Chiral gap and collective excitations in monolayer graphene from strong coupling expansion of lattice gauge theory

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Using the strong coupling expansion of the compact and noncompact U(1) lattice gauge theories for monolayer graphene, we show analytically that fermion band gap and pseudo-Nambu-Goldstone exciton (π exciton) are dynamically generated due to chiral symmetry breaking. The mechanism is similar to the generation of quark mass and pion excitation in quantum chromodynamics (QCD). We derive a formula for the π-exciton analogous to the Gell-Mann-Oakes-Renner (GOR) relation in QCD. Experimental confirmation of the GOR relation on a suspended monolayer graphene would be a clear evidence of chiral symmetry breaking.

Graphene is a monoatomic layer of carbon atoms with a honeycomb lattice structure.[1,2] A novel feature of graphene is that electrons and holes at low energy have a linear-dispersion relation around two independent "Dirac points" in the momentum space.[3] Then the charge carriers on graphene can be described by massless Dirac quasiparticles.[4] The system has, however, a critical difference from relativistic electrons;[3] the Fermi velocity v_F of the electrons on graphene is about 300 times smaller than the speed of light c. This leads to an effective enhancement of the Coulomb interaction among Dirac quasiparticles. In such a strong coupling situation, electrons and holes on graphene may form an exciton condensate and create a gap in the fermion spectrum leading to semimetal-insulator transition. To show unambiguously that undoped monolayer graphene suspended in vacuum becomes an insulator is one of the important theoretical challenges.[5] Also, this problem has much in common with the dynamical breaking of chiral symmetry in strongly coupled relativistic field theories such as quantum chromodynamics (QCD).[6] So far, various theoretical methods such as the Schwinger-Dyson equation,[7–9] renormalization-group equations,[10] and lattice Monte-Carlo methods[11,12] have been applied to study the dynamical formation of the fermion gap in low-energy effective theories of graphene.

The purpose of this Rapid Communication is to shed lights on the strong coupling regime of graphene at zero temperature from an analytic method of strong coupling expansion (see Refs. 13 and 14 for its recent applications in QCD). We start with a "braneworld" or "reduced QED" model of graphene[8,10] in which (2+1)-dimensional Dirac fermions are coupled to (3+1)-dimensional Coulomb field. After discretizing this model on a square lattice with compact U(1) gauge field and staggered fermion,[11,12] we carry out an expansion by the inverse Coulomb coupling and derive an effective action for the fermions. The exciton condensate (chiral condensate) and the fermion gap (chiral gap) are obtained analytically from the resultant effective action. Properties of the pseudo-Nambu-Goldstone (NG) excitation associated with the exciton condensation are also studied. In particular, we derive a mass formula similar to the Gell-Mann-Oakes-Renner (GOR) relation in QCD.[15]

Low-energy Euclidean action for Dirac quasiparticles on a graphene interacting with the U(1) gauge field is described by[8,10]

$$S_E = \sum_f \int dx^{(3)} \bar{\psi}_f (D[A_4] + m) \psi_f + \frac{1}{2g^2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2,$$

(1)

where the natural unit ($\hbar = c = 1$) is taken. Since this is an effective theory for quasiparticles in the first Brillouin zone of the original honeycomb lattice, it has an intrinsic momentum cutoff $p_\Lambda \lesssim \pi/a_{\text{Hc}}$ with $a_{\text{Hc}} = 1.42$ Å being the honeycomb lattice spacing.

The three- and four-dimensional Euclidean coordinates are denoted by $x^{(3)} = (\tau, x_1, x_2)$ and $x^{(4)} = (\tau, x_1, x_2, x_3)$, respectively. The Dirac spinor ψ_f has four components corresponding to 2 (the number of sublattices) $\times 2$ (the number of Dirac points). The "flavor index" f runs from 1 up to the number of flavors N. In this Rapid Communication we specifically focus on $N = 2$ case, which corresponds to the monolayer graphene with the up and down spins of electrons. The Dirac operator is defined as $D[A_4] = \gamma_4(\partial_4 + iA_4) + v_F(\gamma_1\partial_1 + \gamma_2\partial_2)$, where A_4 is a temporal component of the gauge field. The gauge coupling constant for the suspended graphene is $g^2 = e^2/\epsilon_0$ with e being the electric charge and ϵ_0 being the vacuum permittivity. g^2 is reduced by the factor $2/(1+\varepsilon)$ on a substrate with ε being the dielectric constant of the substrate.[10] The Hermitian γ matrices obey the standard relation $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$. The Fermi velocity reads $v_F = (3/2)ta_{\text{Hc}} = 3.02 \times 10^{-3}$ in the unit of light velocity, with the hopping parameter $t \simeq 2.8$ eV,[17] obtained from the spectral slope observed on substrate. The bare mass m corresponds to an explicit band gap which may be formed artificially on epitaxially grown graphene on substrate[18] or on graphene nanoribbon and nanomesh.[19]

Due to the small Fermi velocity, electron interactions are dominated by the Coulomb interaction so that the spatial components of the gauge field, $A_{j=1,2,3}$, can be neglected. With scaled variables, $\tau \to \tau/v_F$ and $A_4 \to v_F A_4$, Dirac particles have an effective mass $m_* = m/v_F$ and an effective coupling $g_*^2 = g^2/v_F$, which is about 300 times larger than the Coulomb coupling strength in the vacuum. In the chiral limit ($m \to 0$), Eq. (1) is invariant under U(4) chiral transformation with 16 generators,[20] $(1, \vec{\sigma}) \otimes (1, \gamma_3, \gamma_5, \gamma_3\gamma_5)$ with $\gamma_5 = \gamma_4\gamma_1\gamma_2\gamma_3$. Absence of γ_3 in $D[A_4]$ is the reason for such large chiral symmetry.

A regularized form of Eq. (1) on a hypothetical square lattice with a lattice spacing $a = \pi/p_\Lambda$ reads[12]

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

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

Here all the dimensionful quantities are scaled by a. The U(1) gauge action S_G is written in terms of a timelike link variable $U_4(x) = \exp[i\theta(x)]$ with $-\pi < \theta \leq \pi$. The fermionic action S_F is written in terms of the staggered fermion χ through

$$M(x) = \sum_b \bar{\chi}_b(x)\chi_b(x), \quad (4)$$

$$V_\mu^+(x) = \sum_b \eta_\mu(x)\bar{\chi}_b(x)U_\mu(x)\chi_b(x+\hat{\mu}), \quad$$

$$V_\mu^-(x) = \sum_b \eta_\mu(x)\bar{\chi}_b(x+\hat{\mu})U_\mu^\dagger(x)\chi_b(x) \quad (5)$$

with $\mu = 1,2,4$ and $U_{1,2}(x) = 1$. b is the staggered flavor index which runs from 1 to $N/2$ since 2^3 doublers emerging from one staggered fermion on a three-dimensional square lattice can be identified with four Dirac components times two "flavors."[11,12] The monolayer graphene corresponds to $N=2$. The staggered phase factors η_μ are $\eta_4(x)=1$, $\eta_1(x)=(-1)^\tau$, $\eta_2(x)=(-1)^{\tau+x_1}$, and $\eta_3(x)=(-1)^{\tau+x_1+x_2} \equiv \epsilon(x)$.

In the chiral limit, fermion action for each flavor in S_F is invariant under $U(1)_V \times U(1)_A$ chiral transformations; $[\chi_b(x),\bar{\chi}_b(x)] \xrightarrow{V} [e^{i\xi_V}\chi_b(x), e^{-i\xi_V}\bar{\chi}_b(x)]$ and $[\chi_b(x),\bar{\chi}_b(x)] \xrightarrow{A} [e^{i\xi_A\epsilon(x)}\chi_b(x), e^{i\xi_A\epsilon(x)}\bar{\chi}_b(x)]$. These are remnants of global $U(4)$ chiral symmetry of Eq. (1).[21] Under the $U(1)_A$ rotation, we have $M(x) \to e^{2i\xi_A\epsilon(x)}M(x)$ and $V_\mu^\pm(x) \to V_\mu^\pm(x)$ so that the chiral condensate $\langle\bar{\chi}\chi\rangle$ serves as an order parameter for the spontaneous symmetry breaking, $U(1)_V \times U(1)_A \to U(1)_V$.

We define an expansion parameter, $\beta \equiv 1/g_*^2$, so that the strong coupling limit corresponds to $\beta \to 0$. (By taking $v_F \sim 0.003$, β in the vacuum is estimated as 0.04 while that on the SiO_2 substrate is 0.1.) Then, the partition function expanded by $S_G \sim O(\beta)$ becomes

$$Z = \int [d\chi d\bar{\chi}][d\theta] \left[\sum_{n=0}^{\infty} \frac{(-S_G)^n}{n!} e^{-S_F} \right] = \int [d\chi d\bar{\chi}]e^{-S_\chi}. \quad (6)$$

The θ integration can be analytically performed order by order in β for general N.[16] When the link variables $e^{i\theta}$ cancel with each other, the fermion self-interactions up to $2N$-Fermi term are induced. Hereafter, we will focus only on the monolayer case ($N=2$).[22] Up to $O(\beta)$, we obtain
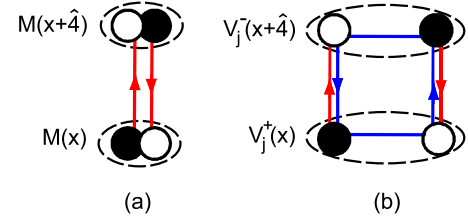

FIG. 1. (Color online) Induced four-fermion interaction in the strong coupling expansion. The open (filled) circle represent $\chi(\bar{\chi})$. (a) In the LO, the timelike links in S_F cancel with each other to leave a spatially local interaction. (b) In the NLO, the timelike links in S_F are canceled by those in S_G to leave a spatially nonlocal interaction.

$$S_\chi = \sum_{x^{(3)}} \left\{ \frac{1}{2} \sum_{j=1,2} [V_j^+(x) - V_j^-(x)] + m_* M(x) \right\}$$
$$- \frac{1}{4} \sum_{x^{(3)}} M(x)M(x+\hat{4})$$
$$+ \frac{\beta}{8} \sum_{x^{(3)}} \sum_{j=1,2} [V_j^+(x)V_j^-(x+\hat{4}) + (V_j^+ \leftrightarrow V_j^-)]. \quad (7)$$

The second line in Eq. (7) is the leading-order (LO) term of $O(\beta^0)$, which is local (nonlocal) in space (time) as shown in Fig. 1(a). The third line is the next-to-LO (NLO) term of $O(\beta)$, which is nonlocal in both space and time as shown in Fig. 1(b). Note that the gauge-field propagating along the third spatial dimension x_3 starts to appear at $O(\beta^3)$ in the strong coupling expansion. The nonlocal four-Fermi interactions in Eq. (7) can be linearized by the extended Stratonovich-Hubbard transformation:[14] $\exp(\alpha AB) \sim \int[d\varphi d\varphi^*]\exp[-\alpha(|\varphi|^2 - A\varphi - B\varphi^*)]$, where A and B are fermion bilinears and α is a positive constant. By introducing two complex auxiliary fields $\phi(x)$ and $\lambda(x)$ corresponding to the LO and NLO terms and integrating out the fermion fields, we arrive at $Z = \int[d\phi d\phi^*][d\lambda d\lambda^*]e^{-S_{\mathrm{eff}}(\phi,\lambda)}$, where the axial $U(1)_A$ rotation induces the transformation, $\phi(x) \to e^{-2i\xi_A\epsilon(x)}\phi(x)$ and $\lambda(x) \to \lambda(x)$.

In the mean-field approximation, where fluctuations of ϕ and λ are neglected, free energy per unit space-time lattice cell at zero temperature, $F_{\mathrm{eff}}(\phi)$, can be obtained after eliminating λ by using the stationary condition $[\delta S_{\mathrm{eff}}(\phi,\lambda)/\delta\lambda = 0]$

$$F_{\mathrm{eff}}(\phi) = \frac{1}{4}|\phi|^2 - \frac{1}{2}\int_k \ln[G^{-1}(\boldsymbol{k};\phi)]$$
$$- \frac{\beta}{4} \sum_{j=1,2} \left[\int_k G(\boldsymbol{k};\phi)\sin^2 k_j \right]^2 + O(\beta^2). \quad (8)$$

Here $G^{-1}(\boldsymbol{k};\phi) = \Sigma_{j=1,2}\sin^2 k_j + |m_* - \phi/2|^2$ is the two-dimensional bosonic propagator with an effective mass, $m_* - \phi/2$ and $\int_k \equiv \frac{1}{\pi^2}\int_{-\pi/2}^{\pi/2}dk_1\int_{-\pi/2}^{\pi/2}dk_2$. Alternative way to derive Eq. (8) is to treat the $O(\beta)$ term of Eq. (7) as a first-order perturbation.

The free energy $F_{\mathrm{eff}}(\phi)$ in the chiral and strong coupling limits ($m=0$, $\beta=0$) is shown in Fig. 2 for illustration. From
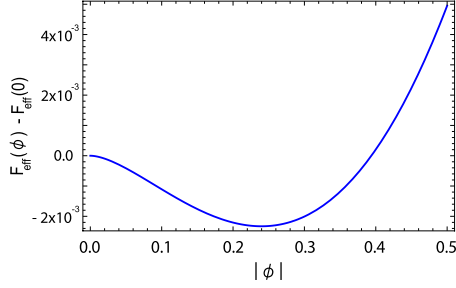
FIG. 2. (Color online) The free energy $F_{\text{eff}}(\phi)$ in the lattice unit as a function of $|\phi|$ for $\beta=0$ and $m=0$.

Eq. (8), we find that $F_{\text{eff}}(\phi \to \infty) \sim |\phi|^2$ due to the tree-level term while $F_{\text{eff}}(\phi \to 0) \sim \text{const} + |\phi|^2 \ln |\phi|^2$ due to the fermion one-loop term. Therefore, we can exactly show, in the case when $N=2$, that dynamical chiral symmetry breaking takes place in the strong coupling limit. Since the $O(\beta)$ correction from the third term in Eq. (8) grows as $|\phi|$ increases, the chiral condensate, $\sigma \equiv |\langle \bar{\chi}\chi \rangle|$, is a decreasing function of β. Up to the linear terms in β and m, we have

$$\sigma \simeq (0.240 - 0.297\beta + 0.0239ma)a^{-2}, \qquad (9)$$

where we recover the lattice spacing a. If we employ $a^{-1} \sim a_{\text{Hc}}^{-1} = 1.39$ keV as a typical cutoff scale of our effective theory, we obtain $\sigma \simeq [(0.680 - 0.421\beta + \frac{1.39m}{\text{eV}})$ keV$]^2$. Note that our approach is limited to the strong coupling regime so that it is inappropriate to extract the critical coupling β_c for semimetal-insulator transition from Eq. (9). The total fermion mass M_F is a sum of the dynamical mass and the bare mass in $G(\mathbf{k}; \phi)$,

$$M_F \equiv (\sigma a^2/2)(v_F/a) + m, \qquad (10)$$

which reduces to $(0.523 - 0.623\beta)$ eV$+3.05m$ for $a \sim a_{\text{Hc}}$.

Let us now consider collective excitations: a phase fluctuation of the order parameter ("π-exciton") analogous to the pion in QCD, and an amplitude fluctuation of the order-parameter ("σ-exciton") analogous to the σ meson in QCD. In terms of the auxiliary fields, the former (the latter) corresponds to $\phi_\pi(x)[\phi_\sigma(x)]$ in the decomposition, $\phi(x) = \sigma + \phi_\sigma(x) + i\epsilon(x)\phi_\pi(x)$. Propagators of the collective modes within the one-loop approximation in the strong coupling limit ($\beta=0$) reads

$$D_{\phi_{\sigma,\pi}}^{-1}(\mathbf{p}, i\omega_*)$$
$$= \frac{1}{2} - \frac{1 + \cosh \omega_*}{8} \int_k H(\mathbf{k},\mathbf{p};\sigma)G(\mathbf{k};\sigma)G(\mathbf{k}+\mathbf{p};\sigma),$$
$$(11)$$

where $H(\mathbf{k},\mathbf{p};\sigma) = \sum_{j=1,2} \sin k_j \sin(k_j+p_j) \pm (m_* + \sigma/2)^2$ with the $+(-)$ sign corresponding to the π exciton (the σ exciton). The $O(\beta)$ correction to the above expression can also be obtained. The actual dispersion relation without the scale transformation of the time variable τ is derived from the pole of the Euclidean propagator, $D_{\phi_{\sigma,\pi}}^{-1}(\mathbf{p}, i\omega/v_F) = 0$.

In the chiral limit, $D_{\phi_\pi}^{-1}(\mathbf{0},0) = 0$ is identical to the gap equation, $\partial F_{\text{eff}}(\sigma)/\partial\sigma = 0$ so that the π exciton is indeed a
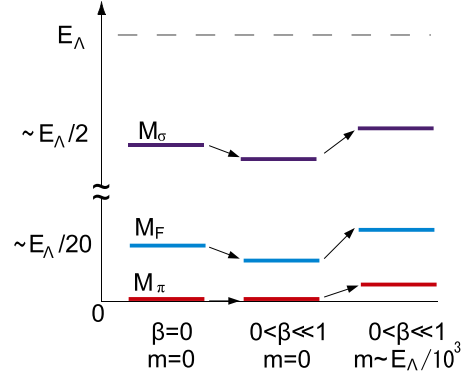

FIG. 3. (Color online) Typical mass gaps for the fermion (M_F), the π exciton (M_π), and the σ exciton (M_σ). The cutoff energy of our effective theory reads $E_\Lambda = v_F(\pi/a) \lesssim v_F(\pi/a_{\text{Hc}}) \sim 10$ eV.

NG boson associated with dynamical breaking of chiral symmetry. For the leading order in m, the π-exciton mass, $M_\pi = \omega_\pi(\mathbf{p}=0)$, reads

$$M_\pi \simeq 2\sqrt{\frac{m}{M_F^{m=0}}}\left(\frac{v_F}{a}\right). \qquad (12)$$

As long as $0 \le m < 2$ meV is satisfied for $a \sim a_{\text{Hc}}$, $M_\pi < M_F$ holds so that the π exciton is the lightest mode in the system. The relation, $M_\pi \propto \sqrt{m}$, is similar to the GOR relation for the pion obtained from current algebra in QCD.[6,15] Indeed, the axial Ward-Takahashi identity for the present system is $\langle [\partial_\mu J_\mu^{\text{axial}}(x) - 2mP(x)]P(y) - 2M(y)\delta_{xy}\rangle = 0$ with the axial current $J_\mu^{\text{axial}}(x) \equiv \frac{i}{2}\epsilon(x)[V_\mu^-(x) - V_\mu^+(x)]$ and the pseudoscalar density $P(x) \equiv i\epsilon(x)M(x)$. Saturating this identity by the π exciton and using Eq. (12),[6] we obtain, in the leading order of m,

$$(F_\pi^\tau M_\pi)^2 = m\sigma, \quad F_\pi^\tau = \sigma a^2 (8v_F a)^{-1/2}, \qquad (13)$$

where σ takes the value in the chiral limit ($m=0$) and the temporal "pion-decay constant" F_π^τ is defined by the matrix element, $\langle 0|J_4^{\text{axial}}|\pi\rangle = 2F_\pi^\tau \omega_\pi$. The dispersion relation for the π exciton is also obtained from Eq. (11). At low momentum with $\beta=m=0$, we have $\omega_\pi \simeq v_\pi|\mathbf{p}|$ with the pion velocity $v_\pi = 4.69v_F = 0.0141$. As for the mass of the σ exciton, we obtain $M_\sigma \simeq (1.30 - 0.47\beta)(v_F/a) + 22.6m$ by solving $D_{\phi_\sigma}^{-1}(\mathbf{0}, iM_\sigma/v_F) = 0$. This is comparable to the cutoff energy scale of the present lattice, $E_\Lambda \equiv v_F(\pi/a)$. Thus the result is not universal unlike the π-exciton case and analogous to the situation for the broad σ meson in QCD.[6] Shown in Fig. 3 is a qualitative summary of the spectra of the fermion and collective excitations obtained in this study.

As shown in Refs. 12, 23, and 24, one may employ a noncompact formulation of the gauge action, $S_G^{(\text{NC})} = \frac{1}{2g_*^2}\sum_{x^{(4)}}\sum_{j=1,2,3}[\theta(x) - \theta(x+\hat{j})]^2$ in order to avoid anomalous phase transition from magnetic monopole condensation.[25] Within the NLO, we find that the noncompact results are obtained by the rescaling, e.g., $\sigma^{(\text{NC})}(\beta) = \sigma^{(\text{C})}(2\beta) + O(\beta^2)$. Our relations $\sigma^{(\text{NC})}(\beta=0) = \sigma^{(\text{C})}(\beta=0)$ and $\sigma^{(\text{NC})}(\beta) < \sigma^{(\text{C})}(\beta)$ in the strong coupling region are consistent with the recent lattice Monte Carlo simulations.[24]

In this Rapid Communication, we performed an analytical study of the monolayer graphene in the strong coupling regime of U(1) lattice gauge theory. An effective action at zero temperature for the Dirac quasiparticles is derived up to next-to-leading order of the strong coupling expansion. Dynamical breaking of chiral symmetry and associated formation of a chiral gap are found. We showed that the π exciton (similar to the pion in QCD) behaves as a pseudo-Nambu-Goldstone boson in the strong coupling regime. A mass formula for the π-exciton analogous to the Gell-Mann-Oakes-Renner relation in QCD is derived. If the GOR-type mass formula of the π exciton can be experimentally confirmed, e.g., through transport phenomena, it would be a good evidence for the dynamical chiral symmetry breaking in monolayer graphene.

There are numerous problems to be examined in the future. Generalization of our approach with the tadpole improvement[23,24] can be performed. To study the renormalization effect on v_F, we need to consider the excitonic fluctuations acting on Dirac quasiparticles. These fluctuations are also important for thermal phase transition of graphene from insulator to semimetal. To study universal low-energy behavior of the graphene, it would be useful to construct a chiral effective theory for light π excitons, a noncovariant analog of the chiral perturbation theory in QCD.[26] To be more faithful to the U(4) chiral symmetry at low energies in Eq. (1), we should employ lattice gauge theory with domain-wall or overlap fermion. Finally, to study multilayer graphene, where the interlayer electron hopping depends on how the layers are stacked, it would be important to develop a lattice gauge theory preserving the original honeycomb structure.

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