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 non-singlet chiral symmetry
  - protects mass renormalization
- strictly local action
  - only nearest neighbor hopping
  - fast for simulations

Graphene electronic structure remarkable

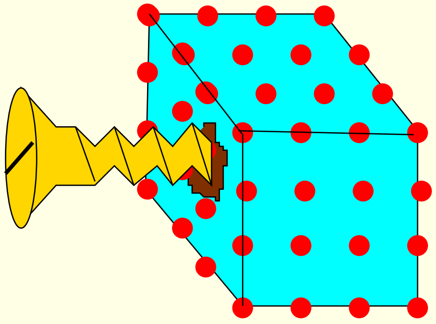
- low excitations described by a massless Dirac equation
  - two ‘‘flavors’’ of excitation
  - versus four of naive lattice fermions

- massless structure robust
  - relies on a ‘‘chiral’’ symmetry
  - tied to a 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
  - lattice symmetries survive quantization
- Classical $U(1)$ chiral symmetry broken by quantum effects
  - any valid lattice formulation must not have $U(1)$ 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

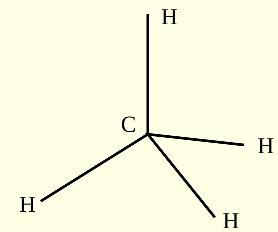
Carbon has 6 electrons

- two tightly bound in the 1s orbital
- second shell: one $2s$ and three $2p$ orbitals

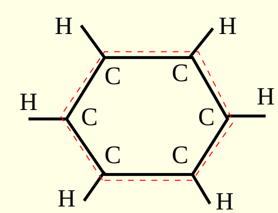
In a molecule or crystal, external fields mix the $2s$ and $2p$ orbitals

Carbon likes to mix the outer orbitals in two distinct ways

- 4 sp^3 orbitals in a tetrahedral arrangement
  - methane CH_4, diamond C_∞

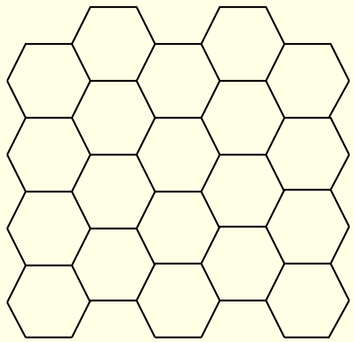


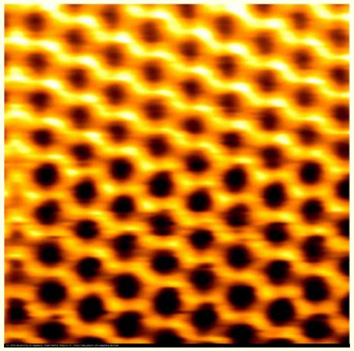
- 3 sp^2 orbitals in a planar triangle plus one p
  - benzene C_6H_6, graphite C_∞
  - the sp^2 electrons tightly held in “sigma” bonds
  - the p electron can hop around in “pi” orbitals



Review of graphene structure

A two dimensional hexagonal planar structure of carbon atoms





- http://online.kitp.ucsb.edu/online/bblunch/castroneto/
- A. H. Castro Neto et al., arXiv:0709.1163

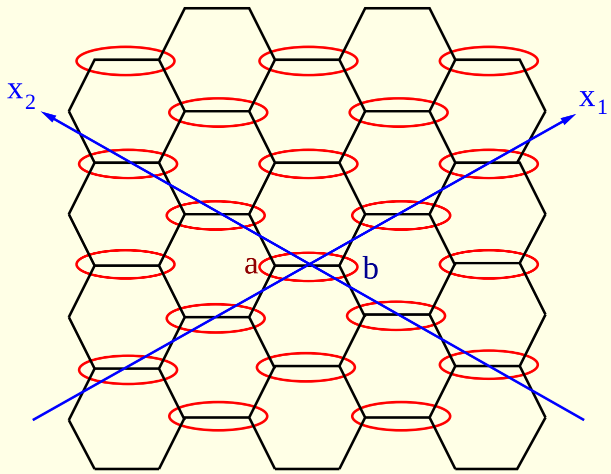
Held together by strong “sigma” bonds, sp^2

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

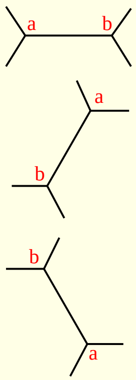
- “a” on the left end of a horizontal bond
- “b” on the right end
- all hoppings are between type a and type b atoms

Label sites by non-orthogonal coordinates x_1 and x_2

- axes at 30 degrees from horizontal

Hamiltonian

$$H = K \sum_{x_1,x_2} a^\dagger_{x_1,x_2} b_{x_1,x_2} + b^\dagger_{x_1,x_2} a_{x_1,x_2}$$
$$+ a^\dagger_{x_1+1,x_2} b_{x_1,x_2} + b^\dagger_{x_1-1,x_2} a_{x_1,x_2}$$
$$+ a^\dagger_{x_1,x_2-1} b_{x_1,x_2} + b^\dagger_{x_1,x_2+1} a_{x_1,x_2}$$



- hops always between a and b sites

Go to momentum (reciprocal) space

- $a_{x_1,x_2} = \int_{-\pi}^{\pi} \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} \; e^{ip_1 x_1} \; e^{ip_2 x_2} \; \tilde{a}_{p_1,p_2}.$
- $-\pi < p_\mu \leq \pi$

Hamiltonian breaks into two by two blocks

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

- where $\quad z = 1 + e^{-ip_1} + e^{+ip_2}$

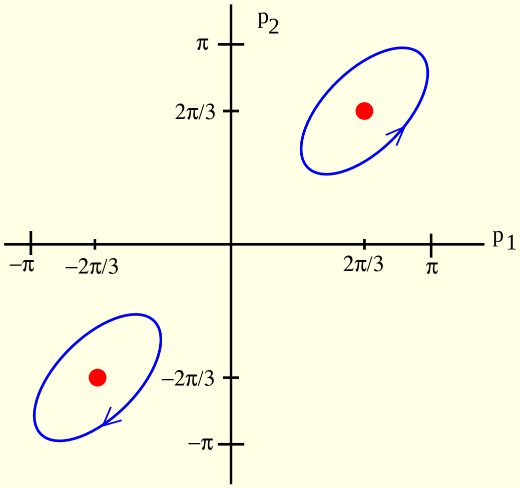
$$\tilde{H}(p_1, p_2) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix}$$

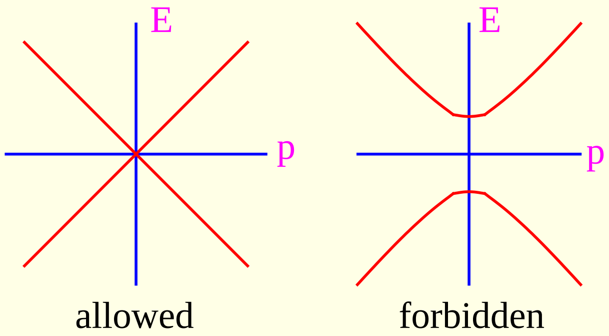
Fermion energy levels at $E(p_1, p_2) = \pm K|z|$

- energy vanishes only when $|z|$ does
- exactly two points $\quad p_1 = p_2 = \pm 2\pi/3$

Topological stability

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

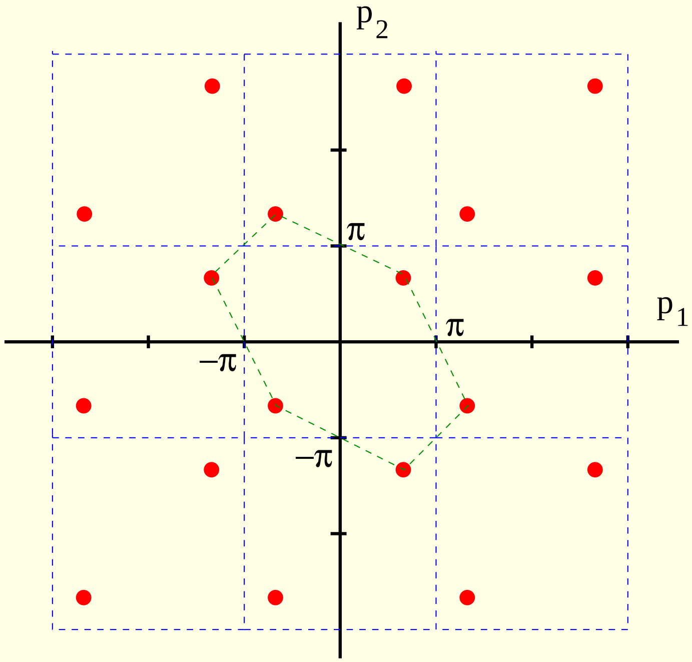


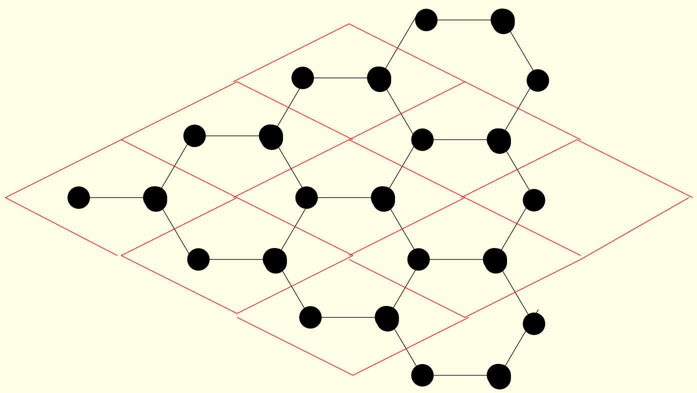


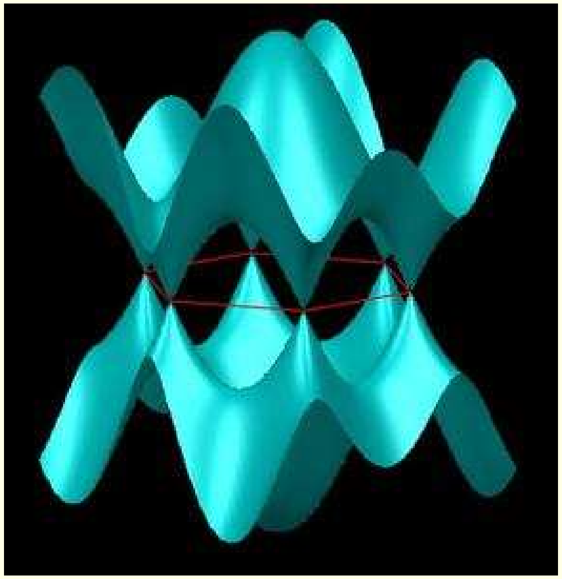
No band gap allowed

- Graphite is black and a conductor

Hexagonal structure hidden in deformed coordinates







Thomas Szkopek

Connection with chiral symmetry

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

No-go theorem

- periodicity of Brillouin zone
- non-trivial wrapping around one zero must unwrap around another
- two zeros is the minimum possible

Four dimensions

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

- require "γ_5 Hermiticity"
  - $\gamma_5 D \gamma_5 = D^\dagger$
- work with Hermitean "Hamiltonian" $H = \gamma_5 D$
  - not the Hamiltonian of the three dimensional Minkowski theory

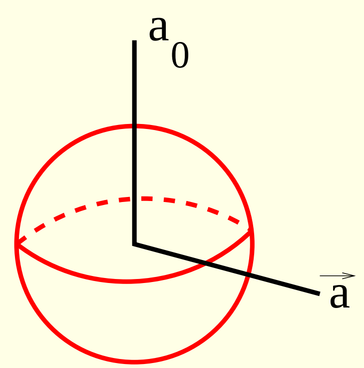
Require same form as the two dimensional case

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

- four component momentum, (p_1, p_2, p_3, p_4)

To keep topological argument

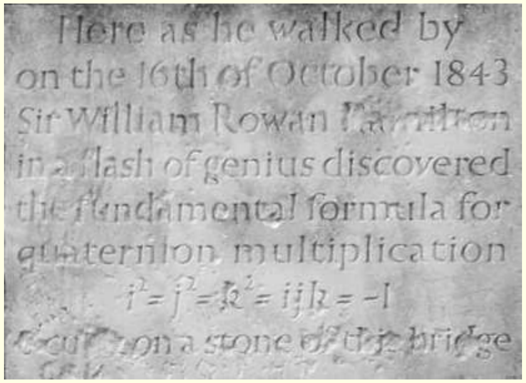
- extend z to quaternions
- $z = a_0 + i\vec{a} \cdot \vec{\sigma}$
  - $|z|^2 = \sum_\mu a_\mu^2$



$\tilde{H}(p_\mu)$ 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
- extend $1 + e^{-ip_1} + e^{ip_2}$ to a sum of quaternion pieces

$$
\begin{aligned}
z = & B(4C - \cos(p_1) - \cos(p_2) - \cos(p_3) - \cos(p_4)) \\
& + i\sigma_x(\sin(p_1) + \sin(p_2) - \sin(p_3) - \sin(p_4)) \\
& + i\sigma_y(\sin(p_1) - \sin(p_2) - \sin(p_3) + \sin(p_4)) \\
& + i\sigma_z(\sin(p_1) - \sin(p_2) + \sin(p_3) - \sin(p_4))
\end{aligned}
$$

- B and C are constants to be determined

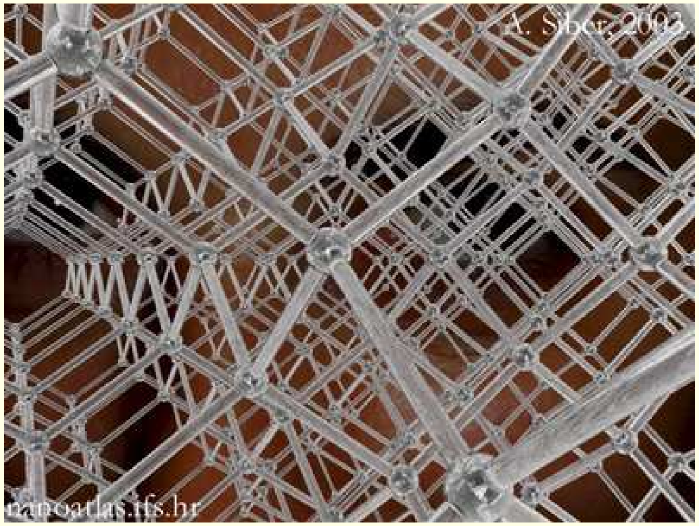
Zero at $|z| = 0$ requires all components to vanish, four relations

$$\begin{aligned}
\sin(p_1) + \sin(p_2) - \sin(p_3) - \sin(p_4) &= 0 \\
\sin(p_1) - \sin(p_2) - \sin(p_3) + \sin(p_4) &= 0 \\
\sin(p_1) - \sin(p_2) + \sin(p_3) - \sin(p_4) &= 0 \\
\cos(p_1) + \cos(p_2) + \cos(p_3) + \cos(p_4) &= 4C
\end{aligned}$$

- 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

- $p_\mu = \tilde{p} + q_\mu$
- $\tilde{p} = \mathrm{acos}(C)$
- define $S = \sin(\tilde{p}) = \sqrt{1 - C^2}$

The quaternion becomes

$$
\begin{aligned}
z = & BS(q_1 + q_2 + q_3 + q_4) \\
& + iC\sigma_x(q_1 + q_2 - q_3 - q_4) \\
& + iC\sigma_y(q_1 - q_2 - q_3 + q_4) \\
& + iC\sigma_z(q_1 - q_2 + q_3 - q_4) + O(q^2)
\end{aligned}
$$

Introduce a gamma matrix convention

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

$$
\gamma_4 = -\sigma_y \otimes 1 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}
$$

$$
\gamma_5 = \sigma_z \otimes 1 = \gamma_1\gamma_2\gamma_3\gamma_4 = \mathrm{diag}(1, 1, -1, -1)
$$

The Dirac operator becomes

$$\begin{aligned}\tilde{D} =& C(q_1 + q_2 - q_3 - q_4) i\gamma_1 \\ &+ C(q_1 - q_2 - q_3 + q_4) i\gamma_2 \\ &+ C(q_1 - q_2 + q_3 - q_4) i\gamma_3 \\ &+ BS(q_1 + q_2 + q_3 + q_4) i\gamma_4 + O(q^2)\end{aligned}$$

Reproducing the Dirac equation if we take

$$\begin{aligned}k_1 &= C(q_1 + q_2 - q_3 - q_4) \\ k_2 &= C(q_1 - q_2 - q_3 + q_4) \\ k_3 &= C(q_1 - q_2 + q_3 - q_4) \\ k_4 &= BS(q_1 + q_2 + q_3 + q_4)\end{aligned}$$

Position space rules from identifying $e^{ip\sigma}$ terms with hopping

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

Notes

- a mixture real and imaginary coefficients for the γ's
- γ_5 exactly anticommutes with D
- D is purely anti-Hermitean
- γ_4 not symmetrically treated to $\vec{\gamma}$

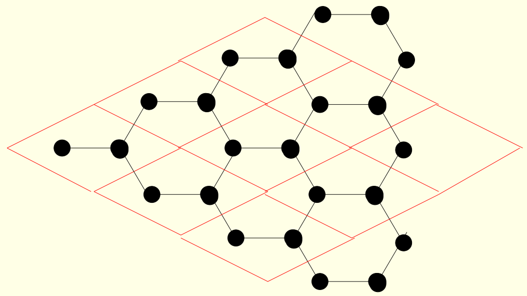
The k coordinates should be orthonormal

- the q's are not in general

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

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

- allows gauging with simple plaquette action
- Borici: $B = 1$, $C = S = 1/\sqrt{2}$



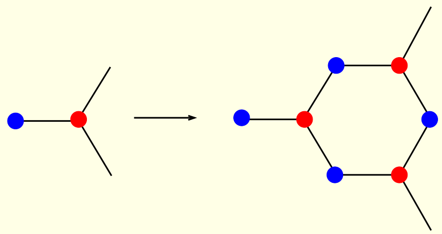
Alternative choice for B and C from graphene analogy

- 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 θ satisfies $\cos(\theta) = -1/4$
  - $\theta = \pi - \mathrm{acos}(1/2) = 104.4775\ldots$ degrees
- 4-d generalization of the diamond lattice

The physical lattice structure

Graphene: one bond splits into two in two dimensions

- $\theta = \pi - \mathrm{acos}(1/2) = 120$ degrees

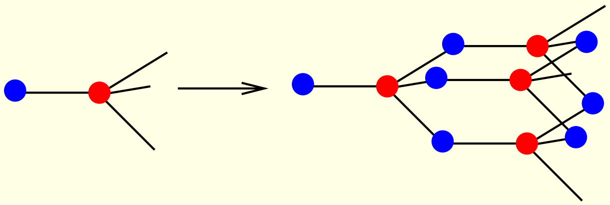
iterating 

- smallest loops are hexagons

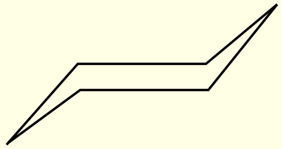
Diamond: one bond splits into three in three dimensions

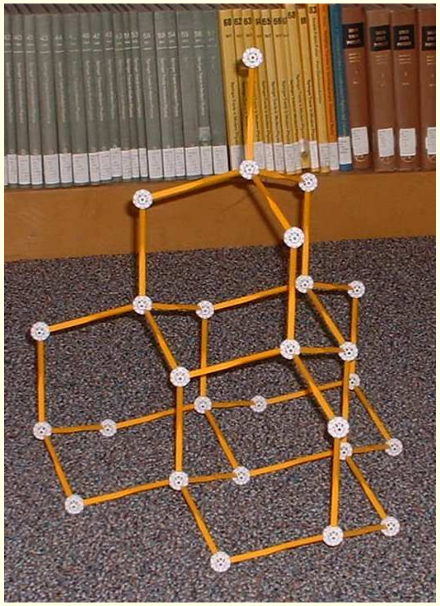
- tetrahedral environment
- $\theta = \pi - \mathrm{acos}(1/3) = 109.4712\ldots$ degrees

iterating



- smallest loops are cyclohexane chairs

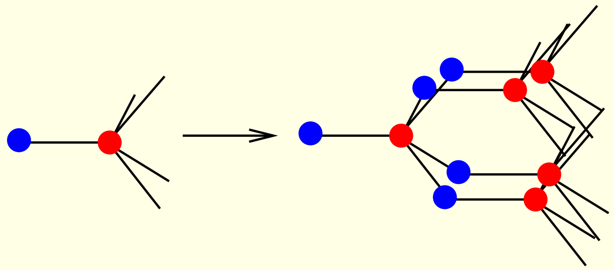




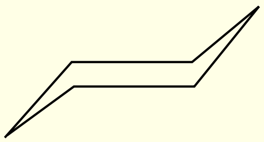
4-d graphene: one bond splits into four

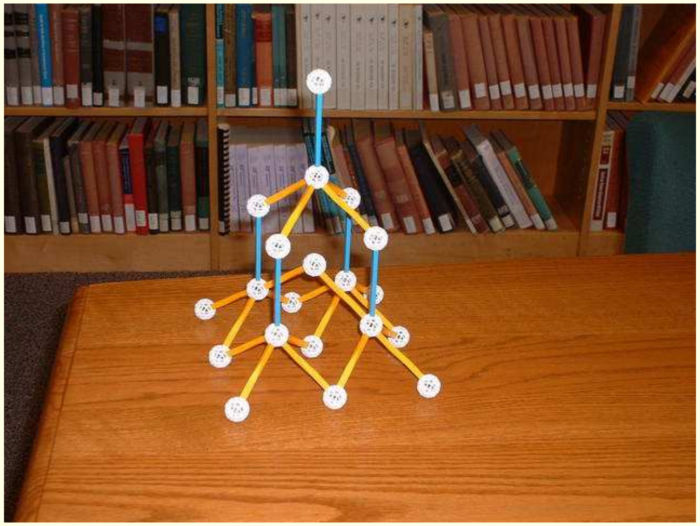
- 5-fold symmetric environment
- $\theta = \pi - \mathrm{acos}(1/4) = 104.4775\ldots$ degrees

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
  - π_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 "pentahedral" symmetry

192 element hypercubic symmetry group reduced to 48 elements

- natural time axis along major hypercube diagonals
- 24 element tetrahedral symmetry in space
  - permutation 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

Do we need additional parameters to tune? Bedaque, Buchoff, Tibursi, Walker-Loud

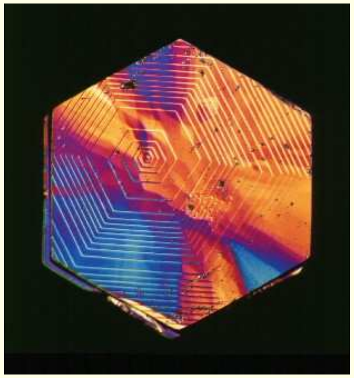
- no full space-time symmetry
  - speed of light for fermions and gluons may differ
  - In general the gauge action requires both 4 and 6 link terms
- for $BS = C$ four link terms should be adequate
- $C = \cos(\pi/5)$, $B = \sqrt{5}$
  - approximate "pentahedral" symmetry
  - 4-d generalization of diamond
  - 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 gauge topology
- four component versus one component fermion field
- two versus four flavors
  - rooting approximation not required for two light flavors



Summary

Extension of graphene and diamond lattices in 2 and 3 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