Study on the Electronic Properties of Graphene based on Strong Coupling Expansion of Lattice Gauge Theory

格子ゲージ理論の強結合展開によるグラフェン物性の研究

arXiv:1003.1769 [cond-mat.str-el]

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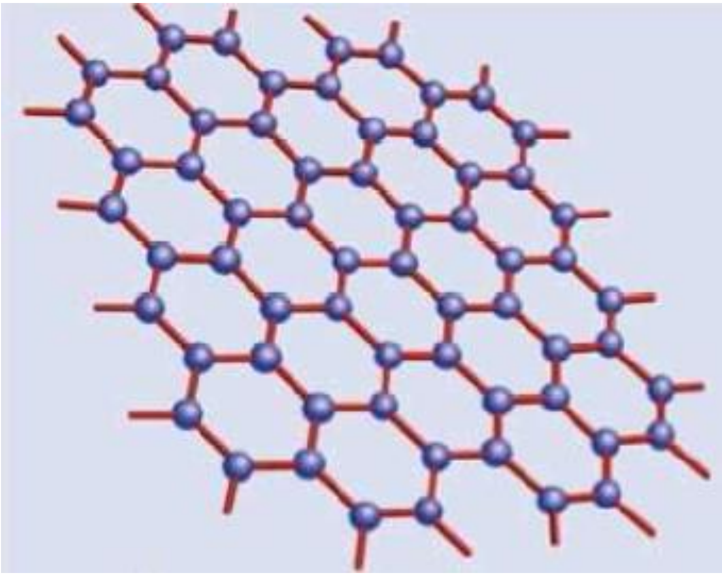
Apr. 28, 2010 @駒場

What is graphene?

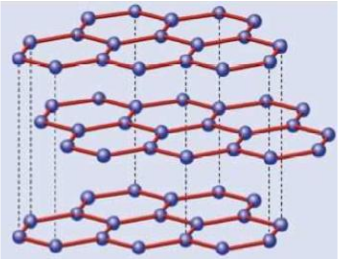
Graphene = Single atomic layer of carbon atoms

Honeycomb lattice structure

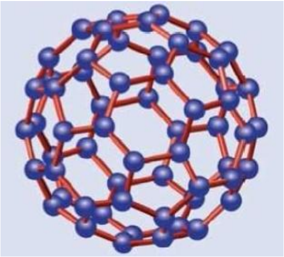
→ Building block of many kinds of carbon materials.



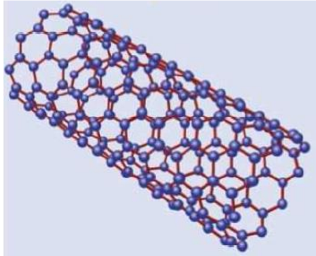
graphene



graphite



fullerene



nanotube

[Castro Neto et al., 2009]

2D electron system easy to process and observe.

History of graphene

1947: Band structure of graphene [Wallace,1947]

purely theoretical?
(unstable structure)

PHYSICAL REVIEW VOLUME 71, NUMBER 9 MAY 1, 1947

The Band Theory of Graphite

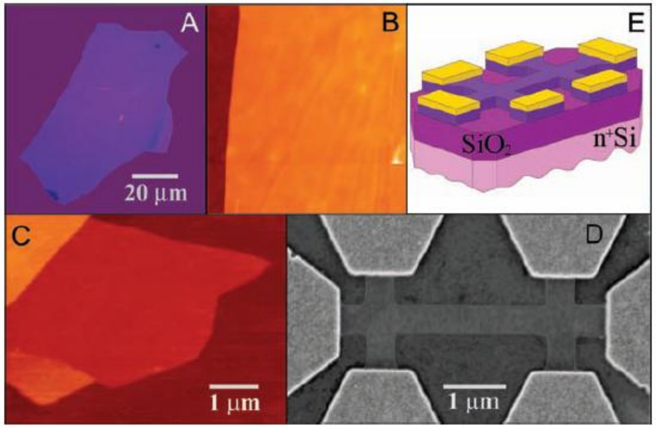
P. R. WALLACE*
National Research Council of Canada, Chalk River Laboratory, Chalk River, Ontario

(Received December 19, 1946)

The structure of the electronic energy bands and Brillouin zones for graphite is developed using the "tight binding" approximation. Graphite is found to be a semi-conductor with zero activation energy, i.e., there are no free electrons at zero temperature, but they are created at higher temperatures by excitation to a band contiguous to the highest one which is normally filled. The electrical conductivity is treated with assumptions about the mean free path. It is found to be about 100 times as great parallel to as across crystal planes. A large and anisotropic diamagnetic susceptibility is predicted for the conduction electrons; this is greatest for fields across the layers. The volume optical absorption is accounted for.

Many theoretical studies…

2004: Isolation of monolayer graphene
[Novoselov *et al.*,2004]



Today:

2D electron system easy to process and observe

One of the largest research interests

(on both theoretical and experimental side)

Outline

1. Introduction

2. Review of low-energy effective gauge theory

3. Strong coupling expansion on lattice

4. Collective excitations

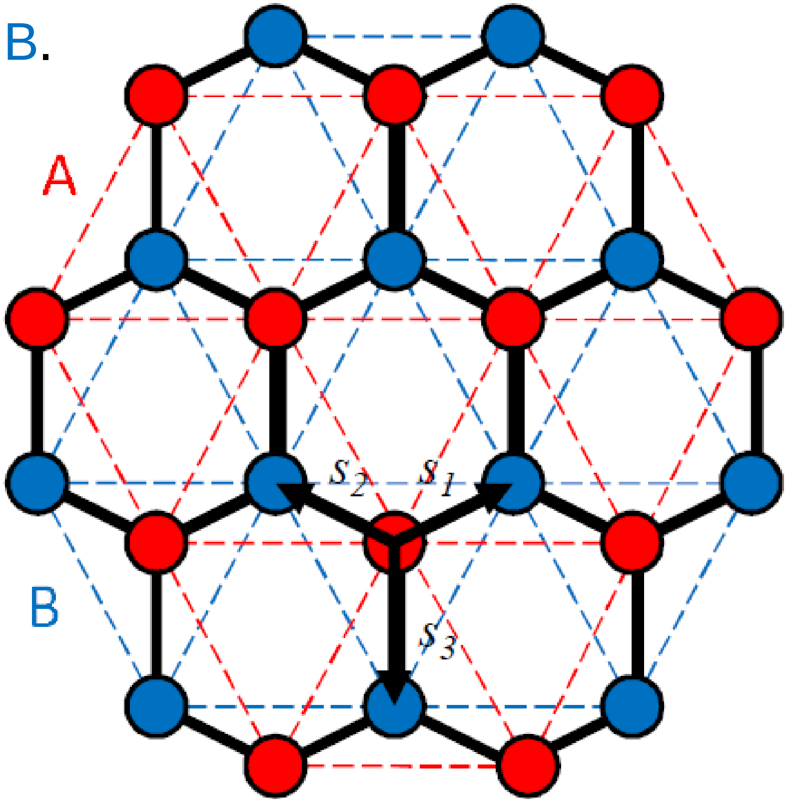
5. Summary

2.

Review of low-energy effective gauge theory

Lattice structure

Introduce triangular sublattices A and B.



Here we consider only nearest-neighbor hopping t.

Tight-binding Hamiltonian:

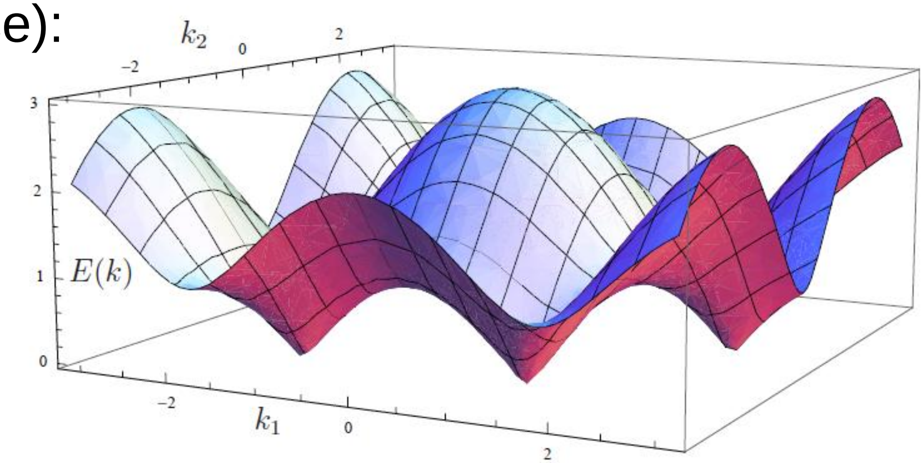
$$H_0 = -t \sum_{\vec{r}\in A} \sum_{i=1,2,3} \left[a^\dagger(\vec{r}) b(\vec{r}+\vec{s}_i) + b^\dagger(\vec{r}+\vec{s}_i) a(\vec{r}) \right]$$

t ~ 2.8eV (hopping parameter) a~1.42 Å (interatomic spacing) [Wallace, 1947]

Linear dispersion

The energy eigenvalue vanishes at two Fermi (Dirac) points (in momentum space):

$$\vec{K}_{\pm} = \left(\pm \frac{4\pi}{3\sqrt{3}a}, 0 \right)$$



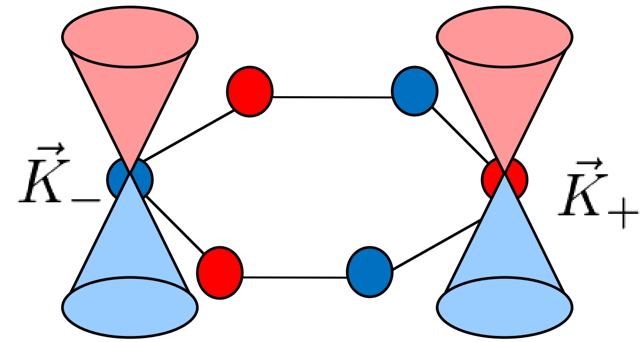
The dispersion relation is linearized around Dirac points.

$$E(\vec{K}_{\pm} + \vec{p}) = \pm v_F |\vec{p}| + O((p/K)^2)$$

[Wallace, 1947]

"Fermi velocity"

$$v_F = (3/2) a_{\rm hc} t \sim c/300$$



Dirac fermions on graphene

Linear dispersion

$$E(\vec{K}_{\pm} + \vec{p}) = \pm v_F |\vec{p}| + O((p/K)^2)$$

Electrons/holes are described as "2-dimensional" massless 4-component Dirac fermions. [Semenoff, 1984]

Dirac eq.: $$\left(\gamma_0 \partial_t - v_F \vec{\gamma} \cdot \vec{\partial}\right) \psi = 0$$

$$\psi_\sigma(\vec{p}) = \begin{pmatrix} a_\sigma(\vec{K}_+ + \vec{p}) \\ b_\sigma(\vec{K}_+ + \vec{p}) \\ b_\sigma(\vec{K}_- + \vec{p}) \\ a_\sigma(\vec{K}_- + \vec{p}) \end{pmatrix}$$

Dirac point d.o.f.= "*pseudospin*"

Sublattice symmetry= "*chiral symmetry*"

Spin d.o.f.= "*flavor*"

Monolayer graphene = 2-flavor x 4 components

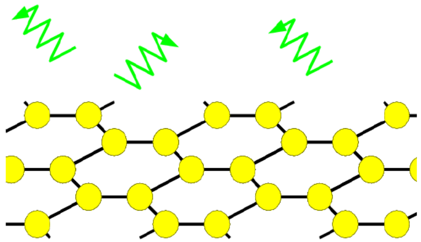
- EFT has U(4) symmetry generated by 16 generators:

$$\{1, \vec{\sigma}\} \otimes \{1, \gamma_3, \gamma_5, \gamma_3\gamma_5\}$$

Effective gauge theory

[Son,2007]

- Euclidean action interacting with U(1) gauge field:



- Fermions in 3-dim.

interaction with gauge field

$$S_F = \sum_f \int dx^{(3)} \bar{\psi}_f \left[\gamma_4(\partial_4 + iA_4) + v_F(\gamma_1\partial_1 + \gamma_2\partial_2) + m\right]\psi_f$$

Explicit band gap
(induced e.g. by substrate)

- U(1) gauge field in 4-dim.

$$S_G = \frac{1}{2g^2}\sum_{j=1,2,3}\int dx^{(4)}(\partial_j A_4)^2$$

Here,

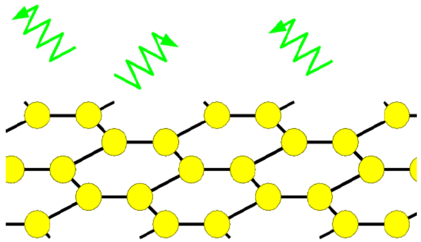
Small Fermi velocity ⇒ Instantaneous Coulomb interaction

⇒ Magnetic field effects are neglected.

$$F_{ij} = 0 \qquad \partial_4 A_i = 0$$

Effective gauge theory

[Son,2007]



- Temporal scale transformation:

$$\tau \to \tau / v_F \qquad A_4 \to v_F A_4$$

- Fermions in 3-dim.

interaction with gauge field

$$S_F = \sum_f \int dx^{(3)} \bar{\psi}_f \left[\gamma_4 (\partial_4 + iA_4) + (\gamma_1 \partial_1 + \gamma_2 \partial_2) + m_* \right] \psi_f$$

Explicit band gap
(induced e.g. by substrate)

$$m_* = m / v_F$$

- U(1) gauge field in 4-dim.

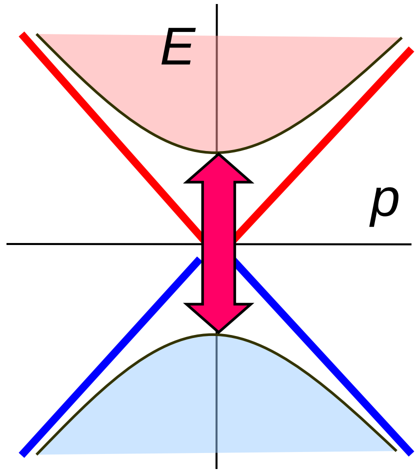
$$S_G = \frac{\beta}{2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2$$

- Small Fermi velocity implies large effective Coulomb coupling:

$$g_*^2 \equiv \beta^{-1} = \frac{g_{\mathrm{QED}}^2}{v_F} (\sim 300 g_{\mathrm{QED}}^2)$$

⇨ Strong coupling expansion around β=0 will work well.

Physics at strong coupling (1)



Graphene: Dynamical gap generation

Insulating phase

Similar mechanism

QCD: Spontaneous chiSB

Dynamical quark mass

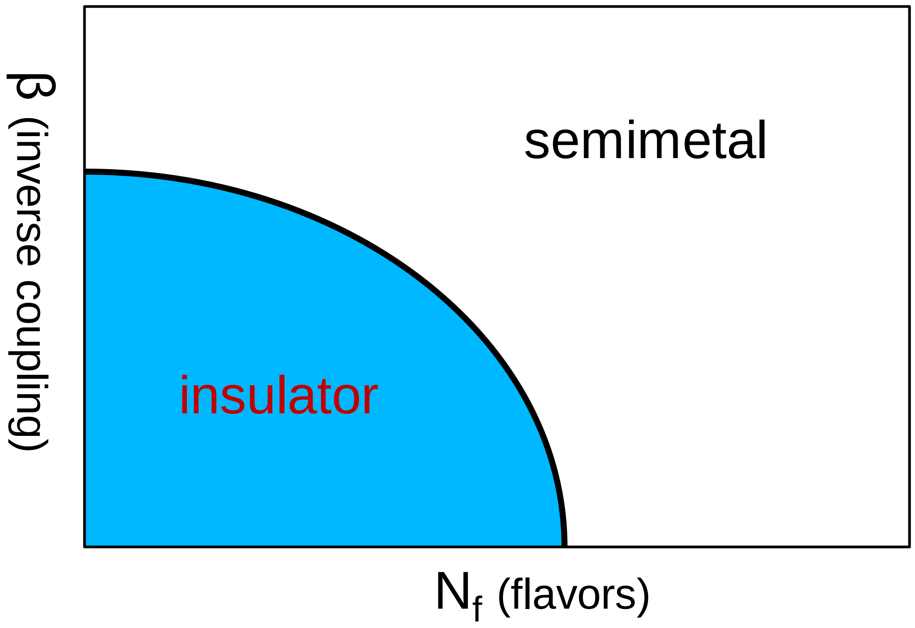
Strong Coupling gauge theory (e.g. QCD)		*Graphene (low-energy)*	
Gauge field	A_μ^a	Electric field	A_μ
Coupling constant	g^2	Effective coupling	g_*^2
Quarks	$q(= u, d, \ldots)$	Quasi-electrons	ψ
Chiral condensate	$\langle \bar{q} q \rangle$	Exciton condensate / CDW	$\langle \bar{\psi} \psi \rangle$
Flavors		Layers x Spin d.o.f.	

Physics at strong coupling (2)

Possible phase diagram:

(Proposed by [Son,2007])

What will occur on the graphene in the strong coupling regime?



Related works:

- Schwinger-Dyson eq. [Khveschchenko,2001,2009] [Gamayun et al.,2009]
- RGE [Son,2007] (1/N expansion) [Herbut et al.,2009]
- Lattice Monte Carlo [Hands & Strouthos,2009] (Thirring-like model) [Drut & Lahde,2009]

Physics at strong coupling (2)

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(Proposed by [Son,2007])

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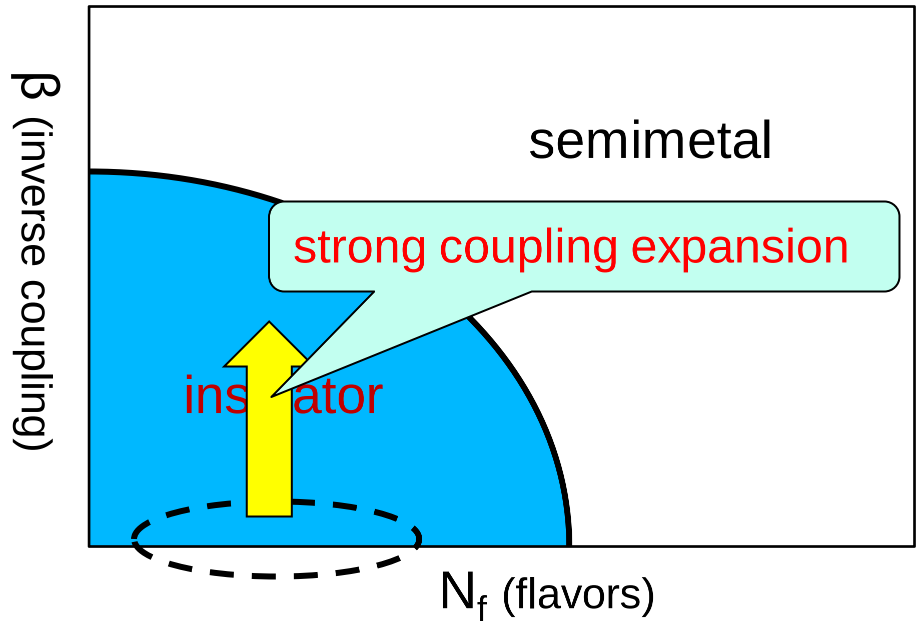


This work:

Strong coupling expansion of U(1) lattice gauge theory

➡ analytic calculations of

- Fermion dynamical gap at/around

  β=0 (strong coupling), m=0 (chiral limit), V=∞ (infinite volume)

- Collective excitations

  (Pseudo-)NG mode, Higgs-like mode

3.

Strong coupling expansion on lattice

Regularization on a square lattice

- Gauge field:

  U(1) Link variables: $U_4(x) = e^{i\theta(x)} \quad (-\pi \leq \theta < \pi)$

  $U_j(x) = 1$ (*j*=1,2,3)

- Fermions:
  - Described by a single staggered fermion χ

    2^3 = 4 x 2 [Hands & Strouthos, 2008]

    doublers components "flavors"(spin)

  - Global chiral symmetry:

$$\mathrm{U(1)_V}: \quad \chi(x) \to e^{i\theta_V}\chi(x), \quad \bar{\chi}(x) \to \bar{\chi}(x)e^{-i\theta_V}$$ (vector)

$$\mathrm{U(1)_A}: \quad \chi(x) \to e^{i\epsilon(x)\theta_A}\chi(x), \quad \bar{\chi}(x) \to \bar{\chi}(x)e^{i\epsilon(x)\theta_A}$$ (axial)

continuum	staggered
~~$(\mathrm{U}(4) \longrightarrow)$~~	$\mathrm{U(1)_V} \times \mathrm{U(1)_A} \xrightarrow{\chi\mathrm{SB}} \mathrm{U(1)_V}$

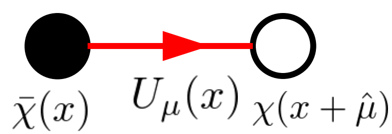
Lattice gauge action

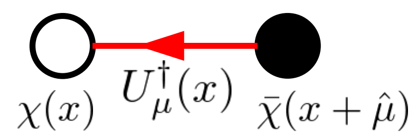
[Drut & Lahde, 2009]

- $$S_F = \sum_{x^{(3)}} \left[\frac{1}{2} \sum_{\mu=1,2,4} \left(V_\mu^+(x) - V_\mu^-(x) \right) + m_* M(x) \right]$$

Hopping operators: (kinetic terms)

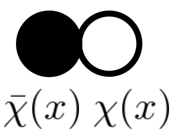
$$V_\mu^+(x) = \eta_\mu(x) \bar{\chi}(x) U_\mu(x) \chi(x+\hat{\mu}) \qquad V_\mu^-(x) = \eta_\mu(x) \bar{\chi}(x+\hat{\mu}) U_\mu^\dagger(x) \chi(x)$$





Mesonic operator: (mass term)

$$M(x) = \bar{\chi}(x) \chi(x)$$

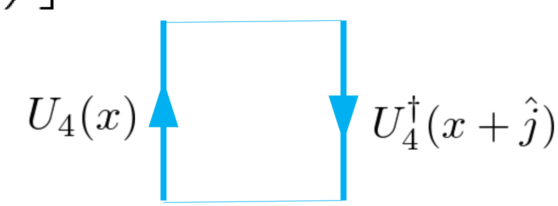


- $$S_G = \beta \sum_{x^{(4)}} \sum_{j=1,2,3} \left[1 - \mathrm{Re} \left(U_4(x) U_4^\dagger(x+\hat{j}) \right) \right]$$

plaquette

$U_j(x) = 1$ (j=1,2,3)

$(\beta = 1/g_*^2)$



Strong coupling expansion

See e.g. [Drouffe & Zuber, 1983]

Expansion parameter: $\beta \equiv 1/g_*^2$

Link integration is performed order by order: $\left[S_G \sim O(\beta)\right]$

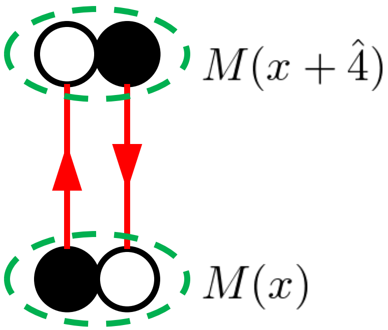
$$Z = \int [d\chi d\bar{\chi}][d\theta] \left[\sum_{n=0}^{\infty} \frac{(-S_G)^n}{n!} e^{-S_F}\right] = \int [d\chi d\bar{\chi}] e^{-S_\chi}$$

Only the terms in which link variables cancel remain:

4-fermi couplings are induced by the link integration.

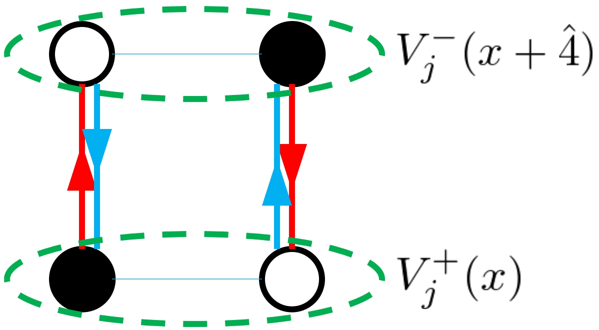
LO[O(1)]

(no plaquette)



NLO[O(β)]

(1 plaquette)



Fermionic effective action

$$S_\chi = \sum_{x^{(3)}} \left[\frac{1}{2} \sum_{j=1,2} \left(V_j^+(x) - V_j^-(x) \right) + m_* M(x) \right]$$

$$- \frac{1}{4} \sum_{x^{(3)}} M(x) M(x+\hat{4})$$

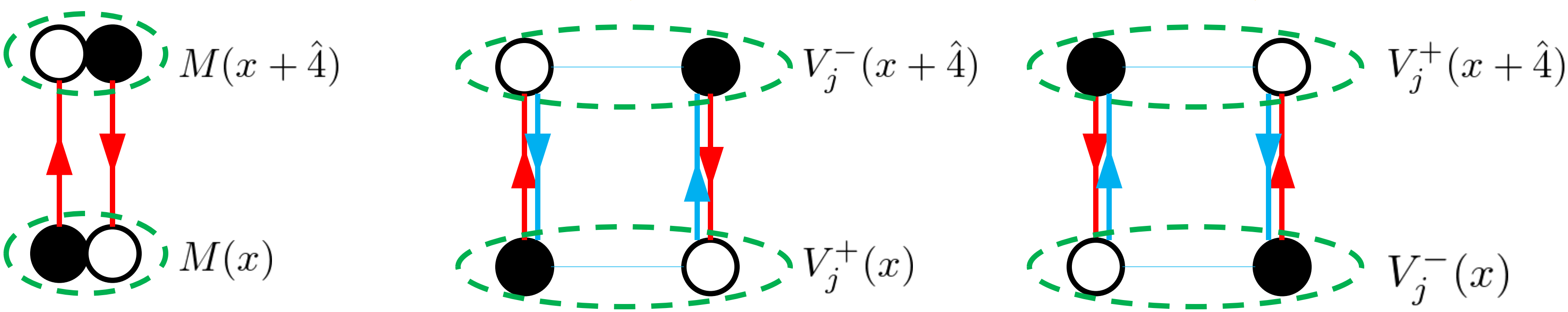
O(1)

$$+ \frac{\beta}{8} \sum_{x^{(3)}} \sum_{j=1,2} \left[V_j^+(x) V_j^-(x+\hat{4}) + V_j^-(x) V_j^+(x+\hat{4}) \right]$$

O(β)

LO[O(1)]

NLO[O(β)]



Auxiliary fields

Linearize the 4-fermi couplings [Miura et al.,2009]

by "Extended Stratonovich-Hubbard transformation":

$$\exp\left[\alpha AB\right] = \frac{1}{\pi\alpha}\int d\lambda d\lambda^* \exp\left[-\alpha\left(|\lambda|^2 - A\lambda - B\lambda^*\right)\right]$$

$$\exp\left[\frac{1}{4}\sum_{x^{(3)}} M(x)M(x+\hat{4})\right] = \int [d\phi][d\phi^*] \exp\left[-\frac{1}{4}\sum_{x^{(3)}}\left[|\phi(x)|^2 - M(x)(\phi(x)+\phi^*(x-\hat{4}))\right]\right]$$

"auxiliary field" : $\phi(x) \equiv \phi_\sigma + i\epsilon(x)\phi_\pi$

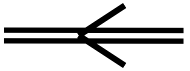
Scalar
$M(x) = \bar{\chi}(x)\chi(x)$

Pseudoscalar
$P(x) = \bar{\chi}(x)i\epsilon(x)\chi(x)$

Free energy at T=0

- Propagator under background

$$G^{-1}(\vec{k};\phi) \equiv \sum_{j=1,2} \sin^2 k_j + {M_F}^2 \quad =$$



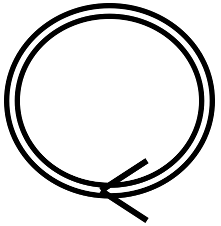
- Dynamical fermion mass $M_F = \left| m_* - \frac{\phi}{2} \right|$

- Integration over the fermionic fields gives

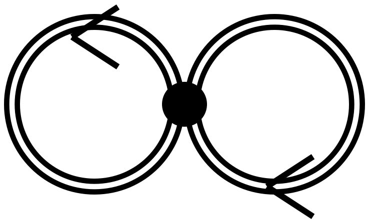
$$F_{\text{eff}}(\phi) = \frac{1}{4}|\phi|^2 - \frac{1}{2}\int_{\vec{k}} \ln\left[G^{-1}(\vec{k};\phi)\right] - \frac{\beta}{4}\sum_{j=1,2}\left[\int_{\vec{k}} G(\vec{k};\phi)\sin^2 k_j\right]^2 + O(\beta^2)$$

Tree level

1-loop [O(1)]

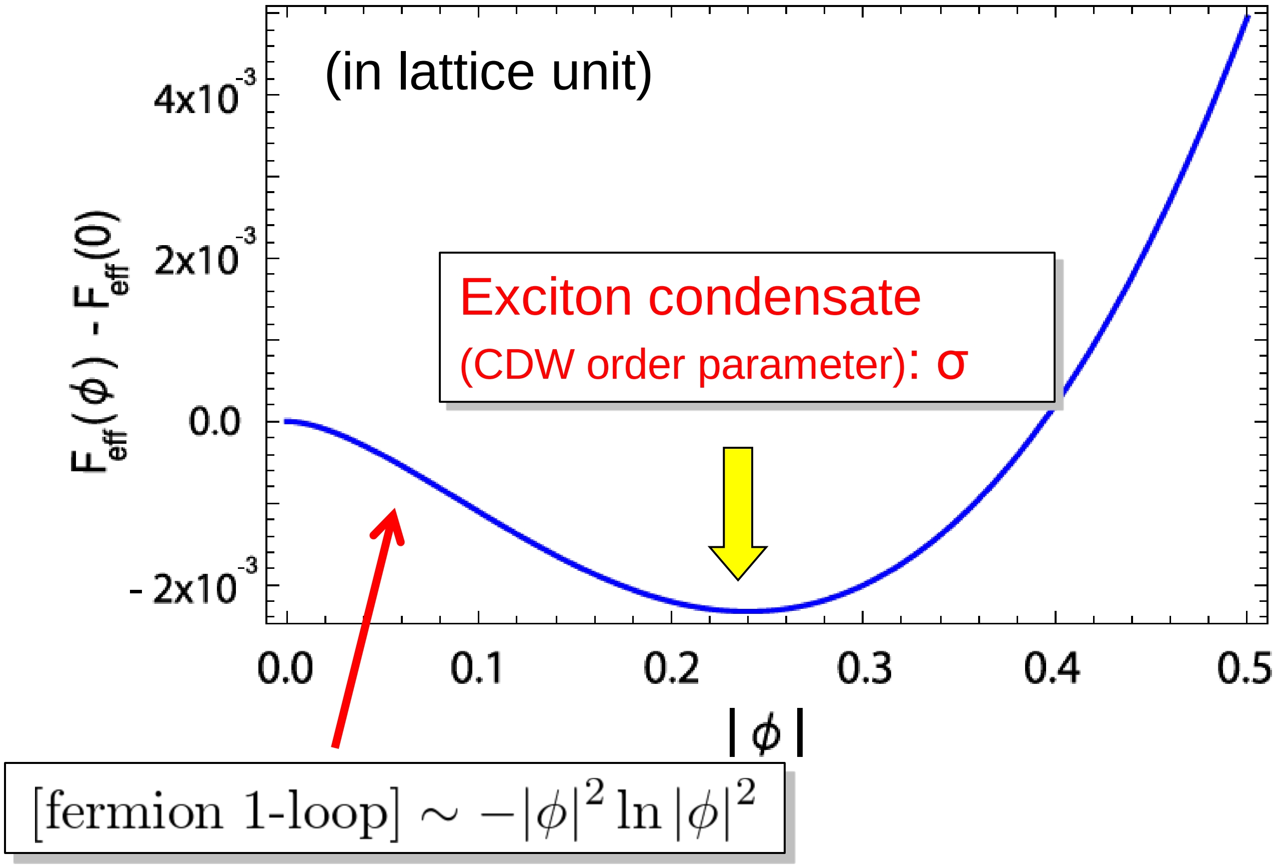


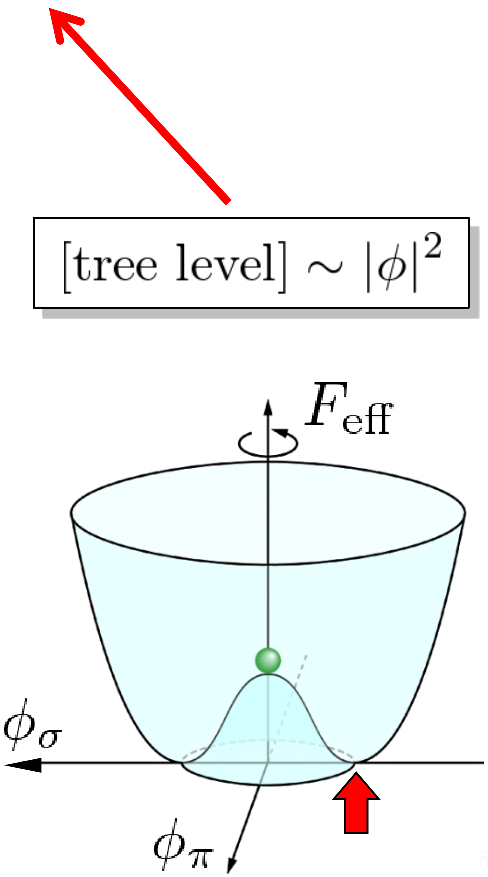
2-loop [O(β)]



Strong coupling limit

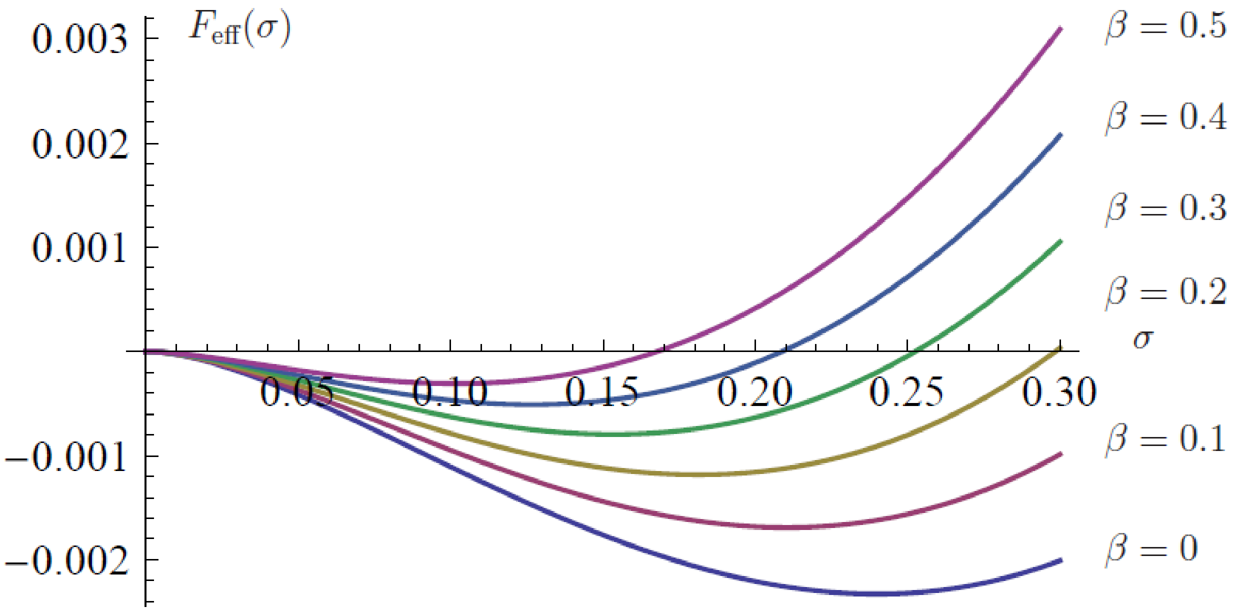
- Free energy in the strong coupling limit ($\beta=0$) & chiral limit ($m=0$)

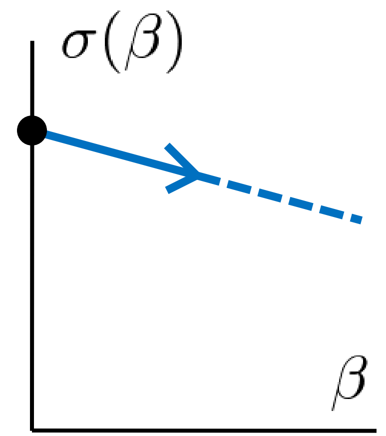




- "Chiral symmetry" is spontaneously broken in the strong coupling limit.

Finite coupling region





- Exciton condensate (in lattice unit):

$$|\langle \bar{\chi}\chi \rangle| = \sigma = 0.240 - 0.297\beta$$

- By setting the lattice spacing $a \sim a_{\rm honeycomb} = 1.42\text{Å}$

➡ Dynamical gap $M_F \equiv \frac{v_F}{a}\frac{\sigma a^2}{2} \simeq (0.523 - 0.623\beta)\text{eV}$

Non-compact gauge action

So far we have worked with compact gauge action:

$$S_G^{\mathrm{C}} = \frac{1}{g_*^2} \sum_{x^{(4)}} \sum_{j=1,2,3} \left[1 - \mathrm{Re}\left(U_4(x) U_4^\dagger(x+\hat{j}) \right) \right]$$

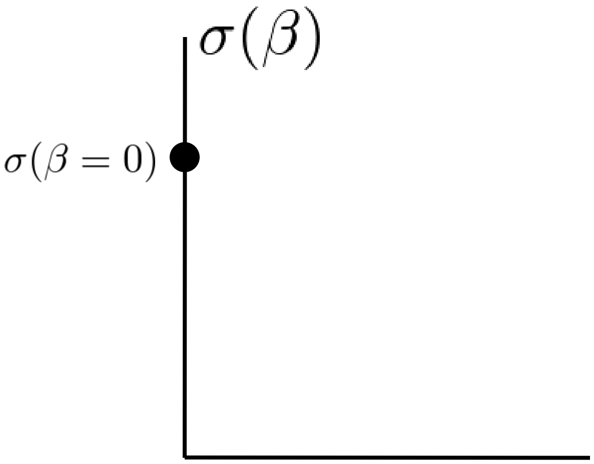
What about the non-compact gauge action ? [Drut & Lahde, 2010]

$$S_G^{\mathrm{NC}} = \frac{\beta}{2} \sum_{x^{(4)}} \sum_{j=1,2,3} \left[\theta(x) - \theta(x+\hat{4}) \right]^2$$

<u>Strong coupling expansion:</u>

LO : The gauge term does not contribute at β=0.

$$\Rightarrow \sigma^{\mathrm{C}}(\beta=0) = \sigma^{\mathrm{NC}}(\beta=0)$$



NLO effect…?

Non-compact link integration

e.g.) Integration over $\theta(x)$ and $\theta(x+\hat{j})$

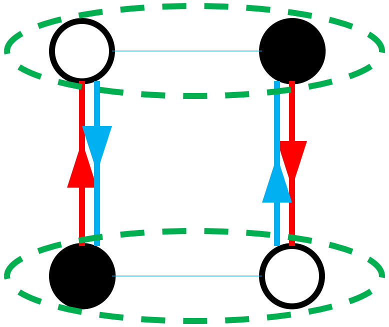
From non-compact plaquette

$$\int_{-\pi}^{\pi}\frac{d\theta(x)}{2\pi}\int_{-\pi}^{\pi}\frac{d\theta(x+\hat{j})}{2\pi}\exp\left[-\frac{1}{2}\left(V_4^+(x)-V_4^-(x)+V_4^+(x+\hat{j})-V_4^-(x+\hat{j})\right)\right]\theta(x)\theta(x+\hat{j})$$

$$=\int_{-\pi}^{\pi}\frac{d\theta(x)}{2\pi}\theta(x)\left[1-\frac{1}{2}\bar{\chi}(x)e^{i\theta(x)}\chi(x+\hat{4})+\frac{1}{2}\bar{\chi}(x+\hat{4})e^{-i\theta(x)}\chi(x)+\frac{1}{4}M(x)M(x+\hat{4})\right]$$

$$\times\int_{-\pi}^{\pi}\frac{d\theta(x+\hat{j})}{2\pi}\cdots$$

$$\left(\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\theta e^{\pm i\theta}=\pm i\right)$$



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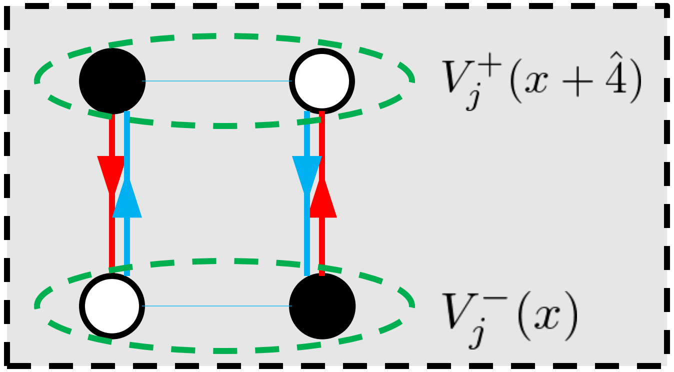


One plaquette also works as its c.c.

The NLO effect is doubled: $\Delta S_\chi^{NC}=2\times\Delta S_\chi^{C}$

Non-compact gauge action

So far we have worked with compact gauge action:

$$S_G^{\mathrm{C}} = \frac{1}{g_*^2} \sum_{x^{(4)}} \sum_{j=1,2,3} \left[1 - \mathrm{Re}\left(U_4(x) U_4^\dagger(x+\hat{j}) \right) \right]$$

What about the non-compact gauge action ? [Drut & Lahde, 2010]

$$S_G^{\mathrm{NC}} = \frac{\beta}{2} \sum_{x^{(4)}} \sum_{j=1,2,3} \left[\theta(x) - \theta(x+\hat{4}) \right]^2$$

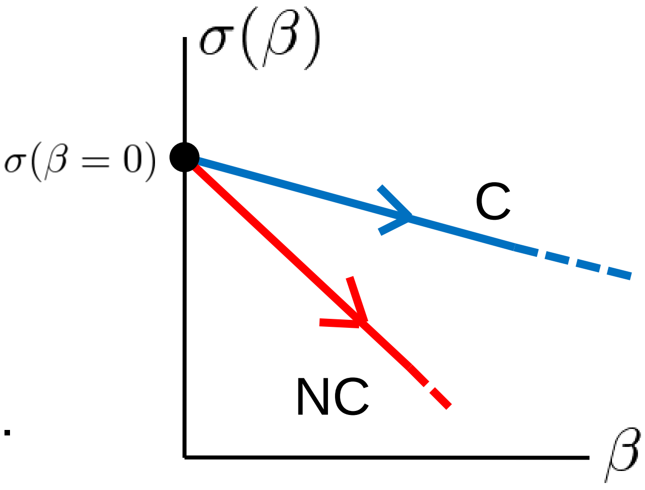
<u>Strong coupling expansion:</u>

LO : The gauge term does not contribute at β=0.

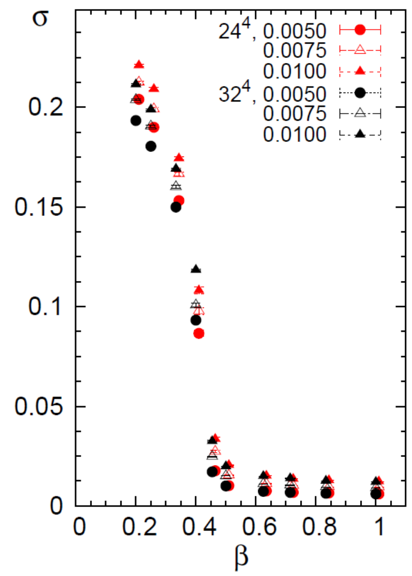
$$\Rightarrow \quad \sigma^{\mathrm{C}}(\beta = 0) = \sigma^{\mathrm{NC}}(\beta = 0)$$

NLO : one plaquette also contributes as its c.c.

⇒ $\sigma^{NC}(\beta)$ drops twice as fast as $\sigma^{C}(\beta)$.



MC simulations vs. Strong coupling expansion (SCE)

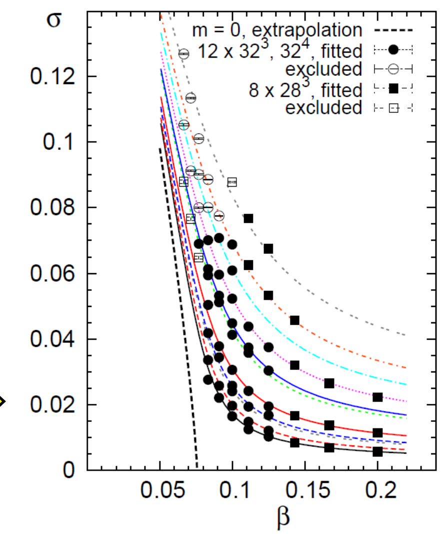


Monte Carlo results:

[Drut & Lahde, 2010]

w/ compact gauge action

w/ non-compact gauge action



[both without “tadpole improvement”]

<u>Comparison:</u>

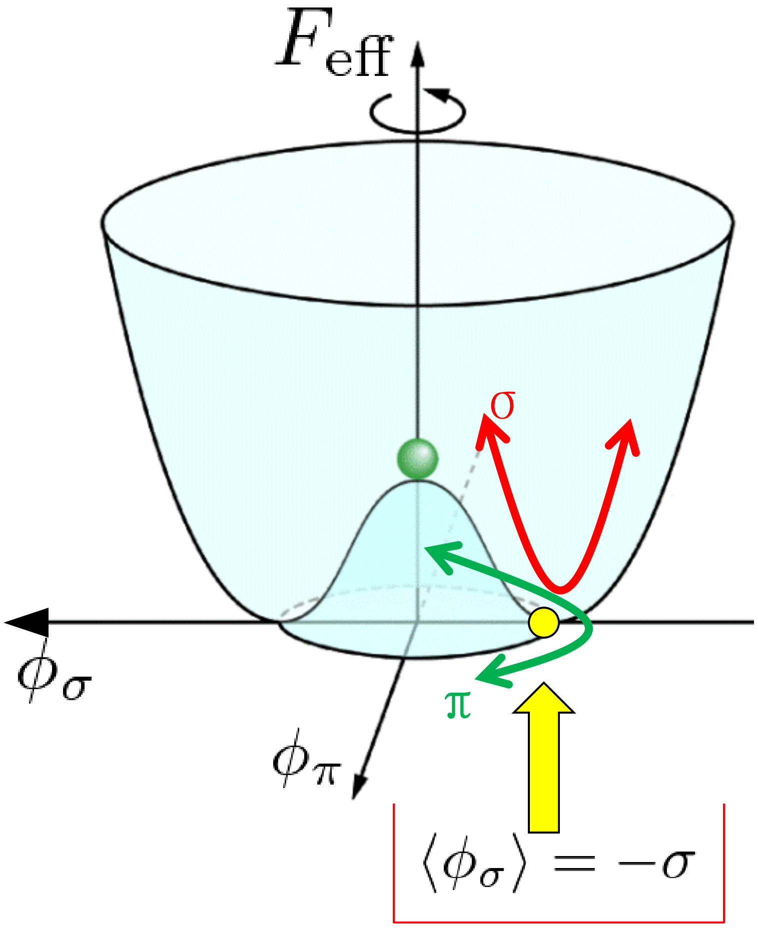
- $\sigma_{MC}(\beta \to 0)$: consistent with $\sigma_{SCE}(\beta=0)=0.240$
- $\sigma_{MC}(\beta\neq 0;$ compact$) > \sigma_{MC}(\beta\neq 0;$ non-compact$)$: consistent with SCE result

4.

Collective excitations

Collective excitations (excitons)

- Fluctuations of the order parameter ϕ



π -mode: phase fluctuation mode

"pseudoscalar" type

$$\langle P \rangle = \langle \bar{\chi} i \epsilon \chi \rangle$$

σ -mode: amplitude fluctuation mode

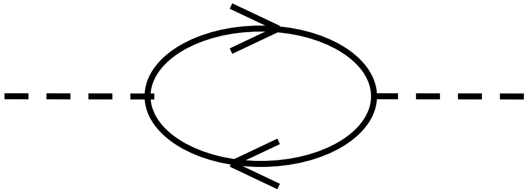
"scalar" type

$$\langle M \rangle = \langle \bar{\chi} \chi \rangle$$

Dispersion relation

- Boson propagators (with fermion 1-loop):

$$D^{-1}_{\phi_{\sigma,\pi}}(x,y) = \left.\frac{\delta^2 S_{\rm eff}[\phi]}{\delta\phi_{\sigma,\pi}(x)\delta\phi_{\sigma,\pi}(y)}\right|_{\phi_\sigma=-\sigma,\phi_\pi=0}$$



$$\Rightarrow \quad D^{-1}_{\phi_{\sigma,\pi}}(\vec{p}, i\omega_*) = \frac{1}{2} - \frac{1+\cosh\omega_*}{8}\int_{\vec{k}} \frac{\sum_j \sin k_j \sin(k_j+p_j) \pm m_\sigma^2}{\left[m_\sigma^2 + \sum_j \sin^2 k_j\right]\left[m_\sigma^2 + \sum_j \sin^2(k_j+p_j)\right]}$$

+:π / −:σ

(for β=0)

- Dispersion relation is given by an imaginary pole of the propagator:

$$D^{-1}_{\phi_{\sigma,\pi}}(\vec{p}, i\omega_{\sigma,\pi}(\vec{p})/v_F) = 0$$

(temporal scale restored)

$\Rightarrow$ Excitation energy (mass): $M_{\sigma,\pi} = \omega_{\sigma,\pi}(\vec{p}=0)$

π -mode

$$M_\pi \simeq \frac{2v_F}{a}\sqrt{\frac{m}{M_F(m=0)}} \xrightarrow{m=0} 0$$

"NG boson" from chiSB

$$\left(= 8.40\sqrt{\frac{m}{M_F(m=0)}}\mathrm{eV}\right)$$

$$\equiv \frac{1}{F_\pi^\tau}\sqrt{m\sigma}$$

"pion decay constant"

$$\langle 0|J_4^{\mathrm{axial}}|\pi\rangle \equiv 2F_\pi^\tau \omega_\pi$$

- Similar to Gell-Mann--Oakes--Renner(GOR) relation for pion in QCD:

$$M_\pi \propto \sqrt{m}$$

cf.) for pions:

$$m_\pi = \frac{1}{f_\pi}\sqrt{m_q \sigma}$$

Experimental observation would give a good evidence of chiSB .

σ -mode

$$M_\sigma \simeq \frac{v_F}{a}(1.30 - 0.47\beta) \simeq (5.47 - 1.97\beta)\mathrm{eV}$$

- Quite a heavy mass

  -- comparable to the cutoff energy $\Lambda \equiv v_F \dfrac{\pi}{a} = 13\mathrm{eV}$

↓

Similar to:

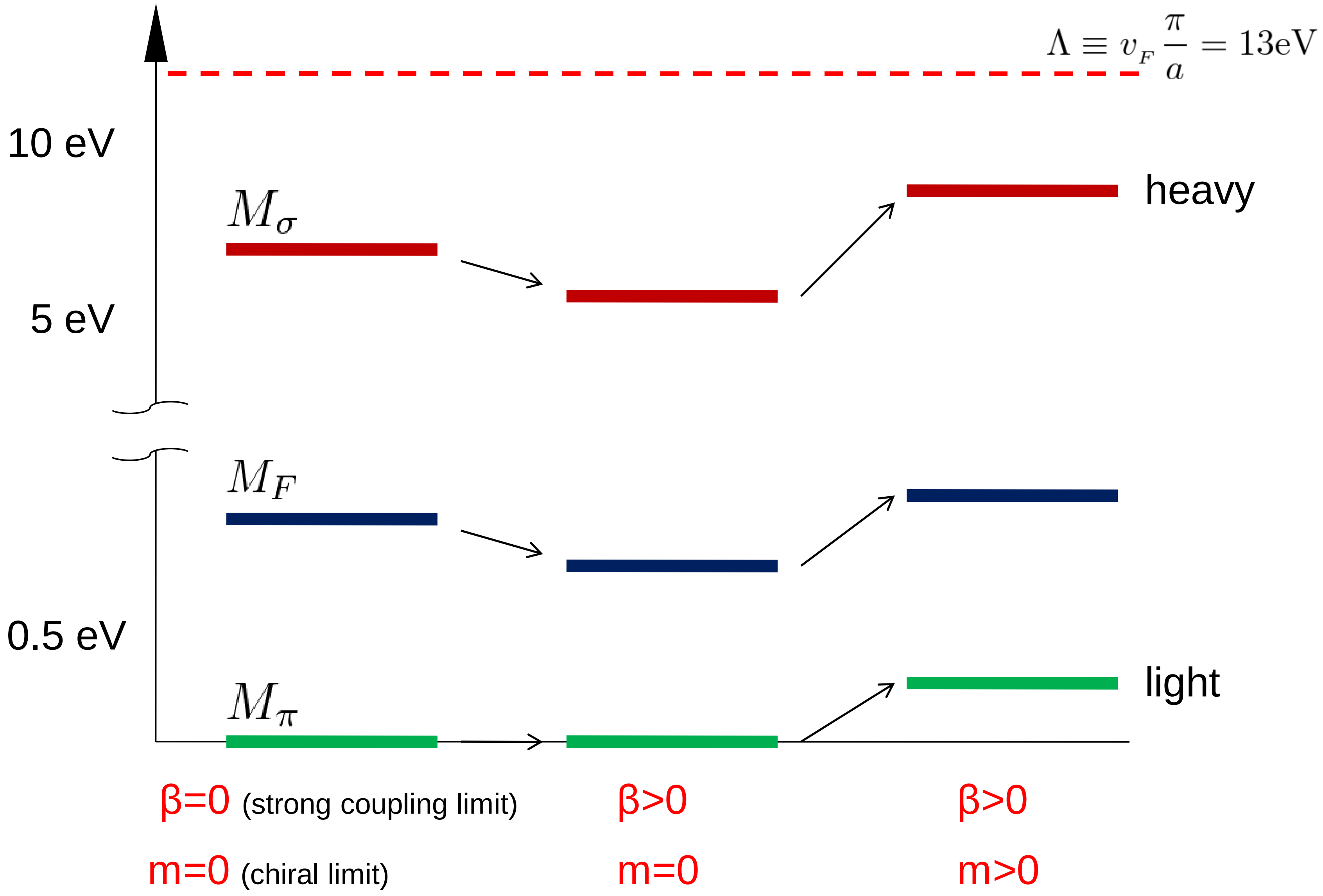
σ-meson in QCD

Higgs particle in electroweak theory

5.

Summary

Excitation spectra



Conclusion

- Monolayer graphene is treated analytically by strong coupling expansion of the U(1) "mixed dimension" model on lattice.

- Chiral symmetry is broken in the strong coupling regime, i.e. the fermionic quasiparticles receive a dynamical gap.

$$|\langle\bar{\chi}\chi\rangle| = (0.240 - 0.297\beta)a^{-2}$$

$$M_F \equiv \frac{v_F}{a}\frac{\sigma a^2}{2} \simeq (0.523 - 0.623\beta)\mathrm{eV}$$

- Compact and non-compact gauge formulations are compared. Difference starts to appear from NLO.

- Collective excitation modes are examined. π(phase fluctuation)-exciton behaves as a NG boson.

$$M_\pi \simeq \frac{2v_F}{a}\sqrt{\frac{m}{M_F^{m=0}}} \quad \propto \sqrt{m} \qquad\qquad M_\sigma \simeq (5.47 - 1.97\beta)\mathrm{eV}$$

$$= 8.40\sqrt{\frac{m}{M_F^{m=0}}}\mathrm{eV}$$

Future prospects

- Finite temperature analysis
- NNLO calculation in strong coupling expansion
- Exact U(4) symmetry e.g. by overlap fermion.
- Larger N_f
- Effective theory for π -excitons (like chiPT for pions)
- Fermions with original honeycomb lattice structure

Thank you.

Low-energy effective theory

Electrons/holes on graphene show linear dispersion around two "Dirac points":

$$E(\vec{K}_\pm + \vec{p}) = \pm v_F |\vec{p}| + O((p/K)^2)$$

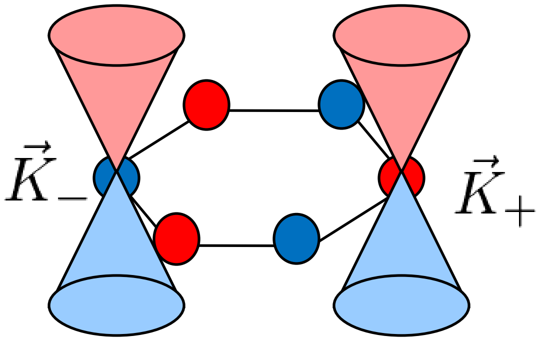
[Wallace, 1947]

"Fermi velocity"

$$v_F = (3/2) a_{\rm hc} t \sim c/300$$

a_{hc}=1.42 Å (interatomic spacing)

t = 2.8eV (hopping parameter)



Electrons/holes are described as massless Dirac fermions.

4 = 2 x 2

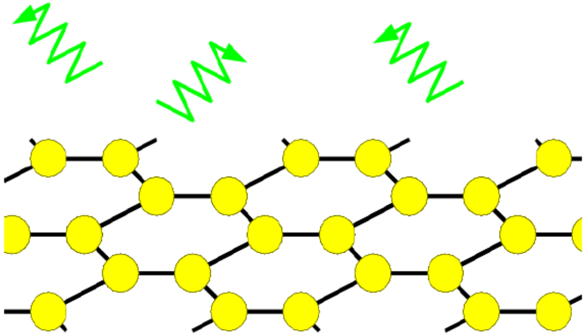
components DPs sublattices

$$\psi_\sigma(\vec{p}) = \begin{pmatrix} a_\sigma(\vec{K}_+ + \vec{p}) \\ b_\sigma(\vec{K}_+ + \vec{p}) \\ b_\sigma(\vec{K}_- + \vec{p}) \\ a_\sigma(\vec{K}_- + \vec{p}) \end{pmatrix}$$

(Spin up/down is considered as "flavor": N_f=2)

Mixed dimension model

Incorporate Coulomb interaction.



Low-energy effective action [Son, 2007]

(2+1)-dim. fermionic field:

$$S_F = \sum_f \int dx^{(3)} \bar{\psi}_f \left[\gamma_4(\partial_4 + iA_4) + v_F(\gamma_1\partial_1 + \gamma_2\partial_2) + m\right] \psi_f$$

(3+1)-dim. U(1) gauge (electric) field:

$$S_G = \frac{1}{2g^2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2$$

$g^2 = \frac{e^2}{\epsilon_0}$ (for suspended graphene)

Assume "instantaneous" Coulomb interaction → Magnetic components (A_i) neglected

Effectively strong coupling

Scale transformation in the temporal direction:

$$\tau \to \tau / v_F \qquad A_4 \to v_F A_4$$

$$S_F = \sum_f \int dx^{(3)} \bar{\psi}_f \left[\gamma_4(\partial_4 + iA_4) + (\gamma_1\partial_1 + \gamma_2\partial_2) + m_*\right] \psi_f$$

$$m_* = m/v_F$$

$$S_G = \frac{1}{2{g_*}^2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2$$

Effectively strong Coulomb coupling.

$$g_*^2 = \frac{e^2}{v_F \epsilon_0} = \frac{g_{QED}^2}{v_F} (\sim 300 g_{QED}^2)$$

→ Perturbative approach cannot be applied.

Treated as strong coupling U(1) gauge theory.

Strong coupling nature

What will occur in the strong coupling regime?

Strong Coulomb coupling

⇩

Spontaneous chiSB ...?

e-h pair: exciton condensate $\langle\bar{\psi}\psi\rangle$

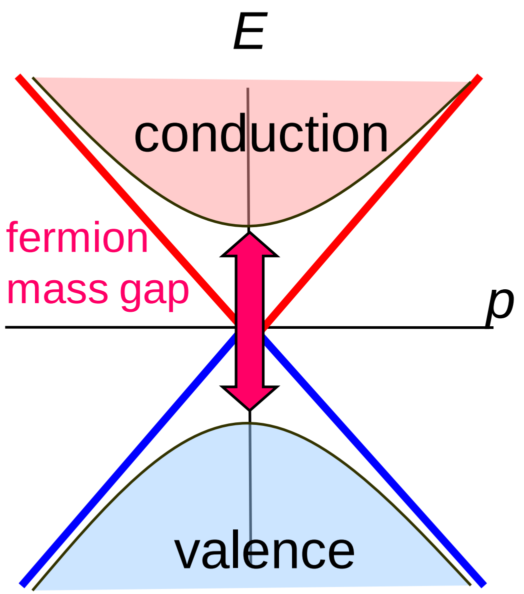
⇩

Dynamical mass gap ...?

⇩

Insulator ...?

?



Semimetal-insulator transition (in graphene)

⇕ *Similar mechanism*

Dynamical mass generation (of quarks [QCD])

Correspondence

Strong Coupling gauge theory (e.g. QCD)	*Graphene (low-energy)*
Gauge field A_μ^a	Electric field A_μ
Coupling constant g^2	Effective coupling g_*^2
Quarks $q(= u, d, \ldots)$	Quasi-electrons ψ
Chiral condensate $\langle \bar{q} q \rangle$	Exciton condensate $\langle \bar{\psi} \psi \rangle$
Flavors	Layers x Spin d.o.f.

Our approach

Lattice gauge theory

Strong coupling expansion

(Powerful approach in QCD)

→

Properties of graphene:

Dynamical mass gap

Collective excitations

Symmetries

Continuum theory is invariant under U(4) transf. generated by

$$\{1, \vec{\sigma}\} \otimes \{1, \gamma_3, \gamma_5, \gamma_3\gamma_5\}$$

Subgroups:

global gauge transf.

$$\mathrm{U(1)_V}: \quad \psi \to e^{i\theta_V}\psi, \quad \bar{\psi} \to \bar{\psi}e^{-i\theta_V}$$

chiral transf. (at chiral limit *m*=0)

$$\mathrm{U(1)_A}: \quad \psi \to e^{i\gamma_5\theta_A}\psi, \quad \bar{\psi} \to \bar{\psi}e^{i\gamma_5\theta_A}$$

Lattice regularized theory is invariant only under

global gauge transf.

$$\mathrm{U(1)_V}: \quad \chi(x) \to e^{i\theta_V}\chi(x), \quad \bar{\chi}(x) \to \bar{\chi}(x)e^{-i\theta_V}$$

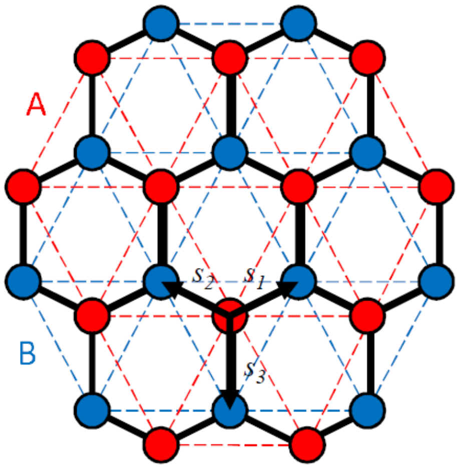
"chiral" transf. (at chiral limit *m*=0)

$$\mathrm{U(1)_A}: \quad \chi(x) \to e^{i\epsilon(x)\theta_A}\chi(x), \quad \bar{\chi}(x) \to \bar{\chi}(x)e^{i\epsilon(x)\theta_A}$$

Staggered fermion preserves $U(1)_V x U(1)_A$ symmetry.

Electron spectrum

To describe the behavior of the electrons,
we introduce the tight-binding Hamiltonian.

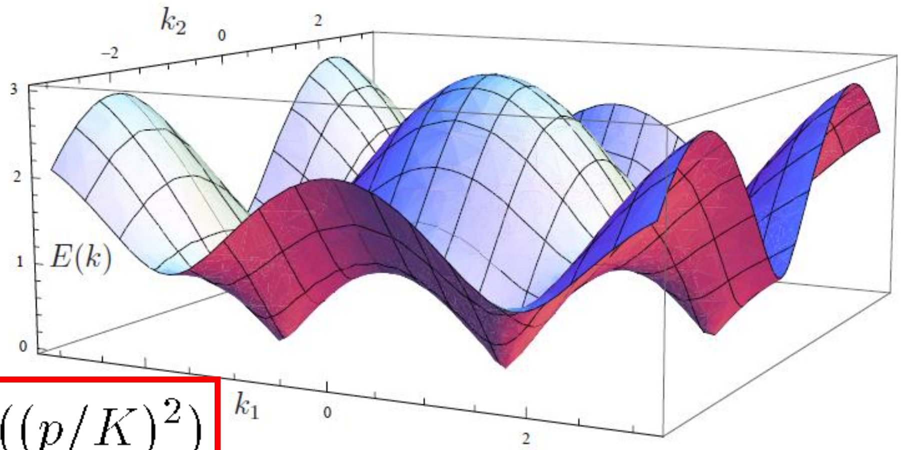


$$H_0 = -t \sum_{\vec{r} \in A} \sum_{i=1,2,3} \left[a^\dagger(\vec{r}) b(\vec{r} + \vec{s_i}) + b^\dagger(\vec{r} + \vec{s_i}) a(\vec{r}) \right]$$

t ~ 2.8eV a~1.42 Å (interatomic spacing)

The energy eigenvalue vanishes at two Fermi (Dirac) points.

$$\vec{K}_\pm = \left(\pm \frac{4\pi}{3\sqrt{3}a}, 0 \right)$$



"Fermi velocity" =(3/2)at ~ 0.00302c

$$E(\vec{K_\pm} + \vec{p}) = \pm v |\vec{p}| + O((p/K)^2)$$

The dispersion relation is linearized around the Dirac points.

Low-energy effective theory

Expanding the operators around the Dirac points,

$$\psi(\vec{p}) \equiv \begin{pmatrix} a(\vec{K}_+ + \vec{p}) \\ b(\vec{K}_+ + \vec{p}) \\ b(\vec{K}_- + \vec{p}) \\ a(\vec{K}_- + \vec{p}) \end{pmatrix}$$

the Hamiltonian is given as

$$H_0 = v \sum_{\vec{p}} \psi^\dagger(\vec{p}) \left(\gamma_0 \vec{\gamma} \cdot \vec{p}\right) \psi(\vec{p})$$

Lagrangian form:

$$L_0 = i \int d^2 r \bar{\psi}(\vec{r}) \left[\gamma^0 \partial_t - v \vec{\gamma} \cdot \vec{\partial}\right] \psi(\vec{r})$$

Low-energy electrons on graphene can be described as (2+1)-D massless Dirac fermions. (except Fermi velocity)

Dirac points → *"pseudospin"*

Spin d.o.f. → *"flavors"*

Strong coupling nature

$$S = i\int dt d^2x \left[\bar{\psi}\gamma^0(\partial_0 - iA_0)\psi - v\bar{\psi}\vec{\gamma}\cdot\vec{\partial}\psi\right] + \frac{1}{2g^2}\int dt d^3x (\partial_i A_0)^2$$

Scale transformation

$$t \to t/v \quad A_0 \to vA_0$$

$$g^2 = e^2/\epsilon_0$$

$$S = i\int dt d^2x \left[\bar{\psi}\gamma^0(\partial_0 - iA_0)\psi - \bar{\psi}\vec{\gamma}\cdot\vec{\partial}\psi\right] + \frac{v}{2g^2}\int dt d^3x (\partial_i A_0)^2$$

Coupling strength ("fine structure constant") becomes

$$\alpha_g = \frac{e^2}{4\pi v\epsilon_0} \sim 300\alpha \sim 2$$

Perturbative approach cannot be applied.

Treated as strong coupling U(1) gauge theory.

Correspondence

SC gauge theory (e.g. QCD)	Graphene (low-energy)
Gauge field A_μ^a	Electromagnetic field A_μ
Coupling constant g^2	$e^2/v\epsilon$
Fermions	Electrons
Chiral condensate $\langle \bar{q} q \rangle$	Exciton cond. $\langle \bar{\psi} \psi \rangle$
Flavors N_f	Layers x Spin d.o.f.

Our approach

Lattice gauge theory

Strong coupling expansion

→ Properties of graphene:

Dynamical mass gap

Collective excitations

(Powerful approach in QCD)

[Nishida, Fukushima & Hatsuda, 2004]

[Miura, Nakano & Ohnishi, 2009]

Lattice regularization

Euclidean Low-energy effective theory [Son,2007]

$$S_F = \int dt d^2x \bar{\psi}_a \left[\gamma_0(\partial_0 + iA_0) + \vec{\gamma}\cdot\vec{\partial} + m_0\right]\psi_a$$

$$S_G = \frac{\beta}{2}\int dt d^3x (\partial_i A_0)^2$$

UV cutoff: $\Lambda = \pi/a \sim 4.36\mathrm{keV}$

⇨ Discretize on the square lattice. (with staggered fermions)

$$\begin{aligned} S_F = &-\frac{1}{2}\sum_{x,t}\eta_0(x,t)\left[\bar{\chi}_a(x,t)e^{i\theta(x,t)}\chi_a(x,t+1) - \bar{\chi}_a(x,t+1)e^{-i\theta(x,t)}\chi_a(x,t)\right] \\ &-\frac{1}{2}\sum_{x,t}\sum_{j=1,2}\eta_j(x,t)\left[\bar{\chi}_a(x,t)\chi_a(x+\hat{j},t) - \bar{\chi}_a(x+\hat{j},t)\chi_a(x,t)\right] \\ &-m_0\sum_{x,t}\bar{\chi}_a(x,t)\chi_a(x,t) \end{aligned}$$

a=1,…N: layer index

$$S_G = \beta\sum_{x,t}\sum_{j=1,2,3}\left[1 - \frac{1}{2}\left(e^{i\theta(x,t)}e^{-i\theta(x+\hat{j},t)} + e^{-i\theta(x,t)}e^{i\theta(x+\hat{j},t)}\right)\right]$$

Link variable (compact form): $e^{i\theta} \sim 1 + iA_0$

Formulation of fermions

Tight-binding Hamiltonian:

Creation/annihilation operators $a_\sigma(\vec{r}), \quad b_\sigma(\vec{r})$

$\sigma = \pm$: original spin d.o.f.

Low energy effective theory:

Dirac spinor form

$$\psi_\sigma(\vec{p}) = \begin{pmatrix} a_\sigma(\vec{K}_+ + \vec{p}) \\ b_\sigma(\vec{K}_+ + \vec{p}) \\ b_\sigma(\vec{K}_- + \vec{p}) \\ a_\sigma(\vec{K}_- + \vec{p}) \end{pmatrix}$$

Dirac point d.o.f.

= "*pseudospin*"

Square lattice regularization:

Staggered fermion χ

2^3 doublers = 4 (spinor d.o.f.) x 2 (spin d.o.f.)

Monolayer graphene is described by a single staggered fermion.

Leading order: O(1)

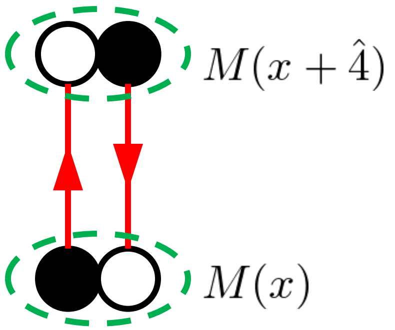
e.g.) Integration over $\theta(x)$

$$\int_{-\pi}^{\pi} \frac{d\theta(x)}{2\pi} \exp\left[-\frac{1}{2}\left(V_4^+(x) - V_4^-(x)\right)\right]$$

$$= \int_{-\pi}^{\pi} \frac{d\theta(x)}{2\pi} \left[1 - \frac{1}{2}\bar{\chi}(x) U_4(x) \chi(x+\hat{4})\right]\left[1 + \frac{1}{2}\bar{\chi}(x+\hat{4}) U_4^\dagger(x) \chi(x)\right]$$

$$= 1 - \frac{1}{4}\bar{\chi}(x)\chi(x+\hat{4})\bar{\chi}(x+\hat{4})\chi(x) = \exp\left[\frac{1}{4} M(x) M(x+\hat{4})\right]$$

$$S_\chi^0 = -\frac{1}{4}\sum_{x^{(3)}} M(x) M(x+\hat{4}) + \sum_{x^{(3)}}\left[\frac{1}{2}\sum_{j=1,2}\left(V_j^+(x) - V_j^-(x)\right) + m_* M(x)\right]$$



4-fermi term:

Local in spatial directions

Non-local in temporal direction

Next-leading order: O(β)

e.g.) Integration over $\theta(x)$ and $\theta(x+\hat{j})$

from plaquette

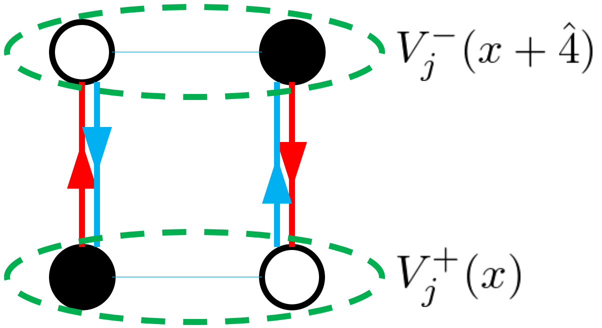
$$\int_{-\pi}^{\pi}\frac{d\theta(x)}{2\pi}\int_{-\pi}^{\pi}\frac{d\theta(x+\hat{j})}{2\pi}\exp\left[-\frac{1}{2}\left(V_4^+(x)-V_4^-(x)+V_4^+(x+\hat{j})-V_4^-(x+\hat{j})\right)\right]U_4^\dagger(x)U_4(x+\hat{j})$$

$$=\int_{-\pi}^{\pi}\frac{d\theta(x)}{2\pi}\int_{-\pi}^{\pi}\frac{d\theta(x+\hat{j})}{2\pi}U_4^\dagger(x)U_4(x+\hat{j})\times\left[1-\frac{1}{2}\bar{\chi}(x)U_4(x)\chi(x+\hat{4})\right]\left[1+\frac{1}{2}\bar{\chi}(x+\hat{4})U_4^\dagger(x)\chi(x)\right]$$
$$\times\left[1-\frac{1}{2}\bar{\chi}(x+\hat{j})U_4(x+\hat{j})\chi(x+\hat{j}+\hat{4})\right]\left[1+\frac{1}{2}\bar{\chi}(x+\hat{j}+\hat{4})U_4^\dagger(x+\hat{j})\chi(x+\hat{j})\right]$$

$$=-\frac{1}{4}\bar{\chi}(x)\chi(x+\hat{4})\bar{\chi}(x+\hat{j}+\hat{4})\chi(x+\hat{j})=\frac{1}{4}V_j^+(x)V_j^-(x+\hat{4})$$

$$\Delta S_\chi=\frac{\beta}{8}\sum_{x^{(3)}}\sum_{j=1,2}[V_j^+(x)V_j^-(x+\hat{4})+V_j^-(x)V_j^+(x+\hat{4})]$$

j=3 does not contribute.



4-fermi term:

Non-local both in spatial and temporal directions

Mean-field approximation

Mean-field approximation:

$$\phi(x) \equiv \phi_\sigma + i\epsilon(x)\phi_\pi$$

Scalar

$$M(x) = \bar{\chi}(x)\chi(x)$$

Pseudoscalar

$$P(x) = \bar{\chi}(x)i\epsilon(x)\chi(x)$$

Integrate out fermion bilinear.

Effective potential:

$$F_{\text{eff}}(\phi,\lambda) = -\frac{1}{N_s^2 N_\tau}\ln Z(\phi,\lambda)$$

$$= \frac{1}{4}|\phi|^2 + \frac{\beta}{2}|\lambda|^2 - \frac{1}{2}\int_{\vec{k}} \ln\left[\left|\frac{\phi}{2} - m_*\right|^2 + \left(1 + \frac{\beta\lambda_2}{2}\right)^2 \sum_{j=1,2}\sin^2\left(k_j - \frac{\beta\lambda_1}{2}\right)\right]$$

Stationary condition

By solving the stationary condition for λ , it is rewritten as a function of ϕ :

$$\frac{\partial F_{\mathrm{eff}}(\phi,\lambda)}{\partial \lambda_1} = 0 \Rightarrow \lambda_1 = 0 + O(\beta)$$

$$\frac{\partial F_{\mathrm{eff}}(\phi,\lambda)}{\partial \lambda_2} = 0 \Rightarrow \lambda_2 = \int_{\vec{k}} \frac{\sin^2 k_i}{|\phi/2 - m_*|^2 + \sum_j \sin^2 k_j} + O(\beta)$$

$$G^{-1}(\vec{k};\phi) \equiv \sum_{j=1,2} \sin^2 k_j + \underbrace{\left| m_* - \frac{\phi}{2} \right|^2}_{\text{“effective mass”}}$$

Effective potential:

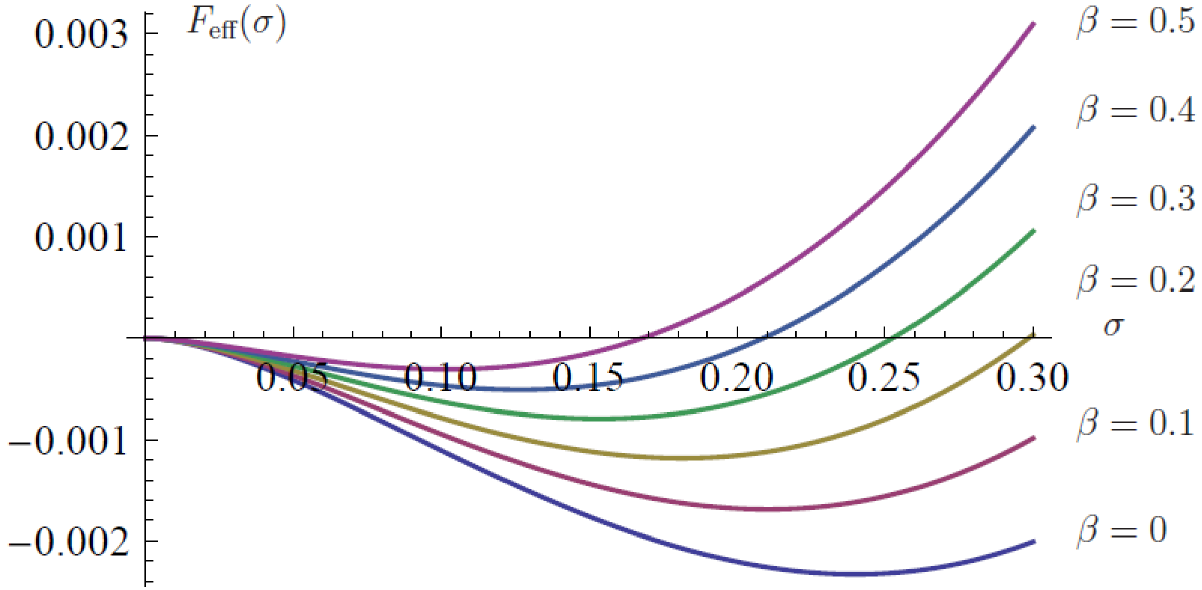
$$F_{\mathrm{eff}}(\phi) = -\frac{1}{N_s^2 N_\tau} \ln Z(\phi)$$

$$= \frac{1}{4}|\phi|^2 - \frac{1}{2}\int_{\vec{k}} \ln\left[G^{-1}(\vec{k};\phi)\right] - \frac{\beta}{4}\sum_{j=1,2}\left[\int_{\vec{k}} G(\vec{k};\phi)\sin^2 k_j\right] + O(\beta^2)$$

Effective potential with varying β

At the chiral limit, the effective potential is

$$F_{\text{eff}} = \frac{\sigma^2}{4} - \frac{2}{L^2}\sum_k^{\pi} \ln\left[\frac{\sigma^2}{4} + \sum_j \sin^2 k_j\right] - \frac{\beta}{2}\left[\frac{4}{L^2}\sum_k^{\pi} \frac{\sin^2 k_1}{(\sigma/2)^2 + \sum_j \sin^2 k_j}\right]^2$$



Solving the stationary condition analytically, we obtain

$$\sigma(\beta) = 0.24 - 0.30\beta + O(\beta^2)$$

($\beta \ll 1$)

Non-compact link integration

e.g.) Integration over $\theta(x)$ and $\theta(x+\hat{j})$

From non-compact plaquette

$$\int_{-\pi}^{\pi}\frac{d\theta(x)}{2\pi}\int_{-\pi}^{\pi}\frac{d\theta(x+\hat{j})}{2\pi}\exp\left[-\frac{1}{2}\left(V_4^+(x)-V_4^-(x)+V_4^+(x+\hat{j})-V_4^-(x+\hat{j})\right)\right]\theta(x)\theta(x+\hat{j})$$

$$=\int_{-\pi}^{\pi}\frac{d\theta(x)}{2\pi}\theta(x)\left[1-\frac{1}{2}\bar{\chi}(x)e^{i\theta(x)}\chi(x+\hat{4})+\frac{1}{2}\bar{\chi}(x+\hat{4})e^{-i\theta(x)}\chi(x)+\frac{1}{4}M(x)M(x+\hat{4})\right]$$

$$\times\int_{-\pi}^{\pi}\frac{d\theta(x+\hat{j})}{2\pi}\cdots \qquad \left(\int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\theta e^{\pm i\theta}=\pm i\right)$$

$$=\frac{1}{4}\left[V_j^+(x)V_j^-(x+\hat{4})+V_j^-(x)V_j^+(x+\hat{4})\right]+(\text{irrelevant terms})$$

One plaquette also works as its c.c.

⇨ The NLO effect is doubled: $\Delta S_\chi^{NC}=2\times\Delta S_\chi^{C}$

With non-compact formulation, σ(β) drops twice as fast as that with compact formulation.