PROCEEDINGS OF SCIENCE

Chiral symmetry of graphene and strong coupling lattice gauge theory

Yasufumi Araki[*(a)] **and Tetsuo Hatsuda**[(a,b)]
[(a)] *Department of Physics, The University of Tokyo, Tokyo 113-0033, Japan*
[(b)] *Institute for the Physics and Mathematics of the Universe (IPMU), The University of Tokyo, Chiba 277-8568, Japan*
E-mail: araki@nt.phys.s.u-tokyo.ac.jp, hatsuda@phys.s.u-tokyo.ac.jp

We model the electrons on a monolayer graphene in terms of the compact and non-compact U(1) lattice gauge theories. The system is analyzed by the strong coupling expansion and is shown to be an insulator due to dynamical gap formation in/around the strong coupling limit. This is similar to the spontaneous chiral symmetry breaking in strong coupling gauge theories. The results from the compact and non-compact formulations are compared up to the next-to-leading order of the strong coupling expansion. Excitonic modes and their dispersion relations in the insulating phase are also investigated: it is found that there arises a pseudo-Nambu–Goldstone mode obeying the Gell-Mann–Oakes–Renner type formula.

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[*]Speaker.

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1. Introduction

After its first experimental discovery in 2004 [1], graphene (monoatomic layer material of carbon atoms) has widely attracted theoretical and experimental attention [2]. Due to its hexagonal lattice structure, charge carriers on a graphene reveal a linear dispersion relation around two "Dirac points" in momentum space [3], so that quasiparticles at low energies can be described as two species of massless Dirac fermions in (2+1)-dimensions [4]. The symmetry between two triangular sublattices of graphene is referred to as the "chiral symmetry".

In the low-energy effective theory of graphene, the effective Coulomb interaction between charge carriers is enhanced by 300 times due to the small Fermi velocity v_F. Such a strong Coulomb interaction may turn a suspended graphene in the vacuum from semimetal to insulator by the formation of a finite spectral gap of quasiparticles [5]. This mechanism is similar to the spontaneous chiral symmetry breaking and associated fermion mass generation in quantum chromodynamics (QCD). Various attempts have been made so far to study the gap formation in monolayer graphene by using the Schwinger–Dyson equation [6, 7, 8], the $1/N$ expansion [9, 10, 11], the exact renormalization group [12], and the lattice Monte Carlo simulations [13, 14, 15, 16]. These works are mainly focused on the critical region of semimetal-insulator transition or on the behavior for large number of flavors.

In this work, we rather focus on the strong coupling region of the system and study the low-energy effective theory discretized on a square lattice [18, 19]. By using the strong coupling expansion of the compact and non-compact formulations of the gauge field, we study the gap formation due to the spontaneous "chiral symmetry" breaking as well as the dispersion relations for collective excitations. Typical energy scale of the emergent excitations are also estimated with the use of the intrinsic length scale of the original honeycomb lattice.

2. Low-energy effective theory of graphene

2.1 Effective action in the continuum limit

With the annihilation operators of the electrons on the two triangular sublattices of graphene (a_σ and b_σ) near the two Dirac points $\mathbf{K}_\pm$, we can construct a 4-component spinor in the momentum space, $\psi_\sigma(\mathbf{p}) \equiv (a_\sigma(\mathbf{K}_+ + \mathbf{p}), b_\sigma(\mathbf{K}_+ + \mathbf{p}), b_\sigma(\mathbf{K}_- + \mathbf{p}), a_\sigma(\mathbf{K}_- + \mathbf{p}))^T$. Here $\sigma = \uparrow, \downarrow$ denotes the original spin of the electrons. The Euclidean effective action for graphene is then written as [7, 10]

$$S_E = \sum_\sigma \int dx^{(3)}\ \bar{\psi}_\sigma \left(D[A] + m\right) \psi_\sigma + \frac{1}{2g^2} \sum_{j=1,2,3} \int dx^{(4)} (\partial_j A_4)^2, \tag{2.1}$$

where the Dirac operator reads $D[A] = \gamma_4(\partial_4 + iA_4) + v_F \sum_{i=1,2} \gamma_i \partial_i$. This is analogous to the action in "reduced QED" [20], in which the fermion ψ in (2+1)-dimensions is interacting with the U(1) gauge field A in (3+1)-dimensions. The Hermitian γ matrices obey the anticommutation relation $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$. The gauge coupling constant is defined by $g^2 = 2e^2/\varepsilon_0(1+\varepsilon)$, with the electric charge e, the dielectric constant of vacuum ε_0, and the dielectric constant of substrate ε. Due to the small Fermi velocity of quasiparticles, $v_F = 3.02 \times 10^{-3}$, one may adopt the "instantaneous approximation" in which the spatial component $\mathbf{A}$ is neglected. From the absence of the z-component in

the Dirac operator, this model possesses a continuous global U(4) symmetry generated by 16 generators $\{1,\gamma_3,\gamma_5,\gamma_3\gamma_5\}\otimes\{1,\vec{\sigma}\}$, which is the extension of the continuous U(1) charge symmetry and the discrete Z_2 sublattice exchange symmetry of the original honeycomb lattice. The explicit chiral symmetry breaking term is represented by the mass m in Eq.(2.1).

After performing the scale transformation in the temporal direction, $x_4 \to x_4/v_F$, $A_4 \to v_F A_4$, the Dirac operator becomes independent of v_F. This scale transformation changes the mass m into the effective mass $m_* = m/v_F$, while the Coulomb coupling strength is enhanced as $g_*^2 = g^2/v_F$ which is about 300 times larger than that of QED. Since the inverse effective coupling strength $\beta = 1/g_*^2$ is 0.0369 in the vacuum-suspended graphene, the expansion by β (strong coupling expansion) would work well.

2.2 Regularization on a square lattice

We discretize the low energy action Eq.(2.1) on a square lattice with a lattice spacing a. Since the original honeycomb lattice has a lattice spacing $a_{\rm Hc} \sim 1.4$Å, we make an approximate identification, $a \sim a_{\rm Hc}$, so that we can carry out the strong coupling expansion. The quasiparticles in monolayer graphene are described with a single staggered fermion χ, because its eight doublers can be identified as 4(spinor components) $\times$ 2(spin) degrees of freedom. As a consequence, the lattice action for fermions on graphene is written as [14]

$$S_F = \sum_{x^{(3)}} \left[\frac{1}{2} \sum_{\mu=1,2,4} \left(V_\mu^+(x) - V_\mu^-(x) \right) + m_* M(x) \right] \tag{2.2}$$

with fermionic bilinears $M(x) = \bar{\chi}(x)\chi(x), V_\mu^+(x) = \eta_\mu(x)\bar{\chi}(x)U_\mu(x)\chi(x+\hat{\mu}), V_\mu^-(x) = \eta_\mu(x)\bar{\chi}(x+\hat{\mu})U_\mu^\dagger(x)\chi(x)$, where $\mu = 1,2,4$. The staggered phase factors η_μ corresponding to the Dirac γ-matrices are $\eta_4(x) = 1, \eta_1(x) = (-1)^{x_4}, \eta_2(x) = (-1)^{x_4+x_1}$. U_μ is the U(1) link variable, where the temporal link is defined as $U_4(x) = \exp[i\theta(x)]$ $(-\pi \le \theta < \pi)$, while the spatial links $U_{1,2,3}$ are set to unity as a result of the instantaneous approximation. In the staggered fermion formulation, the global chiral symmetry U(4) shrinks to $\mathrm{U(1)_V} \times \mathrm{U(1)_A}$, with the ordinary $\mathrm{U(1)_V}$ charge symmetry, and the axial $\mathrm{U(1)_A}$ symmetry generated by $\varepsilon(x) \equiv (-1)^{x_1+x_2+x_4}$.

As for the pure gauge action, we consider two types of formulation. One is the compact formulation which consists of plaquettes made of U(1) compact link variables:

$$S_G^{(\mathrm{C})} = \beta \sum_{x^{(4)}} \sum_{j=1,2,3} \left[1 - \mathrm{Re}\left(U_4(x) U_4^\dagger(x+\hat{j}) \right) \right]. \tag{2.3}$$

The other is the non-compact formulation with the gauge angle θ:

$$S_G^{(\mathrm{NC})} = \frac{\beta}{2} \sum_{x^{(4)}} \sum_{j=1,2,3} \left[\theta(x) - \theta(x+\hat{j}) \right]^2. \tag{2.4}$$

The compact formulation has photon self-interactions which are absent in the non-compact formulation and in the continuum theory.

3. Strong coupling expansion

Expanding the partition function Z by the inverse coupling strength β and integrating out the link variables order by order, we obtain the effective action S_χ in terms of fermions [17]:

$$Z = \int [d\chi d\bar{\chi}][d\theta] \left[\sum_{n=0}^{\infty} \frac{(-S_G)^n}{n!} e^{-S_F} \right] = \int [d\chi d\bar{\chi}] e^{-S_\chi}. \tag{3.1}$$

Since the link integration selects the terms in which the link variable cancel with its complex conjugate, various 4-fermi interaction terms are induced as shown in Fig.1. With the compact formulation, we obtain the leading order (LO) and the next-to-LO (NLO) effective action, $S_\chi^{(0)}$ and $S_\chi^{(1)\mathrm{C}}$ respectively, as

$$S_\chi^{(0)} = \sum_{x^{(3)}} \left[\frac{1}{2} \sum_{j=1,2} \left(V_j^+(x) - V_j^-(x) \right) + m_* M(x) \right] - \frac{1}{4} \sum_{x^{(3)}} M(x) M(x+\hat{4}), \tag{3.2}$$

$$S_\chi^{(1)\mathrm{C}} = \frac{\beta}{8} \sum_{x^{(3)}} \sum_{j=1,2} \left[V_j^+(x) V_j^-(x+\hat{4}) + V_j^-(x) V_j^+(x+\hat{4}) \right]. \tag{3.3}$$

Since the pure gauge term S_G vanishes in the strong coupling limit ($\beta = 0$), the compact formulation and the non-compact one give the same result in the LO. In the NLO, the effective action from the non-compact formulation, $S_\chi^{(1)\mathrm{NC}}$, is twice that from the compact one, $S_\chi^{(1)\mathrm{C}}$, so that observables of the both formulations are related as $\mathscr{O}^{\mathrm{NC}}(\beta) = \mathscr{O}^{\mathrm{C}}(2\beta)$.

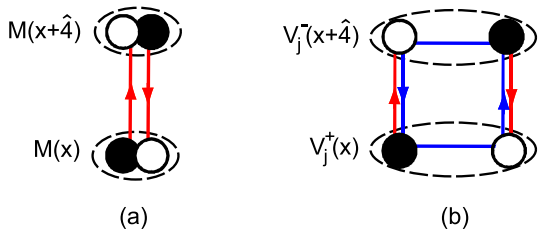

Figure 1: Induced four-fermion interaction in the strong coupling expansion. The open and filled circles represent fermion fields χ and $\bar{\chi}$, respectively. (a) In the LO, the time-like links (red arrows) in the fermion action S_F cancel with each other to leave a spatially local interaction. (b) In the NLO, the time-link links in S_F are canceled by the time-like links in a plaquette S_G (blue arrows) to leave a spatially non-local interaction.

In order to linearize the induced 4-fermi terms and to integrate out the fermions, we introduce complex bosonic auxiliary fields by the Stratonovich–Hubbard transformation. As for the LO 4-fermi terms in Eq.(3.2), we introduce an auxiliary field $\phi(x) = \phi_\sigma(x) + i\varepsilon(x)\phi_\pi(x)$. Another auxiliary field $\lambda = \lambda_1 + i\lambda_2$ is introduced to linearize the NLO terms in Eq.(3.3); the mean field value of λ is determined by requiring the stationary condition of the effective action. Then we arrive at the LO and the NLO effective potential (free energy) written in terms of ϕ as

$$F_{\mathrm{eff}}^{(0)}(\phi) = \frac{1}{4}|\phi|^2 - \frac{1}{2} \int_{\mathbf{k}} \ln \left[G^{-1}(\mathbf{k};\phi) \right], \tag{3.4}$$

$$F_{\mathrm{eff}}^{(1)\mathrm{C}}(\phi) = -\frac{\beta}{4} \sum_{j=1,2} \left[\int_{\mathbf{k}} G(\mathbf{k};\phi) \sin^2 k_j \right]^2. \tag{3.5}$$

with the bosonic effective propagator defined as $G^{-1}(\mathbf{k};\phi) \equiv |\phi/2 - m_*|^2 + \sum_{j=1,2} \sin^2 k_j$ and the momentum integration as $\int_{\mathbf{k}} \equiv (2\pi)^{-2} \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2$. Fig.2 shows $F_{\rm eff}^{(0)}$ in the chiral limit ($m = 0$): Its minimum corresponds to the chiral condensate (the order parameter of chiral symmetry breaking) $\sigma \equiv |\langle \bar{\chi}\chi \rangle| = |\langle \phi \rangle|$, so that the spontaneous "chiral symmetry" breaking takes place in the strong coupling limit. The effective mass of fermions reads $M_F = m + (v_F/a)(\sigma a^2/2)$, from the mass term of the effective action.

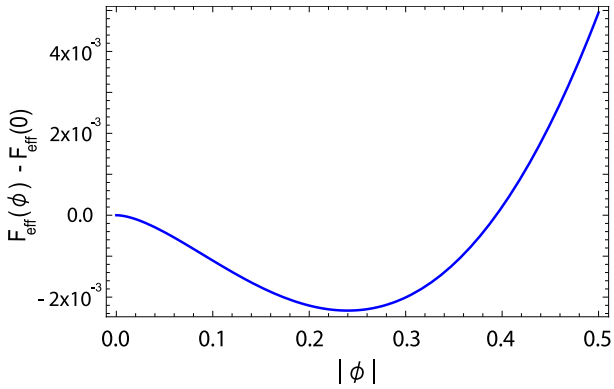

Figure 2: The free energy in the strong coupling limit, $F_{\rm eff}^{(0)}(\phi)$, in the lattice unit as a function of $|\phi|$, in the chiral limit ($m = 0$).

Since $F_{\rm eff}^{(1)}$ is an increasing function of $|\phi|$, the chiral condensate σ drops as β grows. In other words, the chiral symmetry tends to be restored as the coupling strength becomes weaker. Up to the linear terms in β and m, we can calculate σ with the compact formulation as

$$\sigma^{\rm C}(\beta, m) \simeq (0.240 - 0.297\beta + 0.0239\, ma)a^{-2}, \tag{3.6}$$

As we mentioned, the condensate in the non-compact formulation is simply obtained as $\sigma^{\rm NC}(\beta) = \sigma^{\rm C}(2\beta)$ up to NLO. The behavior that $\sigma^{\rm NC}(\beta)$ drops faster than $\sigma^{\rm C}(\beta)$ is consistent with the results of the Monte Carlo simulation for the same lattice model [16]. Taking $a^{-1} \simeq a_{\rm Hc}^{-1} = 1.39$ keV as a typical cutoff scale of our system, we obtain $\sigma^{\rm C}(\beta, m) \simeq \left[\left(0.680 - 0.421\beta + \frac{1.39\, m}{\rm eV}\right) {\rm keV}\right]^2$. The dynamical fermion mass is estimated from the value of the chiral condensate as $M_F \simeq (0.523 - 0.623\beta)$ eV $+ 3.05m$, which is much smaller than the momentum cutoff scale $E_\Lambda \sim \pi v_F/a = 13$eV of the original honeycomb lattice as long as the bare mass m is small enough.

4. Collective Excitations

Here we study the fluctuations of the order parameter $\phi(x)$ around the symmetry broken state $\langle \phi \rangle = -\sigma$: the phase fluctuation ("π-exciton") corresponds to $\phi_\pi(x)$ and the amplitude fluctuation ("σ-exciton") corresponds to $\phi_\sigma(x)$. Propagators of those modes, $D_{\phi_{\sigma,\pi}}$ are derived from the second derivative of the effective action $S_{\rm eff}[\phi]$ with respect to the corresponding fields $\phi_{\sigma,\pi}$. Their excitation energies are obtained from the imaginary pole of the propagator, $D_{\phi_{\sigma,\pi}}^{-1}(\mathbf{p} = 0, \omega = iM_{\sigma,\pi}/v_F) = 0$.

As for the π-exciton, we obtain a mass formula in the leading order of m as

$$M_\pi \simeq \frac{2v_F}{a}\sqrt{\frac{m}{M_F(m=0)}}. \tag{4.1}$$

Since M_π vanishes in the chiral limit ($m = 0$), this mode serves as a pseudo-Nambu–Goldstone (NG) boson emerging from the spontaneous breaking of chiral symmetry. From the axial Ward–Takahashi identity corresponding to the infinitesimal local chiral transformation, a simple relation can be derived, $(F_\pi^\tau M_\pi)^2 = m\sigma$, which is analogous to the Gell-Mann–Oakes–Renner relation for the pion in QCD [21]. Here the temporal "pion decay constant" F_π^τ is defined by the matrix element, $\langle 0|J_4^{\rm axial}(0)|\pi(p)\rangle = 2F_\pi^\tau p_\pi^\tau$, with the axial current $J_\mu^{\rm axial}(x) \equiv \frac{i}{2}\varepsilon(x)\left[V_\mu^-(x) - V_\mu^+(x)\right]$.

By solving the pole equation numerically, the σ-exciton is found to be a massive mode with $M_\sigma \simeq (1.30 - 0.47\beta)(v_{_F}/a) + 22.6m$. Since M_σ acquires a large value comparable to the cutoff scale E_Λ, application of the low-energy effective theory in this channel is not quite justified.

5. Conclusion

We have investigated the behavior of monolayer graphene analytically in/around the limit of strong Coulomb coupling, by means of the strong coupling expansion of U(1) lattice gauge theory. As for the pure gauge action, we have compared the results from the compact and non-compact formulations. In either case, we find that "chiral symmetry" (the sublattice exchange symmetry in the original honeycomb lattice) is spontaneously broken in the strong coupling limit with equal magnitude of the chiral condensate. As the coupling strength becomes weaker, chiral condensate from the non-compact formulation drops faster than that from the compact one. These results up to NLO in the strong coupling expansion agree qualitatively with the extrapolation of the numerical results of the lattice Monte Carlo simulations.

We have also examined the collective excitations associated with the chiral symmetry breaking in our approach and have derived their dispersion relations. The phase fluctuation of the chiral condensate, the "π-exciton", behaves as a pseudo-NG boson, like the pion in QCD. Experimental observation of such mode in vacuum-suspended graphene would be a good evidence for the spontaneous chiral symmetry breaking in the strong coupling regime. The amplitude fluctuation of the chiral condensate, the "σ-exciton," acquires a large mass comparable to the intrinsic cutoff scale E_Λ, so that it needs further investigation without the low-energy approximation.

There are several directions to be investigated in future: Behavior of the present model on a square lattice at finite temperature and finite chemical potential still remains an open problem both analytically and numerically. Formulating the strong coupling expansion on a honeycomb lattice would be of great importance. Extension of our strong coupling approach to the analysis of bilayer graphene, which has been attracting attentions recently [22], would be also of interest.

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