Topological Order in Superconductivity and Carbon Nano-Structures

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Plan of talk today

♦ (Part of ) Target Phenomena

♦ Topological Aspect of QHE

♦ Topological Aspect of Superconductors
  - Dirac Monopoles and Topological Numbers (Simple case)
  - Generic Consideration: Non-Abelian Gauge Structures
  - Zero Bias Conductance Peak and local Time Reversal Symmetry Breaking
  (Peierls Instability of edge states)

♦ Topological Aspects of Carbon Nano-Structures
  - Topological Consideration of Zero Modes Edge states
  - Localized Spin moments: generalized Kondo Problem
  - Localized Spin Moments as a Local Chiral Symmetry Breaking
  (Peierls Instability of edge states)
Zero Bias Conductance Peak in Anisotropic Superconductivity

Zero Energy Boundary States of Anisotropic Superconductivity

Localized Boundary State in Carbon Sheet (1)

Tight-binding Model Calculation

Localized Boundary State in Carbon Sheet (2)

Local Spin Density Functional Appr. Calculation

FIG. 1. Contour plots of spin density $n_1(r) - n_2(r)$ (a) on a plane perpendicular to a graphite flake with zigzag edges and (b) on a plane including the graphite flake. In (a) the edges are perpendicular to the plane and C atoms on the plane are depicted by shaded circles. Positive and negative values of the spin density are shown by solid and dashed lines, respectively. Each contour represents twice (or half) the density of the adjacent contour lines.

FIG. 2. Top views of fully optimized BNC heterosheets, (a) BNC-I and (b) BNC-II. White, shaded, and black circles denote C, B, and N atoms, respectively. The rectangle in each figure denotes the unit cell.

B, N, and C atoms have been observed indeed [8–10]. Second, the phase separation of graphite and BN regions leading to the striped structures above is energetically favorable. In fact, we have performed the total-energy calculations for graphite, BN, BC, and NC heterosheets by DFT. The calculated bond energies of B-C and N-C are smaller than that of graphite by 1.52 and 0.81 eV, respectively. On the other hand, the bond energy of B-N is smaller than that of graphite only by 0.31 eV. Third, undulation

“Magnetic Ordering in Hexagonally Bonded Sheets with First-Row Elements”,
Appearance of Topological Order in Condensed Matter
(X.G. Wen)

- Quantum Hall Effects (Integer & Fractional)
  - Energy Gap and Quatization of Hall Conductance
  - Topological Characterization of Hall Conductance
  - Bulk ↔ Edge
  - Integer ↔ Fractional: Composite Fermion Picture

- Spin Chain with Integral Spin
  - Energy Gap with Topological Origin
  - Kennedy Triplet with finite Length Spin Chains (Edge States)

- Polyacetylene: (SSH Model)

- High-$T_C$, Chiral Spin State, Anyon-Superconductivity, Fractionalization

- Chirality Order in Itinerant Magnetism

- Polarization of Insulators, KSV formula

- Anisotropic Superconductivity & Superfluidity
  - Dirac Monopoles and Topological Origin of Zero Bias Peaks

- Carbon Nano-Structures
  - Various Shape of Edges and Localized Zero Modes
Hofstadter’s Butterfly and the Topological Integers

Energy spectrum of the square lattice (2D) with magnetic field \( \phi \) per plaquette

\[
H = \sum_{\langle ij \rangle} c_i^\dagger e^{i\theta_{ij}} c_j + h.c.
\]

\[
\sum_{j \in \langle i,j \rangle} \theta_{ij} = 2\pi \phi_i = 2\pi \Phi
\]

Diagram is self similar: Fractal

\( n \): Hall conductance in unit \( \frac{e^2}{h} \) when the Fermi energy is at the gap.
Topological Aspect of the Quantum Hall Effect

Bulk $\leftrightarrow$ Edge states (Explicit observable)

(Almost always) with topological ordered states

Laughlin’s unknown integer $n$ has several topological expressions.

$\sigma_{xy}$ as a topological Invariant by bulk states

- Chern number, $C$, TKNN’82, PRL 49, 405
  - Total vorticity of the relative phase of the Bloch function
    on the Brillouin zone.

$\sigma_{xy}$ as a topological Invariant by edge states

- Intersection number, $I$, Y.H.’93, PRB48, 11853, PRL 71, 3697
  - Intersection number of the zero of the Bloch function (Edge States)
    on the complex energy surface with a closed loop (an energy band).

The above 2 Different Topological Integers are Equal.

\[ C = I \]

Bulk and Edge descriptions are equivalent.
TKNN Formula (Chern number)
(TKNN’82, PRL 49, 405)

\[ \sigma_{x'y}^{j, \text{bulk}} = -\frac{e^2}{h} C, \quad C = \sum_{\ell=0}^{j} c_\ell \]

\[ c_\ell = \frac{1}{2\pi i} \int_{T_{MBZ}} d\vec{S}_k \cdot \vec{B}^\ell \]

\[ \vec{B}^\ell = \text{rot}_k \vec{A}^\ell \]

\[ \vec{A}^\ell = \langle \psi^\ell | \nabla_k \psi^\ell \rangle \]

|\psi^\ell (\vec{k})\rangle = \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_q \end{pmatrix}: \text{Bloch function of the lowest } \ell \text{-th band. } (\sum_{k=1}^{q} |\Psi_k|^2 = 1).

\[ T_{MBZ}: \text{(Magnetic) Brilluine zone: topologically Torus} \]

\[ \rightarrow \text{No boundary } \rightarrow C = 0 \text{ by the Stokes Theorem?} \]

\[ \text{No! Look for singularities!} \]
**Chern number and Vortex** (Kohmoto ’85, Hatsugai ’93)

\[ H(k) |\psi^\ell(\vec{k})\rangle = e^{i \xi_{AB}} |\psi^\ell(\vec{k})\rangle^B \]

\[ \vec{B}^\ell,A = \vec{B}^\ell,B \]

\[ \vec{A}^\ell,A = i \vec{\nabla} \xi_{AB} + \vec{A}^\ell,B \]

\[ c_\ell^A = c_\ell^B \]

The Chern number is invariant

- Gauge fixing to calculate \( C \)
  - Take, say, \( \psi_q \) to be real positive! It fails when \( \psi_q = 0 \) !!
  - Need to take different gauge then, say, \( \psi_1 \) to be real positive!

**Patch work of the \( T_{MBZ} \) to calculate \( C \)**

\[ T_{MBZ} = Z \cup NZ \]

\[ Z = \cup_m R_m, \quad NZ = T_{MBZ} \setminus Z \]

where \( R_\ell \) include a zero of \( \psi_q(k) \).
Chern number and Vortex (Cont.)

\[ |\psi\rangle^Z = |\psi\rangle e^{-i \text{Im log} |\psi\rangle_1}, \quad \mathcal{A}^Z = Z \langle \psi | \nabla \psi \rangle^Z = \langle \psi | \nabla \psi \rangle - i \nabla \text{Im log} |\psi\rangle_1 \quad \psi \in Z \]

\[ |\psi\rangle^{NZ} = |\psi\rangle e^{-i \text{Im log} |\psi\rangle_q}, \quad \mathcal{A}^{NZ} = NZ \langle \psi | \nabla \psi \rangle^{NZ} = \langle \psi | \nabla \psi \rangle - i \nabla \text{Im log} |\psi\rangle_q \quad \psi \in NZ. \]

This is well-defined since \(|\psi\rangle_1\) is non zero in \(Z\) and \(|\psi\rangle_q\) is non zero in \(NZ\).

Applying the Stokes theorem in each region, \(c_\ell = \frac{1}{2\pi i} \int dS_k \cdot \text{rot}_k \vec{A}^Z\)

\[ = \frac{1}{2\pi i} \int_{\partial Z} dr \cdot (\vec{A}^Z - \vec{A}^{NZ}) \]

\[ = - \sum_m \frac{1}{2\pi} \int_{\partial R_m} dr \cdot \vec{v}(\vec{k}) \]

\[ v(\vec{k}) = \nabla \text{Im log} \frac{|\psi\rangle_1}{|\psi\rangle_q} \]

The Chern number \(c_\ell\) is given by the total vorticity.
Chern number (Cont.)

|ψ⟩^Z = |ψ⟩e^{-i\text{Im log} j_1} |ψ\rangle^N_Z = |ψ⟩e^{-i\text{Im log} j_q}

This is well-defined since |ψ⟩^1 is non-zero in \( Z \) and |ψ⟩^q is non-zero in \( NZ \).

Applying the Stokes theorem in each region,

\[ c_\ell = \frac{1}{2\pi i} \int_{Z} d\mathbf{s}_k \cdot \text{rot}_k \mathbf{A}^Z \]
\[ + \frac{1}{2\pi i} \int_{NZ} d\mathbf{s}_k \cdot \text{rot}_k \mathbf{A}^{NZ} \]
\[ = \frac{1}{2\pi i} \oint_{\partial Z} d\mathbf{r} \cdot (\mathbf{A}^Z - \mathbf{A}^{NZ}) \]
\[ = -\sum_m \frac{1}{2\pi} \oint_{\partial R_m} d\mathbf{r} \cdot \mathbf{v}(\mathbf{k}) \]

\[ \mathbf{v}(\mathbf{k}) = \vec{\nabla} \text{Im log} \frac{|\psi\rangle^1}{|\psi\rangle^q} \]

The Chern number \( c_\ell \) is given by the total vorticity.
Apply it to the Superconductivity
**Bogoliuov-de Gennes Hamiltonian (simple case)**

\[
H[\{c_i, c_i^\dagger\}] = \sum_{ij} t_{ij}^\sigma c_i^\sigma c_j^\sigma - \mu \sum_{i\sigma} c_i^\dagger c_{i\sigma} + \sum_{ij} \left( \Delta_{ij} c_i^\dagger c_j^\downarrow + \Delta_{ij}^* c_j^\dagger c_i^\downarrow \right)
\]

\[
= \sum_{ij} c_i^\dagger h_{ij} c_j + \text{const.} \quad c_i = \begin{pmatrix} c_i^\uparrow \\ c_i^\downarrow \end{pmatrix}, \quad h_{ij} = \begin{pmatrix} t_{ij} & \Delta_{ij} \\ \Delta_{ji}^* & -\tilde{t}_{ji} \end{pmatrix}
\]

♦ Bilinear in Fermion operators \(\{d_i^\sigma\}\) after the unitary transformation

\[
\begin{align*}
    d_i^\uparrow &= c_i^\uparrow \\
    d_i^\downarrow &= c_i^\dagger \\
    d_i^\dagger &= c_i^\uparrow \\
\end{align*}
\]

\[
H[\{d_i, d_i^\dagger\}] = H[\{c_i, c_i^\dagger\}]
\]

♦ Analogue of the QHE with flux \(\phi = \frac{1}{2}\)

♦ Topological Argument is applied

♦ Hall conductance \(\sigma_{xy}\) in \(\{d_i^\sigma\}\)

\(\leftrightarrow\) Spin Hall conductance \(\sigma_{xy}^{\text{spin}}\) in \(\{c_i^\sigma\}\)
Possible Order Parameters

\[ H^{BdG} = \sum_{ij} t_{ij}^\sigma c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_i c_{i\uparrow}^\dagger c_{i\downarrow} + \sum_{ij} \left( \Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \Delta_{ij}^* c_{j\downarrow} c_{i\uparrow} \right) \]

\[ \sum_{ij} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \Delta_{ij}^* c_{j\downarrow} c_{i\uparrow}) \]

\[ = \sum_{i < j} \Delta_{ij} \left( c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \right) + h.c. \]  

Parity Even: (Singlet) \[ \Delta_{ij} = \Delta_{ji} \]

Parity Odd: (Triplet) \[ \Delta_{ij} = -\Delta_{ji} \]

Singlet:

- **s-wave**
- \[ d_{x^2-y^2} \]
- **high-\(T_C\)**

Quasiparticle dispersion

- **Uniform gap on the Fermi line**
- **4 Dirac Nodes**
- **Gap opening**

Laughlin

T-breaking
Possible Order Parameters – cont.—

Triplet:

Chiral $p$ wave with chemical potential $\mu$

1 Dirac Node at zone boundary

$\mu = 0$

$\mu = -0.5$, Gap Opening

$\mu = -4$, One Dirac Node at zone corner

$\mu = -5$, Gap Opening Again
Chern Number in the Superconductivity

\[ H^{BdG} = \sum_k c^\dagger(k) h(k) c(k), \quad c^\dagger(k) = (c^\dagger_\uparrow(k), c_\downarrow(k)) \]

\[ h(k) = \begin{pmatrix} \epsilon^\dagger(k) & \Delta(k) \\ \Delta^*(k) & -\epsilon^\dagger(-k) \end{pmatrix}, \quad e^\sigma(k) = \sum_j e^{-i k \cdot r_j} t^\sigma(j) \]
\[ \Delta(k) = \sum_j e^{-i k \cdot r_j} \Delta(j) \]

The Chern number \( C \) for the negative energy state \( |k\rangle, h(k)|k\rangle = -E(k)|k\rangle, \)

\[
C = \frac{1}{2\pi i} \int_{T^2} dS_k \cdot B_k
\]

\[ B_k = \text{rot}_k A_k \]
\[ A_k = \langle k | \nabla_k | k \rangle \]

\[ \text{The spin Hall conductance} \quad \sigma_{xy}^{\text{spin}} = -\frac{e^2}{h} C \]

\[ \text{\( C \) is a topological integer \( \rightarrow \) stable against small perturbation} \]

To change \( C \), the energy gap has to collapse

\[ \text{\( \rightarrow \) Use it to characterize the superconducting state!} \]

Characterization by the topological order
Chern Number and the Winding Number

\[ C = -N_{\text{winding}} \]

\[ N_{\text{winding}} = \sum_{\ell} \frac{1}{2\pi} \oint_{\partial R_{\ell}} dk \cdot \nabla_k \text{Im} \log \frac{|k\rangle_1}{|k\rangle_2} \]

The summation is over the poles of \( \frac{|k\rangle_1}{|k\rangle_2} \) (\( R_{\ell} \) is a small area around each pole)

Example:

\[ d_{x^2-y^2} + id_{xy} \]

\[ C = 2 \text{sgn} \frac{\Delta_{x^2-y^2}}{\Delta_{xy}} \]

Sentil-Marston-Fisher
Morita-Hatsugai
Read-Green
Berry’s parametrization in the Superconductivity

\[ h(k) = \begin{pmatrix} \epsilon(k) & \Delta(k) \\ \Delta^*(k) & -\epsilon(k) \end{pmatrix} = R(k) \cdot \sigma \]

\[ R(k) = (R_x(k), R_y(k), R_z(k)) = (\text{Re} \ \Delta(k), -\text{Im} \ \Delta(k), \epsilon(k)) \]

\[ \sigma = (\sigma_x, \sigma_y, \sigma_z) : \text{Pauli matrices} \]

Map from \( k \) to \( R \) as \( R = R(k) \).

\[ h(R)|R\rangle_{\pm} = E_{\pm}(R)|R\rangle_{\pm}, \quad E_{\pm}(R) = \pm R \quad (= \pm |R|) \]

\[ |R\rangle = \frac{1}{\sqrt{2R(R - R_z)}} \begin{pmatrix} R_z - R \\ R_x + iR_y \end{pmatrix} = \begin{pmatrix} \sin \frac{\theta}{2} \\ e^{i\phi} \cos \frac{\theta}{2} \end{pmatrix} \]

\[ |R\rangle = |R\rangle_- \text{ is the negative energy state and } (R, \theta, \phi) \text{ is the polar coordinate.} \]
Chern Number and the Covering Number

By the Gauss’ Theorem

\[ C = - \int_{R(T^2)} dV \delta_R(R) = -N_{\text{covering}} \]

\[ N_{\text{covering}} = N(R(T), \mathcal{O}) \]

How many times the surface \( R(T^2) \) wraps around the origin \( \mathcal{O} \)

→ New Different but equivalent topological Expression for the Chern number!
\( R(T^2) \) for \( d_{x^2} - y^2 + i d_{xy} \) case

\[
R = R(k) = (\text{Re} \ \Delta(k), -\text{Im} \ \Delta(k), \epsilon(k))
\]

\[
\Delta(k) = 2 \Delta_{x_2 - y_2} (\cos k_x - \cos k_y) + 2i \Delta_{xy} (\cos(k_x + k_y) - \cos(k_x - k_y))
\]
$R(T^2)$ for $d_{x^2-y^2} + i d_{xy}$ case

$R = R(k) = (\text{Re} \Delta(k), -\text{Im} \Delta(k), \epsilon(k))$

$\Delta(k) = 2\Delta_{x_2-y_2}(\cos k_x - \cos k_y) + 2i\Delta_{xy}(\cos(k_x + k_y) - \cos(k_x - k_y))$

$\Delta_{x_2-y_2} = t$

$\Delta_{xy} = t$

$\mu = -t,$

$t = 1$
$R(T^2)$ for $d_{x^2-y^2} + id_{xy}$ case

$R = R(k) = (\text{Re} \Delta(k), -\text{Im} \Delta(k), \epsilon(k))$

$\Delta(k) = 2\Delta_{x^2-y^2}(\cos k_x - \cos k_y) + 2i\Delta_{xy}(\cos(k_x + k_y) - \cos(k_x - k_y))$

It’s doubly covered!
Chiral $p$ case

$\mathbf{R} = \mathbf{R}(\mathbf{k}) = (\text{Re} \, \Delta(\mathbf{k}), -\text{Im} \, \Delta(\mathbf{k}), \epsilon(\mathbf{k}))$

$\Delta(\mathbf{k}) = 2i \Delta_x (\sin k_x + i \sin k_y)$

$\Delta_x = -t$

$\mu = -t,$

$t = 1$
Chiral $p$ case

$R = R(k) = (\text{Re } \Delta(k), -\text{Im } \Delta(k), \epsilon(k))$

$\Delta(k) = 2i \Delta_x (\sin k_x + i \sin k_y)$

Self-Intersection!
Inside and Outside of the surface Interchange!

Always Orientable

$\Delta_x = -t$
$\mu = -t,$
$t = 1
Chiral \( p \) case

Self-Intersection!  
Inside and Outside of the surface Interchange!  

\[
R = R(k) = (\text{Re} \, \Delta(k), -\text{Im} \, \Delta(k), \epsilon(k))
\]

\[
\Delta(k) = 2i \Delta_x (\sin k_x + i \sin k_y)
\]
Topological Aspects of (Generic) Superconductors

Generalization for Generic Superconductors

Singlet and Triplet

Unitary order and Nonunitary order

Non-Abelian Gauge Structure

Abelian Chiral Anomaly

(Text Book Example)
Generic BdG Hamiltonian

\[ H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} c_i^{\sigma_1} c_j^{\sigma_2} c_j^{\sigma_3} c_i^{\sigma_4}, \]

\[ \Rightarrow \mathcal{H} = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ij} (\Delta_{ij}^{\sigma_4\sigma_3*} c_j^{\sigma_3} c_i^{\sigma_4} + \Delta_{ij}^{\sigma_1\sigma_2} c_i^{\sigma_1} c_j^{\sigma_2}) \]

\[ \Delta_{ij}^{\sigma_1\sigma_2} = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} \langle c_j^{\sigma_3} c_i^{\sigma_4} \rangle = -\Delta_{ji}^{\sigma_2\sigma_1} \]

\[ = \sum'_{k} (c_k^\uparrow, c_k^\downarrow, c_{-k}^\uparrow c_{-k}^\downarrow) \left( \begin{array}{cccc} \epsilon_k & 0 & \Delta_{k}^{\uparrow\uparrow} & \Delta_{k}^{\uparrow\downarrow} \\ 0 & \epsilon_k & \Delta_{k}^{\downarrow\uparrow} & \Delta_{k}^{\downarrow\downarrow} \\ \Delta_{k}^{\uparrow\uparrow*} & \Delta_{k}^{\downarrow\uparrow*} & -\epsilon_k & 0 \\ \Delta_{k}^{\uparrow\downarrow*} & \Delta_{k}^{\downarrow\downarrow*} & 0 & -\epsilon_k \end{array} \right) \left( \begin{array}{c} c_{k}^{\uparrow} \\ c_{k}^{\downarrow} \\ c_{-k}^{\uparrow} \\ c_{-k}^{\downarrow} \end{array} \right) \]

\[ h_k = \left( \begin{array}{cc} \epsilon_k 1_{22} & \Delta_{k} \\ \Delta_{k}^{\dagger} & -\epsilon_k 1_{22} \end{array} \right), \quad \Delta_{-k} = -\tilde{\Delta}_{k} \]

\[ \Delta_{k} = \begin{cases} \psi_k i\sigma_y & \text{for singlet, } \psi_{-k} = \psi_k, \tilde{\Delta}_{k} = -\Delta_{k} \\ (d_{k} \cdot \sigma)i\sigma_y & \text{for triplet, } d_{-k} = -d_{k}, \tilde{\Delta}_{k} = \Delta_{k} \end{cases} \]
Particle-Hole Symmetry and Unitarity

\[ E_k : \begin{pmatrix} u_k \\ v_k \end{pmatrix} \leftrightarrow -E_k : C \begin{pmatrix} u_k \\ v_k \end{pmatrix}, \quad C = \begin{cases} \rho_x K & \text{for singlet} \\ -i\rho_y K & \text{for triplet} \end{cases} \quad (K\varphi = \varphi^*) \]

\[ h_k^2 = \epsilon_k^2 + \begin{pmatrix} \Delta_k \Delta_k^\dagger & 0 \\ 0 & \Delta_k^\dagger \Delta_k \end{pmatrix} \]

\[ \Delta_k \Delta_k^\dagger \propto 1_2 ? : \begin{cases} \text{Yes : Unitary :} \\ \text{No : Nonunitary :} \end{cases} \begin{cases} \text{Singlet} \\ \text{Triplet with } q_k = 0 \\ \text{Triplet with } q_k \neq 0 \end{cases} \]

\[ E_k = \begin{cases} \pm \sqrt{\epsilon_k^2 + |\Delta_k|^2} : \text{(Unitary)} \\ \pm \sqrt{\epsilon_k^2 + |d_k|^2 \pm q_k} : \text{(Nonunitary)} \end{cases} \]

Quasiparticles are doubly degenerated in unitary order!

\[ q_k = id_k \times d_k^* \quad (\text{real}) \]

\[ (\sigma \cdot q_k)u_\pm = \pm q_k u_\pm, \quad q_k = |q_k| \]
Chern Numbers for Unitary states

Degeneracy $\Rightarrow$ Fixing the phases is not enough to define Chern numbers.

Define Non-Abelian Berry’s connection (Wilczek-Zee)

$$|k\alpha\rangle = |\alpha\rangle, \quad \alpha = 1, \ldots, M$$

$$A_i^{\alpha\beta} = \langle\alpha|\partial_i|\beta\rangle, \quad A^{\alpha\beta} = A_i^{\alpha\beta} dk_i, \quad \partial_i = \partial_{k_i}, i = x, y, z$$

$$(\mathcal{A})^{\alpha\beta} \equiv A^{\alpha\beta},$$

$$\mathcal{F} \equiv d\mathcal{A} + \mathcal{A} \wedge \mathcal{A} = \frac{1}{2!} F_{ij} dk_i \wedge dk_j, \quad F_{ij} = \partial_i A_j - \partial_j A_i + [A_i, A_j]$$

Base change of the degenerate states induces the followings

$$|\alpha\rangle \rightarrow |\tilde{\alpha}\rangle = |\alpha\rangle \omega^{\alpha\tilde{\alpha}}, \quad \omega : \text{unitary}$$

$$\tilde{\mathcal{A}} = \omega^\dagger \mathcal{A} \omega + \omega^\dagger d\omega$$

$$\tilde{\mathcal{F}} = \omega^\dagger \mathcal{F} \omega$$

$$\text{Tr} \tilde{\mathcal{F}} = \text{Tr} \mathcal{F} \quad \Leftarrow \text{Independent of the bases}$$
Chern Numbers for Unitary states (Cont.)

Further the following quantity is an integer

**The first Chern number (Chiral Anomaly)**

\[
C_i(k_i) = \frac{1}{2!} \epsilon_{ijk} \frac{1}{2\pi i} \int_{T_{jk}^2} \text{Tr} \mathcal{F}
\]

\[
C_x(k_x) = \frac{1}{2\pi i} \int_{T_{yz}^2} dk_y dk_z B_x
\]

\[
C_y(k_y) = \frac{1}{2\pi i} \int_{T_{zx}^2} dk_z dk_x B_y
\]

\[
C_z(k_z) = \frac{1}{2\pi i} \int_{T_{xy}^2} dk_x dk_y B_z
\]

Integers!

\[
B_x = \text{Tr} F_{yz}, \quad B_y = \text{Tr} F_{zx}, \quad B_z = \text{Tr} F_{xy}
\]

\[
T_{xy}^2(yz, zx) : 2D \text{ Brillouin zone fixed by } k_z, (y, x)
\]
Dirac Monopoles for Unitary States (Basis)

$\Delta_k = |\Delta_k| \Delta_k^0$, \( \Delta_k^0 \): Unitary

$\Rightarrow$ Eigenvalues are pure phases: $\Delta_k^0 |\alpha\rangle_\sigma = e^{-i\phi_\alpha} |\alpha\rangle_\sigma, (\alpha = 1, 2)$

BdG equation:

$$
\begin{pmatrix}
\epsilon_k 1_2 & |\Delta_k| \Delta_k^0 \\
|\Delta_k| (\Delta_k^0)^{-1} & -\epsilon_k 1_2
\end{pmatrix}
\begin{pmatrix}
u \\ \nu
\end{pmatrix}
= E_k
\begin{pmatrix}
u \\ \nu
\end{pmatrix}
$$

$$
\Rightarrow
\begin{pmatrix}
\epsilon_k & |\Delta_k| \\
|\Delta_k| & -\epsilon_k
\end{pmatrix}
\otimes 1_2
\begin{pmatrix}
u \\ \Delta_k^0 \nu
\end{pmatrix}
= E_k
\begin{pmatrix}
u \\ \Delta_k^0 \nu
\end{pmatrix}
$$

$E_k = \pm R_k = \pm \sqrt{\epsilon_k^2 + |\Delta_k|^2}$: doubly degenerate by $1_2$

Orthonormal states ($\alpha = 1, 2$) for the negative energy band

$$
|\psi^-\rangle = \begin{pmatrix} u_- \\ v_-
\end{pmatrix}_\alpha
= \begin{pmatrix} -\sin \frac{\theta}{2} |\alpha\rangle_\sigma \\ e^{i\phi_\alpha} \cos \frac{\theta}{2} |\alpha\rangle_\sigma
\end{pmatrix}
= |R^-\rangle_\rho \otimes |\alpha\rangle_\sigma
$$

with $\epsilon_k = R \cos \theta$, $|\Delta_k| = R \sin \theta$
Dirac Monopoles for Unitary States (Connection)

\[ A_i^{\pm \alpha\beta} = \langle \psi_\alpha^\pm | \partial_i | \psi_\beta^\pm \rangle = \langle R_\alpha^\pm | \partial_i | R_\beta^\pm \rangle \rho \langle \alpha | \beta \rangle_\sigma + \langle \alpha | \partial_i | \beta \rangle_\sigma , \]
\[ = A_i^{\pm \alpha\beta} (\rho) \delta_{\alpha\beta} + A_i^{\alpha\beta} (\sigma), \quad (2 \text{ contributions}) \]

\[ (A_i^\pm (\rho))^{\alpha\beta} = A_i^{\pm \alpha\beta} (\rho) = \langle R_\alpha^\pm | \partial_i | R_\beta^\pm \rangle \rho \]

\[ (A_i (\sigma))^{\alpha\beta} = A_i^{\alpha\beta} (\sigma) = \langle \alpha | \partial_i | \beta \rangle_\sigma = (U^\dagger \partial_i U)_{\alpha\beta}, \quad U = (|1\rangle_\sigma, |2\rangle_\sigma) \]

\[ B_i^\pm = B_i^\pm (\rho) + B_i (\sigma) = B_i^\pm (\rho) \]

Contribution from \( \sigma \) space vanishes due to the “Sum rule”:

\[ B_i (\sigma) = \epsilon_{ijk} \text{Tr} \partial_j (U^{-1} \partial_k U) = -\epsilon_{ijk} \text{Tr} (U^{-1} \partial_j U)(U^{-1} \partial_k U) = 0 \]
Dirac Monopoles for Unitary States

\[ C_z(k_z) = \frac{1}{2\pi i} \int_{T^2_{xy}} B_z = \frac{1}{2\pi i} \int_{T^2_{xy}} dk_x dk_y \sum_{\alpha} (\partial_x(A_y^\pm(\rho))^{\alpha\alpha} - \partial_y(A_x^\pm(\rho))^{\alpha\alpha}) \]

\[ = C_z^{\alpha=1}(k_z) + C_z^{\alpha=2}(k_z) \]

\[ = N_z^{\alpha=1}(k_z) + N_z^{\alpha=2}(k_z) \]

Sum of Two Covering Degrees around the Dirac Monopole at the Origin

\[ T^2_{xy} \Rightarrow (R_1(T^2_{xy}), R_2(T^2_{xy})) \]

1 to 2 map since \( \Delta \) is \( 2 \times 2 \).
Edge State and Zero Modes

1. Zero Bias Conductance Peak

2. Boundary Magnetism of the Carbon Nanotubes
Zero Energy Edge States in Various Physical Systems

- Anisotropic Superconductivity (\( d_{x^2-y^2}\)-wave)

(a) (1, 1, 0) surface

(b) (1, 0, 0) surface
Zero Energy Edge States in Various Physical Systems

Anisotropic Superconductivity (\(d_{x^2-y^2}\)-wave)

(a)

(1, 1, 0) surface

Zero Energy Edge States!

(b)

(1, 0, 0) surface

No Edge States!
Zero Energy Edge States: cont.

Graphite Ribbons (zigzag, bearded, and armchair edges)

- **(a)** Zigzag
- **(b)** Bearded
- **(c)** Armchair
Zero Energy Edge States: cont.

Graphite Ribbons (zigzag, bearded, and armchair edges)

(a) Zigzag

Zero Energy Edge States!

(b) Bearded

Zero Energy Edge States!

(c) Armchair

No Edge States!
When and Why the Zero Energy Edge States Appear?

Accidental?

No!!

⇒

Topological Origin!

♦ Bulk-Edge Correspondence

♦ Particle Hole Symmetry

♦ Topological Stability

Particle Hole Symmetric System

Hamiltonian (in 1D)

\[ \mathcal{H} = \sum_{x,x'} c_x^\dagger h_{x,x'} c_{x'} , \quad (h_{x,x'} = h_{x',x}^\dagger) \]

\[ c_x = \begin{pmatrix} c_{x\uparrow} \\ c_{x\downarrow} \end{pmatrix} : \text{spinor}, \quad h_{x,x'} = \begin{pmatrix} t_{x,x'} & \Delta_{x,x'} \\ \Delta'_{x,x'} & -t_{x,x'} \end{pmatrix} \]

Bulk Hamiltonian (with Translation Symmetry)

\[ \mathcal{H}^{bulk} = \sum_k c_k^\dagger h_k c_k = \sum_k c_k^\dagger \begin{pmatrix} \xi_k & \Delta_k \\ \Delta_k^* & -\xi_k \end{pmatrix} c_k \]

\[ E(k) = \pm \sqrt{\xi_k^2 + |\Delta_k|^2} \]
Berry’s parametrization

\[ h_k = \begin{pmatrix} \xi_k & \Delta_k \\ \Delta_k^* & -\xi_k \end{pmatrix} = R(k) \cdot \sigma \]

\( \sigma : \) Pauli matrices

\[ R(k) = (\text{Re} \, \Delta_k, -\text{Im} \, \Delta_k, \xi_k) \]

♦ Map from \( k \) to \( R \) as \( R = R(k) \).

♦ In 1D, \( k \in S^1 \) (\( k : 0 \rightarrow 2\pi \)), so \( R \) forms a loop \( \ell \)
  - This map is one to one

A loop in \( R \) space characterize the hamiltonian

\[ H^{bulk}[\ell] \]

♦ The system with edges is also constructed by cutting all the matrix elements between the sites 1 and \( N \) in real space.

\[ H^{edge}[\ell] \]
When the Zero Mode Edge States Exist?
(Sufficient Condition)

I. The loop $\ell$ is on the plane cutting the origin $\mathcal{O}$.

II. The loop $\ell$ is continuously deformed to the circle whose origin is at $\mathcal{O}$ without passing through $\mathcal{O}$.
Check for the Anisotropic Superconductivity (\(d_{x^2-y^2}\)-wave)

\(\begin{align*}
\text{(110) surface: the unit cells, loops, and the dispersion}
\end{align*}\)

The origin \(O\) is always inside the loop.
Check for the Anisotropic Superconductivity: cont.

(100) surface: the unit cells, loops, and the dispersion

The origin $O$ is never inside the loop except at $k_y = \pm \pi$. 
Check for the Graphite Ribbons

The origin $O$ is inside the loop when $|k_y| > \frac{2\pi}{3}$. 

Zigzag edge: the unit cells, loops, and the dispersion

\[ \begin{align*}
\kappa_y &= -\frac{2\pi}{3} \\
\kappa_y &= 0 \\
\kappa_y &= \frac{2\pi}{3}
\end{align*} \]
Check for the Graphite Ribbons: cont.

Bearded edge: the unit cells, loops, and the dispersion.

The origin $\mathcal{O}$ is inside the loop when $|k_y| < \frac{2\pi}{3}$.
Check for the Graphite Ribbons: cont.

Armchair edges: the unit cells, loops, and the dispersion

The origin $O$ is always outside the loop.
Boundary Effects in Anisotropic Superconductivity

- Local (Boundary) Time Reversal Symmetry Breaking in $d_{x^2-y^2}$-wave Superconductivity

- As a Peierls Instability of Flat Band Systems

![Graphs](c) and (d)

with $+s$ and with $+is$

Boundary Effects in Carbon Nanotubes

- Dimerization Instability by Lattice deformation (Zero mode edge states are protected by the chiral symmetry for a small deformation)

Small dimerization
zero modes

- Local Spin Moments in the Zig-Zag edges
As a Peierls Instability of Flat Band Systems

Small $U < U_C^{MF}$
No bulk AF order

Large $U > U_C^{MF}$
Bulk is AF ordered

Topological Order

is NOT merely

FANCY

but

USEFUL!