Electron fractionalization in two-dimensional graphene-like structures

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Outline

Fractionalization in 1D: Polyacetylene

Assume a one-dimensional tight-binding model for electrons

Coupling electrons to phonons induces **either** the dimerization pattern

or the dimerization pattern

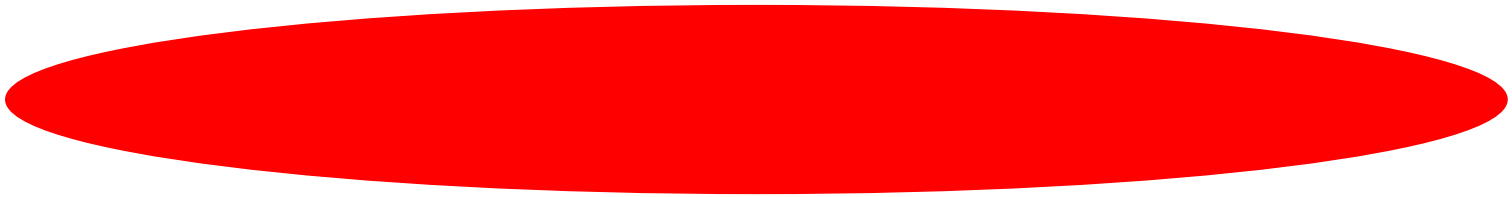
Fractionalization of the electron charge occurs at defects in the dimerization pattern

Ingredient for fractionalization in Polyacetylene

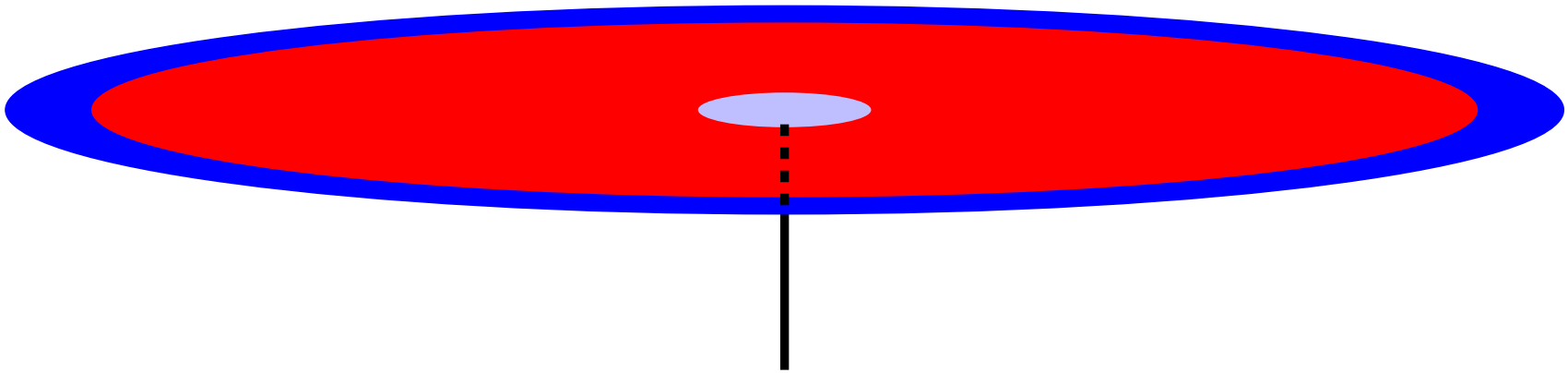
- Polyacetylene has two Fermi points. (The rule in 1D but exceptional in 2D.)
- A perturbation couples the two Fermi points and stabilizes a bond density wave (BDW) for the electrons by opening a single-particle gap at the Fermi energy.
- There are two degenerate BDW associated to the spontaneous breaking of $\mathbb{Z}_2$ translation invariance in the thermodynamic limit.
- There are solitons that interpolate between the two degenerate BDW at a finite energy cost.
- There are single-particle states at the Fermi energy in the background of the soliton.
- The fractional charge is calculated as the difference between the local single-particle density of states with and without the soliton.

Fractionalization in 2D: Fractional Quantum Hall Effect

Incompressible Laughlin state at filling fraction $1/m$, $m = 2n + 1$,



Quasi-hole excited state with charge quantum number e/m



is obtained by adiabatically increasing a flux ϕ from 0 to $\phi_0 = hc/e$ through an infinitesimal solenoid at the origin.

Ingredient for fractionalization in the FQHE

- Time-reversal symmetry is broken.
- The many-body ground state at filling fraction $1/m$, $m = 2n + 1$, is incompressible, i.e., it is featureless as it does not break spontaneously any symmetry.
- The ground state manifold is degenerate in the thermodynamic limit if 2D space is chosen to be a torus: Quantum topological order has emerged.

Polyacetylene versus FQHE

Fractionalization in Polyacetylene (Rebbi and Jackiw 1976, Su, Schrieffer, and Heeger 1979)

- arises out of spontaneous breaking of a symmetry
- and was believed (in the condensed matter community) to be special to 1D (for energetical reasons).

Fractionalization in the FQHE (Laughlin 1983, Halperin 1984, Wen 1990)

- arises out of quantum topological order.

The notion of quantum topological order has played an essential role in attempts to identify examples of quantum-number fractionalization in space larger than 1D (e.g., in high-T_c superconductivity).

3 steps for 2D fractionalization “à la Polyacetylene”

- We seek a model for non-interacting electrons in 2D with two Fermi points.
- We need to open a gap at the Fermi energy by breaking spontaneously a symmetry.
- We need defects in the textured background for the electrons.

Step 1: Two Fermi points in 2D

- We seek a 2D electronic dispersion with a valence and conduction band that touch at two isolated non-equivalent points in the Brillouin zone.
- Choose 2D lattice Λ with sublattices Λ_A and Λ_B

$$H = -\sum_{\langle ij \rangle} t_{\mathbf{r}_i,\mathbf{r}_j} \left(a^\dagger_{\mathbf{r}_i} b_{\mathbf{r}_j} + b^\dagger_{\mathbf{r}_j} a_{\mathbf{r}_i} \right), \qquad t_{\mathbf{r}_i,\mathbf{r}_j} \in \mathbb{R},$$

  and the hopping amplitudes so that valence and conduction bands touch at two points.
- Two possible solutions are

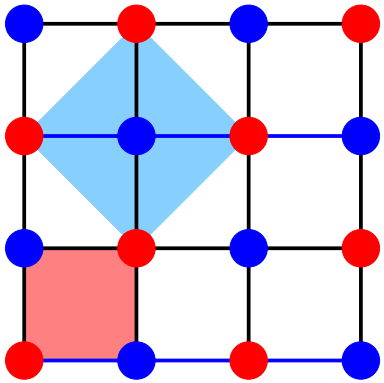
$$\{\Lambda = \text{square lattice}, \qquad t's \text{ give the } \pi \text{ flux phase}\}$$

  or

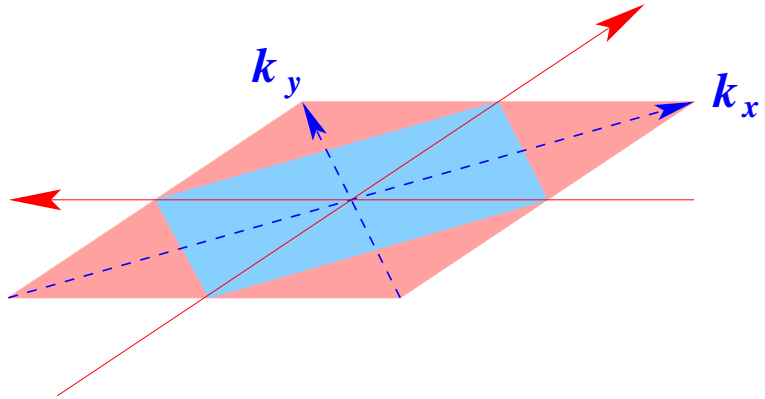
$$\{\Lambda = \text{honeycomb lattice}, \qquad t's \text{ uniform}\}.$$

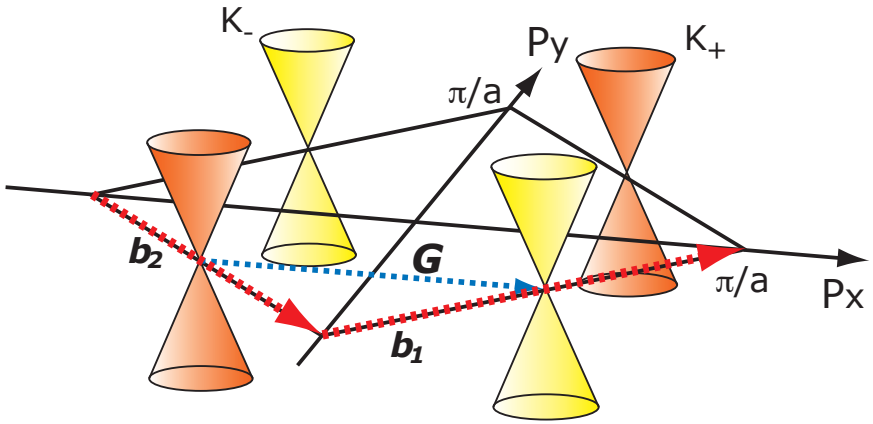
Square lattice with π flux phase

Direct space



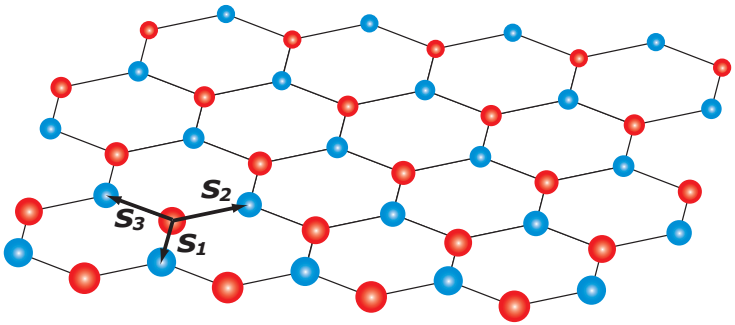
Reciprocal space



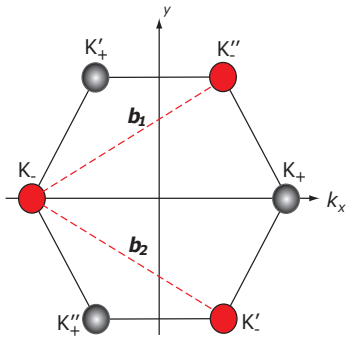


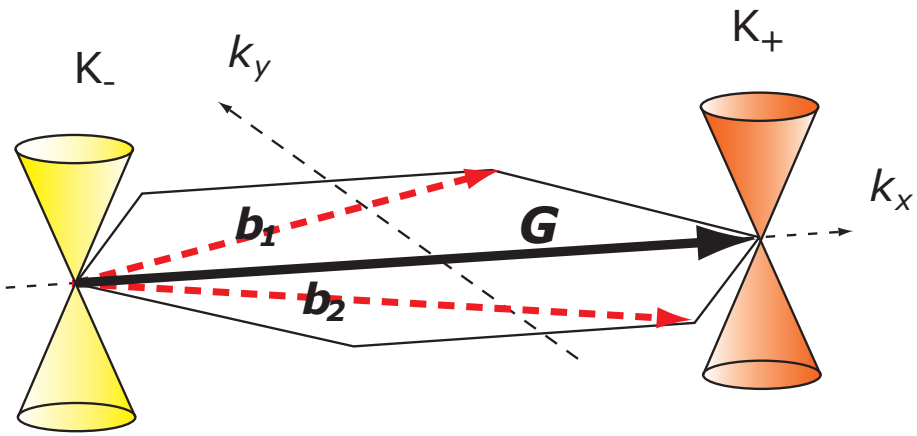
Honeycomb lattice with graphene-like dispersion

Direct space

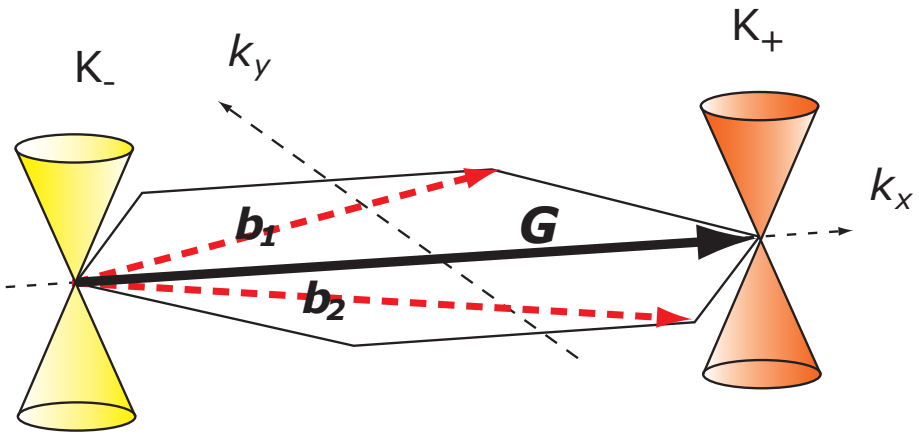


Reciprocal space





Low-energy effective Hamiltonian

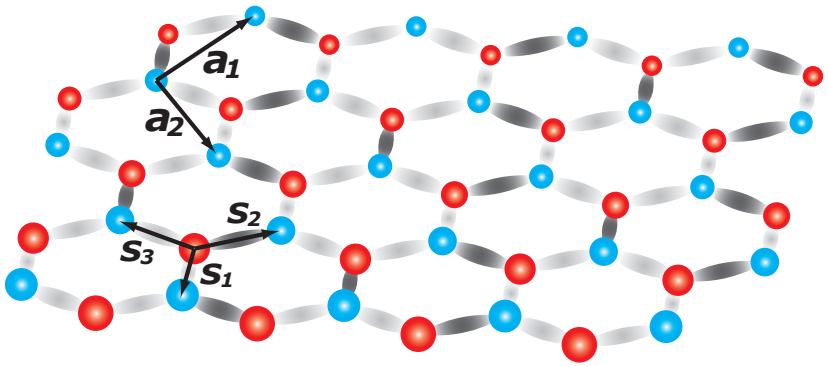


$$H \to \mathcal{H} := \int d^2\boldsymbol{r}\, \Psi^\dagger(\boldsymbol{r})\, \mathcal{K}_D(\boldsymbol{r})\, \Psi(\boldsymbol{r})$$

where

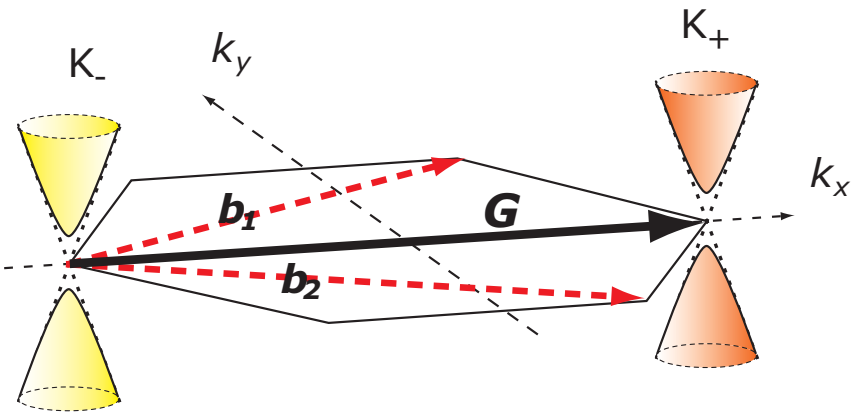
$$\mathcal{K}_D = \begin{pmatrix} 0 & -2i\partial_z & 0 & 0 \\ -2i\partial_{\bar{z}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2i\partial_z \\ 0 & 0 & 2i\partial_{\bar{z}} & 0 \end{pmatrix}, \qquad \Psi(\boldsymbol{r}) = \begin{pmatrix} u_b(\boldsymbol{r}) \\ u_a(\boldsymbol{r}) \\ v_a(\boldsymbol{r}) \\ v_b(\boldsymbol{r}) \end{pmatrix}.$$

Step 2: Opening of a single-particle gap for graphene

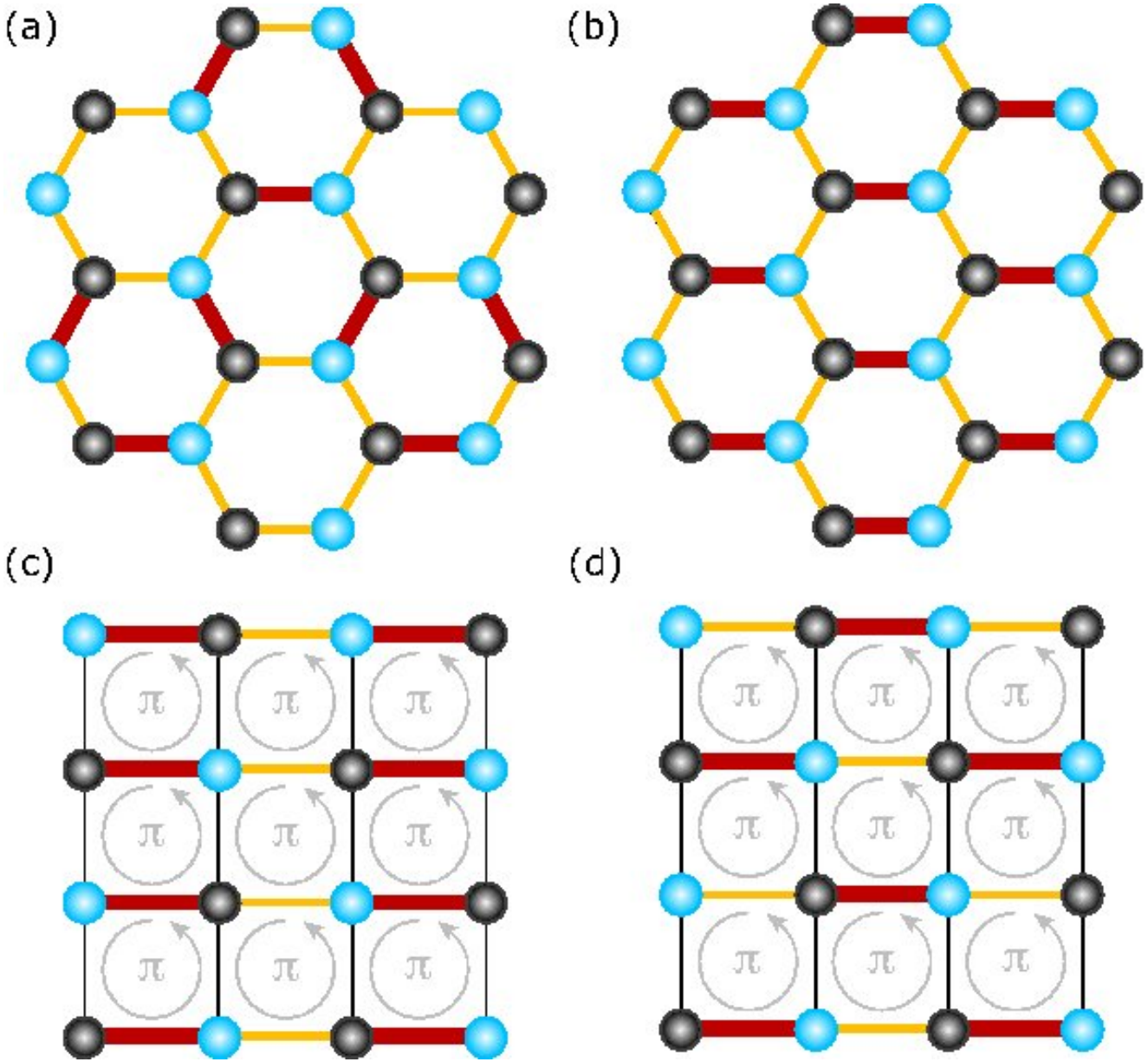


$$H = -\sum_{\boldsymbol{r}\in\Lambda_A}\sum_{i=1}^{3}\left(t+\delta t_{\boldsymbol{r},i}\right)\; a^{\dagger}_{\boldsymbol{r}} b_{\boldsymbol{r}+\boldsymbol{s}_i} + \text{H.c.}$$

with $\delta t_{\boldsymbol{r},i} = \Delta(\boldsymbol{r})\, e^{i\boldsymbol{K}_+\cdot\boldsymbol{s}_i}\, e^{i\boldsymbol{G}\cdot\boldsymbol{r}}/3 + \text{c.c.}$



$$\mathcal{K}_D = \begin{pmatrix} 0 & -2i\partial_z & \Delta(\boldsymbol{r}) & 0 \\ -2i\partial_{\bar{z}} & 0 & 0 & \Delta(\boldsymbol{r}) \\ \bar{\Delta}(\boldsymbol{r}) & 0 & 0 & 2i\partial_z \\ 0 & \bar{\Delta}(\boldsymbol{r}) & 2i\partial_{\bar{z}} & 0 \end{pmatrix}$$


(a)
(b)
(c)
(d)
π

Pattern of symmetry breaking

- Time-reversal and sublattice symmetries are preserved.
- The lattice $\mathbb{Z}_3$ symmetry [the $U(1)$ chiral symmetry in the continuum] is broken by a finite $\Delta \in \mathbb{C}$.
- Sublattice symmetry is broken by a TRS charge density wave μ_s and by a TRS-breaking next-nearest-neighbor hopping η

$$\mathcal{K}_D = \begin{pmatrix} (\mu_s + \eta)(\boldsymbol{r}) & -2i\partial_z & \Delta & 0 \\ -2i\partial_{\bar{z}} & -(\mu_s + \eta)(\boldsymbol{r}) & 0 & \Delta \\ \bar{\Delta} & 0 & -(\mu_s - \eta)(\boldsymbol{r}) & 2i\partial_z \\ 0 & \bar{\Delta} & 2i\partial_{\bar{z}} & (\mu_s - \eta)(\boldsymbol{r}) \end{pmatrix}$$

(Semenoff 1984 and Haldane 1988).

Step 3: $U(1)$ vortices support zero modes

- Take advantage of the fact that $\Delta(\boldsymbol{r})$ has a phase,

  $$\Delta(\boldsymbol{r}) = \Delta_0(r)\, e^{\mathrm{i}(\alpha+n\theta)}, \qquad \Delta_0(r) > 0, \qquad n \in \mathbb{Z}, \qquad z = r\exp(\mathrm{i}\theta).$$

- $\mathcal{K}_D$ has zero modes iff

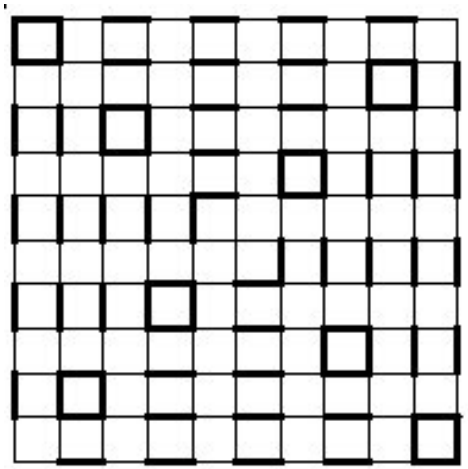
  $$\left(\partial_r - \mathrm{i}r^{-1}\partial_\theta\right)\, u_a(\boldsymbol{r}) + \mathrm{i}e^{\mathrm{i}\theta}\Delta(\boldsymbol{r})\, v_a(\boldsymbol{r}) = 0,$$
  $$\mathrm{i}e^{-\mathrm{i}\theta}\bar{\Delta}(\boldsymbol{r})\, u_a(\boldsymbol{r}) - \left(\partial_r + \mathrm{i}r^{-1}\partial_\theta\right)\, v_a(\boldsymbol{r}) = 0,$$

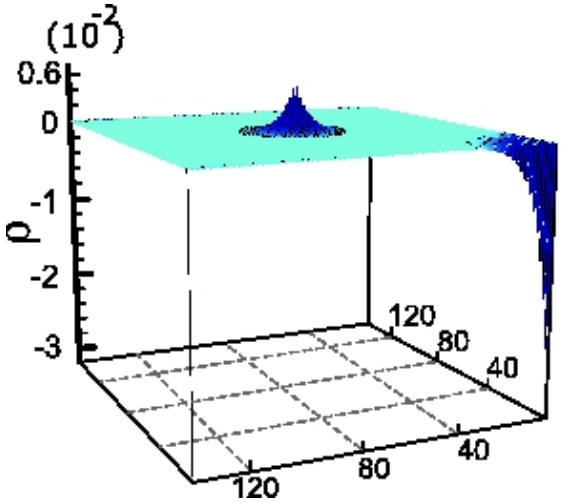
  holds on sublattice Λ_A while the equations obtained from $u_a \to u_b$, $v_a \to v_b$, and $\theta \to -\theta$ must also hold on sublattice Λ_B.
- If $n = -1$, then

  $$u_a(r,\theta) = \frac{e^{\mathrm{i}\left(\frac{\alpha}{2}+\frac{\pi}{4}\right)}}{\sqrt{2\pi}}\, \frac{e^{-\int_0^r dr'\, \Delta_0(r')}}{\sqrt{\int_0^\infty dr\, r\, e^{-2\int_0^r dr'\, \Delta_0(r')}}},$$
  $$v_a(r,\theta) = \bar{u}_a(r,\theta).$$

  is a solution supported on Λ_A.

Comments





Same equations for zero modes were solved in two different contexts:

- When coupling a charge q scalar Higgs field to gauge fields carrying a flux of n/q in 2D space. (Jackiw and Rossi 1981)
- For mid-gap states in a 2D p-wave superconductor. (Read and Green 2000)

Charge is not a conserved quantum number in both cases.

Charge fractionalization

Because we are dealing with a single-particle problem, we can compute the local charge accumulated around a vortex from

$$\nu(\boldsymbol{r},\varepsilon) \equiv \sum_{\varepsilon'} \psi^{\dagger}_{\varepsilon'}(\boldsymbol{r})\psi_{\varepsilon'}(\boldsymbol{r})\delta(\varepsilon-\varepsilon').$$

The charge bound to the vortex is

$$\delta\nu(\boldsymbol{r},\varepsilon) \equiv \nu_{|n|=1}(\boldsymbol{r},\varepsilon) - \nu_{|n|=0}(\boldsymbol{r},\varepsilon).$$

With sublattice symmetry and adiabatic switch-on of a vortex, then

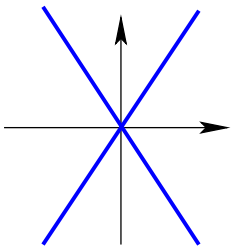
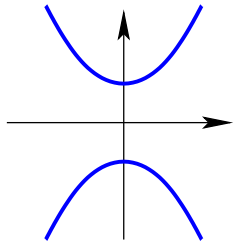
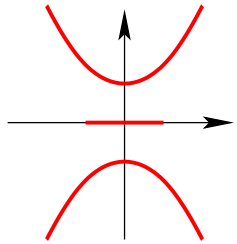
$$\int d^2\boldsymbol{r}\left(2\int_{-\infty}^{0^-} d\varepsilon\,\delta\nu(\boldsymbol{r},\varepsilon) + |\psi_0(\boldsymbol{r})|^2\right) = 0.$$

But the *single* zero mode $\psi_0(\boldsymbol{r})$ is normalized to one and

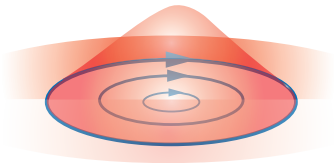
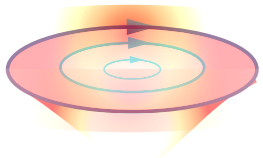
$$\int d^2\boldsymbol{r}\int_{-\infty}^{0^-} d\varepsilon\,\delta\nu(\boldsymbol{r},\varepsilon) = -1/2.$$

Exotic quantum number assignments

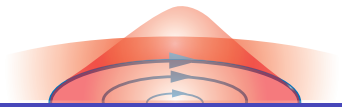
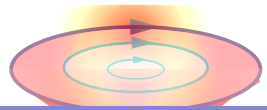
Density of states:

q for spinless fermion: $-e/2$ if unfilled or $+e/2$ if filled.

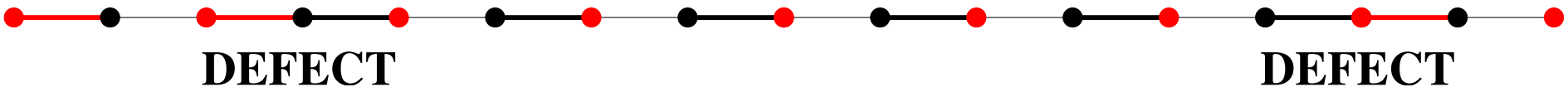



(q, S) for spinfull fermion: $\underbrace{(-e, 0)}_{\text{unfilled}}$ or $\underbrace{(+e, 0)}_{\text{doubly filled}}$ or $\underbrace{(0, \pm 1/2)}_{\text{singly filled}}$.

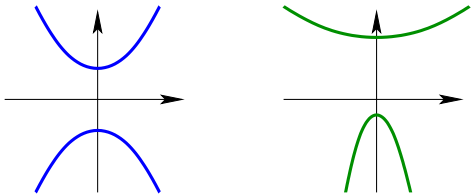



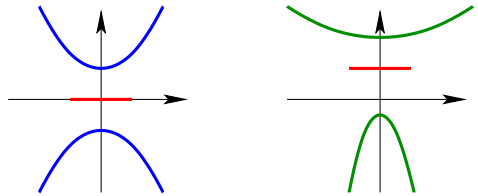
Where is the missing charge $e/2$? We must impose charge neutrality for the vortices:

This is the counterpart to periodic boundary conditions in 1D

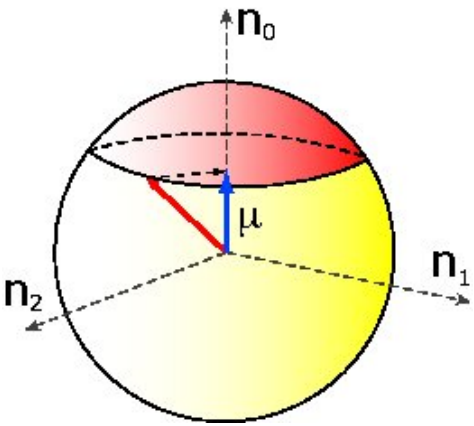


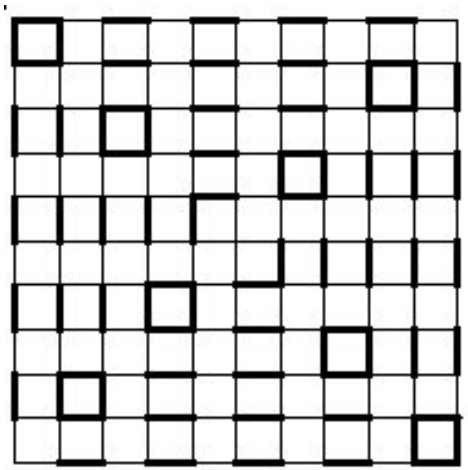
Is the sublattice symmetry essential for fractionalization? No:

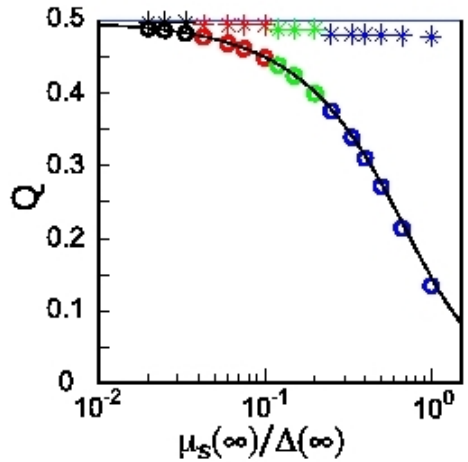




Fractionalization is then irrational (Goldstone and Wilczek 1981, Rice and Mele 1982, Jackiw and Semenoff 1983, Kivelson 1983). In 2D,







$$n_0 = \frac{\mu_s}{m}, \qquad n_1 = \frac{\mathrm{Re}\,\Delta}{m}, \qquad n_2 = \frac{\mathrm{Im}\,\Delta}{m}, \qquad m = \sqrt{\mu_s^2 + |\Delta|^2}$$

Where does $\Delta(\boldsymbol{r})$ come from?

First, we need to open the gap.

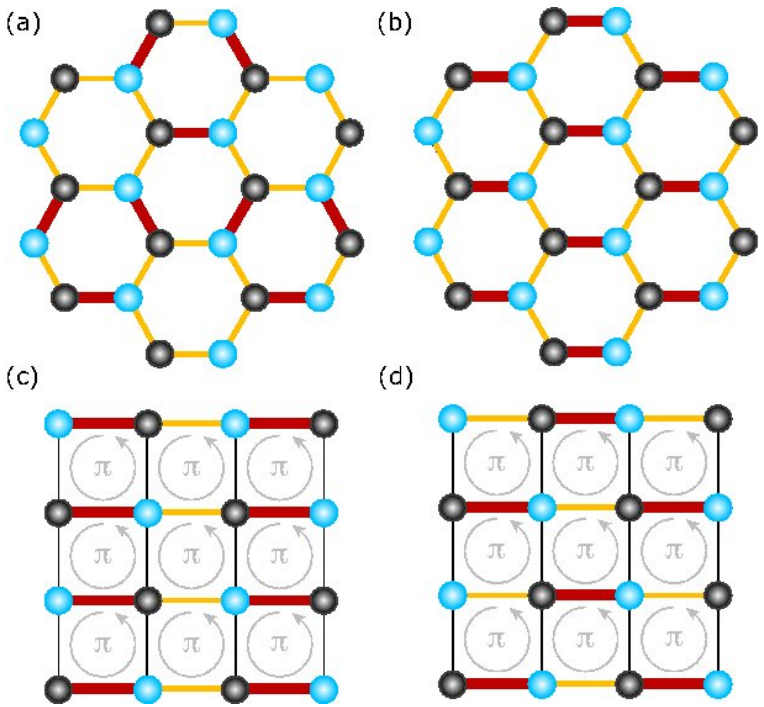
- Phonons do not do the job for graphene because t is very large.
- A repulsive nearest-neighbor interaction V does the job for spinless fermions if $V > V_c^{MF}$ with $V_c^{MF} = 1.906|t|$. However, there are other competing instabilities and the long-range Coulomb interaction has been ignored.

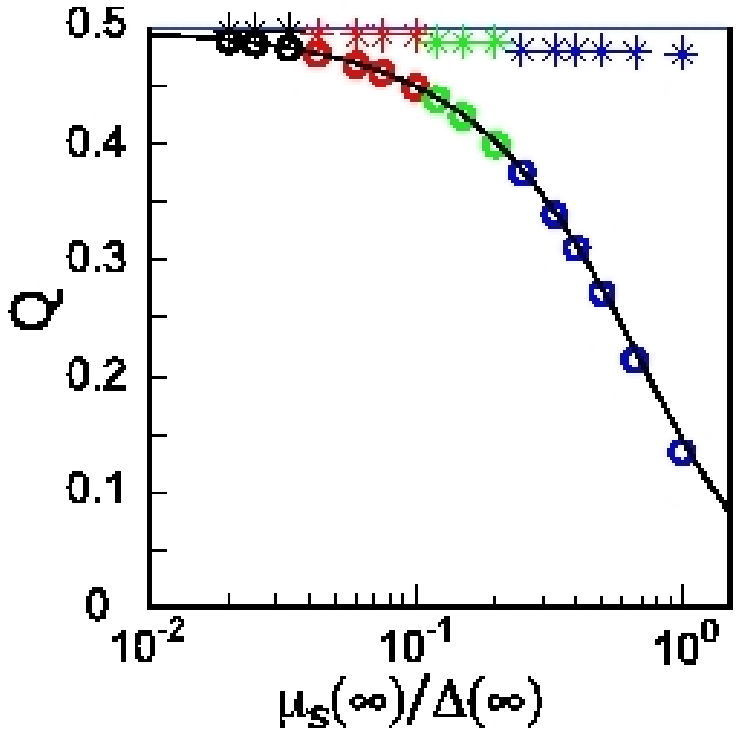
Second, we need vortices.

- Vortices can be generated at finite temperature if their energy cost grows logarithmically with separation at zero temperature.
- At commensuration, vortices are linearly confined at zero temperature. Away from commensuration, vortices are logarithmically confined at zero temperature while mid-gap states survive (Hasegawa et al. 2006).

Can we deconfine the fractional charge at zero temperature?

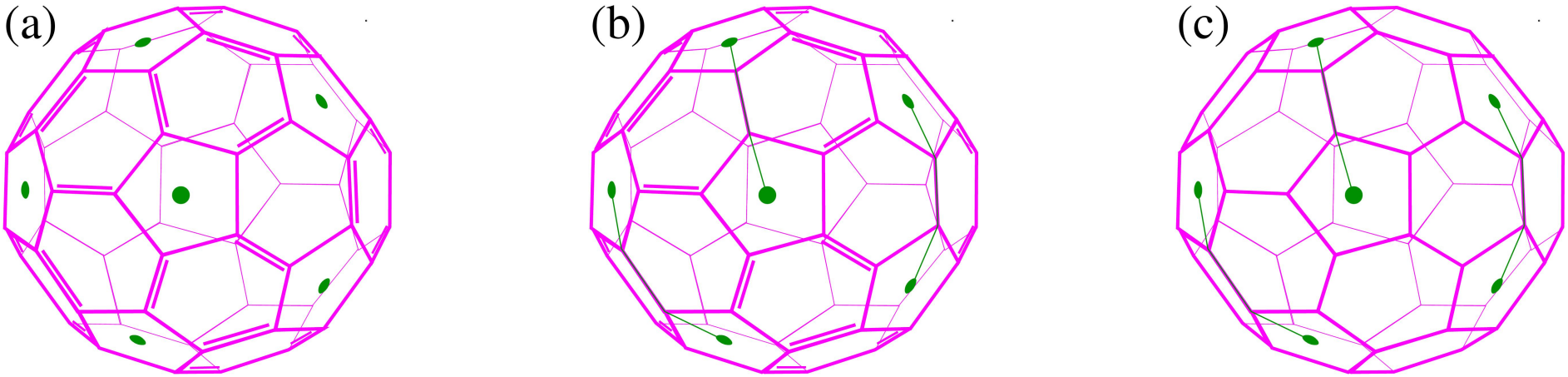
The answer is, at the level of quantum field theory, yes (Jackiw and Pi 2007): Screen the bare vortex logarithmic interactions with dynamical chiral gauge fields. The fractional charge is then always rational, i.e., 1/2, and we recover quantum topological order.





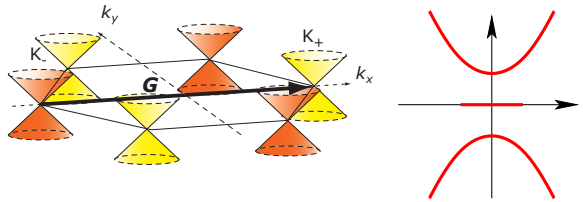
Fullerenes do the job

Building on pioneering work done by Gonzalez, Guinea, Vozmediano (1992 and 1993), Pachos, Stone, and Temme 2008 propose that the Kekulé texture with defective Higgs and chiral gauge fields is geometrically induced at a finite energy cost by wrapping graphene on a sphere (C_{60+6k} fullerenes):

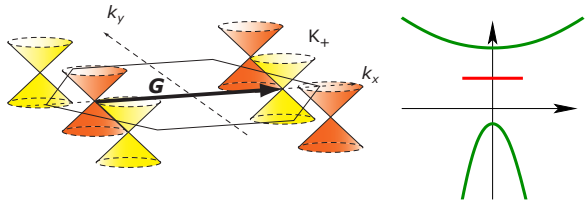


Summary

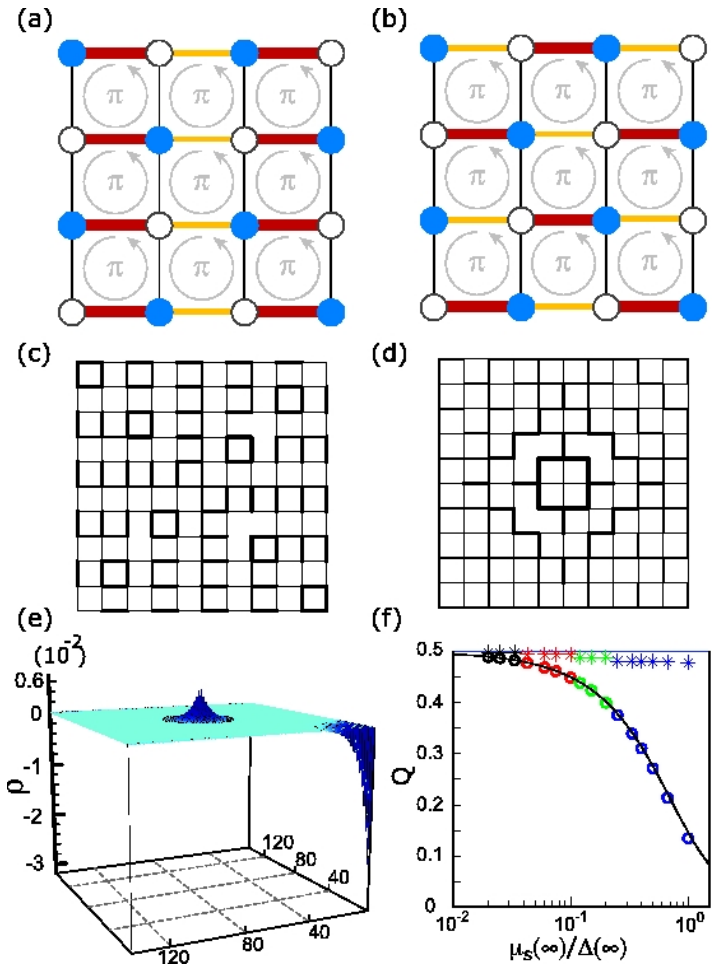
- We found a mechanism for charge fractionalization in 2D similar to that of Polyacetylene in 1D, without breaking time-reversal symmetry or requiring quantum topological order.
- This mechanism demands the existence of two-Fermi points, a bond ordering instability, and vortices in the bond ordering parameter.



- This mechanism is robust to the small breaking of the sublattice symmetry (irrational fractionalization) and is reinforced by the small breaking of the point-group symmetry.



Caption for fractional charge as a function of $\mu(\infty)$



(e) The fermion density profile of (c) for a square lattice with open boundary conditions and 144×144 sites. (f) The fermion number as a function of the scaling variable $\mu_s(\infty)/\Delta(\infty)$ in the presence of the single charge-1 vortex (c) or with the addition of the axial charge-1/2 vortex (d) with core radius $c = 0.01$. The staggered chemical potential μ_s takes the values $0.01t$ (black), $0.03t$ (red), $0.06t$ (green), and $0.1t$ (blue). The thick and thin lines are the theoretical predictions without the axial vortex and $Q = 1/2$, respectively.