Graphene and chiral fermions

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Extending graphene structure to four dimensions gives

- a two-flavor lattice fermion action
- one exact chiral symmetry
  - protects mass renormalization
- strictly local action
  - only nearest neighbor hopping
  - fast for simulations
Graphene electronic structure remarkable

- low excitations described by a massless Dirac equation
  - two “flavors” of excitation
  - versus four of naive lattice fermions
- massless structure robust
  - relies on a “chiral” symmetry
  - involves mapping circles onto circles

Four dimensional extension

- 3 coordinate carbon replaced by 5 coordinate “atoms”
- generalize topology to mapping spheres onto spheres
  - complex numbers replaced by quaternions
Chiral symmetry versus the lattice

- Lattice is a regulator
  - removes all infinities
  - continuum limit defines a field theory
- Classical $U(1)$ chiral symmetry broken by quantum effects
  - a valid lattice formulation must break $U(1)$ axial symmetry
- But we want flavored chiral symmetries to protect masses
  - Wilson fermions break all these
  - staggered require four flavors for one chiral symmetry
  - overlap, domain wall non-local, computationally intensive

Graphene fermions do it in the minimum way allowed!
The graphene structure

A two dimensional hexagonal planar structure of carbon atoms

- http://online.kitp.ucsb.edu/online/bblunch/castroneto/

Held together by strong “sigma” bonds, $sp^2$

One “pi” electron per site can hop around

Consider only nearest neighbor hopping in the pi system
  - tight binding approximation
Fortuitous choice of coordinates helps solve

Form horizontal bonds into “sites” involving two types of atom

- “a” on the left end of a horizontal bond
- “b” on the right end
- all hoppings are between type a and type b atoms

Label “sites” with non-orthogonal coordinates \( x_1 \) and \( x_2 \)

- axes at 30 degrees from horizontal
Hamiltonian

\[ H = K \sum_{x_1, x_2} a_{x_1, x_2}^\dagger b_{x_1, x_2} + b_{x_1, x_2}^\dagger a_{x_1, x_2} + a_{x_1+1, x_2}^\dagger b_{x_1, x_2} + b_{x_1-1, x_2}^\dagger a_{x_1, x_2} + a_{x_1, x_2-1}^\dagger b_{x_1, x_2} + b_{x_1, x_2+1}^\dagger a_{x_1, x_2} \]

- hops always between \( a \) and \( b \) sites

Go to momentum (reciprocal) space

- \( a_{x_1, x_2} = \int_{-\pi}^{\pi} \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} e^{i p_1 x_1} e^{i p_2 x_2} \tilde{a}_{p_1, p_2} \).
- \(-\pi < p_\mu \leq \pi\)
Hamiltonian breaks into two by two blocks

\[
H = K \int_{-\pi}^{\pi} \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} \left( \tilde{a}_{p_1,p_2}^{\dagger} \tilde{b}_{p_1,p_2}^{\dagger} \right) \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix} \begin{pmatrix} \tilde{a}_{p_1,p_2} \\ \tilde{b}_{p_1,p_2} \end{pmatrix}
\]

where

\[
z = 1 + e^{-ip_1} + e^{ip_2}
\]

Hamiltonian energy levels at

\[
E(p_1, p_2) = \pm K |z|
\]

- energy vanishes when \( |z| \) does
- exactly two points \( p_1 = p_2 = \pm 2\pi/3 \)
Topological stability

- contour of constant energy near a zero point
- phase of $z$ wraps around unit circle
- cannot collapse contour without going to $|z| = 0$

No band gap allowed
- Graphite is black and a conductor
Connection with chiral symmetry

- $b \rightarrow -b$ changes sign of $H$
- $\tilde{H}(p_1, p_2) = K \begin{pmatrix} 0 & z \\ \bar{z}^* & 0 \end{pmatrix}$
  - anticommutes with $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
  - $\sigma_3 \rightarrow \gamma_5$ in four dimensions

No-go theorem

Nielsen and Ninomiya (1981)

- periodicity of Brillouin zone
- wrapping around one zero must unwrap elsewhere
- two zeros is the minimum possible
Four dimensions

Feynman path integral in temporal box of length $T$

- $Z = \int (dA \, d\psi \, d\bar{\psi}) e^{-S} = \text{Tr} \, e^{-Ht}$
- “action” $S = \int d^4x \left( \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} D \psi \right)$
  - Wick rotation to imaginary time: $e^{iHT} \rightarrow e^{-HT}$
  - four coordinates $x, y, z, t$

Need Dirac operator $D$ to put into path integral action $\bar{\psi} D \psi$

- properties: $D^\dagger = -D = \gamma_5 D \gamma_5$ “$\gamma_5$ Hermiticity”
- work with Hermitean “Hamiltonian” $H = \gamma_5 D$
  - not the Hamiltonian of the 3D Minkowski theory
Look for analogous form to the two dimensional case

\[ \tilde{H}(p_\mu) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix} \]

- \( z(p_1, p_2, p_3, p_4) \) depends on the four momentum components

To keep topological argument

- extend \( z \) to quaternions
  \[ z = a_0 + i\vec{a} \cdot \vec{\sigma} \]
  - \(|z|^2 = \sum_\mu a_\mu^2|\]

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\[ \tilde{H}(p_\mu) \] now a four by four matrix

- "energy" eigenvalues still \[ E(p_\mu) = \pm K |\tilde{z}| \]
- constant energy surface topologically an \( S_3 \)
  - surrounding a zero should give non-trivial mapping

Introduce gamma matrix convention

\[
[\gamma_\mu, \gamma_\nu]_+ = 2\delta_{\mu\nu}
\]

\[
\vec{\gamma} = \sigma_x \otimes \vec{\sigma} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}
\]

- \( \gamma_4 = -\sigma_y \otimes 1 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \)
- \( \gamma_5 = \sigma_z \otimes 1 = \gamma_1 \gamma_2 \gamma_3 \gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \)
Continuum Dirac action

\[ D = i k_\mu \gamma_\mu \]

\[ \gamma_5 D = H = \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix} \]

\[ z = k_0 + i \vec{k} \cdot \vec{\sigma} \]

Lattice implementation

- not unique
- local action
  - only sines and cosines
  - mimic 2-d case

\[ 1 + e^{-ip_1} + e^{ip_2} = 1 + \cos(p_1) + \cos(p_2) - i(\sin(p_1) - \sin(p_2)) \]
Try

\[ z = B(4C - \cos(p_1) - \cos(p_2) - \cos(p_3) - \cos(p_4)) \]
\[ + i\sigma_x(\sin(p_1) + \sin(p_2) - \sin(p_3) - \sin(p_4)) \]
\[ + i\sigma_y(\sin(p_1) - \sin(p_2) - \sin(p_3) + \sin(p_4)) \]
\[ + i\sigma_z(\sin(p_1) - \sin(p_2) + \sin(p_3) - \sin(p_4)) \]

\( B \) and \( C \) are constants to be determined

- control anisotropic distortions
- similar to non-orthogonal coordinates in graphene solution
Zero of \( z \) requires all components to vanish, four relations

\[
\begin{align*}
\sin(p_1) + \sin(p_2) - \sin(p_3) - \sin(p_4) &= 0 \\
\sin(p_1) - \sin(p_2) - \sin(p_3) + \sin(p_4) &= 0 \\
\sin(p_1) - \sin(p_2) + \sin(p_3) - \sin(p_4) &= 0 \\
\cos(p_1) + \cos(p_2) + \cos(p_3) + \cos(p_4) &= 4C
\end{align*}
\]

- first three imply \( \sin(p_i) = \sin(p_j) \ \forall i, j \)
- \( \cos(p_i) = \pm \cos(p_j) \)
- last relation requires \( C < 1 \)
- if \( C > 1/2 \), only two solutions
  - \( p_i = p_j = \pm \arccos(C) \)
As in two dimensions

- expand about zeros
- identify Dirac spectrum
- rescale for physical momenta

Expanding about the positive solution

- $p_\mu = \tilde{p} + q_\mu$
- $\tilde{p} = \arccos(C)$
Reproduces the Dirac equation $D = i \gamma_{\mu} k_{\mu}$ if we take

$$k_1 = C(q_1 + q_2 - q_3 - q_4)$$
$$k_2 = C(q_1 - q_2 - q_3 + q_4)$$
$$k_3 = C(q_1 - q_2 + q_3 - q_4)$$
$$k_4 = BS(q_1 + q_2 + q_3 + q_4)$$

- here $S = \sin(\tilde{p}) = \sqrt{1 - C^2}$

Other zero at $\tilde{p} = -\arccos(C)$

- flips sign of $\gamma_4$
- the two species have opposite chirality
- the exact chiral symmetry is a flavored one
$B$ and $C$ control distortions between the $k$ and $q$ coordinates

- The $k$ coordinates should be orthogonal
- the $q$’s are not in general

\[
\frac{q_i \cdot q_j}{|q|^2} = \frac{B^2 S^2 - C^2}{B^2 S^2 + 3C^2}
\]

If $B = C/S$ the $q$ axes are also orthogonal

- allows gauging with simple plaquette action
- Borici: $B = 1$, $C = S = 1/\sqrt{2}$
Alternative choice for $B$ and $C$ from graphene analogy

- zeros of $z$ in periodic momentum space form a lattice
- give each zero 5 symmetrically arranged neighbors
  - $C = \cos(\pi/5)$, $B = \sqrt{5}$
- interbond angle $\theta$ satisfies $\cos(\theta) = -1/4$
  - $\theta = \arccos(-1/4) = 104.4775\ldots$ degrees
- 4-d generalization of the diamond lattice
The physical lattice structure

Graphene: one bond splits into two in two dimensions

- $\theta = \arccos(-1/2) = 120$ degrees

- smallest loops are hexagons

![Hexagonal pattern](image-url)
Diamond: one bond splits into three in three dimensions

- tetrahedral environment
- $\theta = \arccos(-1/3) = 109.4712 \ldots$ degrees

iterating

- smallest loops are cyclohexane chairs
4-d graphene “hyperdiamond”: one bond splits into four

- 5-fold symmetric environment
- \( \theta = \arccos(-1/4) = 104.4775 \ldots \) degrees

iterating

- smallest loops are hexagonal “chairs”
Issues and questions

Requires a multiple of two flavors

- can split degeneracies with Wilson terms

Only one exact chiral symmetry

- not the full $SU(2) \otimes SU(2)$
  - enough to protect mass from additive renormalization
  - only one Goldstone boson: $\pi_0$
  - $\pi_{\pm}$ only approximate

One direction treated differently

- $\gamma_4$ has a different phase from the spatial gammas
- with interactions lattice can distort along one direction
- requires tuning anisotropy
Not unique

- only need \( z(p) \) with two zeros

- Here \( C = \cos(\pi/5), \ B = \sqrt{5} \)
  - gives approximate 120 element “pentahedral” symmetry

- Borici’s variation with orthogonal coordinates
  - a linear combination of two naive fermion formulations
• Karsten (1981) and Wilczek (1987)
  • select the time axis as special
  • like spatial Wilson fermions with \( r \rightarrow ir\gamma_0 \)
  • Karsten and Wilczek forms equivalent up to phases

• Tatsuhiro Misumi

\[
D = i\gamma_1 (\sin(p_1) + \cos(p_2) - 1) \\
i\gamma_2 (\sin(p_2) + \cos(p_3) - 1) \\
i\gamma_3 (\sin(p_3) + \cos(p_4) - 1) \\
i\gamma_4 (\sin(p_4) + \cos(p_1) - 1)
\]

• poles at \( p = (0, 0, 0, 0) \) and \( p = (\pi/2, \pi/2, \pi/2, \pi/2) \)
Gauge field topology and zero modes

- the two flavors have opposite chirality
- their respective zero modes can mix through lattice artifacts
  - no longer exact zero eigenvalues of $D$
- similar to staggered, but 2 rather than 4 flavors

Comparison with staggered

- both have one exact chiral symmetry
- both have only approximate zero modes from topology
- four component versus one component fermion field
- two versus four flavors (tastes)
  - no uncontrolled extrapolation to two physical light flavors
Perturbative corrections can shift pole positions

- Capitani, Weber, Wittig
- shift along direction between the poles
- Generalized Karsten/Wilczek operator:
  \[ D = \frac{-i\gamma_4}{\sin(\alpha)} \left( \sum_{\mu=1}^{4} \cos(p_\mu) - \cos(\alpha) - 3 \right) + i \sum_{i=1}^{3} \gamma_i \sin(p_i) \]
- poles at \( \vec{p} = 0 \), \( p_4 = \pm\alpha \)
- alpha gets an additive renormalization
- tune coefficient of \( \overline{\psi}\gamma_4\psi \)

Two operators control asymmetry

- \( \overline{\psi}\gamma_4\partial_4\psi \) and \( \beta_t \)
Point split fields natural

- separate poles at different “bare momenta”

\[
\begin{align*}
  u(q) &= \frac{1}{2} \left( 1 + \frac{\sin(q_4 + \alpha)}{\sin(\alpha)} \right) \psi(q + \alpha e_4) \\
  d(q) &= \frac{1}{2} \Gamma \left( 1 - \frac{\sin(q_4 - \alpha)}{\sin(\alpha)} \right) \psi(q - \alpha e_4)
\end{align*}
\]

- zeros inserted to cancel undesired pole
- not unique
- \( \Gamma \) factor since different poles use different gamma matrices
  - \( \Gamma = i\gamma_4\gamma_5 \) for Karsten/Wilczek formulation
Position space:

\[ u(x) = \frac{1}{2} e^{i\alpha x_4} \left( \psi(x) + i \frac{\psi(x - e_4) - \psi(x + e_4)}{2 \sin(\alpha)} \right) \]

\[ d(x) = \frac{1}{2} \Gamma e^{-i\alpha x_4} \left( \psi(x) - i \frac{\psi(x - e_4) - \psi(x + e_4)}{2 \sin(\alpha)} \right) \]

Gives rise to point-split meson operators; i.e.

\[ \eta'(x) = \frac{1}{8} \left( \bar{\psi}(x - e_4) \gamma_5 \psi(x) - \bar{\psi}(x) \gamma_5 \psi(x - e_4) \right. \]

\[ + \left. \bar{\psi}(x + e_4) \gamma_5 \psi(x) - \bar{\psi}(x) \gamma_5 \psi(x + e_4) \right). \]
Effective Lagrangians and lattice artifacts

- MC, Sharpe and Singleton
- Two possibilities for Wilson fermions as $m_q \to 0$
  - Chiral transition becomes first order
  - Aoki phase
- Two choices here as well
  - $m_{\pi^\pm} > m_{\pi^0}$: $\pi^0$ is normal Goldstone mode
  - $m_{\pi^\pm} < m_{\pi^0}$: 2nd order transition before $m_q \to 0$
- Paired eigenvalues imply a positive fermion determinant
  - Vafa-Witten argument suggests first option
Summary

Extending graphene and diamond lattices to four dimensions:

- a two-flavor lattice Dirac operator
- one exact chiral symmetry
  - protects from additive mass renormalization
  - eigenvalues purely imaginary for massless theory
  - in complex conjugate pairs
- strictly local
  - fast to simulate
Extra Slides
Valence bond theory for carbon

Carbon has 6 electrons
- two tightly bound in the 1s orbital
- second shell: one \(2s\) and three \(2p\) orbitals

In a molecule or crystal, external fields mix the \(2s\) and \(2p\) orbitals

Carbon likes to mix the outer orbitals in two distinct ways
- 4 \(sp^3\) orbitals in a tetrahedral arrangement
  - methane \(CH_4\), diamond \(C_\infty\)
- 3 \(sp^2\) orbitals in a planar triangle plus one \(p\)
  - benzene \(C_6H_6\), graphite \(C_\infty\)
  - the \(sp^2\) electrons in strong “sigma” bonds
  - the \(p\) electron can hop around in “pi” orbitals
Hexagonal structure hidden in deformed coordinates

Thomas Szkopek
Position space rules from identifying $e^{\pm ip}$ terms with hopping

- **on site action:** \[4iBC\overline{\psi}\gamma_4\psi\]
- **hop in direction 1:** \[\psi_j(\gamma_1 + \gamma_2 + \gamma_3 - iB\gamma_4)\psi_i\]
- **hop in direction 2:** \[\psi_j(\gamma_1 - \gamma_2 - \gamma_3 - iB\gamma_4)\psi_i\]
- **hop in direction 3:** \[\psi_j(-\gamma_1 - \gamma_2 + \gamma_3 - iB\gamma_4)\psi_i\]
- **hop in direction 4:** \[\psi_j(-\gamma_1 + \gamma_2 - \gamma_3 - iB\gamma_4)\psi_i\]
- minus the conjugate for a reverse hop

Notes

- a mixture real and imaginary coefficients for the $\gamma$’s
- $\gamma_5$ exactly anticommutes with $D$
- $D$ is purely anti-Hermitean
- $\gamma_4$ not symmetrically treated to $\vec{\gamma}$