Spontaneous mass gap generation in monolayer graphene with strong coupling expansion of square/honeycomb lattice gauge theory

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Abstract. Sublattice symmetry of the honeycomb lattice of monolayer graphene, which can be extended to a continuous chiral symmetry of Dirac fermions in the continuum limit, may be spontaneously broken due to effectively strong Coulomb interaction between electrons on the vacuum-suspended graphene. We analyze this mechanism by strong coupling expansion of lattice gauge theory, which is constructed with the original honeycomb lattice structure. Spontaneous sublattice symmetry breaking in the strong coupling limit is shown, and is compared with the result obtained from the square lattice formulation qualitatively and quantitatively. We also introduce the Kekulé distortion of the honeycomb lattice externally, and show a restoration of the sublattice symmetry at finite distortion amplitude.

1. Introduction
Since its first experimental isolation in 2004 [1], graphene, a 2-dimensional electron system easy to design and observe, has become one of the most active research areas [2]. Monolayer graphene behaves as a semimetal at half-filling, where its charge carriers (quasiparticles) can be described as massless Dirac fermions with a small Fermi velocity [3, 4]. Since the Coulomb interaction between the charged quasiparticles is effectively enhanced by such a small Fermi velocity, exciton condensate may be created and the system may become an insulator in vacuum, where the Coulomb interaction is unscreened. This mechanism is similar to the spontaneous breaking of chiral symmetry, which is a continuous extension of the sublattice symmetry of honeycomb lattice, in the strong coupling gauge theory such as quantum chromodynamics (QCD). Making use of this analogy, it has been studied via various approaches [5]. In our previous work, this mechanism has been verified around the strong coupling limit by the techniques of strong coupling expansion of lattice gauge theory, with an effective model regularized on the square lattice [6].

In this work, we study the mechanism of spontaneous breaking of sublattice symmetry by strong coupling expansion, preserving the exact honeycomb lattice structure of graphene. Results from the honeycomb lattice formulation and the square lattice formulation are compared qualitatively and quantitatively, and the validity of the linear dispersion approximation is discussed. We also investigate the behavior of the system in the presence of external lattice distortion (Kekulé distortion), which can be introduced by external materials or addition of atoms on the layer. Restoration of the sublattice symmetry is shown, at finite distortion amplitude.
2. Strong coupling expansion on the honeycomb lattice

In order to construct an effective lattice gauge theory model of graphene with the original lattice structure, we start from the conventional tight-binding Hamiltonian [3]

\[ H = \hbar \sum_{r \in A} \sum_{i=1,2,3} \left[ a^\dagger(r) b(r + s_i) + b^\dagger(r + s_i) a(r) \right], \]  

with the nearest-neighbor hopping amplitude \( \hbar \). Here, \( a^\dagger(a) \) and \( b^\dagger(b) \) denote creation (annihilation) operators on the triangular sublattices A and B respectively. \( s_i \) \((i = 1, 2, 3)\) corresponds to the relative position between two neighboring sites, where the lattice spacing \( a_{\text{hc}} \equiv |s_i| = 1.42\angstrom \). Its energy eigenvalue \( E(k) = \pm \hbar |\Phi(k)| \), with \( \Phi(k) \equiv \sum_{i=1,2,3} e^{ik\cdot s_i} \), vanishes at two points \( \mathbf{K}_\pm \) in the momentum space, which are called “Dirac points”. The dispersion relation around the Dirac points is gapless and linear in the leading order of momentum, with the Fermi velocity \( v_F = (3/2) a_{\text{hc}} \hbar \) about 300 times smaller than the speed of light. In Lagrangian formalism, we can construct an Euclidean action from the tight-binding Hamiltonian in Eq.(1), which is spatially discrete and temporally continuous, with the temporal scale transformation \( \tau \rightarrow \tau^t/v_F \), as done in Ref.[6]. By discretizing the temporal kinetic term with lattice spacing \( a_{\tau}(\sim a_{\text{hc}}) \) and requiring local U(1) gauge invariance, we obtain a “gauged” honeycomb lattice model [7]

\[ S_F = \frac{1}{2} \sum_{r \in A, r'} \left[ a^\dagger(r, \tau') U_{r'}(r, \tau') a(r, \tau' + a_{\tau}) - \text{H.c.} \right] + \frac{1}{2} \sum_{r \in B, r'} \left[ b^\dagger(r, \tau') U_{r'}(r, \tau') b(r, \tau' + a_{\tau}) - \text{H.c.} \right] + \frac{a_{\tau} \hbar}{v_F} \sum_{r \in A, \tau' \in 1,2,3} \left[ a^\dagger(r, \tau') U_i(r, \tau') b(r + s_i, \tau') + b^\dagger(r + s_i, \tau') U_i^\dagger(r, \tau') a(r, \tau') \right], \]  

where the U(1) link variables read \( U_{r'}(r, \tau') = \exp \left[ ie \int_{r'}^{r' + a_{\tau}} d\tau' A_i \right] \) and \( U_i(r, \tau') = \exp \left[ ie \int_{r'}^{r + s_i} d\tau' \cdot A \right] \), with \( e \) being the electric charge. As a result of discretization, a pair of fermion doublers are generated in the temporal direction, which we identify here as spin (up/down) degrees of freedom. Since the electromagnetic field propagates much faster than the fermions (quasiparticles), we can neglect the retardation (magnetic) effect of the electric field. Therefore, here we set the spatial link variables \( U_i \) to be unity, which is referred to as “instantaneous approximation”.

The kinetic term of the gauge field, \( S_G \), is proportional to the inverse effective coupling strength \( \beta = \epsilon_0 v_F / e^2 \), where \( \epsilon_0 \) is the dielectric constant of vacuum. Since the value of \( \beta \) is 0.037 in the vacuum-suspended graphene, where the Coulomb interaction is unscreened, we expect that the strong coupling expansion by \( \beta \) works well. In this work, we only consider the leading order in the strong coupling expansion, so that the gauge term \( S_G \) does not need to be taken into account. By integrating out the link variables first in the path integral, we obtain the effective action \( S_X \) only in terms of fermions. Since the U(1) link integration drops the terms in which a link variable is not canceled by its complex conjugate, 4-fermi coupling terms, which

Figure 1. The free energy per one pair of A- and B-sites in the strong coupling limit, \( F_{\text{eff}}^{(0)}(\sigma) \), as a function of \( \sigma \). “Honeycomb” shows \( F_{\text{eff}}^{(0)}(\sigma) \) in Eq.(3) with the exact form of \( \Phi(k) \). “Linear” shows \( F_{\text{eff}}^{(0)}(\sigma) \) in Eq.(3) with the linear approximation \( \Phi(k) \approx (3/2)(\pm k_x + ik_y) \). “Square” shows the effective potential obtained by the strong coupling expansion with the square lattice formulation [6] per four square lattice sites, corresponding to a pair of honeycomb lattice sites.
are local in the spatial directions and non-local by one lattice spacing in the temporal direction, are generated from the temporal hopping terms.

In order to treat these 4-fermi terms analytically, we introduce an auxiliary field $\sigma = \langle a^\dagger a - b^\dagger b \rangle$, which denotes the charge density imbalance between two sublattices. Namely, it serves as the order parameter of sublattice (chiral) symmetry breaking, which is referred to as “chiral condensate” in terms of the continuum effective field theory. By the mean-field approximation over the auxiliary field $\sigma$, integration by fermions can be successfully performed and we obtain the free energy per one pair of A- and B-sites in the strong coupling limit,

$$F_{\text{eff}}^{(0)}(\sigma) = \frac{1}{2} \sigma^2 - \int_{k \in \Omega} d\mathbf{k} \ln \left[ \left( \frac{\sigma}{2} \right)^2 + \left| \frac{a_{\mathbf{k}}^\dagger a_{\mathbf{k}}}{v_F} \Phi(\mathbf{k}) \right|^2 \right],$$

where $\int_{k \in \Omega}$ means 2-dimensional momentum integration over the Brillouin zone $\Omega$. The first term, the tree level effect of $\sigma$, becomes dominant at large $|\sigma|$, while the second term, coming from fermion one-loop effect, becomes dominant around $\sigma = 0$. In Fig.1, we compare $F_{\text{eff}}^{(0)}(\sigma)$ in Eq.(3) with the exact form of $\Phi(\mathbf{k})$. $F_{\text{eff}}^{(0)}(\sigma)$ with $\Phi(\mathbf{k})$ approximated by a linear dispersion around the Dirac points, and $F_{\text{eff}}^{(0)}(\sigma)$ obtained from the square lattice formulation [6]. It is shown that the sublattice symmetry is spontaneously broken in the strong coupling limit, with the inter-sublattice charge density imbalance $\sigma = 0.3429$. Qualitatively, the sublattice symmetry breaking structure does not depend on the lattice formulation or the approximation of dispersion relation. It is because the most dominant singularity emerges from the excitations in vicinity of the Dirac points, which are kept unchanged in any approximations. Quantitative difference in $F_{\text{eff}}^{(0)}(\sigma)$ comes from the higher order terms in momentum, which becomes dominant far from the Dirac points in the momentum space.

3. External Kekulé distortion

Let us introduce a so-called “Kekulé distortion” pattern to the honeycomb lattice as an external field, which is characterized by the alternating pattern of strong and weak bonds, similar to a benzene molecule [8, 9, 10]. It is described by the addition of the direction-dependent hopping amplitude, $\delta h_\mathbf{r}(\mathbf{r}) = (\Delta/3)e^{i\mathbf{G}\cdot\mathbf{r}} + e^{i\mathbf{K}_-\cdot\mathbf{r}}e^{-i\mathbf{G}\cdot\mathbf{r}}$, where $\Delta$ denotes the amplitude of the Kekulé distortion and $\mathbf{G} \equiv \mathbf{K}_+ - \mathbf{K}_-$. Since this distortion pattern is periodic by three times the unit lattice in the real space, the Brillouin zone $\Omega$ is split into three hexagonal regions $\Omega_\pm$ and $\bar{\Omega}$, surrounding the Dirac points $\mathbf{k} = \mathbf{K}_\pm$ and the original point $\mathbf{k} = 0$ respectively. By introducing the electromagnetic field and following the strong coupling expansion in the previous section, fermion one-loop effect in $F_{\text{eff}}^{(0)}$ [the second term in Eq.(3)] is modified by the Kekulé distortion. Here we neglect the terms with the order $O(\frac{\Delta}{\hbar} |\mathbf{k}|)$ and consider $\Phi(\mathbf{k})$ to be linear around the Dirac points in the region $\Omega_\pm$.

If we approximate the hexagonal regions $\bar{\Omega} \equiv \Omega_\pm \cup \Omega$, by the circular regions with the same area respectively [with the radius $\rho = (8\sqrt{3}\pi/27a_{2s}^3)^{1/2}$], the momentum integration can be analytically performed, yielding the effective potential

$$F_{\text{eff}}^{(0)}(\sigma) \approx \frac{\sigma^2}{2} - \frac{4\pi}{\sqrt{3}} \left( \frac{3}{4\pi a_{2s}} \right)^2 \left\{ \left[ \frac{\sigma}{2} \right]^2 + \left( \frac{a_{2s}\Delta}{v_F} \right)^2 + a_{2s}^2 \rho^2 \right\} \ln \left[ \left( \frac{\sigma}{2} \right)^2 + \left( \frac{a_{2s}\Delta}{v_F} \right)^2 + a_{2s}^2 \rho^2 \right].$$

![Figure 2. The order parameter for sublattice symmetry breaking $\sigma$ as a function of the Kekulé distortion amplitude $\Delta$. $\sigma$ gets reduced for larger value of $\Delta$ and vanishes at a critical value $\Delta_C$.](image-url)
\[-\left(\left(\frac{\sigma}{2}\right)^2 + \left(\frac{a_{+}\Delta}{v_F}\right)^2\right) \ln \left(\left(\frac{\sigma}{2}\right)^2 + \left(\frac{a_{+}\Delta}{v_F}\right)^2\right)\right) - \frac{1}{3} \ln \left(\left(\frac{3a_{+}h}{v_F}\right)^2\right)\]. \hspace{1cm} (4)

Since the second term in Eq.(4) is suppressed as \(|\Delta| \to \infty\), fermion one-loop effect becomes less dominant at larger \(|\Delta|\). It can be seen that the potential minimum reaches to \(\sigma = 0\) as the distortion amplitude \(|\Delta|\) increases, and finally vanishes at the finite value \(|\Delta_C|\). As seen from Fig.2, this is the second-order phase transition with the mean-field exponent \(z = 1/2\), where \(\sigma \propto |\Delta - \Delta_C|^z\) around \(\Delta = \Delta_C\).

4. Conclusion

In this work, we have shown the behavior of the sublattice symmetry of monolayer graphene analytically at the strong coupling limit of the Coulomb interaction. We have constructed a lattice Euclidean action including the electromagnetic field from the conventional tight-binding Hamiltonian defined on the honeycomb lattice. With the strong coupling expansion techniques of lattice gauge theory, we have derived the effective potential of the system as a function of the charge density imbalance between two sublattices, and have shown that the sublattice symmetry is spontaneously broken at the strong coupling limit. The structure of spontaneous breaking of the sublattice symmetry is same as that shown from the square lattice formulation [6], but they have a certain quantitative difference due to the higher order corrections in momentum neglected in the continuum effective theory.

We have also investigated the effect of external lattice distortion (Kekulé distortion) on the sublattice symmetry. In presence of external Kekulé distortion, we have shown that the spontaneous breaking of the sublattice symmetry gets suppressed and vanishes at a finite distortion amplitude. Since both the sublattice symmetry breaking and the Kekulé distortion generate a spectral gap, the sublattice symmetry gets restored although the gap remains finite at large distortion amplitude. It may be interesting to compare our results with Ref.[10], which concludes that the electron self-energy is independent of Kekulé distortion at large momentum.

Since the effect of Kekulé distortion is studied with the linear dispersion approximation in this work, quantitative accuracy may not be reliable according to the first part of this work, although qualitative symmetry breaking structure can be checked even with such an approximation. Quantitative investigation should be performed with the exact dispersion relation within the whole Brillouin zone. Moreover, higher order corrections in the strong coupling expansion should also be taken into account with the exact honeycomb lattice structure.

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