Chiral Gap and Collective Excitations
in
Monolayer Graphene
from
Strong Coupling Expansion
of
Lattice Gauge Theory

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Dirac fermions on graphene

- Electrons/holes on graphene show linear dispersion near "Dirac points":

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

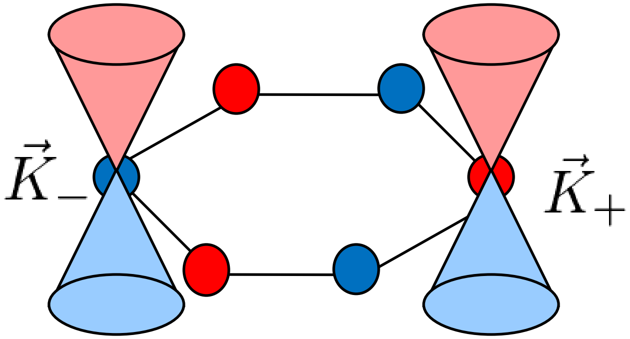
[Wallace, 1947]

"Fermi velocity"

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

a_{hc}=1.42 Å (interatomic spacing)

t = 2.8eV (hopping parameter)

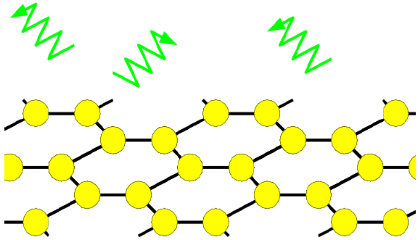


- Electrons/holes are described as massless 4-component Dirac fermions.

[Semenoff, 1984]

Effective gauge theory

[Son,2007]



- Euclidean action in "*Mixed dimensions*" :

  (with temporal scale transformed by v_F)

- ･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.

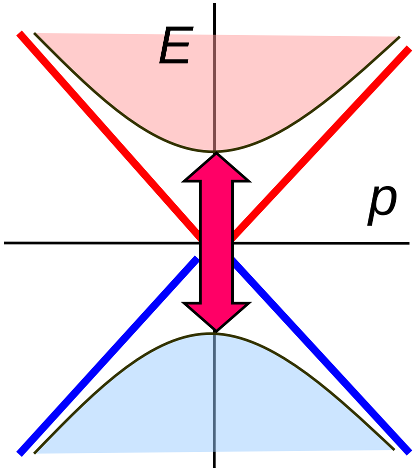
$$S_G = \frac{\beta}{2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2$$

- 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

Physics at strong coupling



Graphene: Dynamical gap generation

Semimetal-insulator transition

Similar mechanism ⇕

QCD: Spontaneous chiSB

Dynamical quark mass

This work:

Strong coupling expansion of U(1) lattice gauge theory in "mixed dimension"

⇨ analytic calculations of

- ▶ Fermion dynamical gap at/around

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

- ▶ Collective excitations

  NG mode, Higgs mode

Regularization on a square lattice

- Gauge field:

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

$U_j(x) = 1$ (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:

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

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

continuum staggered

$$\cancel{(\mathrm{U}(4) \longrightarrow)} \quad \mathrm{U}(1)_\mathrm{V} \times \mathrm{U}(1)_\mathrm{A} \xrightarrow{\chi\mathrm{SB}} \mathrm{U}(1)_\mathrm{V}$$

Lattice gauge action

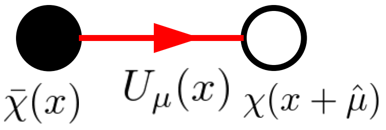
[Drut & Lahde, 2009]

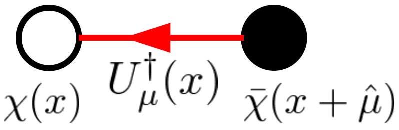
- $$S_F = \sum_{x^{(3)}} \left[\frac{1}{2} \sum_{\mu=1,2,4} \left(V_\mu^+(x) - V_\mu^-(x) \right) + m_* M(x) \right]$$

Hopping operators: (kinetic terms)

$$V_\mu^+(x) = \eta_\mu(x)\bar\chi(x)U_\mu(x)\chi(x+\hat\mu)$$

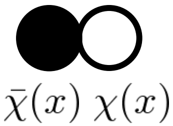
$$V_\mu^-(x) = \eta_\mu(x)\bar\chi(x+\hat\mu)U_\mu^\dagger(x)\chi(x)$$





Mesonic operator: (mass term)

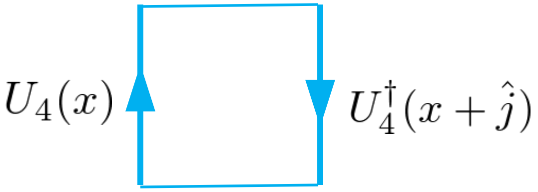
$$M(x) = \bar\chi(x)\chi(x)$$



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

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

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



Strong coupling expansion

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

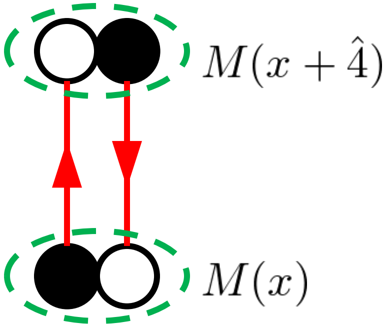
Expansion parameter: $\beta \equiv 1/g_*^2$

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

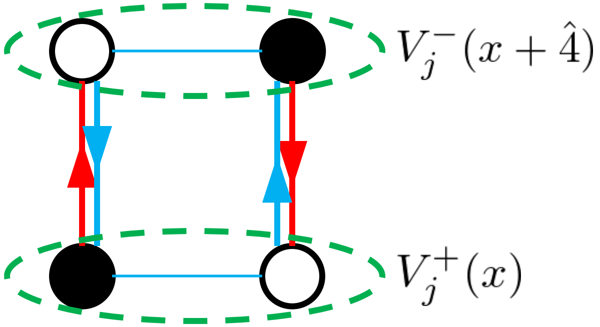
$$Z = \int [d\chi d\bar{\chi}][d\theta] \left[\sum_{n=0}^{\infty} \frac{(-S_G)^n}{n!} e^{-S_F} \right] = \int [d\chi d\bar{\chi}] e^{-S_\chi}$$

Only the terms in which link variables cancel remain:

LO[O(1)]



NLO[O(β)]

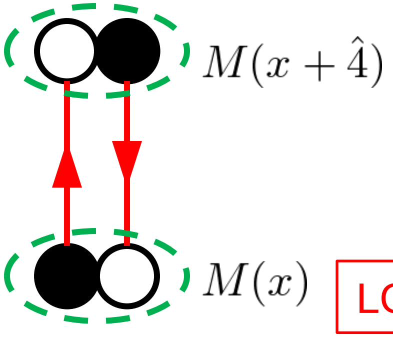


⇨ 4-fermi couplings are induced by the link integration.

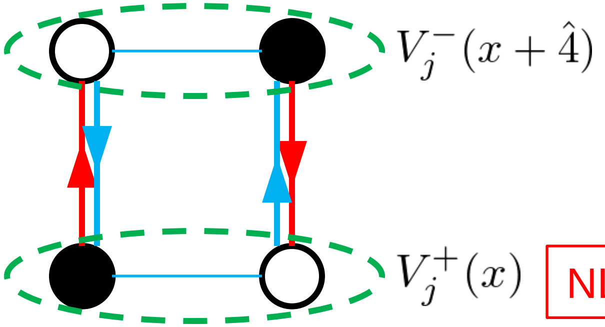
Fermionic effective action

$$\left.\begin{aligned} S_\chi = & \sum_{x^{(3)}} \left[\frac{1}{2} \sum_{j=1,2} \left(V_j^+(x) - V_j^-(x) \right) + m_* M(x) \right] \\ & -\frac{1}{4} \sum_{x^{(3)}} M(x) M(x+\hat{4}) \end{aligned}\right\} \text{O(1)}$$

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



LO[O(1)]



NLO[O(β)]

Auxiliary fields

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

by "Extended Stratonovich-Hubbard transformation":

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

$$\Downarrow$$

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

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

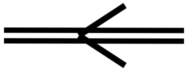
Scalar
$M(x) = \bar{\chi}(x)\chi(x)$

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

Free energy at T=0

- Propagator under background

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



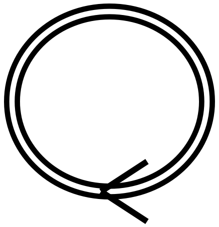
- Dynamical fermion mass $$M_F = \left| m_* - \frac{\phi}{2} \right|$$

- Integration over the fermionic fields gives

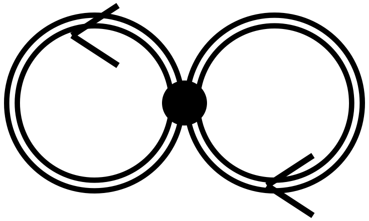
$$F_{\text{eff}}(\phi) = \frac{1}{4}|\phi|^2 - \frac{1}{2}\int_{\vec{k}} \ln\left[G^{-1}(\vec{k};\phi)\right] - \frac{\beta}{4}\sum_{j=1,2}\left[\int_{\vec{k}} G(\vec{k};\phi)\sin^2 k_j\right]^2 + O(\beta^2)$$

Tree level

1-loop [O(1)]

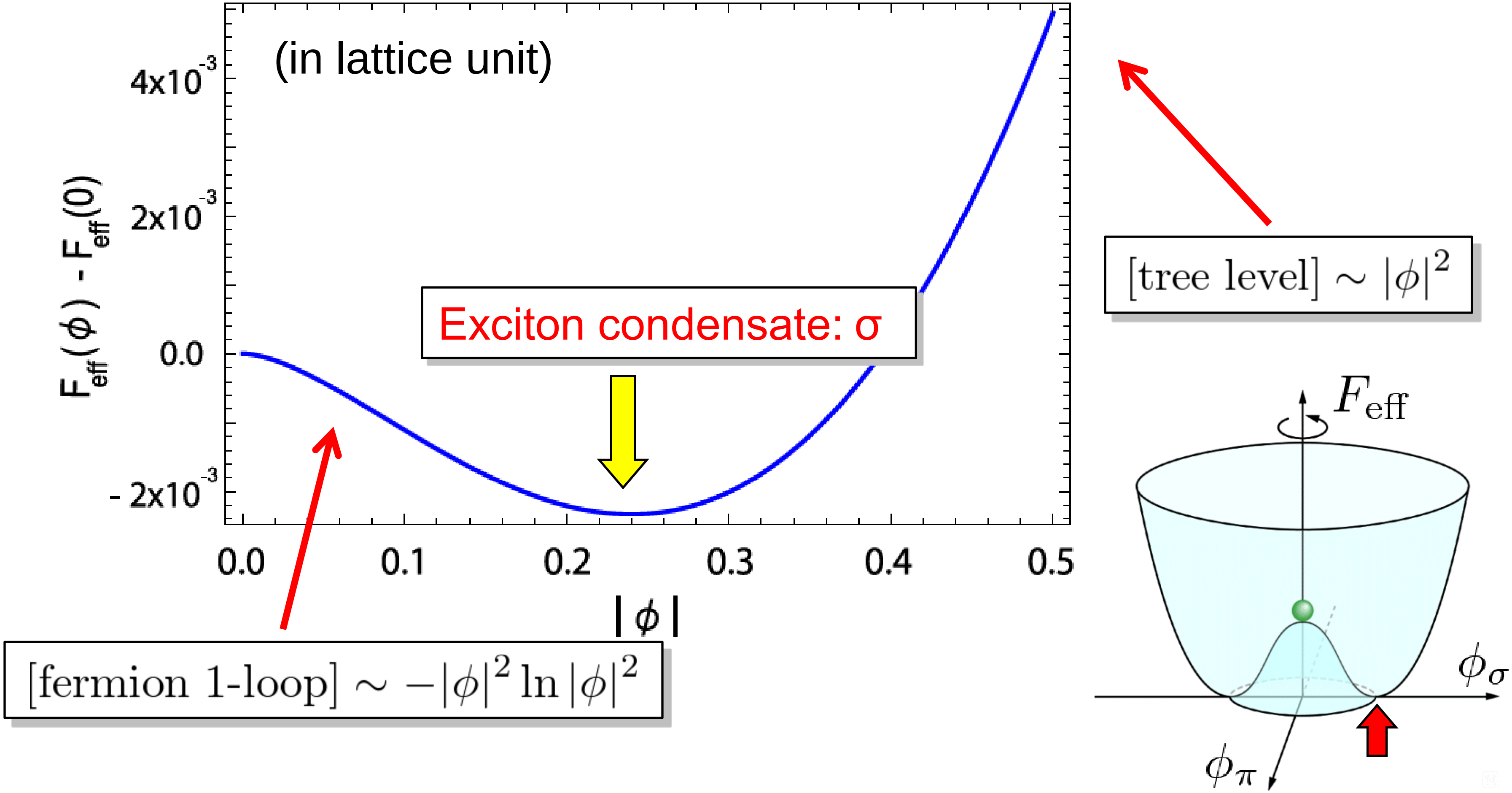


2-loop [O(β)]



Strong coupling limit

- Free energy in the strong coupling limit (β=0) & chiral limit (m=0)



(in lattice unit)

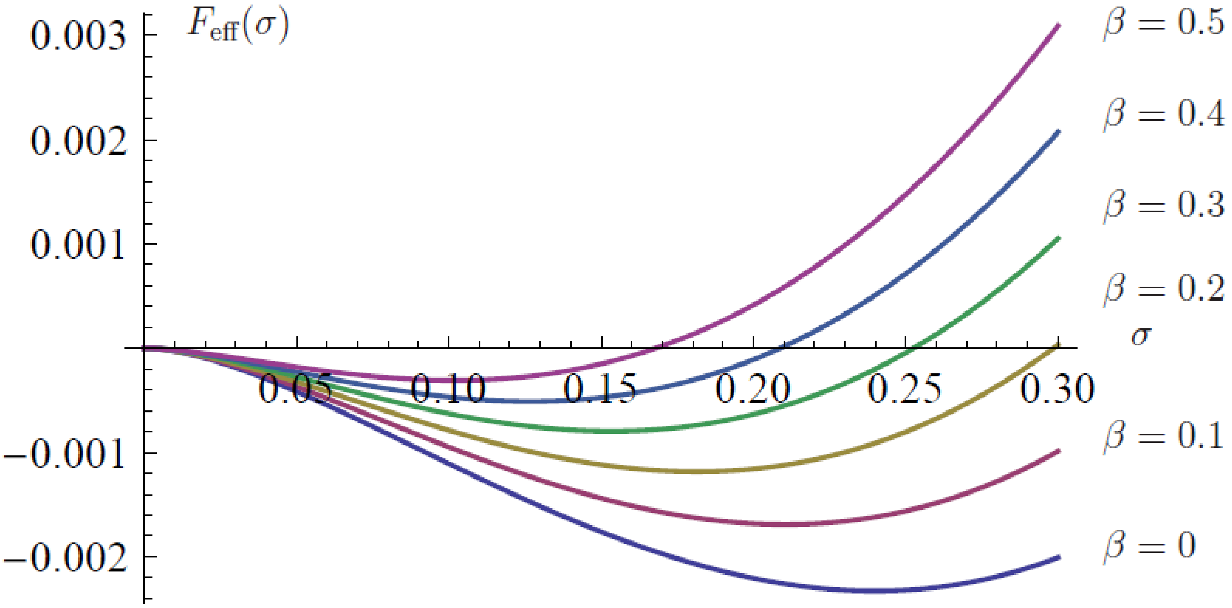
Exciton condensate: σ

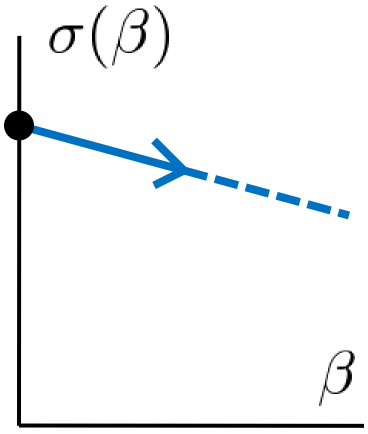
[tree level] $\sim |\phi|^2$

[fermion 1-loop] $\sim -|\phi|^2 \ln |\phi|^2$

- "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 $a \sim a_{\text{honeycomb}} = 1.42\text{Å}$

⇨ 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]

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

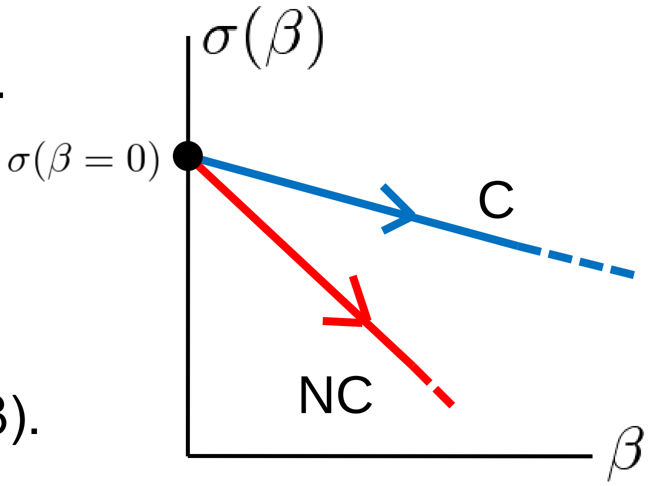
Strong coupling expansion:

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

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

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

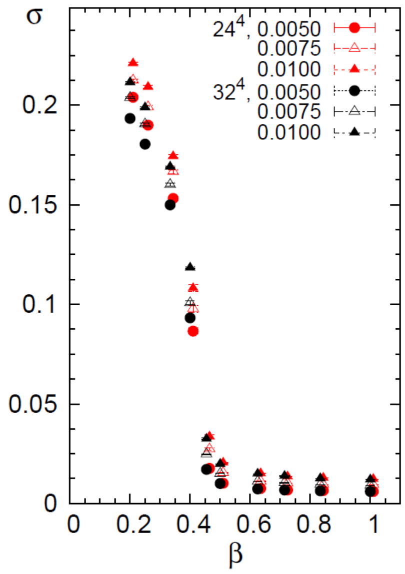
⇒ $\sigma^{\mathrm{NC}}(\beta)$ drops twice faster than $\sigma^{\mathrm{C}}(\beta)$.



MC simulations vs. Strong coupling expansion (SCE)

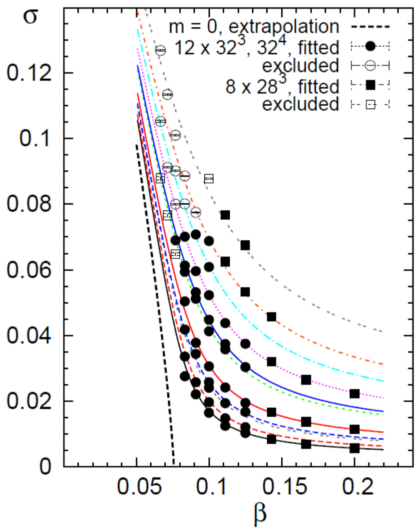
Monte Carlo results:

[Drut & Lahde, 2010]



w/ compact gauge action

w/ non-compact gauge action



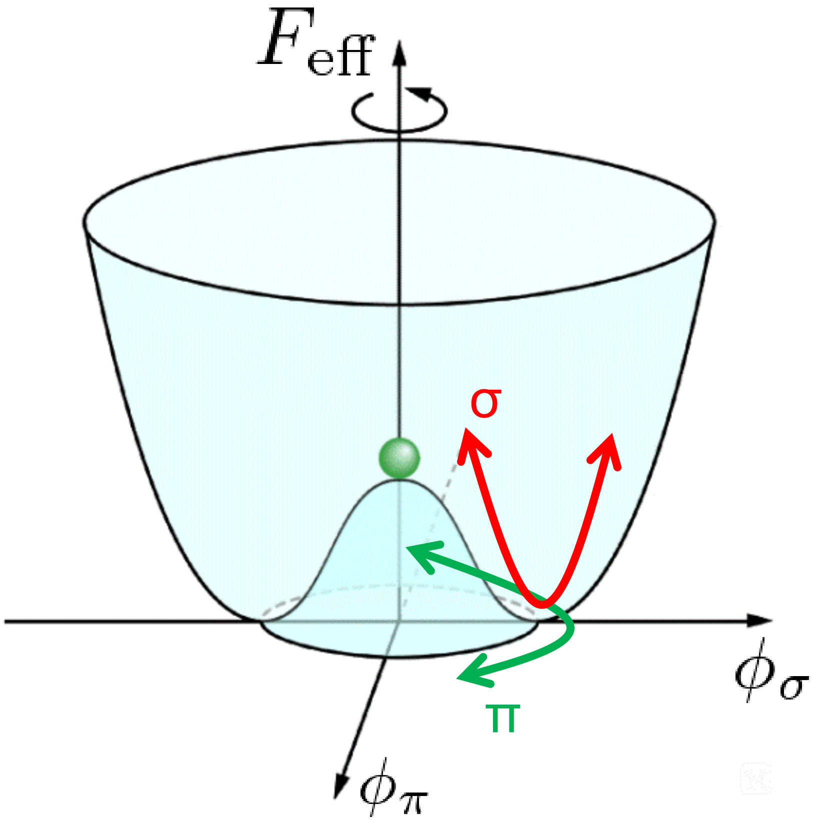
[both without “tadpole improvement”]

Comparison:

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

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

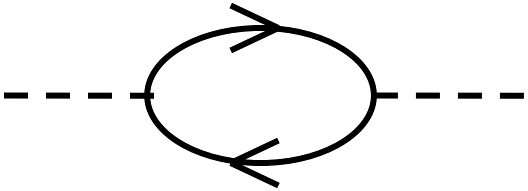
"scalar" type

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

Dispersion relation

- Boson propagators (with fermion 1-loop):

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



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

(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)

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

Two exciton modes

- π -mode:

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

➡ "NG boson"
from chiSB

$$= \sqrt{m\sigma}/F_\pi^\tau$$

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

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

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

Experimental observation would give a good evidence of chiSB .

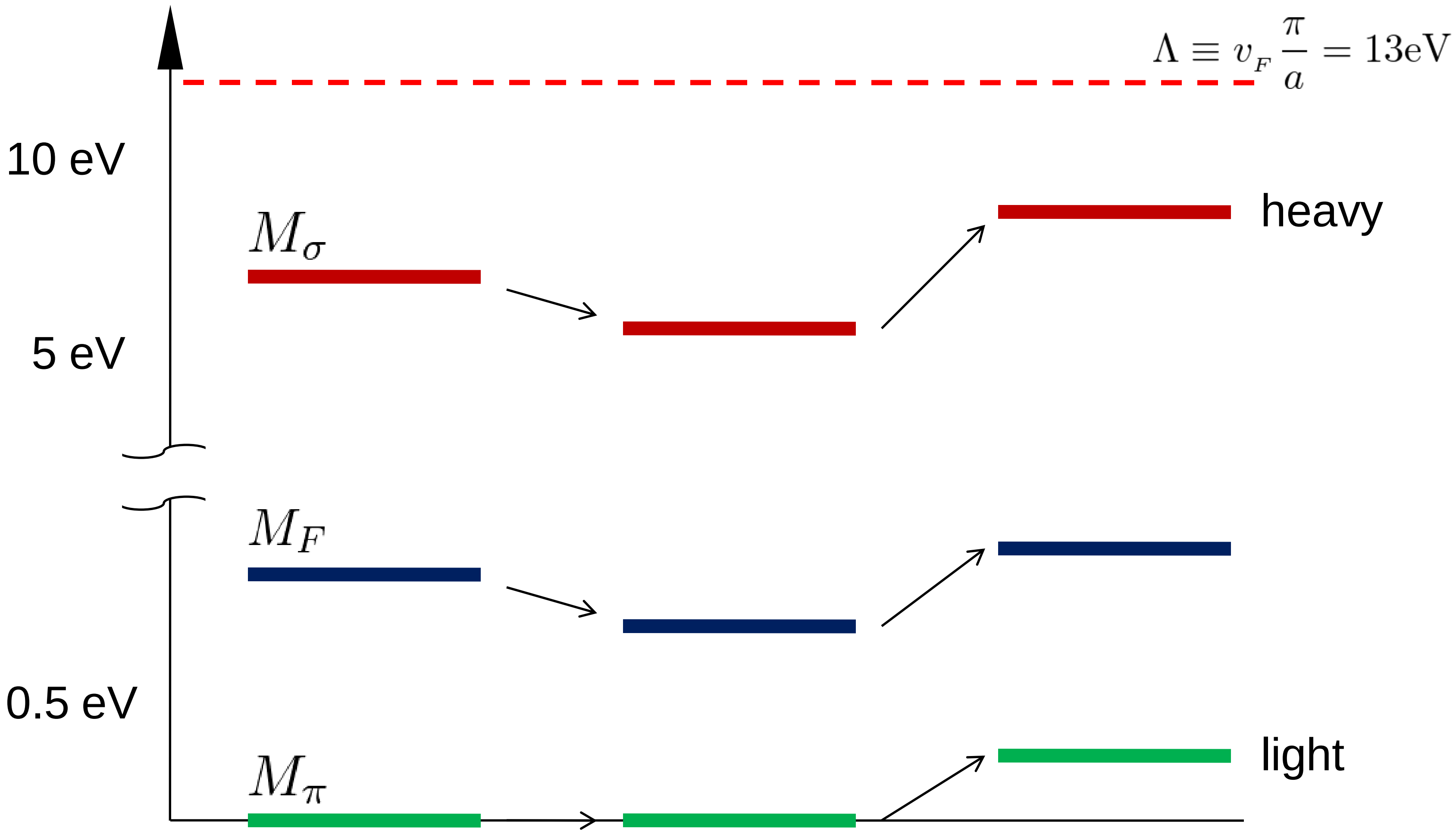
- σ -mode:

$$M_\sigma \simeq (5.47 - 1.97\beta)\text{eV}$$

Quite a heavy mass (comparable to the cutoff energy $\Lambda \equiv v_F \frac{\pi}{a} = 13\text{eV}$)

~ σ -meson in QCD

Excitation spectra



β=0 (strong coupling limit) β>0 β>0

m=0 (chiral limit) m=0 m>0

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.

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

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

Future prospects

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

Thank you.