Graphene, vortices and the index theorem

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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,V)
  - Encode information in these degenerate levels

TOPOLOGICAL DEGENERACY

Anyons
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 $g$.

- **Geometrically induced vortices**: (an effective gauge theory "for free"）， see talks by Franz, Chamon, Jackiw...

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

- Topological quantum computation
  - Kitaev
  - Honeycomb lattice (same as graphene, but with real fermions)
Different geometries of Graphene

Fullerene (C60):

Nanotubes:
The Hamiltonian of graphene is given by

\[ H = -t \sum_{\langle i,j \rangle} a_i^+ a_j = -\frac{t}{2} \sum_{\langle i,j \rangle} (a_i^+ b_j + b_j^+ a_i) \]

\( a_i \) fermionic modes

Fourier transformation:

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

\[ E(\mathbf{k}) = \pm t \sqrt{3 + 2 \cos \mathbf{k} \cdot \mathbf{u} + 2 \cos \mathbf{k} \cdot \mathbf{v} + 2 \cos \mathbf{k} \cdot (\mathbf{u} - \mathbf{v})} \]

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**: \( \sigma^z \) 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 \textbf{pentagon} with no other deformations present.
Results in a \textit{conical configuration}.
To preserve continuity of the spinor field when circulating the pentagon one can introduce \textbf{two additional fields}:

- \textbf{Spin connection} \( Q \):
  \[ \int Q_\mu dx^\mu = -\frac{\pi}{6} \sigma^z \]  
  Mixes \( A \) and \( B \) components

- \textbf{Non-abelian gauge field}, \( A \):
  \[ \int A_\mu dx^\mu = -\frac{\pi}{2} \tau^y \]  
  Mixes + and − spinors

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

\[
\sum_\mu \gamma^\mu \left( p_\mu - iQ_\mu - iA_\mu^k \right) \psi^k = E \psi^k \quad \quad \int A_\mu^k dx^\mu = \pm \frac{\pi}{2}
\]
Graphene: curvature + distortion

Introduce a scalar field in the Dirac equation by introducing a Kekulé distortion on the lattice: 1/3 of hexagons have no double bonds. Centered on them you can cut a $\pi/3$ sector without disturbing the Kekulé pattern.

This creates a single pentagon with no double bonds.

In general: leapfrog fullerene molecules: $C_{60+6k}$

Resulting 4x4 Dirac equation:

$$\begin{pmatrix}
-ie_i^\mu \sigma^i (\nabla_\mu - ieA_\mu) & \Phi \\
\Phi^* & ie_i^\mu \sigma^i (\nabla_\mu + ieA_\mu)
\end{pmatrix}, \quad \Phi = |\Phi| e^{i2e\int A}$$

Graphene: curvature + distortion

\[
\begin{pmatrix}
-ie_i^\mu \sigma^i (\nabla_\mu - ie A_\mu) & \Phi \\
\Phi^* & ie_i^\mu \sigma^i (\nabla_\mu + ie A_\mu)
\end{pmatrix}
\]

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

\[
\gamma^\mu = e_a^\mu \gamma^a, \quad g^{\mu\nu} = e_a^\mu e_b^\nu \eta^{ab}
\]

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

\[
R^\mu_{\nu\rho\sigma} = \partial_\sigma \Gamma^\mu_{\nu\rho} - \partial_\rho \Gamma^\mu_{\nu\sigma} + \Gamma^\lambda_{\nu\rho} \Gamma^\mu_{\lambda\sigma} - \Gamma^\lambda_{\nu\sigma} \Gamma^\mu_{\lambda\rho}
\]

\[
R_{\mu\nu} = R^\rho_{\mu\nu\rho}, \quad R = g^{\mu\nu} R_{\mu\nu}
\]

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

Automatically generated Abrikosov or Nielsen and Olesen vortices
Index Theorem

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

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

Define: $\mathcal{D} = \begin{pmatrix} 0 & P^+ \\ P & 0 \end{pmatrix}, \quad \mathcal{D}^2 = \begin{pmatrix} P^+P & \lambda \\ 0 & PP^+ \end{pmatrix}$

(2x2 Dirac op.)

Define operator: $\gamma_5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

with eigenvalues +1, -1 for $V_+, V_-$

Consider $V_+, V_-$ the dimension of the null subspace of $V_+, V_-$

Then $\text{Tr}(\gamma_5 e^{-t\mathcal{D}^2}) = \sum_{\text{Sp}(P^+)} e^{-t\lambda^2} - \sum_{\text{Sp}(PP^+)} e^{-t\lambda^2} = \nu_+ - \nu_- \equiv \text{index}(\mathcal{D})$

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

\( \mathcal{D} \) can describe a general 2-dimensional **Dirac** operator defined over a **compact** surface coupled with a gauge field.

One can evaluate that

\[
\mathcal{D}^2 = -g^{\mu\nu} \nabla_\mu \nabla_\nu + \frac{i}{4} [\gamma^\mu, \gamma^\nu] F_{\mu\nu} - \frac{1}{4} R
\]

**metric** **covariant derivative** **gauge field** **curvature scalar**

Heat kernel expansion (2-dims):

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

For \( f = \gamma_5 \), \( D = \mathcal{D}^2 \) the only non-zero coefficient is

\[
a_2 = \text{Tr} \left\{ \gamma_5 \left( \frac{i}{4} [\gamma^\mu, \gamma^\nu] F_{\mu\nu} - \frac{1}{4} R \right) \right\} = 2 \iint F \Rightarrow \text{Tr}(\gamma_5 e^{-tD^2}) = \frac{1}{2\pi} \iint F
\]
We have

\[ Tr(\gamma_5 e^{-tD^2}) = \sum_{Sp(P^+P)} e^{-t\lambda^2} - \sum_{Sp(PP^+)} e^{-t\lambda^2} = \nu_+ - \nu_- \equiv \text{index}(D) \]

Also

\[ Tr(\gamma_5 e^{-tD^2}) = \frac{1}{2\pi} \iint F_{xy} d^2 x \]

The Index theorem states: for a (compact) manifold…

\[ \text{index}(D) = \nu_+ - \nu_- = \frac{1}{2\pi} \iint F \]

integer!

It is a topological number: small deformations do not change its value. From this theorem you can obtain the least number of zero modes. The exact number is obtained if \(\nu_+\) or \(\nu_-\) is equal to zero.

[Atiyah and Singer, Ann. of Math. 87, 485 (1968);...]
Index Theorem with Scalar Field

Jackiw & Rossi suggested a version of the index theorem that includes the scalar field:

\[
\text{Index}(D) = \frac{1}{\pi} \int_{\Omega} F + \frac{1}{4\pi i} \int_{\partial \Omega} dr \cdot \frac{\Phi^* \nabla \Phi - \Phi \nabla \Phi^*}{|\Phi|^2}
\]

\[
= \frac{1}{4\pi i} \int_{\partial \Omega} dr \cdot \frac{\Phi^* \partial \Phi - \Phi \partial \Phi^*}{|\Phi|^2}
\]

\[
\nabla \Phi = (\partial - 2ieA)\Phi
\]

E. Weinberg proved this conjecture for flat manifold with open boundary conditions. To show it holds for a compact manifold:

- The gauge and associated scalar bundle are non-trivially twisted. For a sphere need two patches and sew them together with a gauge transformation:

\[
e^{ie\chi} (\partial - ieA) e^{-ie\chi} \quad \text{with} \quad (\partial - ieA) \quad \text{and} \quad e^{i2e\chi} \Phi \quad \text{with} \quad \Phi, \quad \chi \rightarrow \int F
\]

- The curvature: Index is a topo-inv. => not affected by continuous deformations: Bring all vortices close by. For them the manifold looks now flat.
Index Theorem: Euler characteristic

Euler characteristic for lattices on “smooth” surfaces:

\[ \chi = V - E + F = 2(1 - g) - N \]

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

\[
\begin{align*}
V &= (5n_5 + 6n_6 + 7n_7) / 3 \\
E &= (5n_5 + 6n_6 + 7n_7) / 2 \\
F &= n_5 + n_6 + n_7
\end{align*}
\]

From the Euler characteristic formula:

\[ n_5 - n_7 = 6\chi = 12(1 - g) - 6N \]

Fullerenes: \( g = 0, N = 0 \Rightarrow n_5 = 12 \)
Nanotubes: \( g = 0, N = 2 \Rightarrow n_5 - n_7 = 0 \)
Index Theorem: Graphene application

\[ \oint \oint F = \oint A \]
\[ \frac{1}{2\pi} \left( \pm \frac{\pi}{2} \right) (n_5 - n_2) = \pm \frac{3}{2} \chi \]

Stokes's theorem

\[ \text{index}(\mathcal{D}) = \nu_+ - \nu_- = \frac{1}{2\pi} \oint \oint F \]

Thus, one obtains:

\[ \nu_+ - \nu_- = \begin{cases} 
\frac{3}{2} \chi, & \text{for } k = 1 \\
\frac{3}{2} \chi, & \text{for } k = 2 
\end{cases} \]

Least number of zero modes:

\[ 3 \chi = 6(1 - g) - 3N \]
Index Theorem: Graphene application

\[
\text{index}(\mathcal{D}) = \nu_+ - \nu_- = 6(1 - g) - 3N
\]

C60: \(g=0, N=0\)  
Nanotubes: \(g=0, N=2\)

Zero mode pairs  
No zero modes

Scalar vortices have vorticity \( \pi \) so one needs to connect two vortices with a cut to make scalar field \( \Phi \) continuous.

Vortices should have a finite size for large molecules to have a smooth counterpart in the continuous limit.

\( h < 1 \) means that hexagons prefer to have smaller tunneling coupling than pentagons.
Conclusions

- Fullerenes provide Kekule distortion AND vorticity: 
  natural setting with fractionally charged vortices
- How to probe them?

- **Index Theorem** for various graphene configurations.
- Agrees well with known models of *fullerenes* and *nanotubes*.
- Gives conductivity properties for more complex models.
- Predicts **stability** of spectrum under small deformations.

- Relate to **topological models**: 
  - obtain **topologically related degeneracy**: \( 2^{6(1-g)-3N} \)
  - encode and manipulate **quantum information**.
  - apply **reverse engineering** to find new models with specific degeneracy properties.


*Thank you for your attention!*