Chiral symmetry breaking in lattice QED model with fermion brane

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Abstract

We propose a novel approach to the Graphene system using a local field theory of 4 dimensional QED model coupled to 2+1 dimensional Dirac fermions, whose velocity is much smaller than the speed of light. Performing hybrid Monte Carlo simulations of this model on the lattice, we compute the chiral condensate and its susceptibility with different coupling constant, velocity parameter and flavor number. We find that the chiral symmetry is dynamically broken in the small velocity regime and obtain a qualitatively consistent behavior with the prediction from Schwinger-Dyson equations.

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I. INTRODUCTION

The graphene material which is composed of two-dimensional carbon atomic seat has attracted much attention from its specific property [1]. The high conductivity of Graphene has understood by the analogical picture to “relativistic” massless Dirac fermion (quasiparticle) bounded in 2+1 dimension which has been derived in based on tight-binding (TB) model at low energy [2, 3]. In the effective model with massless Dirac fermion, compared with quantum electromagnetic dynamics (QED) in particle physics, the velocity of fermion is 2-orders magnitude smaller than the speed of light [2, 3]. Recent experiments suggest that this magnitude may be changed by a factor [4] due to significant quantum corrections. The spontaneous gap generation at semimetal-insulator transition point (Mott transition) of Graphene has been predicted by Schwinger-Dyson equation and large N model [5–10] in the presence of Coulomb interaction between Dirac fermion before Graphene confirmed in experiments so far, however experimentally there has been no conclusive evidence that semimetal-insulator transition of suspended monolayer Graphene occurs in low temperature even in 20 K [11] (as opposed to this bilayer Graphene posses energy gap structure [12, 13]). It may be that the model is missing an important feature of the dynamics or that the approximations used for the theoretical prediction lead a wrong conclusion. In order to clarify this point it is necessary to carry out an exact calculation based on a solid theoretical approach.

The above effective Dirac fermion system possesses chiral symmetry which could be spontaneously broken by strong effective Coulomb interaction due to enlarged effective fine structure constant \( \alpha_e = e^2/(4\pi v_F) \simeq 2.2 \) at small velocity \( v_F \simeq 1/300 \) estimated as \( v_F = 3ta/2 \) [2] in the natural unit. Here, \( t \) denotes leading hopping parameter of TB model and \( a \) denotes distance among the nearest-neighboring carbon atoms. The semimetal-insulator transition of Graphene is considered as a consequence of the energy gap generation in the phase of chiral symmetry breaking (\( \chi \)SB). This is analogous with the mass-gap generation in 2+1 dimension QED system suggested in 1/N expansion [14], Schwinger-Dyson equation [15] 20 years ago and also several attempts with Monte-Carlo simulation in non-Compact lattice QED [16–18]. However, the present system possesses crucially different points from the 2+1 dimension QED system. Firstly the quasiparticle has different velocity from speed of light in spatial 2 dimension brane and secondly there is Coulomb interaction in spatial 3 dimension but not in spatial 2 dimension. The condensate for scalar bilinear operator \( \langle \bar{\psi}\psi \rangle \) is also as
an order parameter of $\chi_{SB}$ at low temperature in this QED system.

Note that “chiral” symmetry in 2+1 dimension system is defined for the four component Dirac spinor. According to reference [19], four component Dirac spinor is conventionally described as $\psi = (\psi^A, \psi^B)$ where $\psi^{A,B}$ denotes electron wave function (Bloch state) located on sublattices (A,B) in hexagonal Graphene lattice and two independent energy grand points (valleys) $(\pm)$. The subscript means the spin indices of electron. In this notation the chirality of quasiparticle corresponds to valley indices which can be distinguished by $\gamma_5$ projection as well as the particle physics. The gamma matrix is given by tensor structure as $\gamma_0 = \sigma_0 \otimes I_{2 \times 2}$, $\gamma_i = -i \sigma_2 \otimes \sigma_i (i = 1,2,3)$ and $\gamma_5 = i \gamma_0 \gamma_1 \gamma_2 \gamma_3$ constructed by spin and sublattice-valley indices. In the case of monolayer Graphene, chiral symmetry can be regarded as global “flavor” $U(4)$ symmetry of quasiparticle whose generator is given by $\{1, \gamma_5, i \gamma_3, [\gamma_3, \gamma_5]/2\}$ in which the first group generates the rotation operator for sublattice and valley points and second one generates spin rotation (in general multilayer Graphene is described in $U(2N_f)$ symmetry by taking account of layer number $N_{layer}$ as flavor $N_f = N_{spin} \times N_{layer}$ assuming there is no interaction between layers). Using the electron wave function the chiral condensate can be expanded into

$$\langle \bar{\psi} \psi \rangle = \sum_{\sigma} \int [\bar{\psi}_A \psi_B + \bar{\psi}_B \psi_A + h.c.]$$ (1)

which is indeed mixture of different chirality of Graphene [19].

In the leading order of extended TB model into “non-relativistic” QED including Coulomb interaction between quasiparticle, there have been many model calculations of chiral condensate near critical point. For example, the Schwinger-Dyson equation predicts that there is a critical coupling $\alpha_c$ above which the system has a nonzero condensate. In the mean-field approximation, $\alpha_c$ is predicted to be $\alpha_c = 0.5$ [20]. When one-loop vacuum polarization effect is taken into account, the gap equation provides stronger critical coupling $\alpha_c = 0.92$ [8]. The similar critical value has been also obtained by lattice calculation in the Monte-Carlo simulation [21, 22] or strong coupling expansion [23] using “non-relativistic” QED action.

In this paper we propose a new strategy for non-perturbative study of the semimetal-insulator transition of Graphene with QED model. The important difference from the framework of “non-relativistic” QED is that we consider QED action manifestly including both gauge invariant interaction and velocity contribution in the framework of local field theory. In our realistic setup it is possible to rigorously investigate the velocity contribution to $\chi_{SB}$
phomena and compare to actual Graphene. We numerically show that critical behavior when changing velocity and flavor number is qualitatively consistent with Schwinger-Dyson equation.

This paper is organized as the follows: In section II we explain the model of relativistic QED action with fermion brane and in section III we show the detail of setup of our lattice action and simulation. In section IV we show the behavior of chiral condensate and susceptibility when changing the parameters of coupling constant, fermion mass, velocity and flavor number. In section V we summarize and discuss the future works.

II. MODELING THE RELATIVISTIC QED

In the graphene system, since the velocity of the effective Dirac fermion is extremely small, the following action with only the instantaneous Coulomb interaction has been adopted [24]:

\[
S_{\text{Coulomb}} = \int dt d^2 x \bar{\psi} \left[ i \partial_t \gamma_t + i v_F (\partial_x \gamma_x + i \partial_y \gamma_y) \right] \psi + \int dt d^3 x' \bar{\psi} \psi(t, x) \frac{e^2}{8\pi} \frac{\delta(t - t')}{|x - x'|} \gamma_t \psi(t, x').
\]

Introducing the scalar potential \( \phi \) as an auxiliary field, one could equivalently describe the action as

\[
S_{\text{NR}} = \frac{1}{2e^2} \int dt d^3 \vec{E}^2 + \int dt d^2 x \bar{\psi} \left[ i \partial_t + i \phi \right] \gamma_t + i v_F (\partial_x \gamma_x + \partial_y \gamma_y) \psi,
\]

where \( E \equiv -\nabla \phi \).

QED action with fermion bounded on 2+1 dimensional “brane” under gauge invariance in the continuum theory is straightforwardly written as

\[
S = \frac{\beta}{2} \int dt d^3 x (\vec{E}^2 + \vec{B}^2) + \int dt d^2 x \bar{\psi} \left[ i D_t \gamma_t + i v (D_x \gamma_x + D_y \gamma_y) \right] \psi
\]

with fermi-velocity \( v \) as a coefficient of gauge covariant derivative \( D_i = \partial_i + i A_i \) and coupling constant \( \beta = 1/e^2 \) (here we distinguish velocity parameter “\( v \)” from renormalized (physical) velocity “\( v_F \)” as explained below.). Electric and magnetic field can be described as \( \vec{E}_i = F_{it} \), \( \vec{B}_i = \varepsilon_{ijk} F_{jk} / 2 \) \((i = x, y, z)\) with field strength \( F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \), which is defined on 3+1 dimension, while fermion field \( \psi \) is bounded on 2+1 dimension. Second using simultaneous scale transformation for temporal coordinate and temporal gauge field normalization,

\[
t \rightarrow t/v, \quad A_0 \rightarrow A_0 v,
\]
Eq. (4) is represented as

$$S = \frac{\beta}{2} \int dt d^3x (vE^2 + v^{-1}B^2) + \int dt d^2x \bar{\psi} \sum_{\mu=t,x,y} iD_{\mu}\gamma_{\mu}\psi,$$

thus fermi-velocity shows up in the anisotropy of gauge coupling. As a consequence of rescaling we can equivalently deal with kinematic term of massless fermion field as the standard QED. Adopting the rescaled photon field for spatial direction $A_i \rightarrow A_i v$, Eq. (6) can be described as

$$S = \frac{v \beta}{2} \int dt d^3x \left[ \sum_i (\partial_i A_0 - v \partial_0 A_i)^2 \sum_{i,j} + (\partial_i A_j - \partial_j A_i)^2 \right]$$

$$+ \int dt d^2x \bar{\psi} \left[ i(\partial_0 + iA_0)\gamma_t + \sum_{i=x,y} i(\partial_i + ivA_i)\gamma_i \right] \psi,$$

(7)

Taking the non-relativistic limit, which is interpreted as limit of $v \rightarrow 0$ while $v \beta$ is fixed, the spatial photon field can be decoupled in the path integral. Dropping the spatial photon term, non-relativistic action can be derived as

$$S_{NR} = \frac{v \beta}{2} \int dt d^3x E^2 + \int dt d^2x \bar{\psi} \left[ iD_t\gamma_t + i\partial_x\gamma_x + i\partial_y\gamma_y \right] \psi,$$

(8)

so that in this limit time-rescaled version ($t \rightarrow t/v$ and $\phi \rightarrow v\phi$) of the action in Eq. (3) is reproduced.

Here we notice that the relativistic action (6) is a renormalizable local quantum theory. Therefore, the scaling of velocity can be rigorously treated without the contamination from irrelevant operator violating gauge symmetry. The bare fermi velocity $v$ has a renormalization effect due to quantum correction to ultraviolet divergence. Indeed the renormalization group study from relativistic perturbative calculation [25, 26] (and also there is similar discussion in large N [27] and renormalization group [28–30] in spite of non-relativistic action) pointed out that the velocity parameter behaves a logarithmic-divergent scaling due to virtual fermionic loop correction. It turns out that the the renormalized fermi velocity $v_F$ has an infrared fixed point at $v_F = 1$ due to the restoration of Lorentz symmetry. Perturbative analysis has also pointed out that there is an infrared unstable (ultraviolet) fixed point of the running of fermi-velocity above the experimental one (see Figure 1). However, as noticed in [25, 26], such a fixed point is in the strong coupling region where the perturbation theory is not reliable. In addition that recent experimental study using effective spectrum of electron-hole pair in suspended Graphene on SiO$_2$ wafer [4] also shows the effective velocity
FIG. 1: The sketch of renormalization flow of renormalized fermi-velocity \( v_F \) and effective coupling \( \alpha \) with \( \alpha v_F = \text{const.} \) In the perturbation theory there is unstable infrared fixed point at \( \alpha_{\text{fix}} \) which is shown as straight dashed-line. Experimental point represented as cross symbol at \( v_F \sim O(10^{-2}) \). Our lattice calculation aims to prove the wide region of phase structure \((\alpha, v_F)\) shown as the gray zone beyond the region perturbatively reliable.

of Graphene around a few particle region has qualitatively similar behavior of renormalized velocity in the perturbation theory. Therefore, investigation of running behavior of fermi-velocity using non-perturbative calculation with relativistic action would be very important task towards more rigorous discussions than renormalization group study.

III. LATTICE SIMULATION OF THE RELATIVISTIC QED

In our Monte-Carlo study, we employ the conventional non-compact gauge action

\[
S_g = \sum_x \left[ \beta v (\partial_0 \theta_i (x) - \partial_i \theta_0 (x))^2 + \frac{\beta}{v} (\partial_i \theta_j (x) - \partial_j \theta_i (x))^2 \right],
\]

with anisotropic gauge coupling and vector field \( \theta_\mu \). This summation is performed in 4 dimensional coordinate space-time. In this action there are two input parameters, \( \beta \) and \( v \), which correspond to the bare gauge coupling constant and velocity. For the fermion action
on the lattice, we use the staggered type

$$S_f = \sum_{x} \left[ \sum_{\mu} \eta_{\mu}(x) \left\{ \bar{\chi}(x) U_{\mu}(x) \chi(x + \hat{\mu}) - U^\dagger(x - \hat{\mu}) \chi(x - \hat{\mu}) \right\} + m \bar{\chi}(x) \chi(x) \right]$$  \hspace{1cm} (10)

where link variable is defined as $U_{\mu}(x) = \exp(i\theta_{\mu}(x))$, and $\eta_{\mu}(x) = \prod_{i=x+1}^{x-1} (-1)^i$ is Kawamoto-Smit phase factor. In the above equation the staggered fermion is defined in 3 dimensional field, and thus the summation is defined in 3 dimensional coordinate space-time. For comparison the size of z-axis, which is perpendicular coordinate for fermion brane, is set to same $L_z = 8$ as \[21\]. Boundary condition of fermion in temporal direction is anti-periodic boundary associated with finite temperature, and the other directions are set to periodic boundary. In this setup gauge field propagates along z-axis without interaction of fermion. We insert the small mass term with parameter $m$ as a probe to investigate chiral dynamics near chiral limit.

Conveniently staggered fermion in 3 dimensional coordinate automatically satisfies a same flavor $U(4)$ symmetry as monolayer Graphene without additional counter term in the continuum limit \[21\] (due to the lattice artifact it is broken to $U(1) \otimes U(1)$). Lattice size is $30^2 \times 20$, and we perform the Hybrid Monte Carlo (HMC) method with Omelyan integrator using parameter $\lambda_c = 0.1931833$ \[31\] and Hasenbusch accelerator \[32\] with mass parameter $m = 0.05$ to generate gauge configurations with dynamical fermion. We tune the Leapfrog time-stepping parameter $\delta_t = 1/N_t$, where $N_t$ is number of step in unit HMC trajectory, to be that acceptance rate is satisfied with more than 60% in our simulation. From the practical point of view, the rescaling \[5\] has also an advantage of simultaneously covering the region of strong electric coupling and low temperature. Since temporal size is $1/v$ times larger than original action \[4\], the lattice simulation curries out naively equivalent to be at $1/v$ times smaller temperature \[33\] with same computational cost. Note that the physical quantities obtained in this action depends on the effective strong coupling $\alpha = 1/(4\pi\beta v)$ rather than gauge coupling constant $\beta$ since the quantum correction from vertex with $\alpha$ is dominant contribution in this system if velocity is enough small. Correspondingly the loop correction to gauge coupling constant is higher order effect while velocity has logarithmic divergence $(v(\mu) = v(1 + \alpha/4 \ln(\Lambda/\mu))$ with cut-off $\Lambda$) from at least one-loop correction according to the perturbative analysis \[25\]. It turns out that observable are mostly controlled by the theoretical parameter $v$ instead of gauge coupling. Furthermore we introduce the Dirac “mass” term $m\bar{\psi}\psi$ which preserves discrete symmetry (Parity, time-reversal and charge conjugate)
but not chiral symmetry. Scalar condensate of quasiparticle \(\langle \bar{\psi} \psi \rangle\) corresponds to order parameter of chiral transition, and associated from Goldstone theorem the massless Goldstone mode (pion) appearing into QED model plays a significant role of the gap generation in Graphene system \([34]\).

IV. RESULT OF LATTICE SIMULATION

Here we investigate the chiral breaking phenomena with chiral condensate \(\sigma = \langle \bar{\chi} \chi \rangle\) and its susceptibility \(\chi_m = \partial \sigma / \partial m\) behaved as a function of \(\beta v\), \(v\) and \(m\). The disconnected diagram appearing in chiral condensate \(\sigma\) and chiral susceptibility \(\chi_m\) is calculated by the noise method with 200 noise vector. We sample configurations at every 20 HMC trajectories, and employ the Jackknife error estimate with 10 bin-size. Total statistics used in this analysis is around 600–1500 configurations, especially more than 1000 configurations in the strong coupling region \((\beta v < 0.06)\).

Chiral condensate is an order parameter of spontaneous chiral symmetry breaking in which the discontinuous point along the coupling constant regards as second-order critical point in the limit of massless on infinite volume. At the finite mass and lattice volume, if there is critical point associated with spontaneous chiral symmetry breaking in this system, chiral condensate above critical coupling \(\alpha_c\) remains finite value, otherwise below \(\alpha_c\) chiral condensate advances toward zero when approaching \(m = 0\). Figure 2 clearly shows the expected critical behavior that, when mass parameter is decrease, \(\sigma\) at weak coupling region, which is at the large \(\beta v\), goes to zero while at strong coupling region \(\sigma\) remains finite value, and critical coupling is found to be \(\beta v = 0.05–0.06\) at fixed \(v = 0.1\). Chiral susceptibility also shows significant behavior around such critical point. When \(m\) goes down close to zero, peak position of \(\chi_m\) grows up and shifts from weak coupling to strong coupling region. We expect the singularity for critical phenomena at massless point will appear at \(\beta v = 0.05–0.055\), which corresponds to critical coupling \(\alpha_c = 1.45–1.59\). This value is similar order of the prediction in gap equation quoted to \(\alpha_c = 0.92\) \([8]\) or in non-relativistic lattice calculation as \(\alpha_c = 1.02\) \([21]\). Figure 3 also shows a significant change as that below \(\alpha_c\) we can see that \(\sigma\) approaches to zero at chiral limit, especially near \(\alpha_c\) its non-linear behavior, while above \(\alpha_c\) \(\sigma\) does not vanish. At very weak region in which the coupling anisotropy is negligible since \(\beta\) is too large, \(\sigma\) can be described as a perturbative line, and actually in Figure 3 mass dependence
FIG. 2: Chiral condensate (left) and chiral susceptibility (right) of quasiparticle as a function $\beta v$ which corresponds to effective coupling constant $\alpha$ at fixed velocity in $v = 0.1$.

FIG. 3: Mass dependence of chiral condensate at several gauge coupling $\beta$ at fixed velocity in $v = 0.1$. Linear-dashed line shows the leading perturbation result.

of $\sigma$ approaches to the leading perturbative line obtained in lattice perturbation.

To see the contribution of fermi velocity and vacuum polarization of bounded fermion into critical phenomena, we compare the peak position of chiral susceptibility at $v = 0.1$ and $v = 0.05$ (in addition to $v = 0.03$ for full calculation) with and without dynamical fermion at mass parameter $m = 0.0025$ in Figure 4. We notice two points:

1. First, our lattice calculation shows that critical point in full QED is moved to strong region in quenched QED $\beta v \simeq 0.093$ corresponding to $\alpha_c \sim 0.8$, which is about 40–50% strongly shift of coupling constant. Our result is qualitatively consistent behavior with
result in gap equation including frequent vacuum polarization effect of 2+1 dimensional fermion, quoted to be 46% shift from $\alpha_c = 0.5$ (quench) \[20\] to $\alpha_c = 0.92$ \[8\].

2. Secondly, decreasing the velocity from $v = 0.1$ to $v = 0.05$ we see that the critical point $\alpha$ stays almost constant but shifts towards stronger coupling for only about 5–7% in both cases of full QED; peak position of $\chi_m$ is moved as $\beta v \simeq 0.062(v = 0.1) \rightarrow 0.058(v = 0.05)$, and quenched QED; peak position of $\chi_m$ is moved as $\beta v \simeq 0.093(v = 0.1) \rightarrow 0.088(v = 0.05)$. Linearly extrapolating into $v \simeq 1/300$ using $\alpha_c(v) = \alpha_c(v = 0) + cv$ assuming $c$ is constant, we find that the critical point is $\alpha_c(v = 1/300) \sim 1.5$ in the case of full QED ($\alpha_c(v = 1/300) \sim 0.9$ in quenched QED), which is comparable to TB model ($\alpha \sim 2.2$ \[2\]) rather than quenched one. Assuming that the bare velocity $v$ and the renormalized velocity $v_F$ is almost the same, our results suggest the physical point of the Graphene system exists within the symmetry broken phase. To establish the position of the physical point in the phase structure, we have to carry out the renormalization of the effective coupling constant as well as the fermi velocity, which will be left a future work.
V. DISCUSSION

In this paper we have performed the lattice simulation using 4 dimensional non-compact QED with 2+1 dimensional fermion brane including velocity parameter into anisotropic gauge coupling between electric and magnetic fields. Our lattice simulation clearly shows that a consistent behavior associated with chiral symmetry breaking at critical coupling $\alpha_c = 1.45-1.59$ at $v = 0.1$, and furthermore from comparison with different velocity parameter we suggest possibility of quantum correction to the critical phenomena depending on running of velocity parameter in the infrared region. We assert that in our relativistic QED model related to “realistic” Graphene system which includes the fermi-velocity less than 1% speed of light and electromagnetic interaction among electron, the spontaneous chiral symmetry breaking occurs due to small velocity parameter, which plays important role to lead to the strong dynamics of this system rather than gauge coupling as suggested by perturbative argument [25, 26]. Qualitatively the result obtained in our model is similar to model prediction of gap equation [7, 8]. We argue that our model is non-trivial extension of QED model under gauge invariance to relativistic form in contrast to non-relativistic case [3, 21]. Although we have not comprehended the explicit relation between our model and Graphene in low energy region yet, however surprisingly our model also shows the critical behavior of quasiparticle condensate as well as in the non-relativistic calculation [21, 22, 27]. This is strong evidence of that our model realizes the natural extension to relativistic theory of Graphene model beyond TB approximation. We are now proceeding to take into account renormalization of velocity and continuum limit [38] using more detailed parameter search under way. This is a feasible study for one of the most challenging topics of theoretical prediction of semimetal-insulator transition point of suspended Graphene.

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