PP^+ \end{pmatrix}$ $\qquad V = V_+ \oplus V_-$

Same number of zero modes as *D*

Define operator: $\gamma_5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ with eigenvalues +1, -1 for V_+, V_-

Consider $\nu_+,\ \nu_-$ the dimension of the **null** subspace of V_+, V_-

Then $$Tr(\gamma_5 e^{-t\not{D}^2}) = \sum_{Sp(P^+P)} e^{-t\lambda^2} - \sum_{Sp(PP^+)} e^{-t\lambda^2} = \nu_+ - \nu_- \equiv \text{index}(\not{D})$$

Non-zero eigenvalues cancel in pairs. **Expression is *t* independent.**

Index Theorem

$\not{D}$ can describe a general 2-dimensional **Dirac** operator defined over a **compact** surface coupled with a gauge field.

One can evaluate that

$$\not{D}^2 = -g^{\mu\nu}\nabla_\mu\nabla_\nu + \frac{i}{4}[\gamma^\mu,\gamma^\nu]F_{\mu\nu} - \frac{1}{4}R$$

Metric Covariant derivative Gauge field Curvature scalar

Heat kernel expansion

$$Tr(fe^{-tD}) = \frac{1}{4\pi t}\sum_{k\geq 0} t^{k/2} a_k(f,D)$$

For $f = \gamma_5,\ D = \not{D}^2$ the only non-zero coefficient is

$$a_2 = Tr\left\{\gamma_5\left(\frac{i}{4}[\gamma^\mu,\gamma^\nu]F_{\mu\nu} - \frac{1}{4}R\right)\right\} = 2\iint F \Rightarrow Tr(\gamma_5 e^{-t\not{D}^2}) = \frac{1}{2\pi}\iint F$$

Index Theorem

We have

$$Tr(\gamma_5 e^{-t\not{D}^2}) = \sum_{Sp(P^+P)} e^{-t\lambda^2} - \sum_{Sp(PP^+)} e^{-t\lambda^2} = \nu_+ - \nu_- \equiv \mathrm{index}(\not{D})$$

Also

$$Tr(\gamma_5 e^{-t\not{D}^2}) = \frac{1}{2\pi}\iint F_{xy} d^2 x$$

If *D* is defined on compact manifold then RHS is an integer (topological invariant), due to the quantization condition of the Dirac monopoles charge.
Thus, the number of zero modes depends on the gauge field configuration.

Continuous deformations of the gauge field will not change the number of zero modes.

Surface **curvature** does not appear in the above result (only in 2-dims).

Index Theorem

The **Index theorem** states:

$$\boxed{\mathrm{index}(D) = \nu_+ - \nu_- = \frac{1}{2\pi}\iint F}$$

integer!

The integral is taken over the whole compact surface.

For **compact manifolds** the term on the r. h. s. is an **integer**.
It is a **topological number**: small deformations does not change its value.

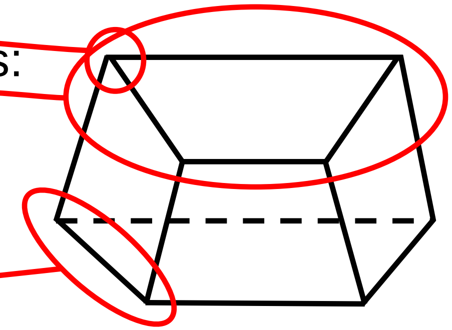
Open boundary conditions can give a discrepancy caused by boundary terms.

From this theorem you can obtain the **least number of zero modes**. The exact number is obtained if ν_+ or ν_- is equal to zero.

[Atiyah and Singer, Ann. of Math. 87, 485 (1968);...]

Index Theorem: Euler characteristic

Euler characteristic for lattices on compact surfaces:



$$\chi = V - E + F = 2(1-g)$$

Consider folding of graphene in a compact manifold. The **minimal** violation is obtained by insertion of **pentagons** or **heptagons** that contribute positive or negative curvature respectively. Consider

- n_5 number of pentagons
- n_6 number of hexagons
- n_7 number of heptagons

$$\Rightarrow \quad V = (5n_5 + 6n_6 + 7n_7)/3$$

$$E = (5n_5 + 6n_6 + 7n_7)/2$$

$$F = n_5 + n_6 + n_7$$

From the Euler characteristic formula:

$$n_5 - n_7 = 12(1-g)$$

Fullerenes: $g = 0 \Rightarrow n_5 = 12$

“Nanotubes”: $g = 1 \Rightarrow n_5 - n_7 = 0$

Index Theorem: Graphene application

$$\iint F = \oint A$$

Stokes's theorem

$$\frac{1}{2\pi}\left(\pm\frac{\pi}{2}\right)(n_5 - n_7) = \pm 3(1-g)$$

$$\boxed{\mathrm{index}(D) = \nu_+ - \nu_- = \frac{1}{2\pi}\iint F}$$

Thus, one obtains: $$\nu_+ - \nu_- = \begin{cases} 3(1-g), \text{ for } k = 1 \\ -3(1-g), \text{ for } k = 2 \end{cases}$$

Least number of zero modes:

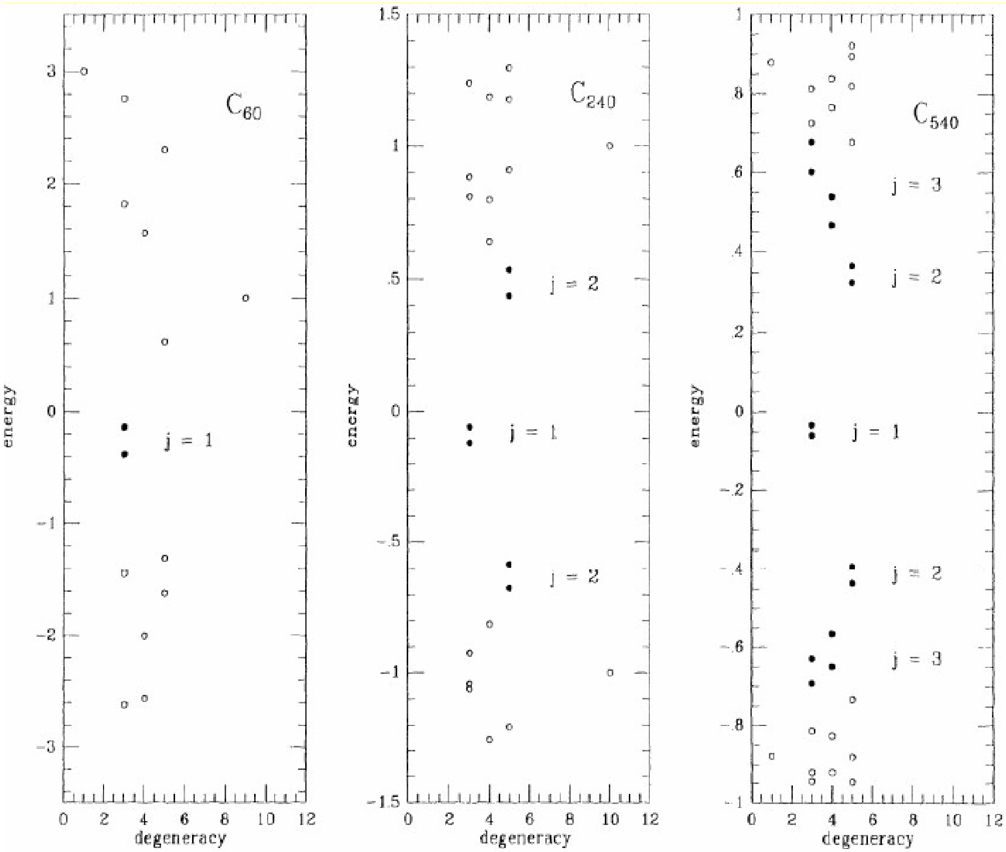
$$\boxed{6\,|1-g\,|}$$

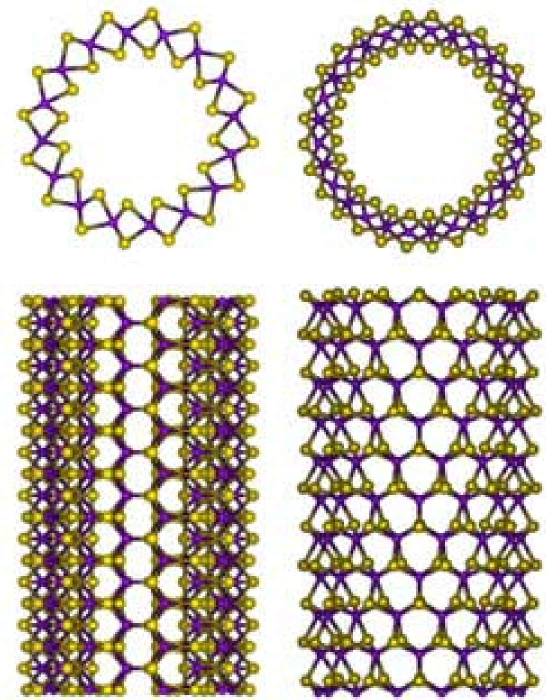
Index Theorem: Graphene application

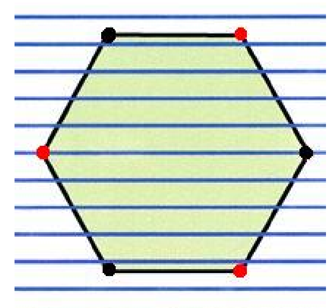
$$\mathrm{index}(D) = \nu_+ - \nu_- = 6\,|1-g\,|$$

C60: g=0

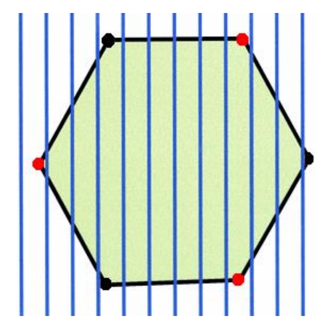
Nanotubes: g=1







Zero mode pairs



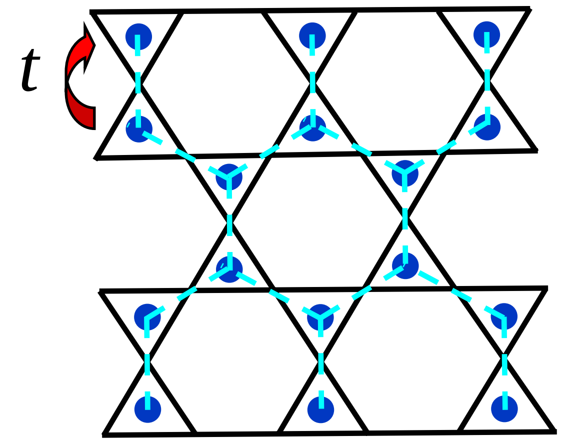
No zero modes

[J. Gonzalez *et al.* Phys. Rev. Lett. 69, 172 (1992)]

Ultra-cold Fermi atoms and optical lattices

Single species ultra cold **Fermi atoms** superposed by **optical lattices** that form a hexagonal lattice.

[Duan *et al.* Phys. Rev. Lett. 91, 090402 (2003)]

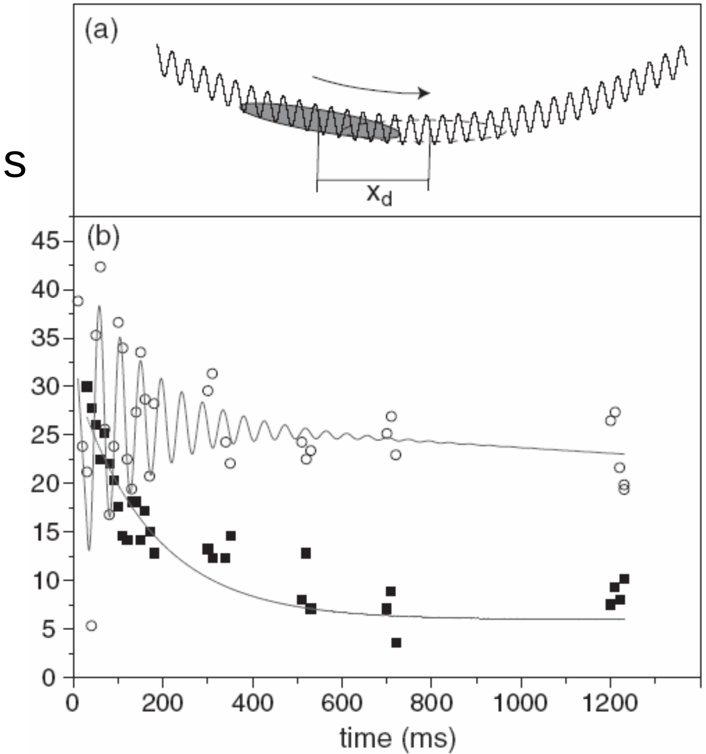


- Very low temperatures: $T \sim 0.1 T_F$
- Arbitrary filling factors: e.g. 1/2

See dependence of conductivity on **disorder**, **impurities** and lattice **defects**: e.g. insert pentagons at the edge of the lattice of effect of empty sites.

Similar **index theorem** can be devised for open boundary conditions.

Measurement of conductivity in Fermi lattices has already been performed in the laboratory:



[Ott *et al.* Phys. Rev. Lett. 92, 160601 (2004)]

Conclusions

- **Index Theorem** for compactified graphene sheets.
- Agrees well with known models of **fullerenes** and **nanotubes**.
- Gives conductivity properties for **higher genus models**:

  sideways connected nanotubes.
- Predicts **stability** of spectrum under small deformations.

- Relate to **topological models**:
  - obtain **topologically related degeneracy:** $2^{6|1-g|}$
  - encode and manipulate **quantum information**.
  - apply **reverse engineering** to find new models with specific degeneracy properties.

- Related experiments with **ultra-cold Fermi atoms** can give insight to the properties of graphene. May be easier to implement than solid state setup.

[cond-mat/0607394]

Thank you for your attention!

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