

Four-dimensional 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

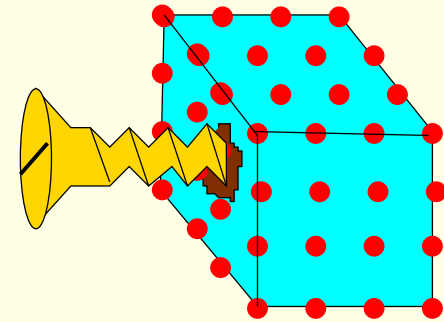


Four dimensional extension

- 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

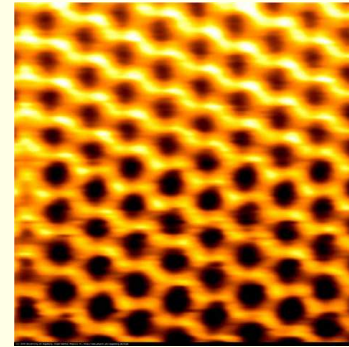
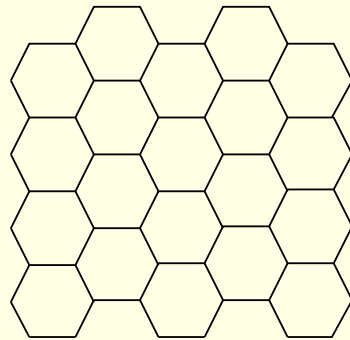
- Lattice is a regulator
 - removes all infinities
 - continuum limit defines a field theory
- Classical $U(1)$ chiral symmetry broken by quantum effects
 - a valid lattice formulation must break $U(1)$ axial symmetry
- But we want flavored chiral symmetries to protect masses
 - Wilson fermions break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



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

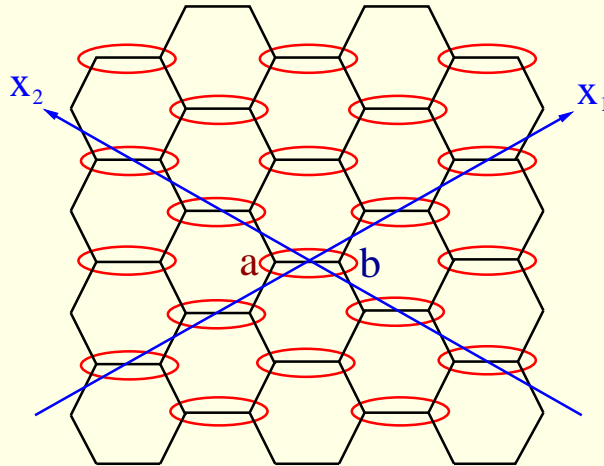
Held together by strong “sigma” bonds, sp^2

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

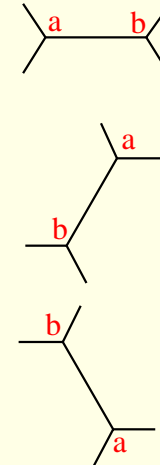
- “ a ” on the left end of a horizontal bond
- “ b ” on the right end
- all hoppings are between type a and type b atoms

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

- axes at 30 degrees from horizontal

Hamiltonian

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



- hops always between a and b sites

Go to momentum (reciprocal) space

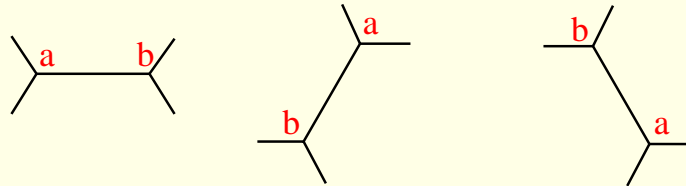
- $a_{x_1, x_2} = \int_{-\pi}^{\pi} \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} e^{ip_1 x_1} e^{ip_2 x_2} \tilde{a}_{p_1, p_2}$.
- $-\pi < p_\mu \leq \pi$

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

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



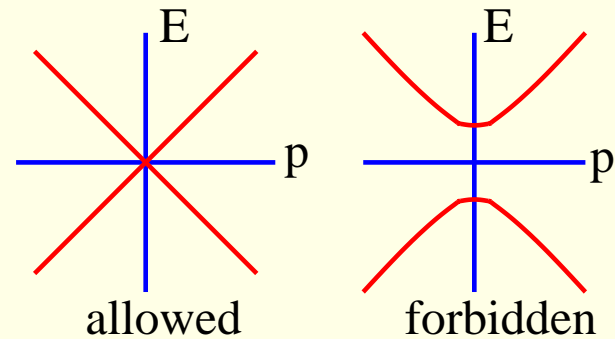
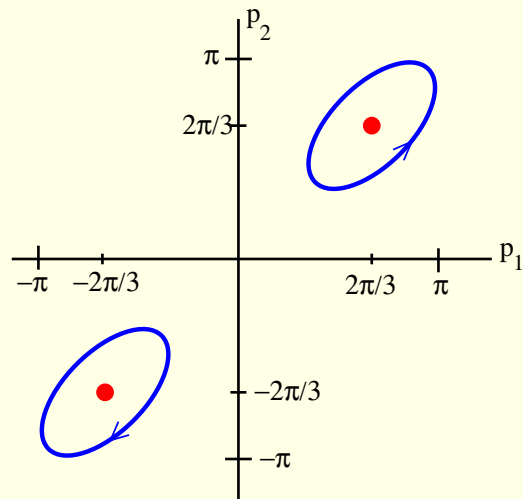
$$\tilde{H}(p_1, p_2) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix}$$

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

- energy vanishes 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
- $\tilde{H}(p_1, p_2) = K \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix}$
 - 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: $D^\dagger = -D = \gamma_5 D \gamma_5$ “ γ_5 Hermiticity”
- work with Hermitean “Hamiltonian” $H = \gamma_5 D$
 - not the Hamiltonian of the 3D Minkowski theory

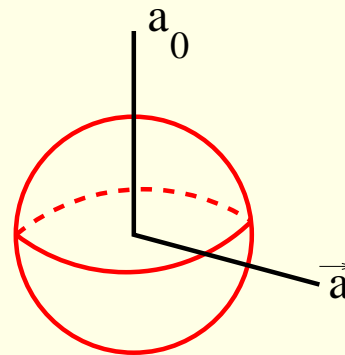
Look for analogous form to the two dimensional case

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

- $z(p_1, p_2, p_3, p_4)$ 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

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

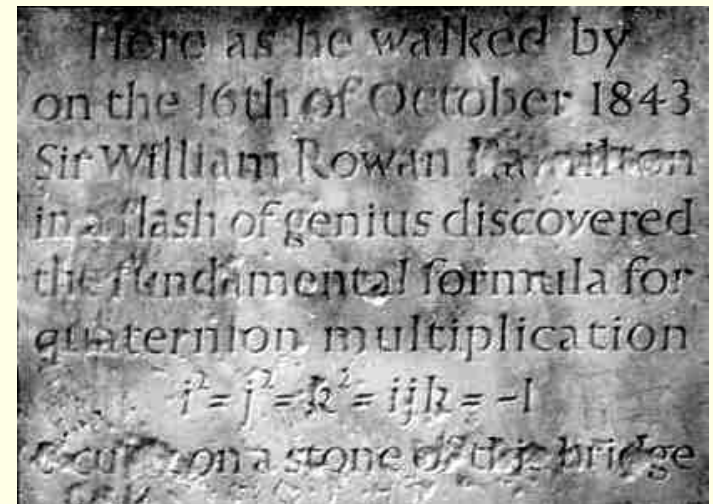
$$\gamma_5 D = H = \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix}$$

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

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

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

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

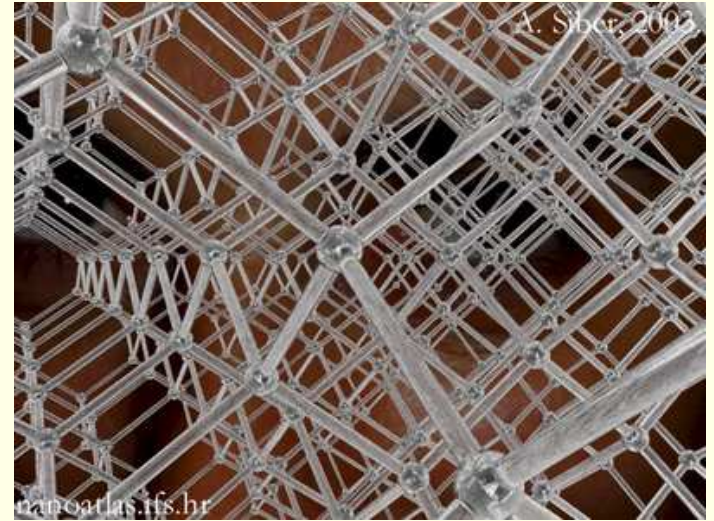
$$\sin(p_1) - \sin(p_2) + \sin(p_3) - \sin(p_4) = 0$$

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

- first three imply $\sin(p_i) = \sin(p_j) \quad \forall i, j$
 - $\cos(p_i) = \pm \cos(p_j)$
- 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 γ_4
- two species of opposite chirality
- the exact chiral symmetry is a flavored one

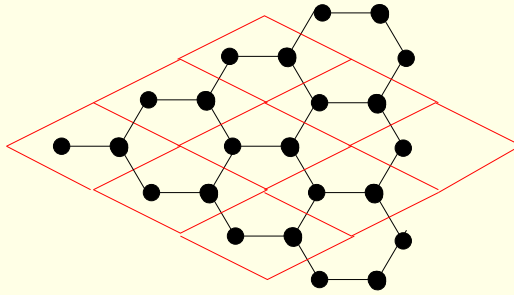
B and C control distortions between the k and q coordinates

- 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

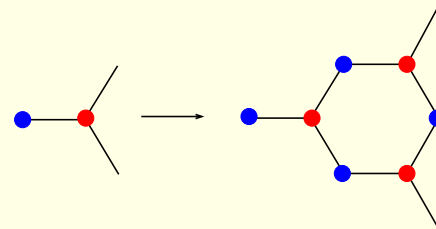
- zeros of z in periodic momentum space form a lattice
- give each zero 5 symmetrically arranged neighbors
 - $C = \cos(\pi/5)$, $B = \sqrt{5}$
- interbond angle θ satisfies $\cos(\theta) = -1/4$
 - $\theta = \text{acos}(-1/4) = 104.4775 \dots$ degrees
- 4-d generalization of the diamond lattice

The physical lattice structure

Graphene: one bond splits into two in two dimensions

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

iterating



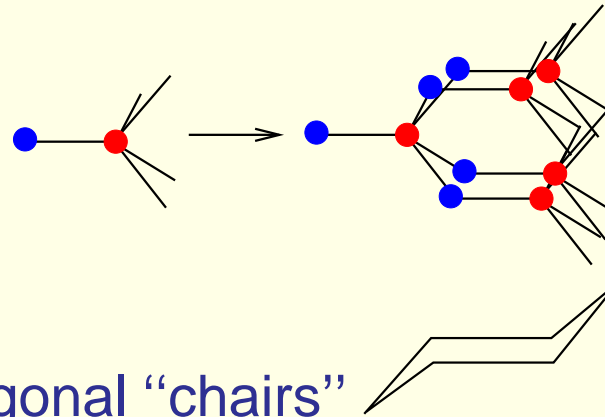
- smallest loops are hexagons



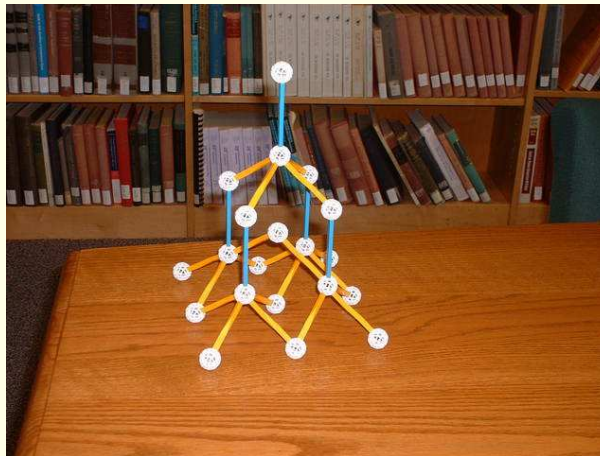
4-d graphene “hyperdiamond”: one bond splits into four

- 5-fold symmetric environment
- $\theta = \arccos(-1/4) = 104.4775 \dots$ 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
 - π_{\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 Wilzcek (1987)
 - select the time axis as special
 - like spatial Wilson fermions with $r \rightarrow ir\gamma_0$
 - both equivalent after phase redefinitions

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
 - no uncontrolled extrapolation to two physical light flavors

Symmetry automatically gives $O(a)$ improvement

- Cichy, Lopez, Jansen, Kujawa, Shindler

Perturbative corrections can shift pole positions

- Capitani, Weber, Wittig
- shift along direction between the poles
- Generalized Karsten/Wilczek operator:

$$D = -i\gamma_4 \left(\sum_{\mu=1}^4 \cos(p_\mu) - \cos(\alpha) - 3 \right) + i \sum_{i=1}^3 \gamma_i \sin(p_i)$$

- poles at $\vec{p} = 0, p_4 = \pm\alpha$
- alpha gets an additive renormalization

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:

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

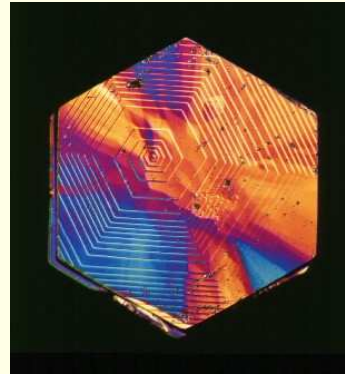
Gives rise to point-split meson operators; i.e.

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

Effective Lagrangians and lattice artifacts

- MC, Sharpe and Singleton
- Two possibilities for Wilson fermions as $m_q \rightarrow 0$
 - Chiral transition becomes first order
 - Aoki phase \leftarrow
- Two choices here as well
 - $m_{\pi_{\pm}} > m_{\pi_0}$: π_0 is normal Goldstone mode \leftarrow ?
 - $m_{\pi_{\pm}} < m_{\pi_0}$: 2nd order transition before $m_q \rightarrow 0$

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

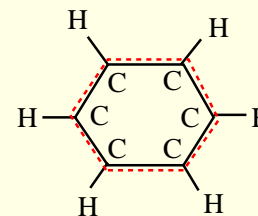
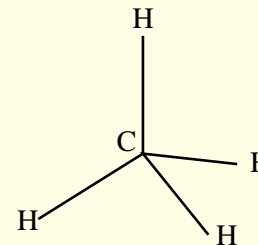
Carbon has 6 electrons

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

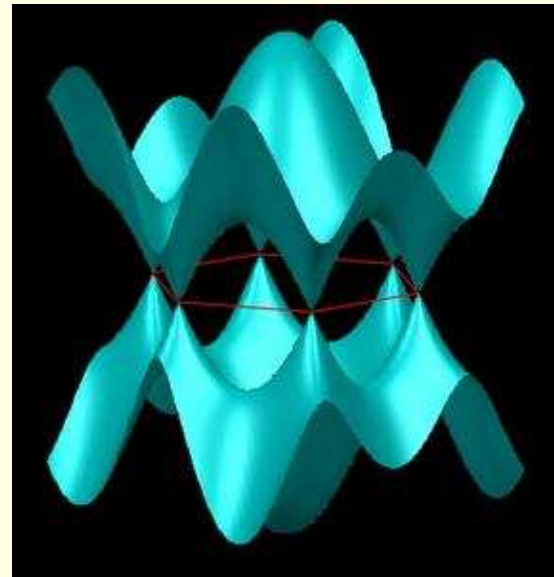
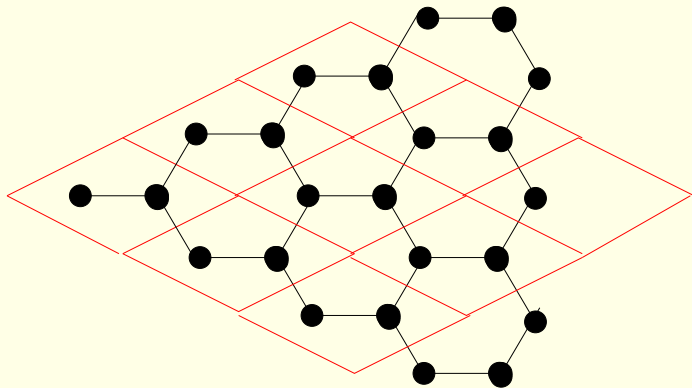
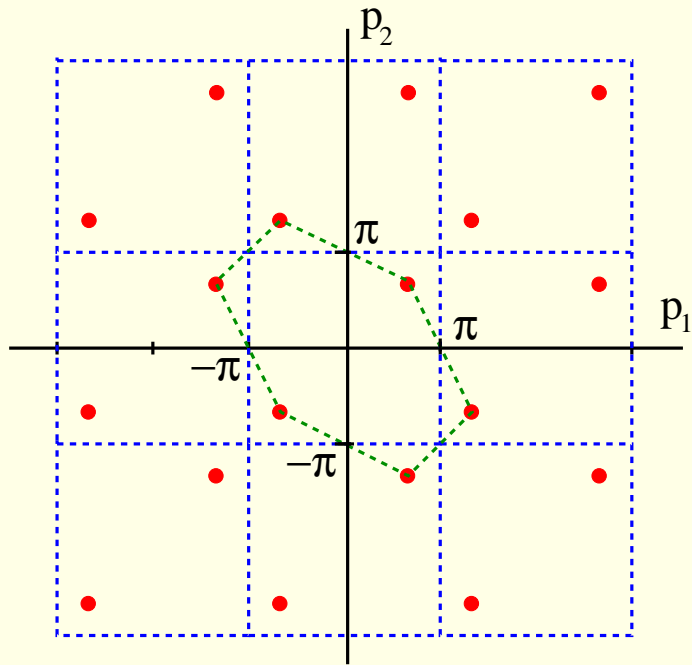
In a molecule or crystal, external fields mix the 2s and 2p orbitals

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: $4iBC\bar{\psi}\gamma_4\psi$
- 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 γ 's
- γ_5 exactly anticommutes with D
- D is purely anti-Hermitian
- γ_4 not symmetrically treated to $\vec{\gamma}$