Dirac Equations
(First-order matrix equations)

$$[\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m]\psi = E\psi$$

Usual (mass term position-independent, homogenous)

Dirac equation: continuum solutions $E > 0$ and $E < 0$

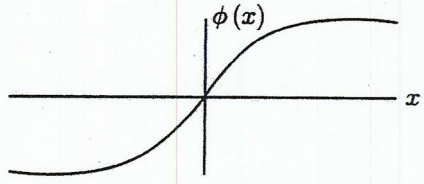
vacuum: $E < 0$ states filled
$E > 0$ states empty
charge $= 0$

Dirac equation in the presence of a defect
(mass term position-dependent, soliton)

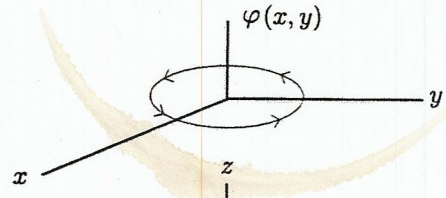
$$[\boldsymbol{\alpha} \cdot \mathbf{p} + \beta\, m\,(\mathbf{r})]\psi = E\psi$$

isolated, normalizable $E = 0$ solution

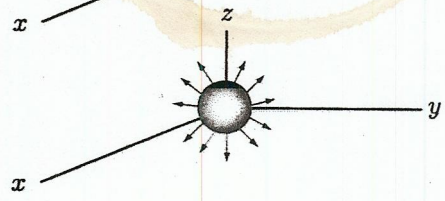
1-d kink



2-d vortex



3-d magnetic monopole



continuum solutions $E > 0, E < 0$
AND isolated, normalizable $E = 0$ solution

"mid-gap" state is found by explicit calculation
is guaranteed by index theorems

Question: for vacuum is mid gap state filled or empty; what is charge?

Answer: double degeneracy of vacuum

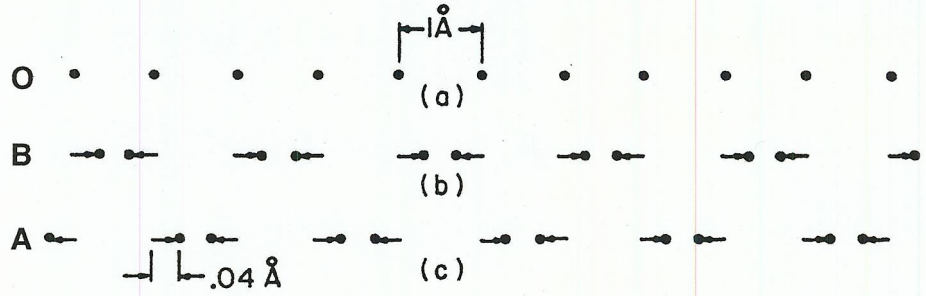
state empty, charge $-1/2$

state filled, charge $+1/2$

observed experimentally in 1-d (polyacetylene)

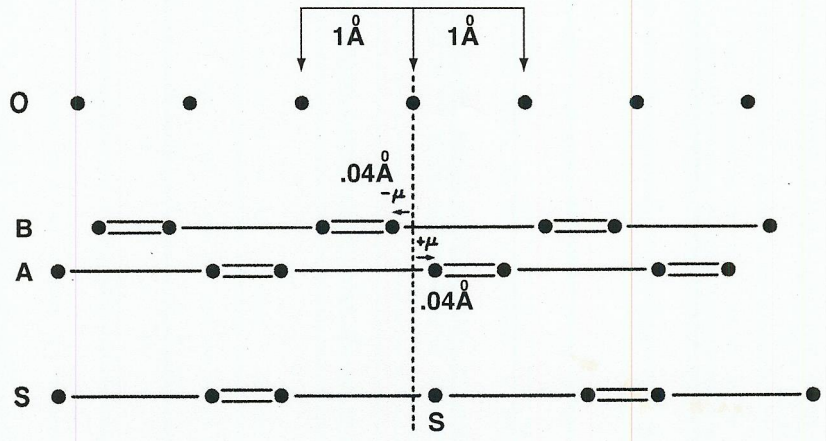
proposed phenomenon in 2-d (graphene)

Polyacetylene Story



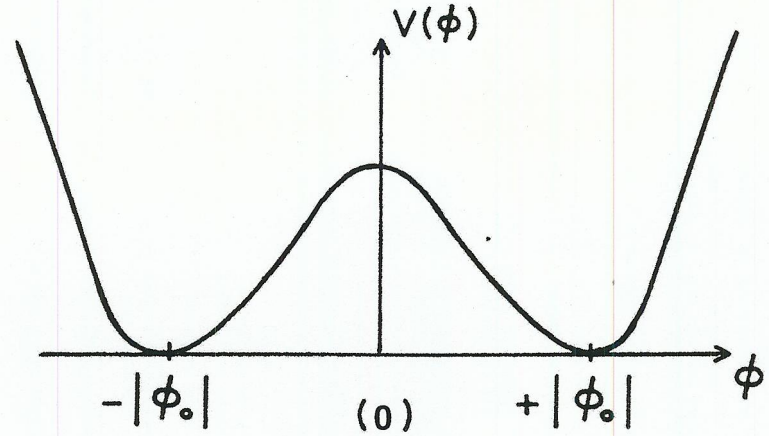
(a) The rigid lattice of polyacetylene; (O) the atoms are equally spaced 1 Å apart. (b), (c) The effect of Peierls' instability is to shift the atoms .04 Å to the left (B) or to the right (A), thus giving rise to a double degeneracy.

Polyacetylene States with Defect

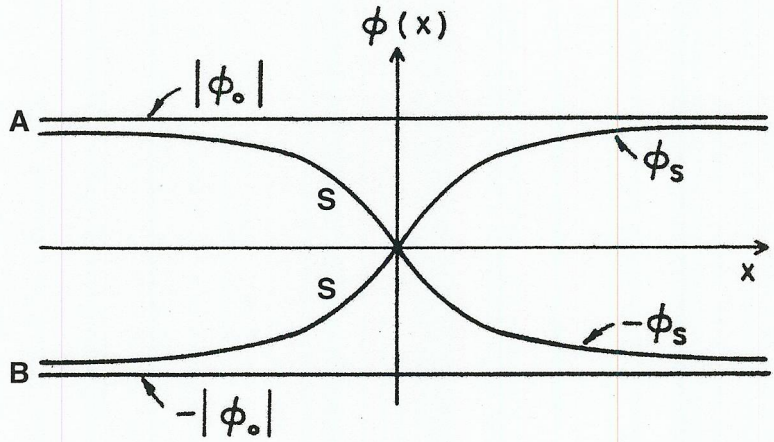


The equally spaced configuration (O) possesses a left-right symmetry, which however is energetically unstable. Rather in the ground states the carbon atoms shift a distance μ to the left or right, breaking the symmetry and producing two degenerate vacua (A, B). A soliton (S) is a defect in the alteration pattern; it provides a domain wall between configurations (A) and (B).

Energetics of Polyacetylene Phonon Field

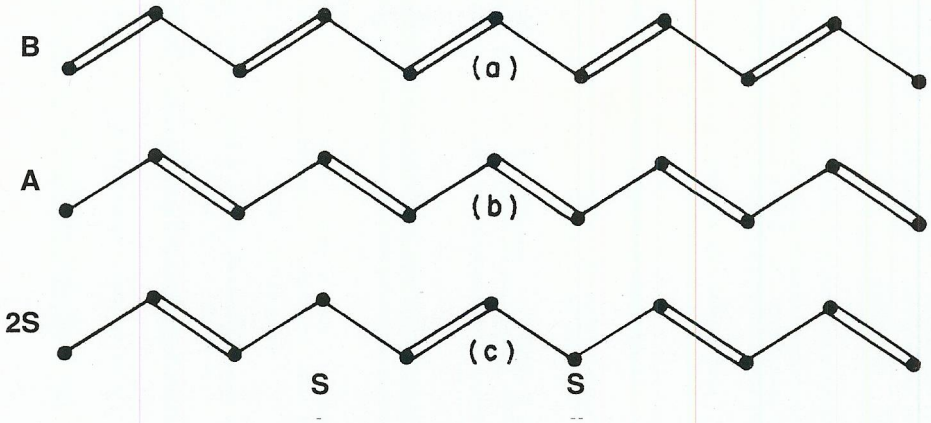


Energy density $V(\phi)$, as a function of a constant phonon field ϕ. The symmetric stationary point, $\phi = 0$, is unstable. Stable vacua are at $\phi = +|\phi_0|$, (A) and $\phi = -|\phi_0|$, (B).



The two constant fields, $\pm\,|\,\phi_0\,|$, correspond to the two vacua (A and B). The kink-soliton fields, $\pm\phi_s$, interpolate between the vacua and represent domain walls.

Polyacetylene Bonding Patterns



Two soliton state carries one fewer link relative to no-soliton vacuum A.

Separate solitons to $\infty \Rightarrow$
split quantum numbers of link $\Rightarrow$
fermion number fractionalization!

Fractional Charge (Analytic Description)

Dirac Hamiltonian matrix $h(\varphi)$
$\Rightarrow$ Dirac equation for fermion dynamics, depending on background field φ.

$$\text{vacuum sector: } h(\varphi_0)\psi_E^v = E\,\psi_E^v$$
$$\text{soliton sector: } h(\varphi_s)\psi_E^s = E\,\psi_E^s$$

negative and positive E continuum solutions:
normalized $E = 0$ mode in soliton sector

negative solutions $\Leftrightarrow$ valence band (positrons)
positive solutions $\Leftrightarrow$ conduction band (electrons)

vacuum charge density:

$$\rho(\mathbf{r}) = \int_{-\infty}^{0} dE\,\rho_E(\mathbf{r}) \qquad \rho_E = \psi_E^\dagger \psi_E$$

renormalized soliton charge:

$$Q = \int d\mathbf{r} \int_{-\infty}^{0-} dE\Big(\rho_E^s(\mathbf{r}) - \rho_E^v(\mathbf{r})\Big)$$

Evaluation simple in the presence of an energy reflection symmetry:
a unitary matrix M that anticommutes with h and maps $E > 0$ on $E < 0$ solutions and vice-versa

$$Mh + hM = 0$$
$$\Rightarrow M\psi_E = \psi_{-E} \Rightarrow \rho_E = \rho_{-E}$$
$$\Rightarrow M\psi_0 = \pm\psi_0$$

Fractional Charge Calculation

completeness: $$\int_{-\infty}^{\infty} dE\, \psi_E^\dagger(\mathbf{r})\psi_E(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$

$$\Rightarrow \int_{-\infty}^{\infty} dE[\rho_E^s(\mathbf{r}) - \rho_E^v(\mathbf{r})] = 0$$

Conjugation ($\rho_E = \rho_{-E}$) and zero mode $\Rightarrow$

$$\int_{-\infty}^{0-} dE\Big(2\rho_E^s(\mathbf{r}) - 2\rho_E^v(\mathbf{r})\Big) + \psi_0^\dagger(\mathbf{r})\psi_0(\mathbf{r}) = 0$$

$$\int_{-\infty}^{0-} dE\Big(\rho_E^s(\mathbf{r}) - \rho_E^v(\mathbf{r})\Big) = -\frac{1}{2}\psi_0^\dagger(\mathbf{r})\psi_0(\mathbf{r})$$

$$Q = -\frac{1}{2}$$

Any dimension! Eigenvalue, not expectation value!

Empty mid-gap state: $Q = -\frac{1}{2}$
Filled mid-gap state: $Q = +\frac{1}{2}$

Rebbi & R.J., *PRD* **13**, 3398 (76);
Su, Schrieffer & Heeger, *PRL* **42**, 1698 (79).

Absent Energy Reflection Symmetry $O(\varepsilon)$

$\Rightarrow$ mid gap state migrates to a non-central position in gap: $\psi_0 \to \psi_x$, $E = O(\varepsilon)$

$\Rightarrow$ charge = irrational number
tends to $-1/2$ as $\varepsilon \to 0$

can be obtained from:

(i) "η" invariant" or "spectral asymmetry"

$$\rho(\mathbf{r}) = -\frac{1}{2} \int_{-\infty}^{\infty} dE \, \text{sign}\,(E)\, \psi_E^{s\dagger}(\mathbf{r}) \psi_E^s(\mathbf{r}) - \frac{1}{2}\, \psi_x^\dagger \psi_x$$

shifted gap state

Niemi & Semenoff, *Phys. Rep.* **135**, 100 (86)

(ii) induced current

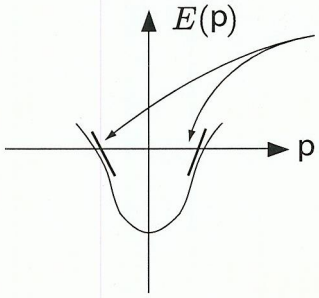
$$< \rho(\mathbf{r}) > = < \psi^\dagger(\mathbf{r})\, \psi(\mathbf{r}) > = -tr\, \gamma^0\, G(\mathbf{r}, \mathbf{r})$$

Goldstone & Wilczek, *Phys. Rev. Lett.* **47**, 987 (81)

for (i) and (ii)

$\rho(\mathbf{r}) = \partial_i k^i(\mathbf{r}) \Rightarrow \int dr\, \rho =$ surface term (topological!)

Polyacetylene Realization



linearization at Fermi level
2 "Dirac Points"

$\Rightarrow$2x2 Dirac Hamiltonian
in 1 spatial dimension

Dirac Hamiltonian

$$H = \underbrace{\psi^\dagger \boldsymbol{\alpha} \cdot \mathbf{p}\, \psi}_{} + \underbrace{\phi\, \psi^\dagger\, \beta \psi}_{} \qquad (2\times 2)$$

linearization at Fermi level

Peierls' instability
ϕ constant $\phi_0 \Rightarrow$ mass $|g|\,\phi_0|$
ϕ soliton $\phi_s \Rightarrow$ zero mode ϕ_0

$$\alpha = \sigma^3, \beta = \sigma^2, p = \frac{1}{i}\frac{d}{dx}$$

$\psi \to e^{i\chi}\psi, \Rightarrow$ Fermi number global symmetry: $J^\mu = \bar{\psi}\,\gamma^\mu\,\psi$

Dirac equation : $h(\phi)\,\psi_E = (\alpha p + \beta\,\phi)\,\psi_E = E\,\psi_E$

$$h\,(\phi_s)\,\psi_0 = 0 \quad \phi_s = \text{kink}$$

NB: σ^1 anticommutes with h

$\sigma^1\,\psi_E = \psi_{-E}$ (energy reflection symmetry)

Conclusion: $Q = \pm\frac{1}{2}$.

Absent energy reflection symmetry: $h \to h + \varepsilon\,\sigma^1$

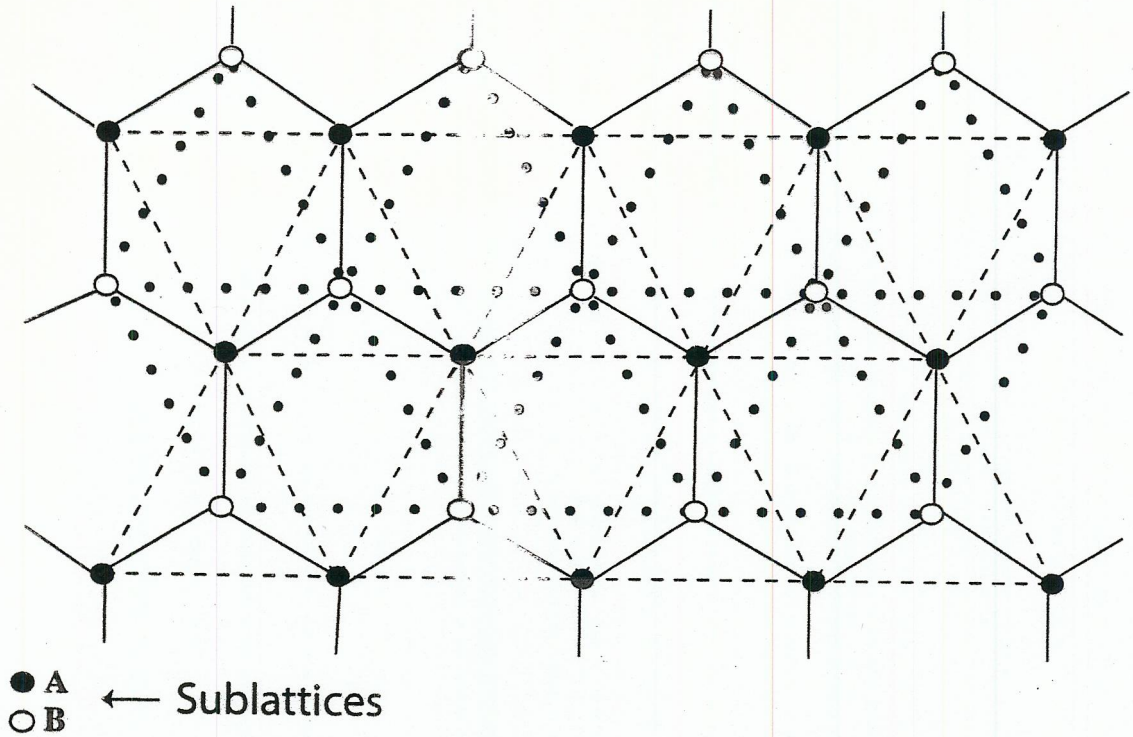
(different adjacent atoms on chain)

$$Q = -\frac{1}{\pi}\,\tan^{-1}\,\frac{\mu}{\varepsilon} \text{ irrational charge } \xrightarrow[\varepsilon \to 0]{} -\frac{1}{2}$$

$$\left(\mu \equiv \varphi(\infty)\right)$$

Graphene Story

Graphene hexagonal lattice

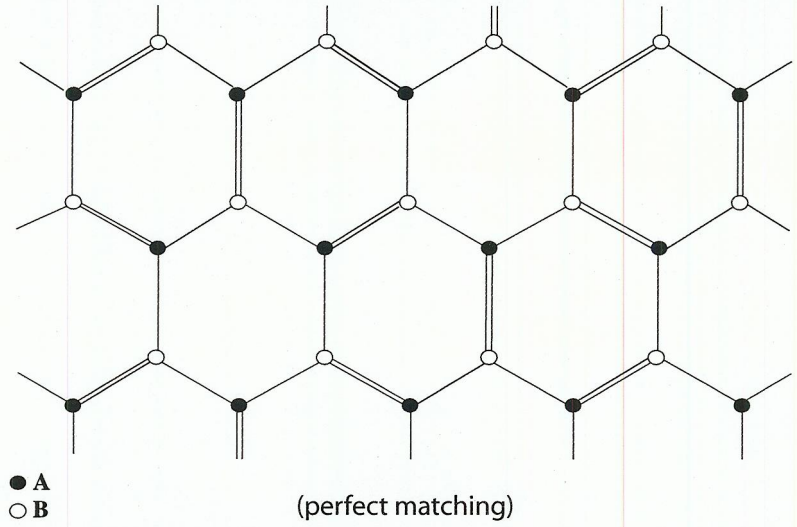


Linearization at Fermi level

2 "Dirac points"

$\Rightarrow$ 4×4 Dirac Hamiltonian in 2 spatial dimensions
(2×2 for each of the two lattices)

Graphene lattice with Kekulé distortion



Dirac Hamiltonian

$$H = \underbrace{\psi^\dagger \boldsymbol{\alpha}\cdot\mathbf{p}\,\psi} + \underbrace{\psi^\dagger \beta\,[\varphi_{re} - i\,\varphi_{im}\,\gamma_5]}\,\psi \qquad (4\times 4)$$

$$\varphi \equiv \varphi_{re} + i\,\varphi_{im}$$

linearization at Fermi level

Kekulé distortion
φ constant $\varphi_0 \Rightarrow$ mass $|\,g\varphi_0\,|$

$$\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix},\ \beta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \gamma_5 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},\ \mathbf{p} = \tfrac{1}{i}\boldsymbol{\nabla}$$

(All vectors are 2-dimensional)

$\psi \to e^{i\chi}\psi \Rightarrow$ Fermi number global symmetry: $J^\mu = \bar{\psi}\gamma^\mu\psi$

Dirac equation : $h(\varphi)\,\psi_E = (\boldsymbol{\alpha}\cdot\mathbf{p} + \beta\,[\varphi_{re} - i\,\varphi_{im}\gamma_5])\,\psi_E = E\,\psi_E$

$$h\,(\varphi_s)\,\psi_0 = 0 \qquad \varphi_s = \text{vortex}$$

NB: $\alpha^3 = \begin{pmatrix} \sigma^3 & 0 \\ 0 & -\sigma^3 \end{pmatrix}$ anticommutes with with h

$\alpha^3\psi_E = \psi_{-E}$ (energy reflection symmetry)

Conclusion : $Q = \pm\frac{1}{2}$

Hou, Chamon & Mudry,

PRL **98**, 186809 (07) [cond-mat/0609740]