First-order chiral transition in the compact lattice theory of graphene and the case for improved actions

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A comparison of the compact and non-compact lattice versions of the low-energy theory of graphene is presented. The compact theory is found to exhibit a chiral phase transition which appears to be of first order, at a critical coupling of $\beta_c = 0.42 \pm 0.01$. We confirm that the non-compact theory exhibits a second-order transition at $\beta_c = 0.072 \pm 0.003$, and determine the effects of UV-divergent tadpole contributions in both cases. Upon tadpole improvement of the non-compact theory we find $\beta_{c1} = 0.163 \pm 0.002$, which strengthens the case for a semimetal-insulator transition in graphene at strong Coulomb coupling. Finally, we highlight the need for systematic studies using improved lattice actions.

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Graphene, a sheet of $sp^2$-bonded carbon, has become an attractive candidate for nanoscale electronics due to its many remarkable and desirable properties\textsuperscript{[1, 2]}. These include high carrier mobility at room temperature, great mechanical and tensile strength, in addition to chemical stability and impermeability. While the hexagonal lattice symmetry suggests that graphene is a semimetallic material exhibiting massless Dirac quasiparticles, the possibility that graphene might become an excitonic insulator due to strong Coulomb interactions has recently been revived\textsuperscript{[3]}

In a series of papers within the Lattice Monte Carlo (LMC) framework\textsuperscript{[4, 5]}, the semimetal-insulator transition, which manifests itself as the spontaneous breaking of a $U(4)$ chiral symmetry, was found to happen at a critical coupling of $\alpha_c \sim 1.1$, which is intermediate between that of graphene on a SiO$_2$ substrate ($\alpha \sim 0.8$) and suspended graphene ($\alpha \sim 2.1$). LMC studies of a closely related Thirring-like model, including the determination of the renormalized Fermi velocity, were reported in Ref.\textsuperscript{[6]}. These results belong to a larger class of LMC studies, such as those of Quantum Electrodynamics in $2+1$ (QED\textsubscript{3})\textsuperscript{[7]} and $3+1$ (QED\textsubscript{4})\textsuperscript{[8]} dimensions, and of four-fermion theories such as the Thirring\textsuperscript{[9]} and Gross-Neveu\textsuperscript{[10]} models.

Spontaneous chiral symmetry breaking in LMC is typically studied using staggered fermions\textsuperscript{[11]}, as chiral symmetry is then partially preserved at finite lattice spacing $a$. In practical LMC simulations the continuum limit is recovered in the vicinity of second-order phase transitions, where the relevant correlation lengths $\xi$ diverge. In the case of graphene, such a continuum description is attainable on the critical line of vanishing bare mass and (inverse) coupling $\beta \geq \beta_c \approx 0.072$, with $\alpha_c = 1/(4\pi\beta_c)$. In the strong coupling phase $\beta < \beta_c$ the Coulomb interaction induces the formation of particle-hole pairs, with a binding energy that yields an intrinsic cutoff scale $\Lambda \sim a^{-1}$, such that the limit $a \rightarrow 0$ is not well defined (or rather, it defines an unstable theory). Keeping $a$ finite, however, one may approach the critical line and recover a well-defined theory, with bound states at strong coupling and massless fermions at weak coupling.

The requirement of exact gauge invariance on the lattice necessitates the use of "gauge links" $U \equiv \exp(i\theta)$, with $\theta$ the lattice gauge field. Gauge links have the side effect of introducing vertices of higher order in $a$, such as photon-photon interactions, which are absent in the continuum theory. Such vertices also yield potentially large "tadpole" contributions, where the naive power-counting in $a$ is cancelled by UV divergences. Consequently, Lattice QCD simulations employ various levels of "improvement"\textsuperscript{[12]}, in order to minimize the impact of such discretization artifacts. We report here a systematic study of the tadpole effects in the graphene theory, which were first pointed out in Ref.\textsuperscript{[13]}, and their impact on the determination of $\beta_c$. We also present a comparison of the non-compact and compact lattice theories of graphene, where the latter case involves photon self-interactions which are absent in the former.

The Euclidean action of the lattice theory of graphene is conventionally split into gauge and fermion components, such that $S_E = S_E^g + S_E^f$. In the compact formulation, the gauge field $\theta$ enters into $S_E^g$ in terms of link variables, giving

\begin{equation}
S_E^{g,c}[\theta] = \beta \sum_{n} \left[ 3 - \sum_{i=1}^{3} \Re \left( U_n U_{n+e_i}^\dagger \right) \right],
\end{equation}

where $\Re(x)$ denotes the real part of $x$, $\beta \equiv 1/g^2$ is the inverse coupling, $n$ a site on the $(3+1)$-dimensional spacetime lattice, and $e_\mu$ a unit vector in the direction $\mu$.

Early on, the analogous compact formulation of QED\textsubscript{4} was found to exhibit a first-order transition\textsuperscript{[14]} where the breaking of chiral symmetry is coincident with the condensation of magnetic monopoles. While the addition of a four-Fermi interaction to QED\textsubscript{4} makes it possible
to isolate the chiral symmetry breaking transition, the resulting theory may belong to a different universality class than continuum QED [12]. In order to avoid this situation for the case of graphene, an attractive option is the non-compact formulation

$$S_{E}^{g,n'}[\theta] = \frac{\beta}{2} \sum_{n} \left[ \sum_{i=1}^{3} \left( \theta_{n} - \theta_{n+e_{i}} \right)^{2} \right],$$

which is free of photon self-interactions, and is known to support a second-order transition which may be identified with the spontaneous breaking of chiral symmetry in the continuum theory. Thus, Eq. (2) has become the standard choice for LMC studies of Abelian gauge theories, such as QED$_{4}$ [7], QED$_{4}$ [8] and we have used it for graphene. The first objective of this study is to characterize the compact version of the low-energy theory of graphene, which differs significantly from QED as the spatial gauge links are constant and the fermions propagate in two spatial dimensions only.

The fermion action $S_{F}$ is identical in the compact and non-compact theories, and in the staggered fermion formulation it is given by

$$S_{F}[\bar{\chi}, \chi, \theta] = -\sum_{n,n'} \bar{\chi}_{n} D_{n,n'}[\theta] \chi_{n'},$$

where $(n, n')$ denotes the sites of a (2+1)-dimensional space-time sublattice, and gauge invariance is retained by coupling the staggered spinors $\chi_{n}$ to the gauge field via link variables in the time direction. The staggered Dirac operator is given by (see e.g. Ref. [10])

$$D_{n,n'}[\theta] = \frac{1}{2} \left[ \delta_{n+e_{0},n'} U_{n} - \delta_{n-e_{0},n'} U_{n'}^{\dagger} \right] + \frac{v}{2} \sum_{i} \eta_{n,n'} \left[ \delta_{n+e_{i},n'} - \delta_{n-e_{i},n'} \right] + m_{0} \delta_{n,n'},$$

where $\eta_{n,0} = (-1)^{n_{0}}$ and $\eta_{n,1} = (-1)^{n_{0}+n_{1}}$. The Fermi velocity $v$ can be absorbed into the remaining parameters, giving $\beta \equiv v/g^{2}$ and $m \equiv m_{0}/v$. Simulations are thus conventionally performed in terms of $(\beta, m)$ and $v = 1$. The mass term acts as a symmetry breaking parameter, without which the chiral condensate $\sigma$ would be zero at finite volume. The limit $m \to 0$ is reached by extrapolation, using an equation of state (EOS) of the form $m = f(\sigma, \beta)$, which describes a second-order transition with critical exponents $\delta$ and $\beta$. A detailed description of the EOS can be found in Ref. [10].

“Tadpole improvement” (TI) is a non-perturbative method due to Lepage and Mackenzie [17] that accounts for the UV divergent tadpole contributions by renormalizing the link field $U$. The effect of the UV modes is encoded in the function $u_{0}$, which depends on the input parameters of the simulation and is to be determined a posteriori. A conventional definition of $u_{0}$ is

$$u_{0} \equiv \langle P \rangle^{1/2}, \quad P = \frac{1}{V} \sum_{n} U_{n} U_{n+e_{1}}^{\dagger},$$

in terms of the plaquette $P$. It should be noted that the power 1/2 (instead of 1/4 as in Lattice QCD) is due to the smaller number of fluctuating gauge links.

Recently, Ref. [13] has reported that $u_{0}(\beta, m)$ deviates significantly from unity, and thus the effects of TI are likely to be significant. Therefore, the second objective of this study is to determine how TI affects the determination of $\delta_{c}$ and the critical exponents. In the non-compact theory, modifications due to TI are restricted to the fermion action, whereas in the compact case the gauge action is affected as well.

As in Ref. [13], we consider the plaquettes in the $(x, t)$ and $(y, t)$ planes, however unlike Ref. [13] we compute $\langle P \rangle$ by summing over the plaquettes in the (2+1)-dimensional fermionic sublattice only. This choice is appropriate for the non-compact theory, and the resulting numerical differences are insignificant for the subsequent analysis. Our results for $P$ are shown in Fig. 1. We find that $P$ is independent of $m$ up to statistical fluctuations, and thus we define $u_{0}(\beta)$ as the average of $P$ over $m$.

In practice, TI amounts to replacing the link field $U$ in Eqs. (11) and (12) according to $U \to U/u_{0}$, where $u_{0}$ is to be determined a posteriori using Eq. (6). If the staggered spinors are rescaled as $\chi \equiv \sqrt{m_{0}} \chi$, one can define an “improved” Dirac operator

$$D_{n,n'}^{I}[\theta] = \frac{1}{2} \left[ \delta_{n+e_{0},n'} U_{n} - \delta_{n-e_{0},n'} U_{n'}^{\dagger} \right] + \frac{v}{2} \sum_{i} \eta_{n,n'} \left[ \delta_{n+e_{i},n'} - \delta_{n-e_{i},n'} \right] + m_{0}' \delta_{n,n'},$$

where

$$\sigma' \equiv \sigma/u_{0}, \quad v' \equiv u_{0}v, \quad m_{0}' \equiv u_{0}m_{0},$$

FIG. 1: (Color online) Plaquettes $(P)$ as a function of $\beta$ for the non-compact (left) and compact (right) theories, for Eq. (11) averaged over the fermionic sublattice. Our notation is $N_{x} \times N_{y}^{2}$, where $N_{x}$ is the extent of the fermion sublattice and $N_{y}$ of that of the bulk dimension. Black datapoints are for a $32^{4}$ lattice, while red (gray) points are for $12 \times 28^{3}$. To illustrate the dependence on $m$, the datapoints have been shifted horizontally relative to $m = 0.010$, and for the compact case the $24^{4}$ data have also been shifted vertically relative to the $32^{4}$ data.
The primal parameters in Eq. (7) represent the input quantities. The primed parameters in Eq. (7) represent the input quantities, while for the non-compact case we have $\beta' \equiv \beta$ if the tadpoles of fermionic origin were ignored. Our results for the non-compact theory are shown in Figs. 2 and 3 for the unimproved and TI cases, respectively. Similarly, the results for the compact theory are given in Figs. 1 and 5. Most of our data for the non-compact case are taken from Ref. [5], except for the data on $32^4$ lattices close to the critical point.

$\chi_4$ (right) for the non-compact theory after TI, together with an EOS fit. Note the significantly reduced scaling violations compared to the unimproved data. The optimal fit is compatible with $\beta = 1$, giving $\beta_0 = 0.163 \pm 0.002$ and $\delta = 2.2 \pm 0.1$. The errors are mostly systematic, due to finite-volume effects and residual scaling violations. The black symbols denote data on $12 \times 32^3$ and $32^4$ lattices, while red (gray) symbols denote data for $12 \times 28^3$ and $28^4$ lattices, respectively. Similarly, the results for the non-compact action in Eq. (2) is not directly modified as it involves no gauge links.

The primed parameters in Eq. (7) represent the input for the LMC calculation. Once $u_0(\beta)$ has been mapped out, the tadpole-improved (unprimed) quantities can be determined. Apart from the rescaling of the chiral condensate according to $\sigma' \rightarrow u_0 \sigma$, we find for the compact case

$$\beta' = \frac{\beta}{\sigma} = \frac{\beta'_{u_0}}{G^2 / u_0^2} = u_0 \beta'_{u_0},$$

while for the non-compact case we have

$$\beta = \frac{\beta}{\sigma} = \frac{\beta'_{u_0}}{G^2 / u_0^2} = \beta'_{u_0},$$

and we note that $m \equiv m_{u_0} / v$ remains unmodified. Both of these results differ from the prescription $\beta = u_0 / \beta'_{u_0}$ which was applied in Ref. [13]. However, such a choice would be valid for the compact theory in the absence of TI for the fermion action. It is noteworthy that the non-compact theory would have $\beta' = \beta$ if the tadpoles of fermionic

FIG. 2: (Color online) Chiral condensate $\sigma$ (left) and susceptibility $\chi_1$ (right) in the non-compact theory after TI, together with an EOS fit to the unimproved lattice data. The fitted parameters are $\beta_0 = 0.072 \pm 0.003$ and $\delta = 2.3 \pm 0.3$, with $\beta \simeq 1$. The data are obtained for lattices of size $12 \times 32^3$ and $32^4$ (circles) and $12 \times 28^3$ (squares). Errors for the individual datapoints were obtained with the standard block-jackknife method. Note the deviations from the EOS (scaling violations) at small $\beta$ and large $m$.

FIG. 3: (Color online) Chiral condensate $\sigma$ (left) and susceptibility $\chi_1$ (right) in the non-compact theory after TI, together with an EOS fit to the unimproved lattice data. The fitted parameters are $\beta_0 = 0.072 \pm 0.003$ and $\delta = 2.3 \pm 0.3$, with $\beta \simeq 1$. The data are obtained for lattices of size $12 \times 32^3$ and $32^4$ (circles) and $12 \times 28^3$ (squares). Errors for the individual datapoints were obtained with the standard block-jackknife method. Note the deviations from the EOS (scaling violations) at small $\beta$ and large $m$.

FIG. 4: (Color online) Chiral condensate $\sigma$ (left) and susceptibility $\chi_1$ (right) in the non-compact theory after TI, together with an EOS fit. Note the significantly reduced scaling violations compared to the unimproved data. The optimal fit is compatible with $\beta = 1$, giving $\beta_0 = 0.163 \pm 0.002$ and $\delta = 2.2 \pm 0.1$. The errors are mostly systematic, due to finite-volume effects and residual scaling violations. The black symbols denote data on $12 \times 32^3$ and $32^4$ lattices, while red (gray) symbols denote data for $12 \times 28^3$. 

such that the tadpole-improved observables may be computed using the original unimproved gauge configurations, provided that the input parameters of the simulation and the spinors are reinterpreted according to Eq. (7). As $u_0 < 1$, the net effect of TI (apart from possible shifts of the critical coupling $\beta_c$) is to make the condensate smaller in the spontaneously broken phase, an effect which increases with decreasing $\beta$. For the compact gauge action in Eq. (1), TI leads to a similar prescription $\sigma' = u_0 \sigma$, while the non-compact action in Eq. (2) is not directly modified as it involves no gauge links.
As the tadpole correction $u_0(\beta) \sim 0.5$ close to the chiral phase transition in the non-compact theory, the effects of TI can potentially be dramatic. We find that the agreement with the EOS improves and the effects of outlying data points are lessened, which is due to decreased scaling violations at small $\beta$. While the net effect on the critical exponents is slight (these remain compatible with the values of Ref. [5]), the change in $\beta_c$ is larger as a consequence of Eq. (9). After TI, we find $\beta^\text{TI}_c \approx 0.27 \pm 0.01$ has been shifted closer to that of the non-compact theory. At $\beta_c$, the data indicate a discontinuous jump of $\Delta \sigma \sim 0.04$ in the condensate.

In conclusion, we find that the effect of TI is not as drastic as reported in Ref. [13], particularly in the non-compact theory, where $\beta_c$ is shifted to a larger (instead of a smaller) value. The predicted semimetal-insulator transition in suspended graphene is therefore unlikely to be an artifact of tadpole effects. While the full chiral symmetry is not realized in LMC simulations with staggered fermions at small $\beta$ (see Refs. [8, 13]), it is known to eventually be restored in the vicinity of the tricritical point ($\beta = \beta_c, m = 0$). However, this conceptual weakness may be inconsequential, as the accuracy of the extrapolation can be systematically improved by obtaining additional data closer to the tricritical point. Nevertheless, simulations with overlap fermions [19] may serve to further clarify this point, and to extend the scope of the present work.

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