Four-dimensional graphene and chiral fermions

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Extending graphene structure to four dimensions gives

- a two-favor 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
  - tied to non-trivial mapping of $S_1$ onto $S_1$

Four dimensional extension

- 3 coordinate carbon replaced by 5 coordinate “atoms”
- generalize topology to mapping $S_3$ onto $S_3$
  - complex numbers replaced by quaternions
Chiral symmetry versus the lattice

- Lattice is a regulator
  - removes all infinities
  - symmetries survive quantization

- 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!
Carbon and valence bond theory for dummies

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
Review of graphene structure

A two dimensional hexagonal planar structure of carbon atoms

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

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

- \( a_{x_1, x_2} = \int_{-\pi}^{\pi} \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} e^{ip_1 x_1} e^{ip_2 x_2} \tilde{a}_{p_1, p_2} \cdot \)
- \( -\pi < p_\mu \leq \pi \)
Hamiltonian breaks into two by two blocks

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

- where

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

\[ \tilde{H}(p_1,p_2) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix} \]

Fermion energy levels at \( E(p_1,p_2) = \pm K|z| \)

- energy vanishes only 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
Hexagonal structure hidden in deformed coordinates
Connection with chiral symmetry

- \( b \rightarrow -b \) changes sign of \( H \)

- \( \tilde{H}(p_1, p_2) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix} \) 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

- periodicity of Brillouin zone

- wrapping around one zero must unwrap elsewhere

- two zeros is the minimum possible
Four dimensions

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

- require “$\gamma_5$ Hermiticity”
  - $\gamma_5 D \gamma_5 = D^\dagger$
- work with Hermitean “Hamiltonian” $H = \gamma_5 D$
  - not the Hamiltonian of the 3D Minkowski theory

Require same form as the two dimensional case

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

- four component momentum, $(p_1, p_2, p_3, p_4)$
To keep topological argument

- extend \( z \) to quaternions

\[
\begin{align*}
\vec{a}_0 + i \vec{a} \cdot \vec{\sigma}
\end{align*}
\]

- \( |z|^2 = \sum_\mu a_\mu^2 \)

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

- “energy” eigenvalues still \( E(p_\mu) = \pm K|z| \)

- constant energy surface topologically an \( S_3 \)

- surrounding a zero should give non-trivial mapping
Implementation

- not unique
- local action
  - only sines and cosines
  - mimic 2-d case
    \[ 1 + e^{-ip_1} + e^{ip_2} = 1 - \cos(p_1) - \cos(p_2) - i(\sin(p_1) - \sin(p_2)) \]
- possible choice

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

- \( B \) and \( C \) are constants to be determined
Zero at $|z| = 0$ 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

- $p_\mu = \tilde{p} + q_\mu$
- $\tilde{p} = \arccos(C)$
- define $S = \sin(\tilde{p}) = \sqrt{1 - C^2}$
The quaternion becomes

\[ z = BS(q_1 + q_2 + q_3 + q_4) \]
\[ + iC\sigma_x(q_1 + q_2 - q_3 - q_4) \]
\[ + iC\sigma_y(q_1 - q_2 - q_3 + q_4) \]
\[ + iC\sigma_z(q_1 - q_2 + q_3 - q_4) + O(q^2) \]

Introduce a gamma matrix convention

\[ \tilde{\gamma} = \sigma_x \otimes \vec{\sigma} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \]
\[ \gamma_4 = -\sigma_y \otimes 1 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \]
\[ \gamma_5 = \sigma_z \otimes 1 = \gamma_1\gamma_2\gamma_3\gamma_4 = \text{diag}(1, 1, -1, -1) \]
The Dirac operator becomes

\[ \tilde{D} = C(q_1 + q_2 - q_3 - q_4)i\gamma_1 \]
\[ + C(q_1 - q_2 - q_3 + q_4)i\gamma_2 \]
\[ + C(q_1 - q_2 + q_3 - q_4)i\gamma_3 \]
\[ + BS(q_1 + q_2 + q_3 + q_4)i\gamma_4 + O(q^2) \]

Reproducing the Dirac equation if we take

\[ k_1 = C(q_1 + q_2 - q_3 - q_4) \]
\[ k_2 = C(q_1 - q_2 - q_3 + q_4) \]
\[ k_3 = C(q_1 - q_2 + q_3 - q_4) \]
\[ k_4 = BS(q_1 + q_2 + q_3 + q_4) \]
Position space rules from identifying $e^{\pm ip}$ terms with hopping

- on site action: $4iBC\bar{\psi}\gamma_4\psi$
- hop in direction 1: $\bar{\psi}_j(+\gamma_1 + \gamma_2 + \gamma_3 - iB\gamma_4)\psi_i$
- hop in direction 2: $\bar{\psi}_j(+\gamma_1 - \gamma_2 - \gamma_3 - iB\gamma_4)\psi_i$
- hop in direction 3: $\bar{\psi}_j(-\gamma_1 - \gamma_2 + \gamma_3 - iB\gamma_4)\psi_i$
- hop in direction 4: $\bar{\psi}_j(-\gamma_1 + \gamma_2 - \gamma_3 - iB\gamma_4)\psi_i$
- 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 $\bar{\gamma}$
The \( k \) coordinates should be orthonormal

- 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

- extend Brillouin zone to include neighboring zones
- zeros of $z$ in 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
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: one bond splits into four
- 5-fold symmetric environment
- $\theta = \cos(-1/4) = 104.4775 \ldots$ degrees

iterating

- smallest loops are again 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
  • $\pi_0$ a Goldstone boson
  • $\pi_{\pm}$ only approximate

Not unique
• only need $z(p)$ with two zeros
• Borici’s variation with orthogonal coordinates
• $C = \cos(\pi/5)$, $B = \sqrt{5}$
  • approximate 120 element “pentahedral” symmetry
192 element hypercubic symmetry group reduced to 48 elements

- natural time axis along major hypercube diagonals
- 24 element tetrahedral symmetry in space
  - permutations of links in positive direction
  - half of these elements have negative parity
- time reversal exchanges positive and negative links
- $2 \times 24 = 48$ element discrete symmetry group
- $O(a^2)$ corrections to Euclidian symmetry
  - Cichy, Gonzalez Lopez, Jansen, Kujawa, Shindler
Additional parameters to tune?  Bedaque, Buchoff, Tibursi, Walker-Loud

- no full space-time symmetry
  - speed of light for fermions and gluons may differ
  - general gauge action requires both 4 and 6 link terms
- for $BS = C$ four link terms should be adequate
- $C = \cos(\pi/5)$, $B = \sqrt{5}$
  - approximate “pentahedral” symmetry
  - 4-d generalization of diamond
  - should constrain 6 link terms
Zero modes from gauge field topology only approximate

- the two flavors have opposite chirality
- their zero modes can mix through lattice artifacts
- 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
  - no uncontrolled extrapolation to two physical light flavors
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
  - should be very fast to simulate