Chiral Symmetry of Graphene and Strong Coupling Lattice Gauge Theory

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What is graphene?

Graphene = Single atomic layer of carbon atoms

Honeycomb lattice structure

Building block of many kinds of carbon materials.





Electronic features of graphene:

[Castro Neto et al., 2009]

Linear dispersion around two "Dirac points". [Wallace, 1947]

 $E(\mathbf{K}_{\pm} + \mathbf{p}) = \pm \boldsymbol{v}_{F} |\mathbf{p}|_{+\mathcal{O}((p/K)^{2})} \quad \text{(gapless)}$

"Fermi velocity" ~c/300

Description as

Massless Dirac fermions

[Semenoff, 1984]

"Chiral symmetry" = sublattice symmetry



Effective gauge theory

 $^{2} \prod_{i=1,2,3}^{2} J$

Euclidean action with Coulomb (U(1) gauge) interaction: ("braneworld", "reduced QED") [Gorbar et al.,2002]

Fermions in 3-dim.

$$S_{F} = \sum_{f} \int dx^{(3)} \bar{\psi}_{f} \left[\gamma_{4}(\partial_{4} + iA_{4}) + (\gamma_{1}\partial_{1} + \gamma_{2}\partial_{2}) + \underbrace{m_{*}}^{\uparrow} \right] \psi_{f}$$

$$\cdot U(1) \text{ gauge field in 4-dim.}$$

$$S_{G} = \frac{\beta}{2} \sum_{f} \int dx^{(4)}(\partial_{j}A_{4})^{2}$$

Small Fermi velocity \square Effectively strong Coulomb coupling $g_*^2 \equiv \frac{1}{\beta} = \frac{g_{\text{QED}}^2}{v_F} (\sim 300g_{\text{QED}}^2)$ (β~0.04)

> Strong coupling expansion around β =0 will work well. (If not screened by substrate)

Physics at strong coupling



<u>This work:</u>

Strong coupling expansion of U(1) lattice gauge theory ("reduced QED")

Analytic calculations of
 Fermion dynamical gap at/around
 β=0 (strong coupling), m=0 (chiral limit), V=∞ (infinite volume)
 Collective excitations
 e.g.) (pseudo-)NG mode (~ pion)

Regularization on a square lattice



Strong coupling expansion

Expansion parameter: $\beta \equiv 1/g_*^2$ (inverse effective coupling) Link integration is performed order by order: $\begin{bmatrix} S_G \sim O(\beta) \end{bmatrix}$ $Z = \int [d\chi d\bar{\chi}] [d\theta] \left[\sum_{n=0}^{\infty} \frac{(-S_G)^n}{n!} e^{-S_F} \right] = \int [d\chi d\bar{\chi}] e^{-S_\chi}$

4-fermi couplings are induced by the link integration.



Strong coupling limit (LO term)

Strong coupling limit (β =0) & chiral limit (m=0)

The gauge term does not contribute at $\beta=0$: $\sigma^{C}(\beta=0) = \sigma^{NC}(\beta=0)$



"Chiral symmetry" is spontaneously broken in the strong coupling limit. (sublattice symmetry)

NLO effect: compact formulation



Exciton condensate (in lattice unit):

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

• By setting the lattice spacing $a \sim a_{\text{honeycomb}} = 1.42 \text{\AA}$

$$\checkmark$$
 Dynamical gap $M_F \equiv rac{v_F}{a} rac{\sigma a^2}{2} \simeq (0.523 - 0.623 eta) \mathrm{eV}$

NLO effect: non-compact form.

In the link integration,

One plaquette also works as its c.c.



Collective excitations (excitons)

Two excitation modes: fluctuations of the order parameter φ



 $\begin{array}{l} \underline{\mathsf{T-mode}} \text{ (phase fluctuation mode)} \\ M_{\pi} \simeq \frac{2v_{F}}{a} \sqrt{\frac{m_{\text{bare}}}{M_{F}(m=0)}} & \stackrel{m=0}{\longrightarrow} 0 \\ & \left(= 8.40 \sqrt{\frac{m}{M_{F}(m=0)}} \mathrm{eV} \right) \end{array}$

Similar to pions in QCD (GMOR relation):

$$M_{\pi} = \sqrt{m_{\scriptscriptstyle \rm bare} \sigma} / f_{\pi}$$

• σ -mode (amplitude fluctuation mode) $M_{\sigma} \simeq (5.47 - 1.97\beta) \text{eV}$

Quite a heavy mass (Higgs-like)

Conclusion

Lattice strong coupling expansion (analytic)

Strong coupling: spontaneous chiSB

 $\square Dynamical spectral gap: M_F = \frac{\sigma}{2} \quad \left[\rightarrow \frac{v_F}{a} \frac{\sigma a^2}{2} \right]$ $\blacktriangleright \text{ Compact vs. Non-compact formulation:}$

 \square Difference starts from NLO: $\sigma^{NC}(\beta) < \sigma^{C}(\beta)$

► Collective excitation modes:

 π (phase fluctuation) \square Pion-like behavior (GMOR rel.)

Future prospects:

- NNLO effect? (now being investigated)
- Finite T? (KT transition in (2+1)-D?)
- Taste breaking? (compare with overlap fermions, ...)
- Anisotropy effects? (graphene under uniaxial strain)
- Gauge theory on the original honeycomb lattice? etc.

Thank you.

Results from Strong coupling expansion



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"
 $v_F = (3/2)a_{hc}t \sim c/300$
 $a_{hc}=1.42$ Å (interatomic spacing)
 $t = 2.8$ eV (hopping parameter)

Electrons/holes are described as massless Dirac fermions.

$$\begin{array}{c} \mathbf{4} = & \mathbf{2} & \mathbf{X} & \mathbf{2} \\ \text{components} & \text{DPs} & \text{sublattices} \end{array} \quad \psi_{\sigma}(\vec{p}) = \begin{pmatrix} a_{\sigma}(\vec{K}_{+} + \vec{p}) \\ b_{\sigma}(\vec{K}_{-} + \vec{p}) \\ b_{\sigma}(\vec{K}_{-} + \vec{p}) \\ a_{\sigma}(\vec{K}_{-} + \vec{p}) \end{pmatrix} \\ \text{(Spin up/down is considered as "flavor": N_{c}=2)} \end{array}$$

Mixed dimension model



Low-energy effective action [Son, 2007]



(2+1)-dim. fermionic field:

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

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

$$S_G = \frac{1}{2g^2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2$$
$$g^2 = \frac{e^2}{\epsilon_0} \text{ (for suspended graphene)}$$

Assume "instantaneous" Coulomb interaction Magnetic components (*A*_i) neglected

Effectively strong coupling

Scale transformation in the temporal direction:

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

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

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

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?



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^a_μ	Electric field A_{μ}
Coupling constant g^2	Effective coupling g_*^2
Quarks $q(=u, d, \ldots)$	Quasi-electrons ψ
Chiral condensate $\langle ar{q}q angle$	Exciton condensate $\langle ar{\psi}\psi angle$
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

 $\begin{array}{l} \{1,\vec{\sigma}\} \otimes \{1,\gamma_3,\gamma_5,\gamma_3\gamma_5\} \\ \text{Subgroups:} \\ \text{global gauge transf.} \\ \text{U}(1)_{\mathrm{V}}: \quad \psi \to e^{i\theta_{\mathrm{V}}}\psi, \quad \bar{\psi} \to \bar{\psi}e^{-i\theta_{\mathrm{V}}} \\ \text{chiral transf. (at chiral limit$ *m* $=0)} \\ \text{U}(1)_{\mathrm{A}}: \quad \psi \to e^{i\gamma_5\theta_A}\psi, \quad \bar{\psi} \to \bar{\psi}e^{i\gamma_5\theta_A} \end{array}$

Lattice regularized theory is invariant only under

global gauge transf.

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

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

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

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.

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

 $t \sim 2.8 \text{eV}$ $a \sim 1.42 \text{ Å}$ (interatomic spacing)

The energy eigenvalue vanishes at two Fermi (Dirac) points. k_2



The dispersion relation is linearized around the Dirac points.

Low-energy effective theory

Expanding the operators around the Dirac points,

he Hamiltonian is given as

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

Lagrangian form:

t

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

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

Dirac points \rightarrow "pseudospin" Spin d.o.f. \rightarrow "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
 $t \to t/v \quad A_0 \to v A_0$
$$g^2 = e^2/\epsilon_0$$

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

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^a_μ	Electromagnetic field A_{μ}
Coupling constant g^2	$e^2/v\epsilon$
Fermions	Electrons
Chiral condensate $\langle \bar{q}q \rangle$	Exciton cond. $\langle \psi \psi \rangle$
Flavors	Layers x Spin d.o.f.
Our approach Lattice gauge theory Strong coupling expansion	Properties of graphene Dynamical mass gap
(Powerful approach in QCD) [Nishida, Fukushima & Hatsuda, 200 [Miura, Nakano & Ohnishi, 2009])4]

Lattice regularization

Euclidean Low-energy effective theory [Son,2007]

$$\begin{split} S_F &= \int dt d^2 x \bar{\psi}_a \left[\gamma_0 (\partial_0 + iA_0) + \vec{\gamma} \cdot \vec{\partial} + m_0 \right] \psi_a \\ S_G &= \frac{\beta}{2} \int dt d^3 x (\partial_i A_0)^2 \\ & \text{UV cutoff: } \Lambda = \pi/a \sim 4.36 \text{keV} \end{split}$$

Discretize on the square lattice. (with staggered fermions)

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

Formulation of fermions

Tight-binding Hamiltonian:

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

1

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

Υ.

Low energy effective theory:

Dirac spinor form

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 directionsNon-local in temporal direction

Next-leading order: $O(\beta)$

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

$$\int_{-\pi}^{\pi} \frac{d\theta(x)}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta(x+\hat{j})}{2\pi} \exp\left[-\frac{1}{2}\left(V_{4}^{+}(x)-V_{4}^{-}(x)+V_{4}^{+}(x+\hat{j})-V_{4}^{-}(x+\hat{j})\right)\right] U_{4}^{\dagger}(x)U_{4}(x+\hat{j})$$

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

$$\times \left[1-\frac{1}{2}\bar{\chi}(x+\hat{j})U_{4}(x+\hat{j})\chi(x+\hat{j}+\hat{4})\right] \left[1+\frac{1}{2}\bar{\chi}(x+\hat{j}+\hat{4})U_{4}^{\dagger}(x+\hat{j})\chi(x+\hat{j})\right]$$

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

$$\Delta S_{\chi} = \frac{\beta}{8}\sum_{x^{(3)}}\sum_{j=1,2} \left[V_{j}^{+}(x)V_{j}^{-}(x+\hat{4})i+V_{j}^{-}(x)V_{j}^{+}(x+\hat{4})\right]$$
i= 2 does not contribute

j=3 does not contribute.



4-fermi term:

Non-local both in spatial and temporal directions

Mean-field approximation

Mean-field approximation:

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 :

$$\frac{\partial F_{\text{eff}}(\phi,\lambda)}{\partial\lambda_1} = 0 \quad \text{if } \lambda_1 = 0 + O(\beta)$$

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

$$\text{Effective potential:}$$

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

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

Effective potential with varying β

At the chiral limit, the effective potential is



Non-compact link integration

$$\begin{array}{l} \text{e.g.) Integration over } \theta(x) \text{ and } \theta(x+\hat{j}) & \text{From non-compact plaquette} \\ \int_{-\pi}^{\pi} \frac{d\theta(x)}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta(x+\hat{j})}{2\pi} \exp\left[-\frac{1}{2}\left(V_{4}^{+}(x) - V_{4}^{-}(x) + V_{4}^{+}(x+\hat{j}) - V_{4}^{-}(x+\hat{j})\right)\right] \theta(x)\theta(x+\hat{j}) \\ = \int_{-\pi}^{\pi} \frac{d\theta(x)}{2\pi} \theta(x) \left[1 - \frac{1}{2}\bar{\chi}(x)e^{i\theta(x)}\chi(x+\hat{4}) + \frac{1}{2}\bar{\chi}(x+\hat{4})e^{-i\theta(x)}\chi(x) + \frac{1}{4}M(x)M(x+\hat{4})\right] \\ & \times \int_{-\pi}^{\pi} \frac{d\theta(x+\hat{j})}{2\pi} \cdots \left(\int_{-\pi}^{\pi} \frac{d\theta}{2\pi}\theta e^{\pm i\theta} = \pm i\right) \\ = \frac{1}{4} \left[V_{j}^{+}(x)V_{j}^{-}(x+\hat{4}) + V_{j}^{-}(x)V_{j}^{+}(x+\hat{4})\right] + (\text{irrelevant terms}) \end{array}$$

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, $\sigma(\beta)$ drops twice as fast as that with compact formulation.