Topological phases created by electron-phonon interaction
or
Continuous deformations in 2D solid state systems

Klaus Ziegler and Andreas Sinner

Universität Augsburg

2DCP School, Tbilisi, September 13, 2019

History: topological invariants in physics

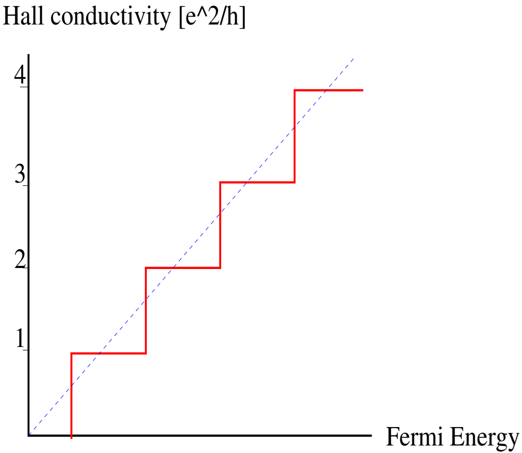
(I) Inertia tensor of rigid bodies

History: topological invariants in physics

(I) Inertia tensor of rigid bodies
(II) vortices in superconductors

History: topological invariants in physics

(I) Inertia tensor of rigid bodies
(II) vortices in superconductors
(III) Quantum Hall effect in a 2D electron gas: Hall steps



Overview

- Basics: spectrum vs. wavefunction
- Graphene with periodic flux
- Topological states in photonic metamaterials
- Theory of deformations
- Graphene-like materials: effect of strain
- Graphene-like materials: electron-phonon interaction
- Saddle-point integration: spontaneous Dirac mass generation
- Transport properties
- Conclusion

References:

A. Sinner and K. Ziegler, Phys. Rev. B 93, 125112 (2016)
K. Ziegler and A. Sinner, EPL 119, 27001 (2017)
K. Ziegler, J. Opt. Soc. Am. B 35, 107 (2018)
A. Sinner and K. Ziegler, Annals of Physics 400, 262 (2019)
A. Sinner and K. Ziegler, arxiv:1908.00442

Topological materials: essential features

- two (or more) bands

Topological materials: essential features

- two (or more) bands
- singular wavefunction

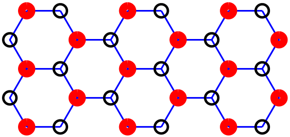
Topological materials: essential features

- two (or more) bands
- singular wavefunction
- topological invariants (e.g. quantized Hall conductivity)

Topological materials: essential features

- two (or more) bands
- singular wavefunction
- topological invariants (e.g. quantized Hall conductivity)

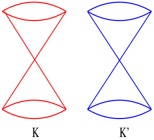
prototype for topological materials: graphene
graphene is a semimetal but not a topological material



Which mechanisms can make graphene a topological material?

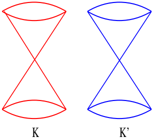
strong homogeneous magnetic field

Graphene: quantized Hall conductor without homogeneous magnetic field



– periodic magnetic flux and nearest-neighbor hopping
(Haldane, PRL '88)

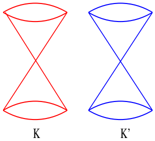
Graphene: quantized Hall conductor without homogeneous magnetic field



– periodic magnetic flux and nearest-neighbor hopping
(Haldane, PRL '88)

– spin-orbit coupling
(Kane/Mele, PRL '05)

Graphene: quantized Hall conductor without homogeneous magnetic field

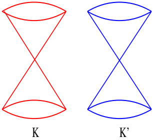


– periodic magnetic flux and nearest-neighbor hopping
(Haldane, PRL '88)

– spin-orbit coupling
(Kane/Mele, PRL '05)

– localized spins (spin texture)
(Hill/Sinner/Z, New Journ. Phys. '11)

Graphene: quantized Hall conductor without homogeneous magnetic field



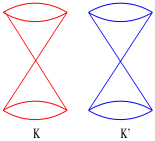
– periodic magnetic flux and nearest-neighbor hopping
(Haldane, PRL '88)

– spin-orbit coupling
(Kane/Mele, PRL '05)

– localized spins (spin texture)
(Hill/Sinner/Z, New Journ. Phys. '11)

– time-periodic driving (Floquet topological insulators)
(Lindner/Refael/Galitski, Nature Phys. '11)

Graphene: quantized Hall conductor without homogeneous magnetic field



– periodic magnetic flux and nearest-neighbor hopping
(Haldane, PRL '88)

– spin-orbit coupling
(Kane/Mele, PRL '05)

– localized spins (spin texture)
(Hill/Sinner/Z, New Journ. Phys. '11)

– time-periodic driving (Floquet topological insulators)
(Lindner/Refael/Galitski, Nature Phys. '11)

– electron-phonon interaction
(Sinner/Z, Annals of Phys. '19)

Topological materials in Nature

Database:

"Out of 26938 stoichiometric materials ... [there are] 2861 topological insulators (TI) and 2936 topological semimetals "

M.G. Vergniory, L. Elcoro, C. Felser, B.A. Bernevig, Z. Wang
The (High Quality) Topological Materials In The World
arXiv:1807.10271 (1958 pages and 4989 figures!)

Spectrum vs. wavefunction I

Haldane's or Bernevig-Hughes-Zhang (BHZ) model
Hamiltonian with Pauli matrices

$$H_{BHZ} = \begin{pmatrix} k_1\sigma_1 + k_2\sigma_2 + m\sigma_3 & 0 \\ 0 & k_1\sigma_1 - k_2\sigma_2 \pm m\sigma_3 \end{pmatrix}$$

doubly degenerate eigenvalues do not depend on the signs of k_2 and m:

$$E_{k_1,k_2} = \pm\sqrt{k^2 + m^2}$$

Spectrum vs. wavefunction I

Haldane's or Bernevig-Hughes-Zhang (BHZ) model
Hamiltonian with Pauli matrices

$$H_{BHZ} = \begin{pmatrix} k_1\sigma_1 + k_2\sigma_2 + m\sigma_3 & 0 \\ 0 & k_1\sigma_1 - k_2\sigma_2 \pm m\sigma_3 \end{pmatrix}$$

doubly degenerate eigenvalues do not depend on the signs of k_2 and m:

$$E_{k_1,k_2} = \pm\sqrt{k^2 + m^2}$$

reason: transformation properties of H

$$(k_1\sigma_1 - k_2\sigma_2 + m\sigma_3)^T = k_1\sigma_1 + k_2\sigma_2 + m\sigma_3$$

and

$$\sigma_1(k_1\sigma_1 - k_2\sigma_2 - m\sigma_3)\sigma_1 = k_1\sigma_1 + k_2\sigma_2 + m\sigma_3$$

The determinant $\det(H - \lambda\sigma_0)$ is invariant

There is more information in the wavefunction!

Spectrum vs. wavefunction II

eigenfunctions of $k_1\sigma_1 + k_2\sigma_2 + m\sigma_3$:

$$\Psi_\pm(k_2) = \begin{pmatrix} 1 \\ -\frac{m\pm\sqrt{k^2+m^2}}{k_1-ik_2} \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{m\pm\sqrt{k^2+m^2}}{k}e^{i\phi} \end{pmatrix}$$

wavefunction has a pole at $k_1 - ik_2 = 0$ for $m \neq 0$!

Spectrum vs. wavefunction II

eigenfunctions of $k_1\sigma_1 + k_2\sigma_2 + m\sigma_3$:

$$\Psi_\pm(k_2) = \begin{pmatrix} 1 \\ -\frac{m\pm\sqrt{k^2+m^2}}{k_1 - ik_2} \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{m\pm\sqrt{k^2+m^2}}{k} e^{i\phi} \end{pmatrix}$$

wavefunction has a pole at $k_1 - ik_2 = 0$ for $m \neq 0$!

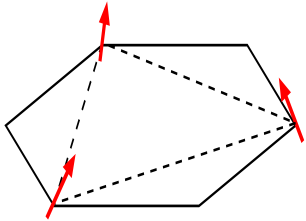
eigenfunctions of $k_1\sigma_1 - k_2\sigma_2 + m\sigma_3$:

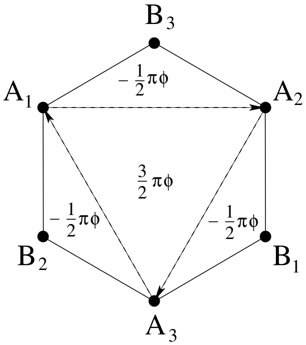
$$\Psi_\pm(-k_2) = \begin{pmatrix} 1 \\ -\frac{m\pm\sqrt{k^2+m^2}}{k_1 + ik_2} \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{m\pm\sqrt{k^2+m^2}}{k} e^{-i\phi} \end{pmatrix}$$

the wavefunctions have a different chirality

Graphene with periodic flux

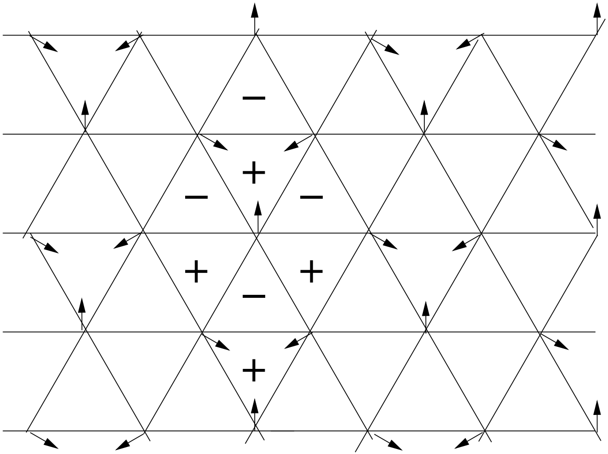
effective flux created by a spin texture





Graphene with periodic flux

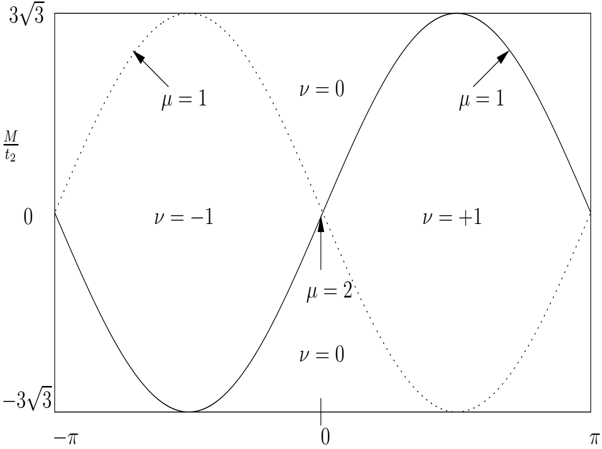
flux on the spin-occupied triangular sublattice



Graphene with periodic flux: phase diagram

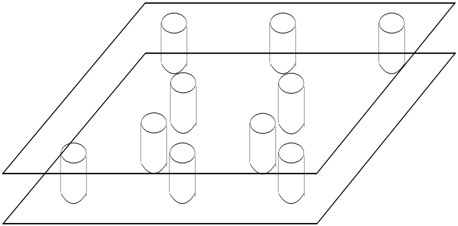
ϕ-m phase diagram

$$\sigma_{xy} = \nu \frac{e^2}{h} \ , \quad \sigma_{xx} \propto \mu \frac{e^2}{h}$$



Topological states in photonic metamaterials

Dirac photons on finite 2D geometries:



Maxwell equations $\longrightarrow$ $H_{Dirac} = i\sigma_x \partial_x + i\sigma_y \partial_y + m\sigma_z$

Topological states in photonic metamaterials

2D electromagnetic field

$$\mathbf{E} = \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = \begin{pmatrix} E_z^R + H_z^R \\ E_z^L + H_z^L \end{pmatrix}$$

Topological states in photonic metamaterials

2D electromagnetic field

$$\mathbf{E} = \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = \begin{pmatrix} E_z^R + H_z^R \\ E_z^L + H_z^L \end{pmatrix}$$

Stokes parameters

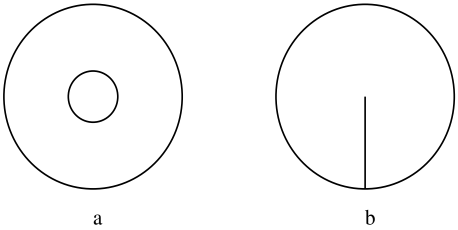
– intensity $I = \mathbf{E} \cdot \mathbf{E}$

– polarization

$$\mathbf{P} = \frac{1}{I} \begin{pmatrix} \mathbf{E} \cdot \sigma_x \mathbf{E} \\ \mathbf{E} \cdot \sigma_y \mathbf{E} \\ \mathbf{E} \cdot \sigma_z \mathbf{E} \end{pmatrix} \qquad |\mathbf{P}|^2 = 1$$

Topological states in photonic metamaterials

1) uniform Dirac mass

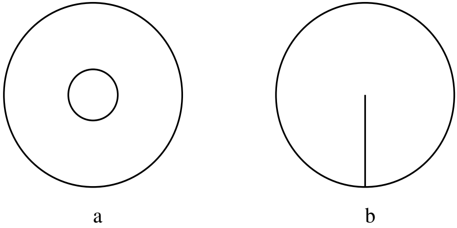


a) two edges:

$$\mathbf{E} = \begin{pmatrix} K_0(\bar{r}) \\ -ie^{i\alpha} sgn(m)\ K_1(\bar{r}) \end{pmatrix} \ , \quad \mathbf{P} = -2sgn(m)\ \frac{K_0(\bar{r})K_1(\bar{r})}{r} \begin{pmatrix} -y \\ x \end{pmatrix}$$

Topological states in photonic metamaterials

1) uniform Dirac mass



a) two edges:

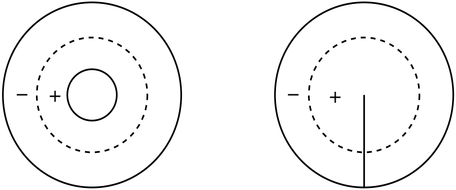
$$\mathbf{E} = \begin{pmatrix} K_0(\bar{r}) \\ -ie^{i\alpha} sgn(m)\ K_1(\bar{r}) \end{pmatrix} \ , \quad \mathbf{P} = -2sgn(m)\ \frac{K_0(\bar{r})K_1(\bar{r})}{r} \begin{pmatrix} -y \\ x \end{pmatrix}$$

b) one edge:

$$\mathbf{E} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\alpha/2} \\ -ie^{i\alpha/2} sgn(m) \end{pmatrix} \frac{e^{-|m|r}}{\sqrt{r}} \ , \quad \mathbf{P} = -sgn(m) \begin{pmatrix} -y \\ x \end{pmatrix} \frac{e^{-2|m|r}}{r^2}$$

Topological states in photonic metamaterials II

2) non-uniform Dirac mass



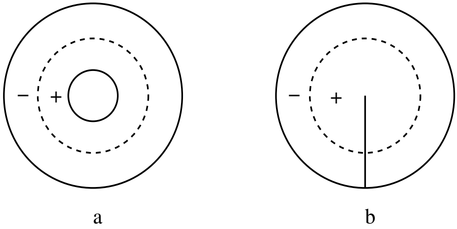
a b

a) two edges:

$$\mathbf{P} = P(\bar{r})\begin{pmatrix} -y \\ x \end{pmatrix}$$

Topological states in photonic metamaterials II

2) non-uniform Dirac mass



a) two edges:

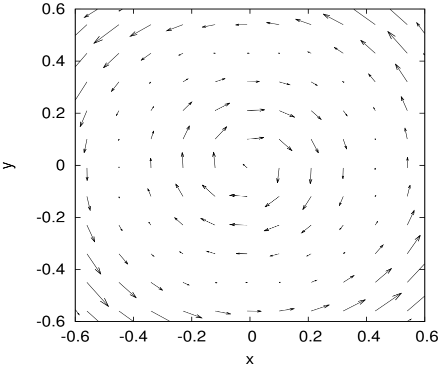
$$\mathbf{P} = P(\bar{r}) \begin{pmatrix} -y \\ x \end{pmatrix}$$

b) one edge:

$$\mathbf{P} = sgn(m_i) \begin{pmatrix} -y \\ x \end{pmatrix} \frac{e^{-2|m_i||r-r_0|}}{r^2}$$

topological states in photonic metamaterials III

polarization of 2a) with two edges: "Skyrmion"



nonzero Berry curvature!

Theory of deformations: a gauge-field approach

classical elasticity theory & quantum theory of electrons

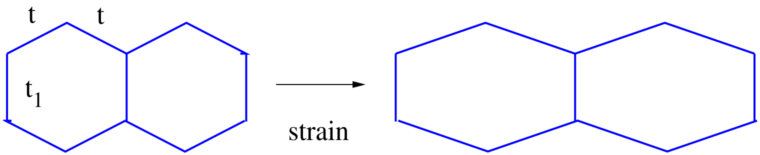
$$\vec{p}_e \rightarrow \vec{p}_e + \frac{e}{c}\vec{A}$$

$\vec{A}$ is not unique (gauge invariance!)
physical quantity: $\nabla \times \vec{A}$

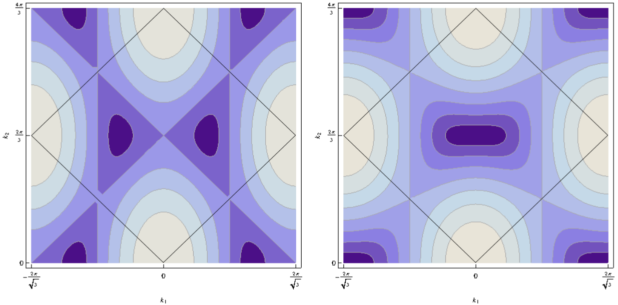
different levels of approximation:
a) classical electrons & classical deformations
b) quantum electrons & classical deformations
c) quantum electrons & quantum deformations (aka phonons)

examples:
a): classical elasticity theory
b): uniform strain
c): electron-phonon interaction

Graphene-like materials: effect of strain

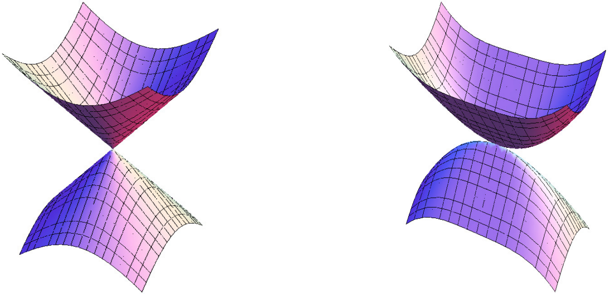


bonds: $t_1 \geq t$ relevant bond ratio: t_1/t



Graphene-like materials: effect of strain

changing $t_1/t = 1 \to 2$

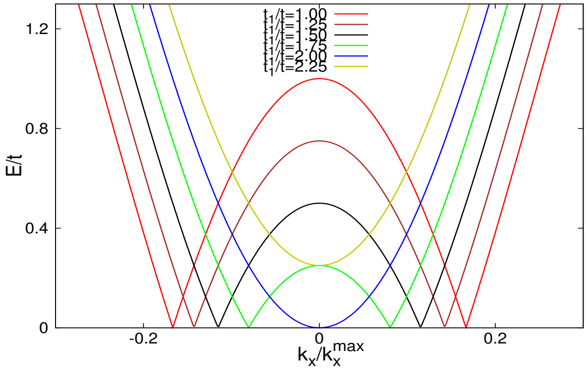


$E_{k_x,k_y}: \quad \pm k$

$$\pm\sqrt{\frac{k_x^4}{4m^2} + c^2 k_y^2}$$

Graphene-like materials: effect of strain

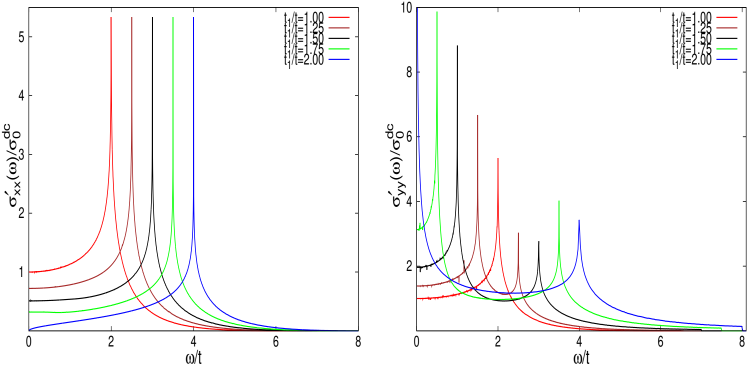
changing $t_1/t = 1...2.25$: the spectrum



a gap opens for $t_1/t > 2$
reminiscent of Landau level formation

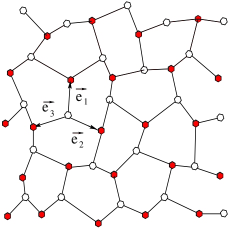
Graphene-like materials under strain: transport properties

changing $t_1/t = 1...2$: the conductivity in x and y direction



divergent conductivity reflects the van Hove singularity at the saddle points

Graphene-like materials: electron-phonon interaction



electronic Hamiltonian

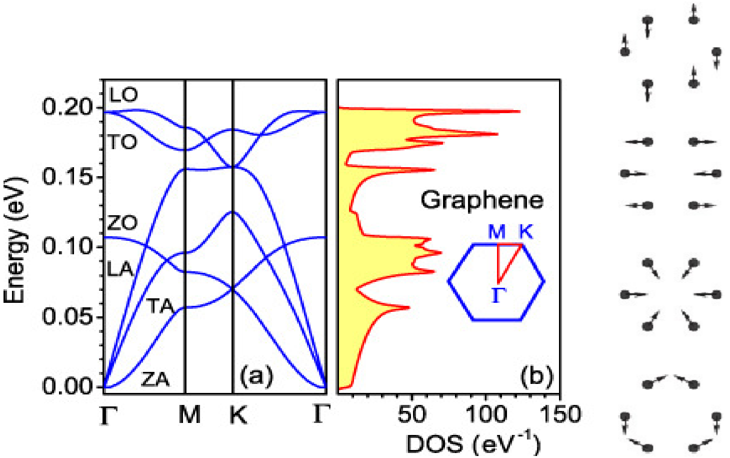
$$H_0 = -t \sum_{\langle rr' \rangle} (c_r^\dagger d_{r'} + d_{r'}^\dagger c_r)$$

electron-phonon Hamiltonian

$$H_2 = \sum_{\langle rr' \rangle} \{\hbar\omega b_{rr'}^\dagger b_{r'r} + \alpha(b_{rr'}^\dagger c_r^\dagger d_{r'} + b_{r'r} d_{r'}^\dagger c_r)\}$$

Graphene-like materials: electron-phonon interaction

Phonon bands predicted by bandstructure calculations for graphene (Basko et al., PRB)



Graphene-like materials: electron-phonon interaction

Functional integral approach: partition function

$$\mathcal{Z} = Tre^{-\beta H} = \int \exp\{-\mathcal{S}[\bar{\psi}, \psi, A]\}\ \mathcal{D}[\bar{\psi}, \psi, A]$$

action ($x = (\mathbf{r}, t)$)

$$\mathcal{S}[\bar{\psi}, \psi, A] = \frac{1}{2g} \int A_\mu^2\ d^3x + \int\ \bar{\psi}[\gamma_\mu \partial^\mu + m + \frac{i}{\sqrt{2}} \gamma_\mu A^\mu]\psi\ d^3x$$

phonons represented by an effective gauge field A_μ

after ψ integration: effective phonon model

$$\mathcal{S}[\bar{\psi}, \psi, A] \to \mathcal{S}[A] = \frac{1}{2g} \int A_\mu^2\ d^3x - \mathrm{tr} \log \left[\gamma_\mu \partial^\mu + m + \frac{i}{\sqrt{2}} \gamma_\mu A^\mu\right]$$

Saddle-point approximation

Saddle-point integration:

mean-field approximation + quantum fluctuations

a) saddle point (variational) condition

$$\delta_A \mathcal{S}[A] = 0$$

with uniform solution A_0

b) fluctuations around the saddle point

$$\mathcal{S}[A_0 + Q] \sim \mathcal{S}_\Delta[A_0] + \mathcal{S}_{CS}[Q] + \mathcal{S}_M[Q]$$

where the Chern-Simons action

$$\mathcal{S}_{CS}[Q] = -2 \sum_\lambda C_\lambda \sum_{\mu,\mu'} \epsilon_{\mu\mu'\lambda} \int \left(\frac{\partial Q_{\mathbf{x}\mu}}{\partial x_\lambda} Q_{\mathbf{x}\mu'} - Q_{\mathbf{x}\mu} \frac{\partial Q_{\mathbf{x}\mu'}}{\partial x_\lambda} \right) d^3\mathbf{x}$$

exists for a system which is neither symmetric nor antisymmetric under parity transformation

Graphene-like materials: electron-phonon interaction

mean-field approximation: effective electronic Hamiltonian

H_0: hopping on the honeycomb lattice

spontaneous symmetry breaking for $g > g_c$:

– phase with modulated strain

$$H_0 + i\Delta \sum_{\mathbf{r}} \cos(\mathbf{G}\cdot\mathbf{r}) c_{\mathbf{r}}^{\dagger} d_{\mathbf{r}} + h.c. \ , \quad \mathbf{G} = \mathbf{K} - \mathbf{K}'$$

Graphene-like materials: electron-phonon interaction

mean-field approximation: effective electronic Hamiltonian

H_0: hopping on the honeycomb lattice

spontaneous symmetry breaking for $g > g_c$:

– phase with modulated strain

$$H_0 + i\Delta \sum_{\mathbf{r}} \cos(\mathbf{G}\cdot\mathbf{r}) c_{\mathbf{r}}^\dagger d_{\mathbf{r}} + h.c. \ , \quad \mathbf{G} = \mathbf{K} - \mathbf{K}'$$

– Haldane phase

$$H_0 + im \sum_{j=1}^{3} \sum_{\mathbf{r}} (c_{\mathbf{r}+\mathbf{c}_j}^\dagger c_{\mathbf{r}} - c_{\mathbf{r}-\mathbf{c}_j}^\dagger c_{\mathbf{r}} - d_{\mathbf{r}+\mathbf{c}_j}^\dagger d_{\mathbf{r}} + d_{\mathbf{r}-\mathbf{c}_j}^\dagger d_{\mathbf{r}})$$

Graphene-like materials: electron-phonon interaction

mean-field approximation: effective electronic Hamiltonian

H_0: hopping on the honeycomb lattice

spontaneous symmetry breaking for $g > g_c$:

– phase with modulated strain

$$H_0 + i\Delta \sum_{\mathbf{r}} \cos(\mathbf{G}\cdot\mathbf{r}) c^\dagger_{\mathbf{r}} d_{\mathbf{r}} + h.c. \ , \quad \mathbf{G} = \mathbf{K} - \mathbf{K}'$$

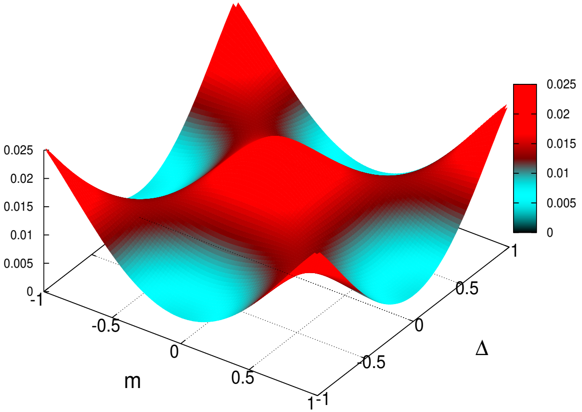
– Haldane phase

$$H_0 + im \sum_{j=1}^{3} \sum_{\mathbf{r}} (c^\dagger_{\mathbf{r}+\mathbf{c}_j} c_{\mathbf{r}} - c^\dagger_{\mathbf{r}-\mathbf{c}_j} c_{\mathbf{r}} - d^\dagger_{\mathbf{r}+\mathbf{c}_j} d_{\mathbf{r}} + d^\dagger_{\mathbf{r}-\mathbf{c}_j} d_{\mathbf{r}})$$

1) order parameters m and Δ break the time-reversal symmetry!
2) both order parameters create a spectral gap!

Graphene-like materials: electron-phonon interaction

mean-field action



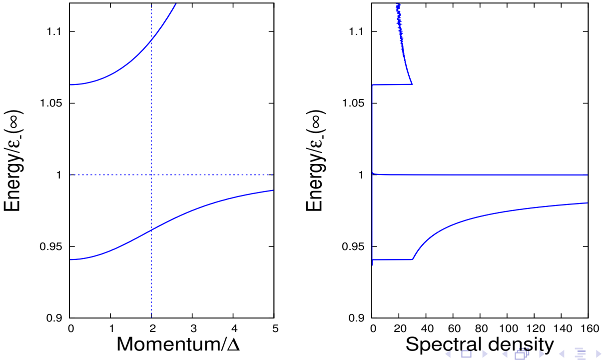
Haldane (m) phase for a single Dirac node

interaction creates two phonon bands with dispersions

$$\hbar\omega \rightarrow \epsilon_{\pm}(p) = \sqrt{f(p) \pm t(p)}$$

where ($a \propto 1/|m|$, $b = const.$)

$$f(p) = \frac{1}{2}\left(p^2 + 2\frac{\Delta}{a} + \frac{b^2}{a^2}\right) \quad , \quad t(p) = \frac{1}{2}\sqrt{\left(p^2 + \frac{b^2}{a^2}\right)^2 + 4\frac{\Delta}{a}\frac{b^2}{a^2}}$$



Linear response to an external field q_ν

current:

$$j_\mu = \bar{\psi}\gamma_\mu\psi$$

external field q_ν couples to the current $\int q_\nu j_\nu d^3x$ in the action

$$\langle j_\mu \rangle_q - \langle j_\mu \rangle_0 \sim q_\nu \frac{\partial^2}{\partial q_\nu \partial q_\mu} \log \mathcal{Z} = q_\nu \langle j_\mu j_\nu \rangle_0$$

which implies the conductivity tensor

$$\sigma_{\mu\nu} = \frac{\langle j_\mu \rangle_q - \langle j_\mu \rangle_0}{q_\nu} = \langle j_\mu j_\nu \rangle_0$$

transport properties

from

$$\langle ... \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\bar{\psi}, \psi, A] ... \exp\{-\mathcal{S}[\bar{\psi}, \psi, A]\}$$

we obtain the Hall conductivity for $\mu \neq \nu$

$$\sigma_{\mu\nu} = \frac{2\pi}{\omega} \int d^3x \; e^{-i\omega\tau} \langle (\bar{\psi}\gamma_\mu \psi)_x (\bar{\psi}\gamma_\nu \psi)_0 \rangle$$

$$= -\frac{4\pi}{\omega g^2} \int d^3x \; e^{-i\omega\tau} \langle Q_{\mu,x} Q_{\nu,0} \rangle$$

Chern-Simons action gives quantized Hall plateaux with

$$C_\lambda = \frac{im}{3} \int \frac{k^2}{(m^2 + k^2)^3} d^3\mathbf{k} \sim \frac{i\pi}{12} \mathrm{sign}(m)$$

one Dirac node

$$\boxed{\sigma_{12} = \frac{1}{2} sgn(m) \frac{e^2}{h}}$$

two Dirac nodes

$$\boxed{\sigma_{12} = sgn(m) \frac{e^2}{h}}$$

Conclusion

- topological invariants due to singularities of the wavefunction
- uniaxial strain moves the Dirac nodes and opens a gap
- electron-phonon interaction: spontaneous Dirac mass creation
- two Dirac nodes get masses with opposite sign
- Chern-Simons action provides quantized Hall plateaux

Outlook

- new phases for double layers with excitons?

JSF Julian Schwinger Foundation

topological materials: essential features III

– two electronic (photonic) bands