Symmetry on honeycomb lattice formulation

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collaboration with Masaki Hirotsu (Osaka) and Tetsuya Onogi (Osaka)

Ref. M. Hirotsu, T. Onogi, ES, Nucl. Phys. B885 (2014) 61. T. Onogi, Lattice 2014.

Quark confinement and the hadron spectrum XIth, St. Petersburg, 7--12 Sep 2014

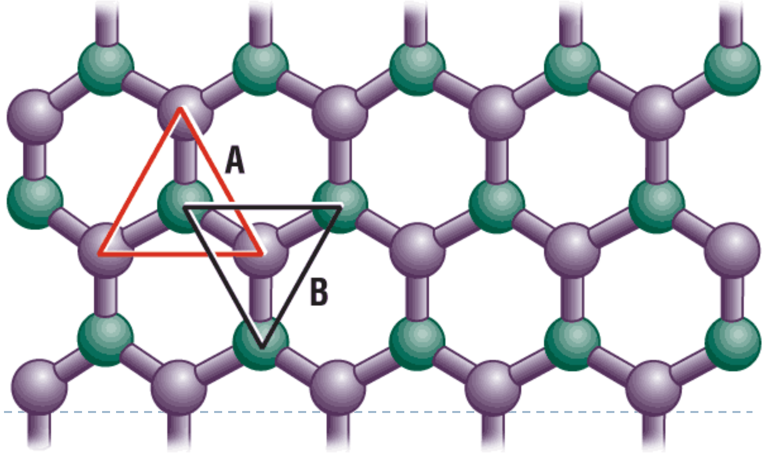
1. Introduction

Honeycomb lattice materials

- One-atom-thick 2D material layered as honeycomb lattice is attractive in condensed matter physics.

  e.g. Graphene, MoS_2, WS_2, WSe_2, ZnO (2D), etc
- Those have unique band structure, dispersion relation, large e mobility, quantum Hall effect.
- Graphene has been one of the most fascinating material since its discovery in 2004 by Novoselov, Geim et al.
- Energy spectrum is similar to massless Dirac particle (quasi-particle)

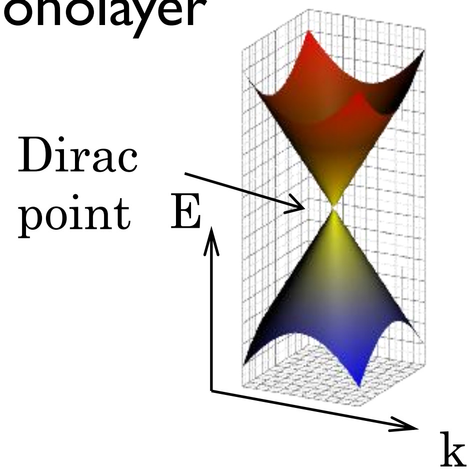
Main motivation:
Theoretical approach for understanding appearance of band gap in Monolayer or multilayer of Graphene.



1. Introduction

Band structure of Graphene

Monolayer

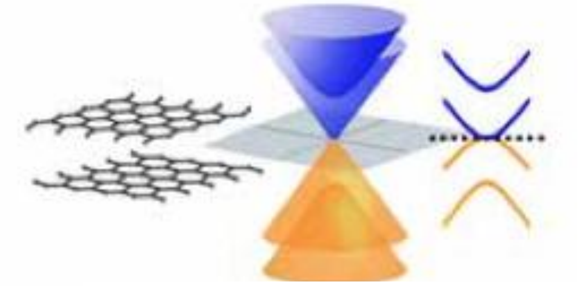


Dispersion relation: $E = \pm vk$

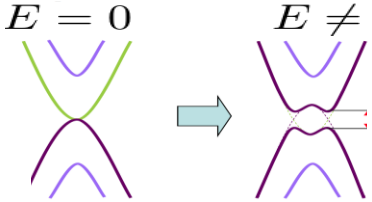
Gapless in Dirac point

Bilayer

Parabolic dispersion



External E field perpendicular to plane



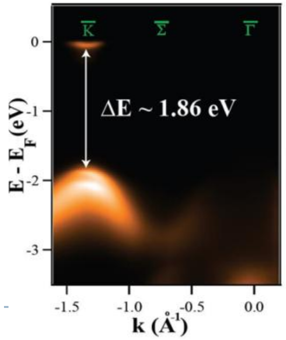
Band gap

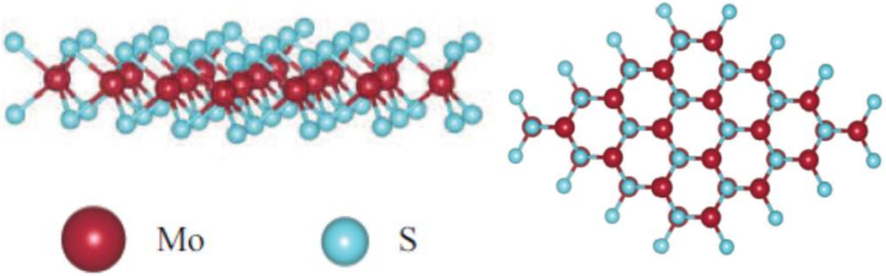
Application: bilayer Graphene is rather useful for semiconductor material.

e.g. Geim, Novoselov, Nature Material 6, 183(2007)

Note: Monolayer MoS_2

- Parabolic dispersion
- Energy gap (~1.8 eV) in Dirac point
- More useful for semiconductor





T. Eknapakul et al., Nano. Lett. 14, 1412(2014)

Symmetry

- Gapless mode

Monolayer Graphene : massless Dirac mode.

Bilayer Graphene : gapless mode with quadratic dispersion.

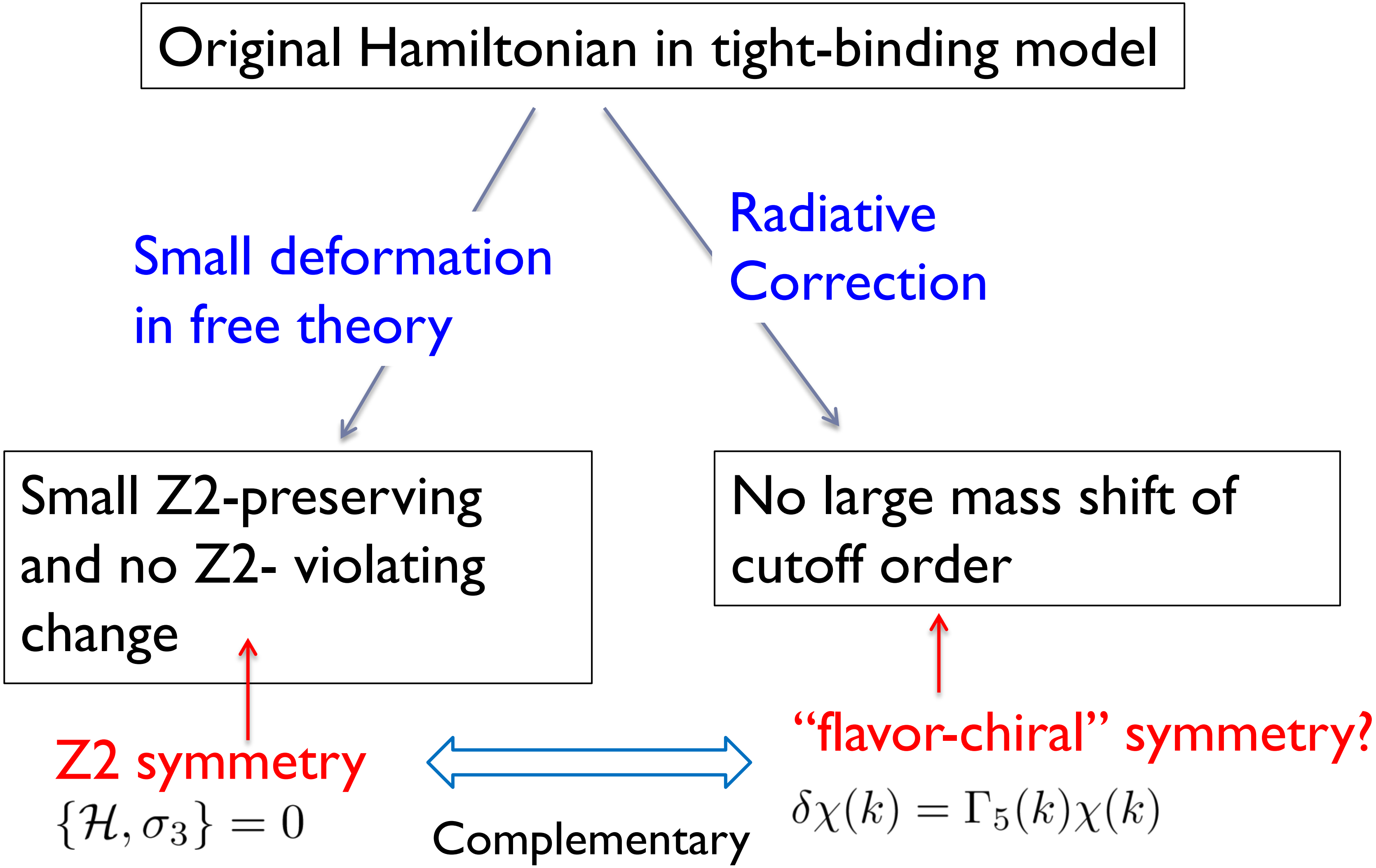
How do we figure out the appearance of gapless mode in Graphene starting from tight-binding model ?

Stability of massless quasi-particle even if there is radiative correction order of cut-off scale (inverse of lattice spacing)

- So far there has been a discussion of Z2 symmetry in free-field near low-energy limit. e.g. Hatsugai-Aoki-Fukui 2006
- Is it also realized when extending into whole energy region ?
- The exact formula of (hidden) symmetry of Honeycomb lattice Hamiltonian is needed.

1. Introduction

Symmetry



Original Hamiltonian in tight-binding model

Small deformation in free theory

Radiative Correction

Small Z2-preserving and no Z2- violating change

No large mass shift of cutoff order

Z2 symmetry

$\{\mathcal{H}, \sigma_3\} = 0$

Complementary

"flavor-chiral" symmetry?

$\delta\chi(k) = \Gamma_5(k)\chi(k)$

2. Tight-binding model

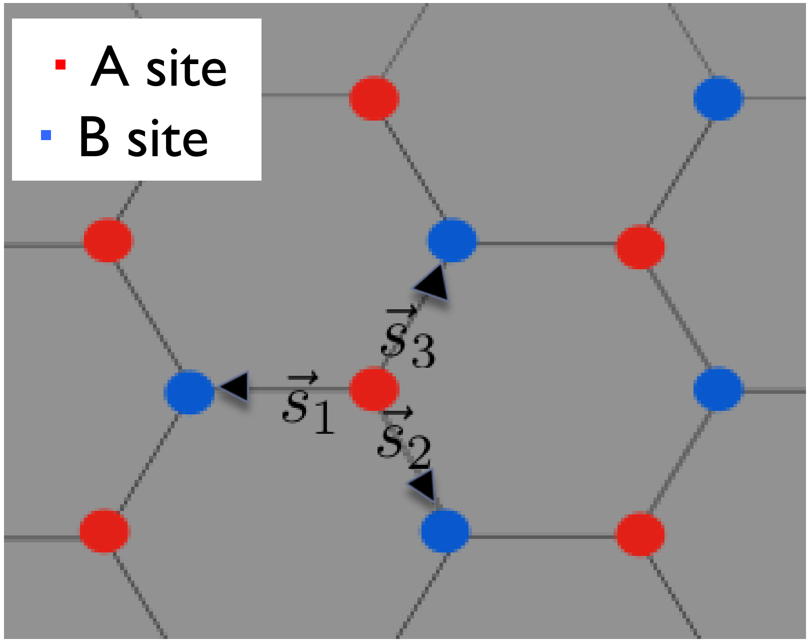
Hamiltonian of Graphene

$$H = t\sum_{\vec{x}}\sum_{i=1}^{3}[a^\dagger(\vec{x})b(\vec{x}+\vec{s}_i)+h.c.]$$
$$+t'\sum_{x}\sum_{j=1}^{6}[a^\dagger(\vec{x})a(\vec{x}+\vec{b}_j)+b^\dagger(\vec{x}+\vec{s}_1)b(\vec{x}+\vec{s}_1+\vec{b}_j)]$$

$t = 2.8\ \mathrm{eV}, \quad t' = 0.1\ \mathrm{eV}$

$a, a^\dagger$: ann., cr. operator at site A

$b, b^\dagger$: ann., cr. operator at site B



Nearest-neighbor bond

$$\begin{cases} \vec{s}_1 = a_0(-1,0), \\ \vec{s}_2 = \frac{a_0}{2}(-1,\sqrt{3}) \\ \vec{s}_3 = \frac{a_0}{2}(1,\sqrt{3}) \end{cases}$$

Fundamental lattice vector for A, B site

$$\begin{cases} \vec{b}_1 = \vec{s_2} - \vec{s_3}, \quad \vec{b}_2 = \vec{s_2} - \vec{s_1}, \\ \vec{b}_3 = \vec{s_3} - \vec{s_1}, \quad \vec{b}_4 = \vec{s_3} - \vec{s_2}, \\ \vec{b}_5 = \vec{s_1} - \vec{s_2}, \quad \vec{b}_6 = \vec{s_1} - \vec{s_3} \end{cases}$$

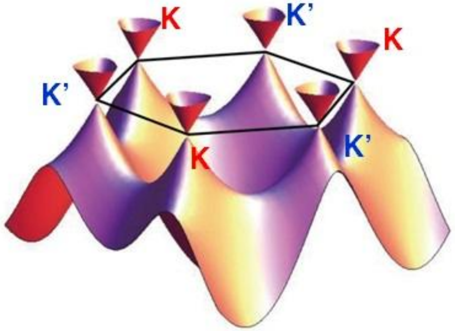
2. Tight-binding model

Energy spectrum

G. W. Semenoff, (1984)

- Leading order

$$H = t\sum_{\sigma}\int \frac{d^2k}{(2\pi)^2}(a^\dagger(k)b^\dagger(k))\begin{pmatrix} 0 & \Phi(k) \\ \Phi^*(k) & 0 \end{pmatrix}\begin{pmatrix} a(k) \\ b(k) \end{pmatrix}$$



$$E = \pm|\Phi(k)| \qquad \Phi(k) = e^{i\vec{k}\cdot\vec{s}_1} + e^{i\vec{k}\cdot\vec{s}_2} + e^{i\vec{k}\cdot\vec{s}_3}$$

Dirac point (E=0): $K_1 = \left(0, \frac{4\pi}{3a_0}\right), K_2 = \left(\frac{2\pi}{\sqrt{3}a_0}, \frac{2\pi}{3a_0}\right)$

- Low-energy limit

$$H_0 = v_F\int \frac{d^2k}{(2\pi)^2}\left[u^\dagger(k)(k_x\sigma_2 + k_y\sigma_1)u(k) - v^\dagger(k)(k_x\sigma_2 + k_y\sigma_1)v(k)\right]$$

$$u(k) = \begin{pmatrix} a(k-K_1) \\ b(k-K_1) \end{pmatrix}, \quad v(k) = \begin{pmatrix} a(k-K_2) \\ b(k-K_2) \end{pmatrix},$$

Massless Dirac fermion with velocity v_F emerges.

$$v_F = \frac{\sqrt{3}}{2}a_0 t \sim c/300$$

Being velocity of 1/300 times speed-of-light, it turns out to be large fine structure constant.

$$\alpha_v = \frac{e^2}{4\pi hc} \times 300$$

Study in strong QED system
e.g. Drut, Lahde (2009-2010),
ES, Onogi, (2012), …

3. Position space formulation

Hamiltonian in position space

- Purpose
  - To find the manifest symmetry prohibiting mass term in Hamiltonian.
  - Analogy to staggered fermion formulation
    - Flavor-chiral rotation in position space formulation in 4D Lagrangian

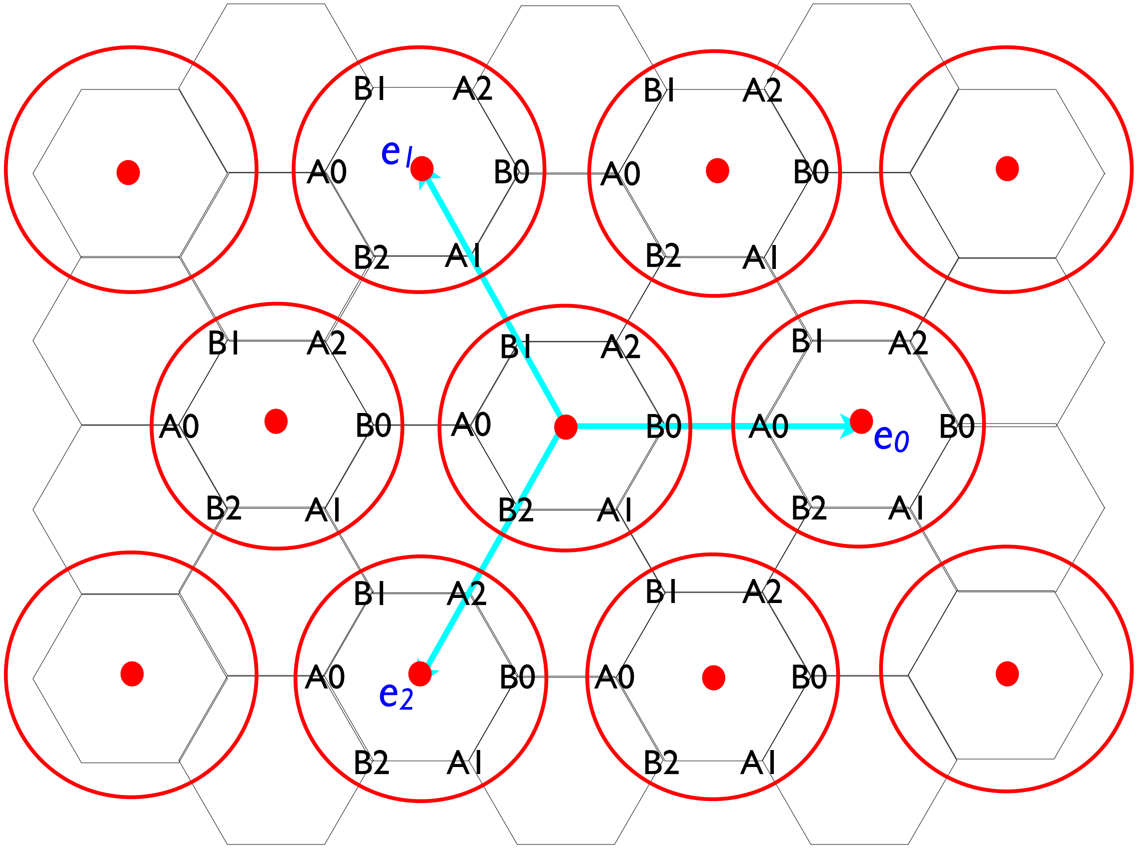
      Kluberg-Stern et al. (1983)
    - Exact symmetry on the lattice
  - In 2+1D system,

    Flavor degree → A,B site index
    Spinor degree → internal degree of A and B site

3. Position space formulation

Labeling site on Honeycomb lattice

- New assignment of Honeycomb lattice index



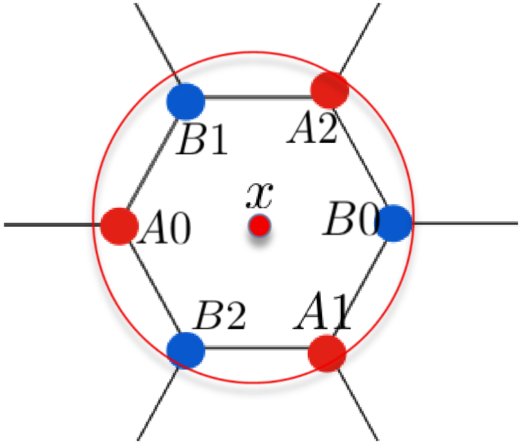
- The center of hexagonal unit cell is fundamental lattice site.
- Inside of hexagonal cell has A,B index and three internal degree.
- $e_{i=0,1,2}$ is the new fundamental lattice vector.

$$\begin{cases} \vec{e}_0 = a(1,0) \\ \vec{e}_1 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2}) \\ \vec{e}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2}) \end{cases}$$

(a : lattice spacing)

3. Position space formulation

Degree of freedom



- Quasi-particle field $\chi_{A\rho}(x)$
  - A, B : two DOFs
  - ρ: internal A,B lattice with three DOFs
  - 2x3 = 6 DOFs tensor structure
- Structure of Dirac operator

$$\underset{\boxed{6\text{x}6}}{\underset{\uparrow}{A_{I\rho,I'\rho'}}} = \sum_{a=0}^{3} \underset{\boxed{2\text{x}2}}{\underset{\uparrow}{(\tau^a)_{II'}}} \otimes \underset{\boxed{3\text{x}3}}{\underset{\uparrow}{(B^a)_{\rho\rho'}}}$$

$$I, I' = A, B \qquad \rho, \rho' = 0, 1, 2$$

Involving the 6x6 matrix, whose structure is similar to the staggered-Dirac operator.

Position space formulation

- Hamiltonian

$$\mathcal{H} = t\sum_{\vec{x}} \chi^\dagger(\vec{x})\Big[(\tau_1 \otimes M)\chi(\vec{x}) - i\sum_{\rho}(\tau_2 \otimes \Gamma_\rho)(\nabla_\rho\chi(\vec{x})) + \frac{1}{2}\sum_{\rho}(\tau_1 \otimes \Gamma_\rho)(\Delta_\rho\chi(\vec{x}))\Big]$$

$$M = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \ \Gamma_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \Gamma_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ \Gamma_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\nabla_\rho\chi(X) \equiv \frac{1}{2}\left[\chi(\vec{x}+\vec{e}_\rho) - \chi(\vec{x}-\vec{e}_\rho)\right]$$

$$\Delta_\rho\chi(X) \equiv \chi(\vec{x}+\vec{e}_\rho) + \chi(\vec{x}-\vec{e}_\rho) - 2\chi(\vec{x})$$

1st : mass term
2nd : kinetic term in honeycomb lattice
3rd : order *a* mass term involving second differential (e.g Wilson term)

It turns out to be manifest locality as well as staggered fermion.

3. Position space formulation

Physical and unphysical mode

- Diagonalization of mass term

One massive mode

Change of basis

$$M = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \xrightarrow{\hspace{3cm}} M^{\mathrm{diag}} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Two zero modes

Integrating out the massive mode, the zero modes remain as physical modes, and then 4 DOFs are physical degree of freedom.
If we take the continuum limit, Hamiltonian is consistent with formula of QED Dirac fermion in 2+1 dimension including Fermi velocity v_F

$$H_{\mathrm{eff}} = v_F \int d^2x \psi^\dagger \Big[(\tau_2 \otimes \sigma_1)\partial_1 + (\tau_2 \otimes \sigma_2)\partial_2 \Big] \psi(x)$$

ψ is 4 component fermion field

4. Hidden symmetry

Global symmetry of H_{eff}

- Global transformation with 4x4 matrix

$$\delta\psi = i\Gamma\psi \qquad H_{\text{eff}} = v_F \int \psi^\dagger \mathcal{H}\psi,\ \mathcal{H} = (\tau_2 \otimes \sigma_1)\partial_1 + (\tau_2 \otimes \sigma_2)\partial_2$$

4 possibilities for [*H*, Γ]=0

$1_{2\times 2} \otimes 1_{2\times 2}$	$\tau_1 \otimes \sigma_3$	$\tau_2 \otimes 1_{2\times 2}$	$\tau_3 \otimes \sigma_3$

Candidate of “Flavor-Chiral” symmetry

- Discrete symmetry on Graphene

Parity transformation: $\vec{x} \to \vec{x}_P,\ A \leftrightarrow B \quad \Rightarrow P = \tau_1 \otimes 1$

Parity conserving mass term $m(\tau_1 \otimes 1_{2\times 2})$ is prohibited by the last two symmetries

However, those symmetry could be violated by lattice artifact

4. Hidden symmetry

Flavor-chiral symmetry on honeycomb

- We look for the exact flavor-chiral symmetry on Hamiltonian.
- “Top-down” approach
  - Seeking the symmetry of χ field in whole energy spectrum

$$\delta\chi(k) = \Gamma_5(k)\chi(k) \qquad \lim_{k\to 0}\Gamma_5(k) = \Gamma_5^{\text{cont}}$$

which also prohibits the mass term, $[H,\Gamma_5]=0$.

  - Low energy: at NNLO

$(\tau_1 \otimes 1)$ series are failed, but $(\tau_3 \otimes \sigma_3)$ series are survived in H_{eff}.

  - Low energy expansion: at N^{3}LO

$(\tau_3 \otimes A)$, $(1 \otimes B)$ series (A,B is arbitrary 3x3 matrix) only appear.

  - Ansatz for $\Gamma_5(k)$

$$\boxed{\delta\chi(\vec{x}) = i\theta\Big[\underbrace{3(\tau_3\otimes X)\chi(\vec{x}) + \frac{1}{2}\sum_\rho(\tau_3\otimes Y_\rho)(\Delta_\rho\chi(\vec{x})) + \frac{1}{i}\sum_\rho(1\otimes Z_\rho)(\nabla_\rho\chi(\vec{x}))}_{\Gamma_5(x)\chi(x)}\Big]}$$

Flavor-chiral symmetry on honeycomb

- Explicit formula of X,Y,Z coefficients

$$X = \begin{pmatrix} 0 & -i & i \\ i & 0 & -i \\ -i & i & 0 \end{pmatrix},$$

$$Y_0 = \begin{pmatrix} 0 & -i & i \\ i & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, Y_1 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, Y_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & -i \\ -i & i & 0 \end{pmatrix},$$

$$Z_0 = \begin{pmatrix} 0 & -1 & 1 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, Z_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, Z_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \end{pmatrix}$$

Continuum limit (mass diagonal basis)

$$\delta\chi(x) \to \tau_3 \otimes \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \Rightarrow \tau_3 \otimes \sigma_3$$

Coincide with global "flavor-chiral sym." in H_{eff}

4. Hidden symmetry

Remarks

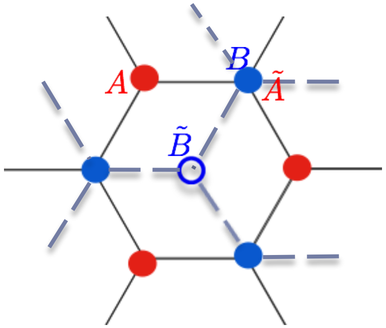
- This formulation easily extends toward multi-hopping interaction. Since multi-hopping interaction is written as polynomial of H, $H_{\text{non-local}} = P(H)$, our argument does not change (in contrast, Z2 symmetry is not applied in more than 2 hopping case, $\{H^2, \sigma_3\} \neq 0$).
- In bilayer case (AB-staking), if we define

$$\begin{cases} \delta\chi = i\theta\Gamma_5\chi \\ \delta\tilde{\chi} = i\tilde{\theta}\Gamma_5\tilde{\chi} \end{cases}$$

χ : electron in tupper-layer

$\tilde{\chi}$: electron in lower-layer

$\theta, \tilde{\theta}$: parameters for "chiral" symmetry



A B Upper layer

$\tilde{A}$ $\tilde{B}$ Lower layer

B sites sit on top of $\tilde{A}$

and in $\theta = \tilde{\theta}$, Hamiltonian is also invariant under flavor-chiral symmetry.

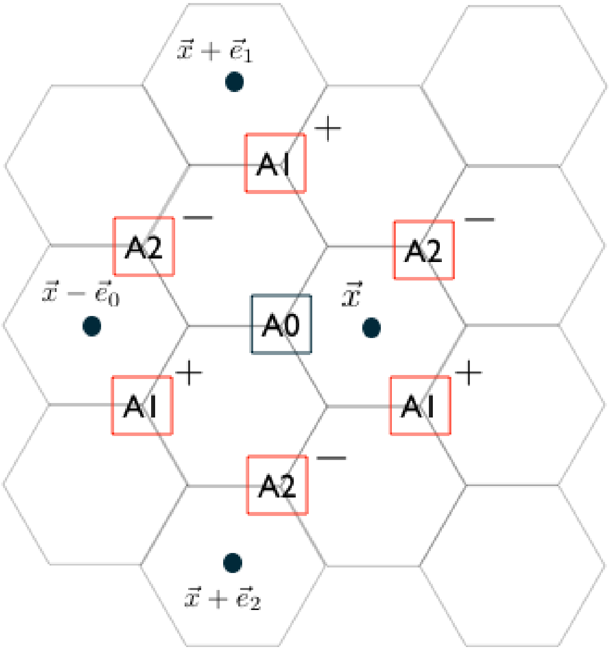
Summary and future work

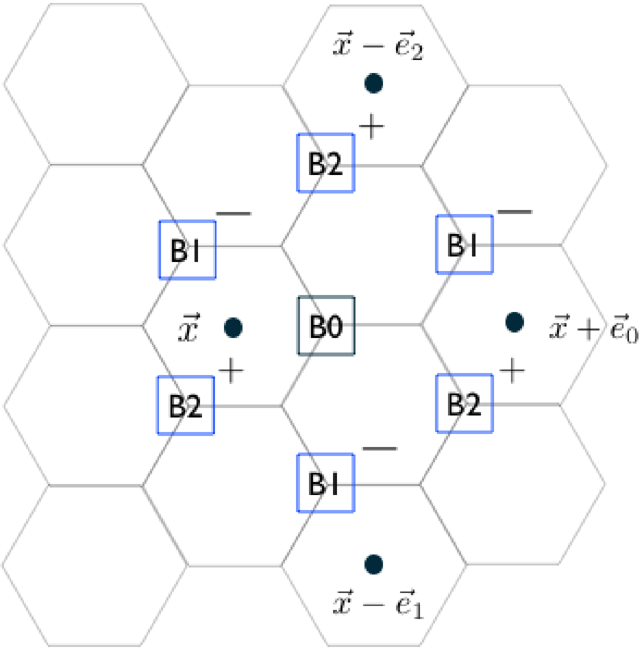
- We show formula of flavor-chiral symmetry on honeycomb lattice.
- Flavor-chiral symmetry is exact even in finite lattice spacing. It may be more realistic formula for Graphene.
- It is also extendable to bilayer case.
- What's the next ?
  - Naively gauge interaction is able to introduce into link variable.
  - The check of consistency is necessary with perturbation.
  - Our goal: Non-perturbative calculation for phase transition, boundary effect (carbon nanotube) and anomalous Hall effect in Monte-Carlo simulation.

Backup

Symmetry in terms of conventional labeling

$$\begin{aligned}\delta a(\vec{x}) = \theta[&a(\vec{x}+\vec{s}_2-\vec{s}_3) - a(\vec{x}-\vec{s}_1+\vec{s}_2) + a(\vec{x}+\vec{s}_3-\vec{s}_1)\\ &-a(\vec{x}-\vec{s}_2+\vec{s}_3) + a(\vec{x}+\vec{s}_1-\vec{s}_2) - a(\vec{x}-\vec{s}_3+\vec{s}_1)]\\ \delta b(\vec{x}) = \theta[&b(\vec{x}+\vec{s}_2-\vec{s}_3) - b(\vec{x}-\vec{s}_1+\vec{s}_2) + b(\vec{x}+\vec{s}_3-\vec{s}_1)\\ &-b(\vec{x}-\vec{s}_2+\vec{s}_3) + b(\vec{x}+\vec{s}_1-\vec{s}_2) - b(\vec{x}-\vec{s}_3+\vec{s}_1)]\end{aligned}$$

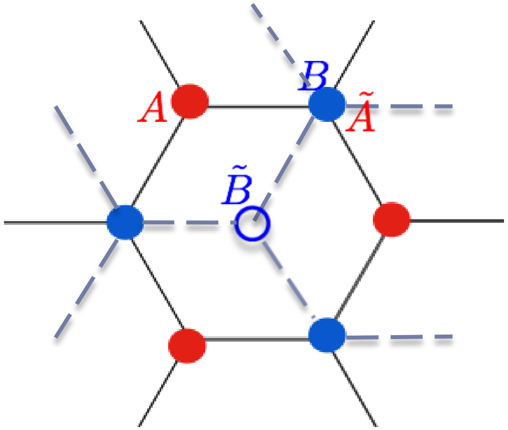




2. Tight-binding model

Bilayer energy spectrum

- AB staking



A B Upper layer

$\tilde{A}$ $\tilde{B}$ Lower layer

B sites sit on top of $\tilde{A}$

Inter-layer hopping Hamiltonian

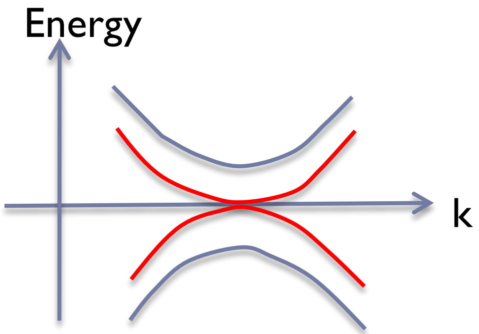
$$H_{\text{inter}} = \int \frac{d^2k}{(2\pi)^2} \left[\left(a^\dagger(k) b^\dagger(k) \right) \begin{pmatrix} 0 & 0 \\ \gamma & 0 \end{pmatrix} \begin{pmatrix} \tilde{a}(k) \\ \tilde{b}(k) \end{pmatrix} + h.c. \right]$$

Energy eigenvalue in AB staking

$$E(k) = \pm \left[\frac{\gamma^2}{2} + |t\Phi(k)|^2 \pm \sqrt{\left(\frac{\gamma^2}{2} + |t\Phi(k)|^2 \right)^2 - |t\Phi(k)|^4} \right]^{1/2}$$

Near Dirac point $|t\Phi(k)| \sim v_F |\vec{k} - \vec{K}|$

$$E(k) \sim \pm \left[\gamma + \frac{v_F^2}{\gamma} (\vec{k} - \vec{K})^2 \right], \quad \pm \frac{v_F^2}{\gamma} (\vec{k} - \vec{K})^2$$



In the same Dirac point, parabolic dispersion emerges.

In order to determine $X,\ Y_\rho,\ Z_\rho$, we employ momentum representation of $\chi(\vec{x}), \chi^\dagger(\vec{x})$

$$\mathcal{H} \;=\; \int \frac{d^2k}{(2\pi)^2}\tilde{\chi}^\dagger(\vec{k})\Big[(\tau_1 \otimes \Lambda) + \sum_\rho e^{ik_\rho}(\tau_- \otimes \Gamma_\rho) + \sum_\rho e^{-ik_\rho}(\tau_+ \otimes \Gamma_\rho)\Big]\tilde{\chi}(\vec{k}) \tag{1}$$

with $\tau_\pm \equiv (\tau_1 \pm i\tau_2)/2$ and $\Lambda \equiv M - 1$, and for chiral transformation $\delta\tilde{\chi}(\vec{k}) = i\theta\tilde{\Gamma}_5(\vec{k})\tilde{\chi}(\vec{k})$ $\tilde{\Gamma}_5(\vec{k})$ is given as

$$\tilde{\Gamma}_5(\vec{k}) = (\tau_3 \otimes X) + \sum_\rho e^{ik_\rho}\gamma_\rho + \sum_\rho e^{-ik_\rho}\gamma_\rho^\dagger, \tag{2}$$

with

$$\gamma_\rho = \frac{\tau_3 + 1}{2} \otimes W_\rho^\dagger + \frac{\tau_3 - 1}{2} \otimes W_\rho. \tag{3}$$

W_ρ is defined as $W_\rho = \frac{1}{2}(Y_\rho + iZ_\rho)$.

Imposing $[\tilde{H}(\vec{k}), \tilde{\Gamma}_5(\vec{k})] = 0$, we obtain following equations;

$$\{\Lambda, X\} + \sum_{\rho} (\Gamma_\rho W_\rho + W_\rho^\dagger \Gamma_\rho) = 0 \tag{1}$$

$$\{\Gamma_\rho, X\} + \Lambda W_\rho^\dagger + W_\rho \Lambda = 0 \tag{2}$$

$$\Lambda W_\rho + W_\rho^\dagger \Lambda + \sum_{\sigma \neq \lambda (\sigma, \lambda \neq \rho)} (\Gamma_\sigma W_\lambda^\dagger + W_\lambda \Gamma_\sigma) = 0 \tag{3}$$

$$\Gamma_\rho W_\rho^\dagger + W_\rho \Gamma_\rho = 0 \tag{4}$$

$$\Gamma_\rho W_\sigma + W_\sigma^\dagger \Gamma_\rho = 0 \ (\rho \neq \sigma). \tag{5}$$