Critical exponents of the semimetal-insulator transition in graphene: A Monte Carlo study

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The low-energy theory of graphene exhibits spontaneous chiral symmetry breaking due to pairing of quasiparticles and holes, corresponding to a semimetal-insulator transition at strong Coulomb coupling. We report a lattice Monte Carlo study of the critical exponents of this transition as a function of the number of Dirac flavors $N_f$, finding $\delta=1.25 \pm 0.05$ for $N_f=0$, $\delta=2.26 \pm 0.06$ for $N_f=2$ and $\delta=2.62 \pm 0.11$ for $N_f=4$, with $\gamma = 1$ throughout. We compare our results with recent analytical work for graphene and closely related systems and discuss scenarios for the fate of the chiral transition at finite temperature and carrier density, an issue of relevance for upcoming experiments with suspended graphene samples.

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Graphene, a single layer of carbon atoms arranged in a honeycomb lattice$^{1,2}$, provides a building block for more complex allotropes such as graphite (graphene sheets attached by van der Waals forces), fullerences (graphene spheres with pentagonal dislocations), and nanotubes (cylindrically rolled-up graphene). In the absence of electron-electron interactions, the valence and conduction bands of graphene are connected by two inequivalent “Dirac points” around which the low-energy excitations are massless quasiparticles with a linear dispersion relation and a Fermi velocity of $v_F = c/300$. Such a semimetallic band structure is, unfortunately, unsuitable for many electronic applications, which depend crucially on the ability to externally modify the conduction properties, as routinely done with semiconducting devices. The quest to engineer a band gap in graphene has thus been propelled to the forefront of current research. Hitherto suggested solutions include gap formation due to interaction with a substrate$^3$, induction of strain$^4$, and geometric confinement by means of nanoribbons or quantum dots$^5$.

The low $v_F$ in graphene indicates that the analog of the fine-structure constant of Quantum electrodynamics (QED) is $\alpha_s \sim 1$, and thus the Coulomb attraction between electrons and holes may play a significant role in defining the ground-state properties. An intriguing possibility is that spontaneous formation of excitons (electron-hole bound states) and the concomitant breaking of chiral symmetry may turn graphene into a Mott insulator. While the strength of the Coulomb interaction precludes a perturbative approach, previous (approximate) analytic studies$^7$ at the neutral point (zero carrier density $n$) and zero temperature $T$ have addressed the appearance of an excitonic gap as a function of $\alpha_s$ (see Fig. 1). Such treatments suggest that the transition into the insulating phase should be governed by essential singularities rather than power laws, a behavior known as Miransky scaling.$^8$

In our recent lattice Monte Carlo (LMC) study,$^9$ indications were found that the chiral transition is of second order, with well-defined critical exponents. Subsequently, in Ref. 10 we provided a rough estimate of the critical exponents as $\delta \sim 2.3$, $\beta_\mu \sim 0.8$, and $\gamma \sim 1$, although a more precise determination was not possible due to insufficient data on large-enough lattices. Nevertheless, Miransky scaling and classical mean-field exponents were found to be disfavored.

The aim of the present work is to provide a more rigorous and comprehensive determination of the quantum critical properties for $N_f=0$, 2, and 4 Dirac flavors, as well as to contrast these results with recent analytical and simulation work for graphene and related theories. We also briefly elaborate on the mechanisms that inhibit exciton formation at nonzero $T$ and $n$ and their connection to other systems.

The LMC studies of Refs. 9–11 suggest that the low-energy theory of graphene is an appropriate starting point for a quantitative analysis. This is defined by the Euclidean action

$$S_E = -\int d^2x dt \bar{\psi}_i D[A_0] \psi_i + \frac{e^2}{2\epsilon^2} \int d^3x dt (\partial_i A_0)^2,$$

with the Dirac operator

$$D[A_0] = \gamma_0 (\partial_0 + i A_0) + v \gamma_i \partial_i + m_0, \quad i = 1, 2,$$

where the $\psi_i$ with $a=1, \ldots, N_f$ are four-component spinors in 2+1 dimensions, $A_0$ is a Coulomb field in 3+1 dimensions, and the case of a graphene monolayer is recovered for $N_f=2$ in the limit $m_0 \to 0$. Furthermore, $\alpha_s = e^2/(4\pi\epsilon_0)$ with the inverse coupling $\beta = v_e / \epsilon^2$ such that screening by a substrate is reflected in the dielectric constant $\epsilon_0$.

The gauge term of Eq. (1) is discretized in the noncompact formulation.$^{9,10}$ The staggered discretization$^{12}$ of the fermionic component of Eq. (1) is preferred as chiral symmetry is then partially retained at finite lattice spacing. As $N$ staggered flavors correspond to $N_f=2N$ continuum Dirac flavors,$^{13}$ the case of $N_f=2$ is recovered for $N=1$, giving

$$S_0[\bar{\chi}, \chi, U_0] = -\sum_{m,n} \bar{\chi}_m K_m n[U_0] \chi_n,$$

where the $\chi_n$ are staggered fermion spinors and the site indices $(m,n)$ are restricted to a 2+1 dimensional sublattice. Invariance under spatially uniform, time-dependent gauge transformations is retained by the link variables $U_{0,m}=U_{n}=\exp(i\theta_n)$, where $\theta_n$ is the lattice gauge field. For $v=1$, the staggered form of Eq. (2) is...
performed at finite appearance of Goldstone modes. Practical simulations are however, the “chiral limit”

described by a critical Coulomb coupling $\alpha_c = (4\pi\beta_c)^{-1}$ and a critical number of fermion flavors $N_f$. The coupling on a SiO$_2$ substrate is denoted by $\alpha_{\text{SiO}_2}$, and for suspended graphene by $\alpha_{\text{susp}}$. Inset: hypothetical phase diagram in the ($n$ and $T$) plane. At low $T$, suspended graphene exhibits semimetallic properties whenever the carrier density $n$ exceeds a characteristic value $n^*$. At the neutral point the semiconducting behavior persists until $T = e_f^0 = h c_F / \sqrt{m t}$, where the transition may be of Kosterlitz-Thouless type or a crossover.

We now seek to characterize the critical exponents of the chiral transition in graphene. The spontaneous breakdown of chiral symmetry in Eq. (1) is signaled by a nonzero condensate $\chi(0)$ of the order parameter. The mass term in Eq. (2) breaks chiral symmetry explicitly, generating a nonvanishing condensate, which is otherwise not possible at finite volume. The appearance of a gap in the quasiparticle spectrum of graphene at a critical coupling $\beta_c$ is then marked by $\sigma = 0$ for $m_0 = 0$. However, the “chiral limit” $m_0 \to 0$ cannot be approached directly as that limit corresponds to a very large fermionic correlation length, especially in the vicinity of $\beta_c$ due to the appearance of Goldstone modes. Practical simulations are performed at finite $m_0$ such that the limit $m_0 \to 0$ is reached by extrapolation for which it is useful to also study the susceptibility $\chi_1 = \partial R / \partial m_0$ and the logarithmic derivative $R = \partial \ln \sigma / \partial \ln m_0$. An instructive way to determine $\beta_c$ and the critical exponents is by fitting an equation of state (EOS) $m_0 = f(\sigma, \beta)$ to simulation data at finite $m_0$. Knowledge of $f(\sigma, \beta)$ with good precision close to the transition then allows for an educated extrapolation to the chiral limit.

We have considered the EOS successfully applied\(^\text{15}\) to lattice QED,
Critical Exponents of the Semimetal-Insulator Transition

model in 2+1 dimensions, where \( \delta = 2.8 \) for \( N_f = 2 \), reaching \( \delta = 7 \) at a critical flavor number of \( N_f = 6.6 \). Extensive LMC studies of QED have found \( \delta \approx 2.2 \) for \( N_f = 0 \), while for QED with dynamical fermions \( \delta = 3.15 \). The case of QED in 2+1 dimensions (QED\(_3\)) is noteworthy as the LMC study of Ref. 18 yielded \( \delta = 2.3 \) for \( N_f = 1 \) and \( \delta = 2.7 \) for \( N_f = 4 \), which are suggestive of our values for graphene, although spontaneous chiral symmetry breaking in QED\(_3\) is difficult to establish as the order parameter can be exponentially suppressed for large \( N_f \).

The gap-equation analysis of Ref. 7 reported \( \beta_1 = 0.16 \) for \( N_f = 0 \) and \( \beta_1 = 0.066 \) for \( N_f = 2 \), which are in qualitative agreement with our results. However, the transition of Ref. 7 is of infinite order and vanishes for \( N_f = 4 \). These discrepancies are smallest for \( N_f = 0 \), where our results approach \( \delta = 1 \). Our observations are thus in line with indications\(^{19}\) that the critical exponents, as obtained from Schwinger-Dyson equation (SDE) analyses, may be dependent on the chosen resummation scheme.

An effective theory containing both the order parameter and the Dirac quasiparticles as dynamical fields has recently been developed in Ref. 20. Based on an expansion to leading order around \( \epsilon = 3 - d \) spatial dimensions, the long-range \( \sim 1/r \) Coulomb tail was found to be irrelevant in the renormalization group (RG) sense such that the chiral transition could then be described using only short-range interactions of the Gross-Neveu-Yukawa form, yielding the estimates \( \gamma \approx 1.25 \) and \( \delta \approx 2.8 \) for the critical exponents at \( N_f = 2 \), in qualitative agreement with our present findings, as well as with large-\( N_f \) calculations of the RG flow.\(^{21}\) However, our results are not compatible with \( \delta = 2 + O(1/N_f) \) found in Refs. 20 and 22, which is surprising as the Gross-Neveu-Yukawa theory is expected to interpolate between \( \delta = 19/5 = 4 \) at \( N_f = 0 \) and \( \delta = 2 \) in the \( N_f \to \infty \) limit.\(^{20}\) It is not clear, as no chiral transition exists in the graphene theory above the critical flavor number \( N_f = 4.8 \),\(^{11}\) how to consistently compare our results with large-\( N_f \) estimates.

What is the fate of the semimetal-insulator transition at nonzero temperature? On the basis of the Mermin-Wagner theorem,\(^{23}\) one expects either a crossover or a Berezinskii-Kosterlitz-Thouless (BKT) transition\(^{24}\) at a critical temperature \( T_c \). The most compelling experimental evidence so far for a BKT transition has been reported in Ref. 25, where graphene samples on a substrate were subjected to transverse magnetic fields up to \( B \approx 30 \) T. In the temperature range of 10–1 K, a growth in the resistivity by a factor of \( \sim 200 \) was observed and attributed to the “magnetic catalysis” predicted in Refs. 26 and 27. At \( B = 0 \), the resistivity of annealed suspended graphene was observed\(^{28}\) to increase by a factor of \( \sim 3 \) over a temperature range of 200–50 K while also changing character from metallic to semiconducting. A study of the low-energy theory of graphene at nonzero \( T \) is thus clearly called for, possibly along the lines of Ref. 29, which considered the Gross-Neveu model in 2+1 dimensions.

At low \( T \), the large extent of the imaginary time dimension renders the system effectively three dimensional such
that a chiral transition may still be observed at a critical density \( n_c \). Interestingly, away from the neutral (unpolarized) point, nonrelativistic Fermi systems (such as the asymmetric Fermi liquid in the context of ultracold atoms and dilute neutron matter\(^{30}\)) can undergo transitions into exotic phases\(^{31-33}\) before reverting to a fully polarized normal state. Whether the low-energy theory of graphene exhibits such phenomena is currently unknown.

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