Graphene and chiral fermions

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BNL & U. Mainz

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

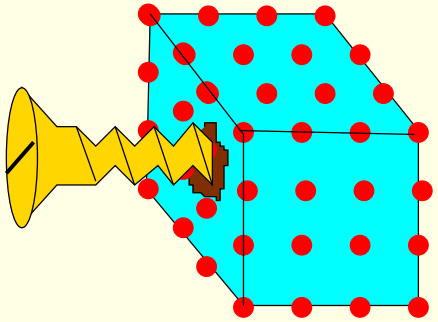
Graphene electronic structure remarkable

- 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

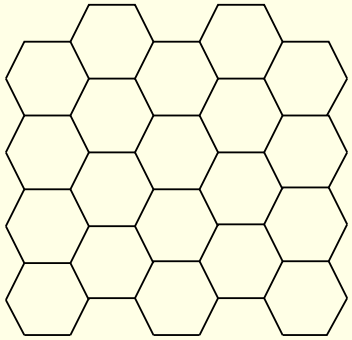


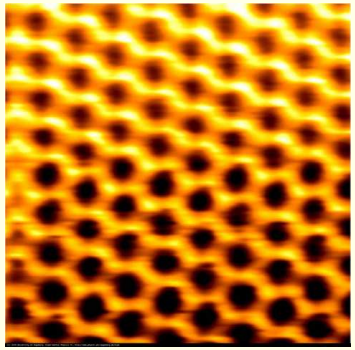
- Lattice is a regulator
  - removes all infinities
  - continuum limit defines a field theory
- Classical $U(1)$ chiral symmetry broken by quantum effects
  - a valid lattice formulation must break $U(1)$ axial symmetry
- But we want flavored chiral symmetries to protect masses
  - Wilson fermions break 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





- A. H. Castro Neto et al., RMP 81,109 [arXiv:0709.1163]
- http://online.kitp.ucsb.edu/online/bblunch/castroneto/

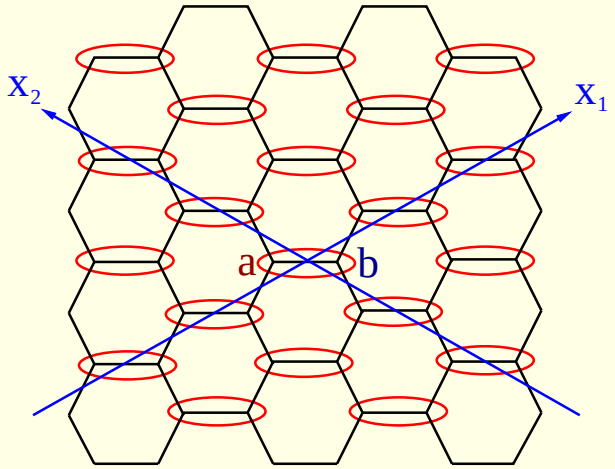
Held together by strong ‘‘sigma’’ bonds, sp^2

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

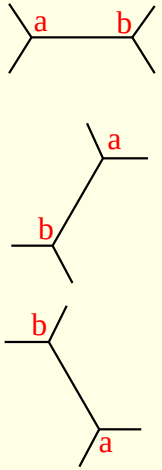
- "a" on the left end of a horizontal bond
- "b" on the right end
- all hoppings are between type a and type b atoms

Label "sites" with non-orthogonal coordinates x_1 and x_2

- axes at 30 degrees from horizontal

Hamiltonian

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



- hops always between a and b sites

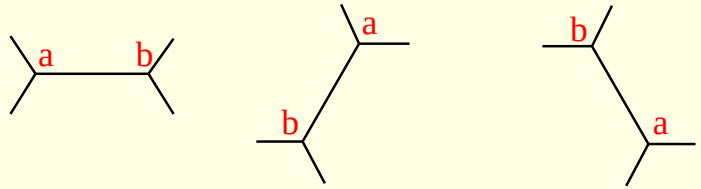
Go to momentum (reciprocal) space

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

Hamiltonian breaks into two by two blocks

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

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



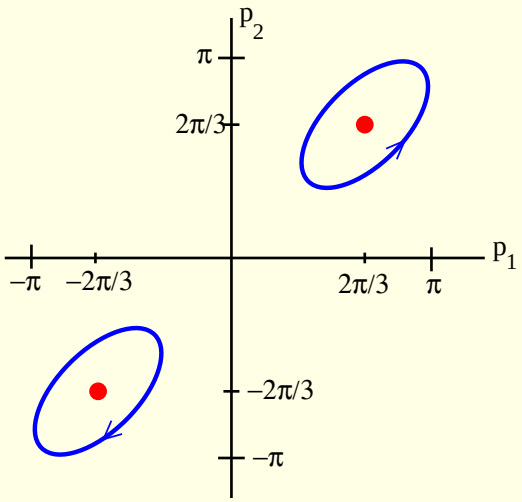
$$\tilde{H}(p_1, p_2) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix}$$

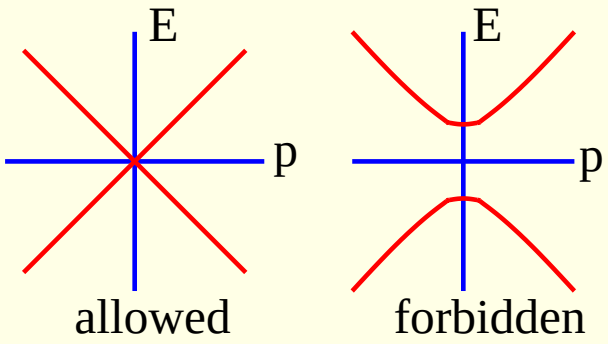
Fermion energy levels at $E(p_1, p_2) = \pm K|z|$

- energy vanishes 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

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

- $Z = \int (dA\, d\psi\, d\overline{\psi}) e^{-S} = \mathrm{Tr}\, e^{-Ht}$
- "action" $S = \int d^4x \left(\frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \overline{\psi} D \psi \right)$
  - 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 $\overline{\psi} D \psi$

- properties: $D^\dagger = -D = \gamma_5 D \gamma_5$ "γ_5 Hermiticity"
- work with Hermitean "Hamiltonian" $H = \gamma_5 D$
  - not the Hamiltonian of the 3D Minkowski theory

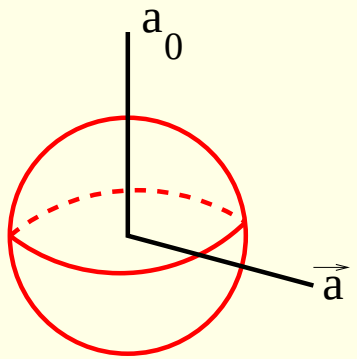
Look for analogous form to the two dimensional case

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

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

To keep topological argument

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



$\tilde{H}(p_\mu)$ 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

Introduce gamma matrix convention

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

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

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

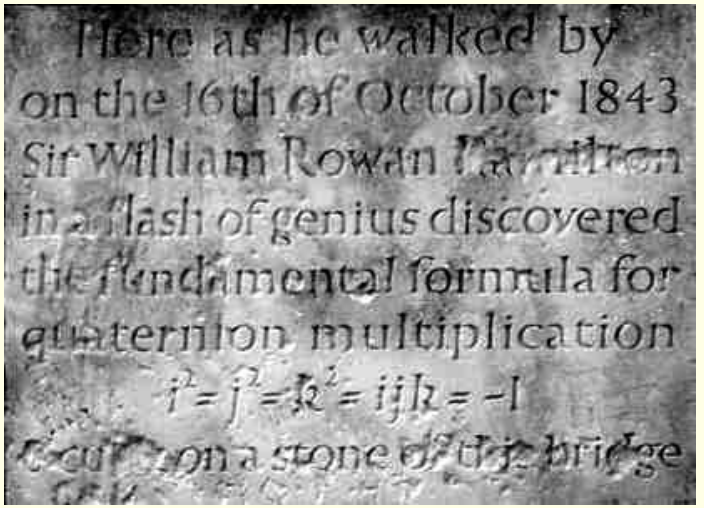
$$\gamma_5 = \sigma_z \otimes 1 = \gamma_1\gamma_2\gamma_3\gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Continuum Dirac action

$$D = ik_\mu \gamma_\mu$$

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

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



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

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

B and C are constants to be determined

- control anisotropic distortions
- similar to non-orthogonal coordinates in graphene solution

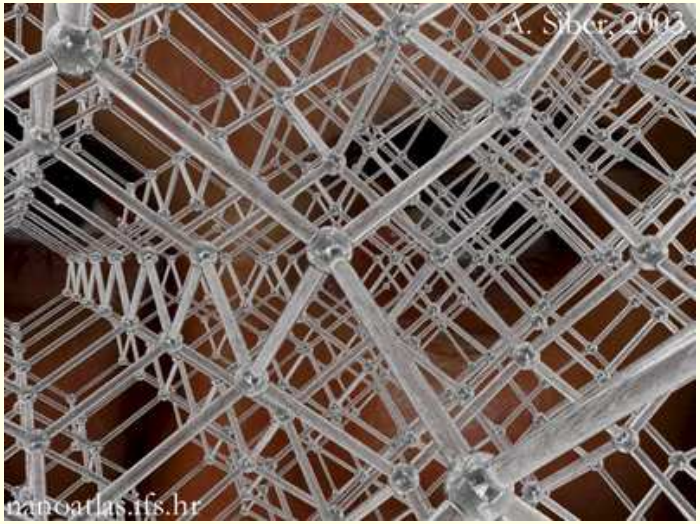
Zero of z requires all components to vanish, four relations

$$\sin(p_1) + \sin(p_2) - \sin(p_3) - \sin(p_4) = 0$$
$$\sin(p_1) - \sin(p_2) - \sin(p_3) + \sin(p_4) = 0$$
$$\sin(p_1) - \sin(p_2) + \sin(p_3) - \sin(p_4) = 0$$
$$\cos(p_1) + \cos(p_2) + \cos(p_3) + \cos(p_4) = 4C$$

- 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

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

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

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

- flips sign of γ_4
- the two species have opposite chirality
- the exact chiral symmetry is a flavored one

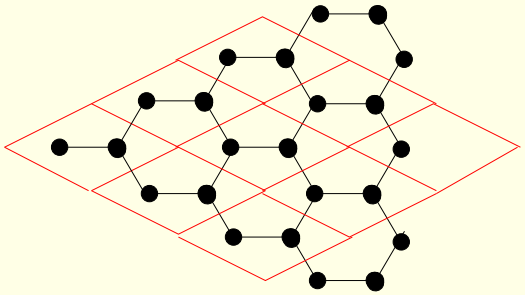
B and C control distortions between the k and q coordinates

- 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

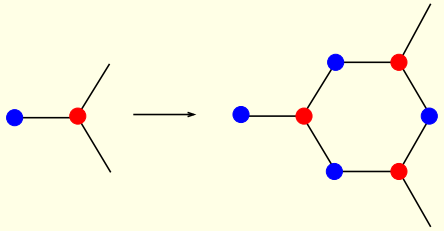
- zeros of z in periodic momentum space form a lattice
- give each zero 5 symmetrically arranged neighbors
  - $C = \cos(\pi/5)$, $B = \sqrt{5}$
- interbond angle θ satisfies $\cos(\theta) = -1/4$
  - $\theta = \mathrm{acos}(-1/4) = 104.4775\ldots$ degrees
- 4-d generalization of the diamond lattice

The physical lattice structure

Graphene: one bond splits into two in two dimensions

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

iterating

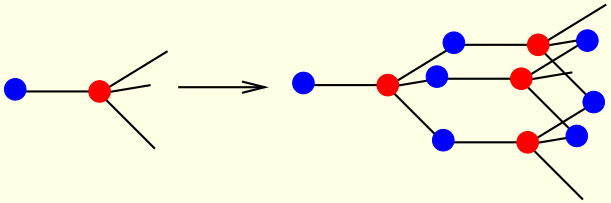


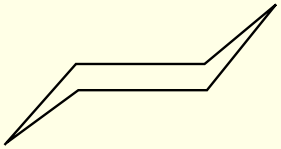
- smallest loops are hexagons

Diamond: one bond splits into three in three dimensions

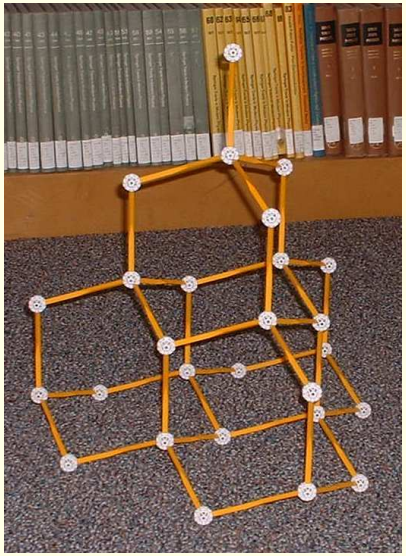
- tetrahedral environment
- $\theta = \mathrm{acos}(-1/3) = 109.4712\ldots$ degrees

iterating





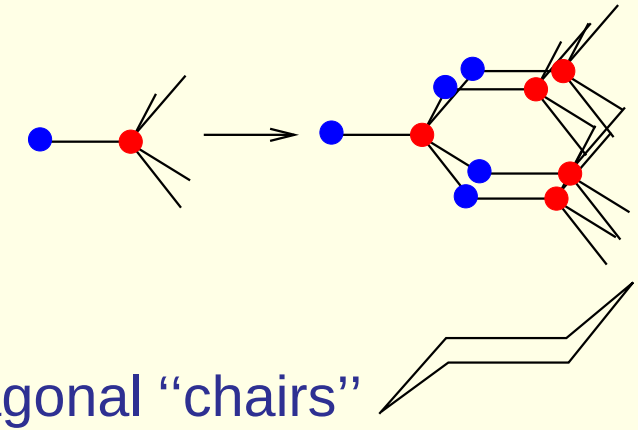
- smallest loops are cyclohexane chairs



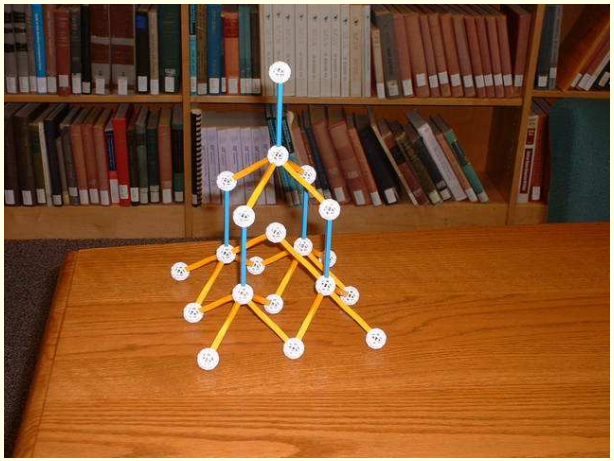
4-d graphene “hyperdiamond”: one bond splits into four

- 5-fold symmetric environment
- $\theta = \mathrm{acos}(-1/4) = 104.4775\ldots$ 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: π_0
  - $\pi_\pm$ only approximate

One direction treated differently Bedaque, Buchoff, Tibursi, Walker-Loud

- γ_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 $r \longrightarrow ir\gamma_0$
  - Karsten and Wilczek forms equivalent up to phases
- Tatsuhiro Misumi

$$\begin{aligned} D = & i\gamma_1(\sin(p_1) + \cos(p_2) - 1) \\ & i\gamma_2(\sin(p_2) + \cos(p_3) - 1) \\ & i\gamma_3(\sin(p_3) + \cos(p_4) - 1) \\ & i\gamma_4(\sin(p_4) + \cos(p_1) - 1) \end{aligned}$$

  - 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 $\overline{\psi}\gamma_4\psi$ dimension 3

Two operators control asymmetry

- $\overline{\psi}\gamma_4\partial_4\psi$ and β_t dimension 4

Point split fields natural

- separate poles at different "bare momenta"

$$u(q) = \frac{1}{2}\left(1 + \frac{\sin(q_4 + \alpha)}{\sin(\alpha)}\right)\psi(q + \alpha e_4)$$

$$d(q) = \frac{1}{2}\Gamma\left(1 - \frac{\sin(q_4 - \alpha)}{\sin(\alpha)}\right)\psi(q - \alpha e_4)$$

- zeros inserted to cancel undesired pole
  - not unique
- Γ factor since different poles use different gamma matrices
  - $\Gamma = i\gamma_4\gamma_5$ for Karsten/Wilczek formulation

Position space:

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

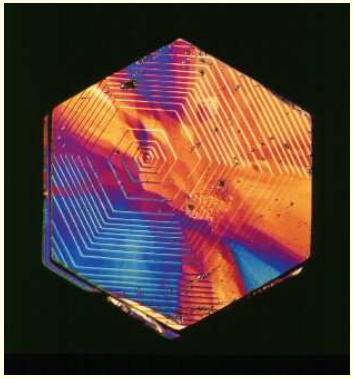
Gives rise to point-split meson operators; i.e.

$$\eta'(x) = \frac{1}{8} \Big(\overline{\psi}(x - e_4)\gamma_5\psi(x) - \overline{\psi}(x)\gamma_5\psi(x - e_4) + \overline{\psi}(x + e_4)\gamma_5\psi(x) - \overline{\psi}(x)\gamma_5\psi(x + e_4) \Big).$$

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 $\longleftarrow$
- Two choices here as well
  - $m_{\pi_\pm} > m_{\pi_0}$: π_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

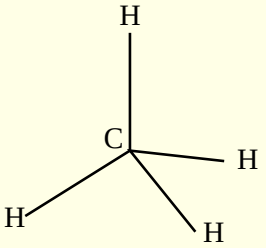
Carbon has 6 electrons

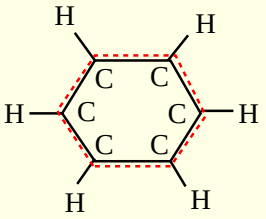
- two tightly bound in the 1s orbital
- second shell: one $2s$ and three $2p$ orbitals

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

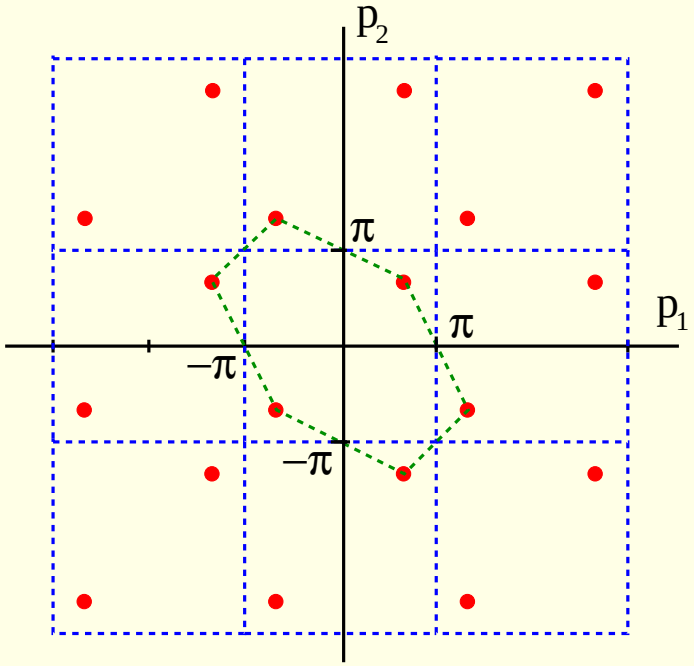
Carbon likes to mix the outer orbitals in two distinct ways

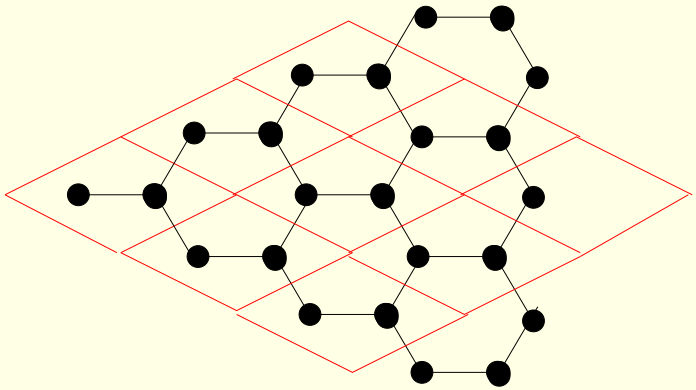
- 4 sp^3 orbitals in a tetrahedral arrangement
  - methane CH_4, diamond C_∞
- 3 sp^2 orbitals in a planar triangle plus one p
  - benzene C_6H_6, graphite C_∞
  - the sp^2 electrons in strong "sigma" bonds
  - the p electron can hop around in "pi" orbitals

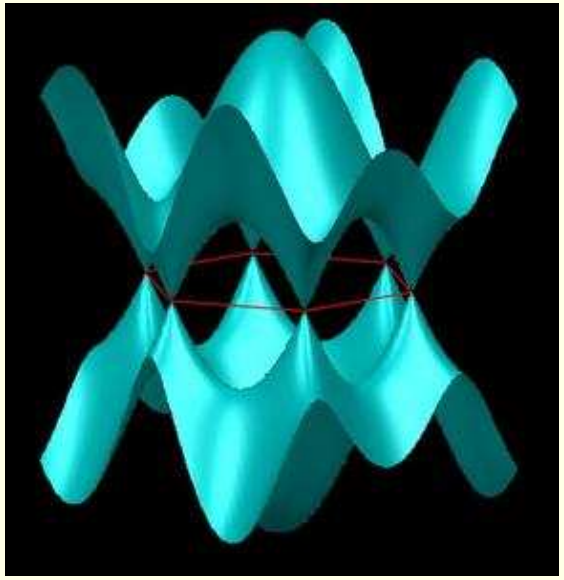




Hexagonal structure hidden in deformed coordinates







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: $\overline{\psi}_j(+\gamma_1+\gamma_2+\gamma_3-iB\gamma_4)\psi_i$
- 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 $\vec{\gamma}$