Interactions and Phase Transitions on Graphene's Honeycomb Lattice

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(Received 16 June 2006; published 2 October 2006)

The low-energy theory of interacting electrons on graphene's two-dimensional honeycomb lattice is derived and discussed. In particular, the Hubbard model in the large-N limit is shown to have a semimetal–antiferromagnetic insulator quantum critical point in the universality class of the Gross-Neveu model. The same equivalence is conjectured to hold in the physical case $N = 2$, and its consequences for various physical quantities are examined. The effects of the long-range Coulomb interaction and the magnetic field are discussed.

DOI: 10.1103/PhysRevLett.97.146401 PACS numbers: 71.10.Fd, 73.43.Nq, 81.05.Uw

A graphite monolayer, or *graphene*, emerged recently as the new frontier in physics of electronic systems with reduced dimensionality [1]. Such two-dimensional or quasi-two-dimensional systems have led to some of the most startling discoveries in condensed matter physics in the recent past, the quantum Hall effects and the metal-insulator transitions in silicon metal oxide semiconductor field effect transistors and Ga-As heterostructures, and the high-temperature superconductivity in cuprates being prime examples. What makes graphene qualitatively new is its semimetallic nature with low-energy quasiparticles behaving as ''relativistic'' Dirac spinors over a good portion of the conducting band. The spinor structure is a general consequence of the bipartite nature of the honeycomb lattice [2]. Indeed, recently observed quantization rules for the Hall conductivity [3] may be understood as a direct consequence of the Dirac nature of its low-energy spectrum [4,5].

The relativistic spectrum and the concomitant linearly vanishing density of states at the Fermi level, similarly as in the superconducting state of cuprates, provide graphene's quasiparticles with an additional protection against the effects of interactions. Nevertheless, a sufficiently strong repulsion is expected to turn the semimetallic state into a gapped insulator, possibly breaking the translational and/or the rotational symmetry in the process. Within the simplest interacting theory defined by the Hubbard model, there is convincing numerical evidence for the quantum phase transition at a large Hubbard U into an antiferromagnet (AF) [6]. On the other hand, the long-range Coulomb interaction remains unscreened in the semimetal (SM) [7] and has been argued to favor the charge-density wave (CDW) at strong coupling [8]. The competition between different instabilities, the universality class, or even the order of the SM–insulator transition and the interplay of interactions with the Landau quantization in the external magnetic field present some of the basic open problems. Although graphene in its natural state may not be near a critical point [9], one can conceive mechanical deformations that would pull it deeper into the strong-coupling regime [10]. Finally, the outcome of the competition between different interactions should have consequences for the selection of the ground state in the magnetic field, even at weak coupling [11].

In the present Letter, some of these issues are addressed by considering the half-filled Hubbard model on a honeycomb lattice, complemented with the additional long-range Coulomb interaction between electrons. The analysis is based on a useful decomposition of Hubbard's on-site interaction on a bipartite lattice into a sum of squares of average and staggered densities, and average and staggered magnetizations. The long-range part of the Coulomb interaction may be represented by a massless scalar gauge field, whereas its main effect on the lattice scale is to provide the repulsion between nearest neighbors. When prepared like this, in the continuum limit such an extended Hubbard model on a honeycomb lattice maps onto a $(2 + 1)$-dimensional field theory of Dirac fermions, with *nine* different couplings. Its apparent complexity notwithstanding, when generalized to a large number of fermion flavors N, the theory admits a simple SM-AF critical point of the Gross-Neveu variety [12]. Coulomb interaction is marginally irrelevant at the critical point. Assuming that the equivalence with the Gross-Neveu model persists down to the physical case of $N = 2$, I infer the values of the critical exponents in the original Hubbard model. A more general phase diagram and the implications of these results for graphene are discussed.

The extended Hubbard model will be defined by the Hamiltonian $H = H_0 + H_1$, where

$$H_0 = -t \sum_{\vec{A},i,\sigma=\pm 1} u_\sigma^\dagger(\vec{A}) v_\sigma(\vec{A} + \vec{b}_i) + \text{H.c.}, \tag{1}$$

$$H_1 = \sum_{\vec{X},\vec{Y},\sigma,\sigma'} n_\sigma(\vec{X}) \left[\frac{U}{2} \delta_{\vec{X},\vec{Y}} + \frac{e^2(1 - \delta_{\vec{X},\vec{Y}})}{4\pi|\vec{X} - \vec{Y}|} \right] n_{\sigma'}(\vec{Y}). \tag{2}$$

The sites $\vec{A}$ denote one triangular sublattice of the honeycomb lattice, generated by linear combinations of the basis vectors $\vec{a}_1 = (\sqrt{3}, -1)(a/2)$, $\vec{a}_2 = (0, a)$. The second sub-

lattice is then at $\vec{B} = \vec{A} + \vec{b}$, with the vector $\vec{b}$ being $\vec{b}_1 = (1/\sqrt{3}, 1)(a/2)$, $\vec{b}_2 = (1/\sqrt{3}, -1)(a/2)$, or $\vec{b}_3 = (-a/\sqrt{3}, 0)$. a is the lattice spacing. Neutralizing background is assumed, as usual.

The doubly degenerate spectrum of H_0 at $E(\vec{k}) = \pm t|\sum_i \exp[\vec{k}\cdot\vec{b}_i]|$ becomes linear and isotropic in the vicinity of two nonequivalent points at the edges of the Brillouin zone at $\pm\vec{K}$, with $\vec{K} = (1, 1/\sqrt{3})(2\pi/a\sqrt{3})$ [2]. Retaining only the Fourier components near $\pm\vec{K}$ one can write the quantum-mechanical action corresponding to H_0 at low energies as $S = \int_0^{1/T} d\tau d\vec{x} L_0$, with the *free* Lagrangian L_0 defined as

$$L_0 = \sum_{\sigma=\pm 1} \bar{\Psi}_\sigma(\vec{x}, \tau)\gamma_\mu \partial_\mu \Psi_\sigma(\vec{x}, \tau), \tag{3}$$

and

$$\Psi_\sigma^\dagger(\vec{x}, \tau) = T\sum_{\omega_n} \int^\Lambda \frac{d\vec{q}}{(2\pi a)^2} e^{i\omega_n\tau + i\vec{q}\cdot\vec{x}} (u_\sigma^\dagger(\vec{K} + \vec{q}, \omega_n), v_\sigma^\dagger(\vec{K} + \vec{q}, \omega_n), u_\sigma^\dagger(-\vec{K} + \vec{q}, \omega_n), v_\sigma^\dagger(-\vec{K} + \vec{q}, \omega_n)), \tag{4}$$

where it was convenient to rotate the reference frame so that $q_x = \vec{q}\cdot\vec{K}/K$ and $q_y = (\vec{K}\times\vec{q})\times\vec{K}/K^2$, and set $\hbar = k_B = v_F = 1$, where $v_F = ta\sqrt{3}/2$ is the Fermi velocity. Choosing $\gamma_0 = I_2 \otimes \sigma_z$ implies $\gamma_1 = \sigma_z \otimes \sigma_y$ and $\gamma_2 = I_2 \otimes \sigma_x$, with I_2 as the 2×2 unit matrix, and $\vec{\sigma}$ as the Pauli matrices. $\Lambda \approx 1/a$ is the ultraviolet cutoff over which the linear approximation for the dispersion holds. The summation convention is adopted hereafter, but *only* over repeated space-time indices. Besides the "relativistic" invariance, L_0 also exhibits a global invariance under the $U(4)$, generated by $\{I_2, \vec{\sigma}\} \otimes \{I, \gamma_3, \gamma_5, \gamma_{35}\}$, where I is the 4×4 unit matrix, $\gamma_3 = \sigma_x \otimes \sigma_y$, $\gamma_5 = \sigma_y \otimes \sigma_y$, and $\gamma_{35} = -i\gamma_3\gamma_5$. This is similar to the emergent "chiral" symmetry of a d-wave superconductor [13].

Generalizing slightly Hamman's decomposition, the first term in H_1 can also be rewritten exactly as

$$\frac{U}{8}\sum_{\vec{A}} \{[n(\vec{A}) + n(\vec{A} + \vec{b})]^2 + [n(\vec{A}) - n(\vec{A} + \vec{b})]^2 - [m(\vec{A}) + m(\vec{A} + \vec{b})]^2 - [m(\vec{A}) - m(\vec{A} + \vec{b})]^2\}, \tag{5}$$

where $n(\vec{A}), m(\vec{A}) = u_+^\dagger(\vec{A})u_+(\vec{A}) \pm u_-^\dagger(\vec{A})u_-(\vec{A})$ are the particle number and the magnetization at the sites $\vec{A}$. Variables at the second sublattice are analogously defined in terms of $v_\sigma(\vec{B})$.

Defining the two *slow* components of the fields as

$$r_\sigma^{1,2}(\vec{x}, \tau) = \int_{|\vec{k}\pm\vec{K}|<\Lambda} \frac{d\vec{k}}{(2\pi)^2} e^{i\vec{k}\cdot\vec{x}} r_\sigma(\vec{k}, \tau), \tag{6}$$

with $r = u, v$, the Dirac field becomes

$$\Psi_\sigma^\dagger(\vec{x}, \tau)e^{i(\vec{K}\cdot\vec{x})\gamma_{35}} = (u_\sigma^{1\dagger}(\vec{x}, \tau), v_\sigma^{1\dagger}(\vec{x}, \tau), u_\sigma^{2\dagger}(\vec{x}, \tau), v_\sigma^{2\dagger}(\vec{x}, \tau)). \tag{7}$$

At low energies one may then approximate

$$r_\sigma(\vec{x}, \tau) \approx r_\sigma^1(\vec{x}, \tau) + r_\sigma^2(\vec{x}, \tau), \tag{8}$$

so that the spin densities on the two sublattices become

$$r_\sigma^\dagger(\vec{x}, \tau)r_\sigma(\vec{x}, \tau) \approx \tfrac{1}{2}\bar{\Psi}_\sigma(\vec{x}, \tau)(I_2 + e^{i2\vec{K}\cdot\vec{x}\sigma_z}\sigma_x) \otimes (\sigma_z \pm I_2)\Psi_\sigma(\vec{x}, \tau), \tag{9}$$

with the plus sign for $r = u$ and the minus for $r = v$.

The notation is now in place to write the low-energy theory of the extended Hubbard model. In the continuum limit ($a \to 0$) the Lagrangian becomes

$$L = L_0 - ia_0\sum_\sigma \bar{\Psi}_\sigma\gamma_0\Psi_\sigma + a_0\frac{|\vec{\nabla}|}{2e^2}a_0 + \sum_{x=d,c,f,a} L_x, \tag{10}$$

with

$$L_x = g_x\left(\sum_\sigma w_{x,\sigma}\bar{\Psi}_\sigma M_x \Psi_\sigma\right)^2 + \tilde{g}_x \sum_{\mu=3,5}\left(\sum_{\sigma\pm 1} w_{x,\sigma}\bar{\Psi}_\sigma M_x\gamma_1\gamma_\mu\Psi_\sigma\right)^2, \tag{11}$$

and $w_{d,\sigma} = w_{c,\sigma} = 1$, $w_{f,\sigma} = w_{a,\sigma} = \sigma$, $M_d = M_f = \gamma_0$, and $M_c = M_a = I$. The short-range couplings are $g_d = -2\tilde{g}_d - e^2/4K = (U + V)a^2/8$, $g_c = -2\tilde{g}_c = (U - V)a^2/8$, $g_f = g_a = -2\tilde{g}_f = -2\tilde{g}_a = -Ua^2/8$. d and c couplings correspond to the first (average density) and the second (staggered density), whereas f and a couplings represent the third (magnetization) and the fourth (staggered magnetization) terms in Eq. (5). The Coulomb interaction is represented by the following: (i) the intra-unit-cell, nearest-neighbor repulsion $V = e^2\sqrt{3}/(a\pi)$ and the $2\vec{K}$ Fourier component $e^2/2K$, and (ii) its long-range part, which is recovered upon Gaussian integration over the scalar gauge field a_0. $|\vec{\nabla}|$ should be understood as $|\vec{q}|$ in Fourier space [14]. Whereas such a separation would be exact for an infinitely long-ranged interaction, it is only an *approximation* for the Coulomb interaction.

The usual power counting implies that all short-range interactions in L are irrelevant and that the charge e is a marginal coupling at the noninteracting fixed point $g_x = \tilde{g}_x = e = 0$. Any critical point would therefore have to lie in the strong-coupling regime. To exert some control over it we may deform the Lagrangian from two to N flavors of the Dirac fields as follows:

$$\bar{\Psi}_+\Psi_+ \to \sum_{\sigma=1}^{N/2} \bar{\Psi}_\sigma \Psi_\sigma, \qquad \bar{\Psi}_-\Psi_- \to \sum_{\sigma=(N/2)+1}^{N} \bar{\Psi}_\sigma \Psi_\sigma, \tag{12}$$

and $g_x \to 2g_x/N$, $\tilde{g}_x \to 2\tilde{g}_x/N$, and $e^2 \to 2e^2/N$. The integration over the Fourier components with $\Lambda/b < q < \Lambda$ and $-\infty < \omega < \infty$ renormalizes then the short-range couplings at $T = 0$ as

$$\beta_x = \frac{dg_x}{d\ln b} = -g_x - C_x g_x^2 + O(1/N), \tag{13}$$

$$\tilde{\beta}_x = \frac{d\tilde{g}_x}{d\ln b} = -\tilde{g}_x + 2\tilde{g}_x^2 + O(1/N), \tag{14}$$

with $C_{c,a} = 4$, $C_{d,f} = 0$, and with the couplings rescaled as $g\Lambda/\pi \to g$. To the leading order in $1/N$ β functions for different interactions thus do not mix [15]. Since the model when $N = \infty$ is exactly solvable by the saddle-point method, the leading order β functions may also be understood as guaranteeing that the solution is cutoff independent [15]. The nonanalyticity of the inverse gauge-field propagator and the gauge invariance of L also dictate that

$$\beta_e = \frac{de^2}{d\ln b} = (z-1)e^2, \tag{15}$$

with z as the dynamical exponent, *exactly* [14]. Relativistic invariance of L is broken when $e \neq 0$, and consequently $z \neq 1$ at finite length scales. Similarly to the bosonic case,

$$z = 1 - \frac{e^2}{2\pi N} + O(1/N^2), \tag{16}$$

and the charge is marginally *irrelevant* to the first order in $1/N$ [7,16].

Besides the trivial fully attractive fixed point, the large-N β functions in Eqs. (13)–(15) exhibit *two critical points* in the attractive plane $e^2 = g_f = g_d = \tilde{g}_x = 0$: (i) at $g_a = -1/4$, $g_c = 0$ and (ii) $g_c = -1/4$, $g_a = 0$. There is also a bicritical point at $g_a = g_c = -1/4$, which directs the flows towards one of the two critical points (Fig. 1). The critical points are related by the symmetry under a change of sign of γ_μ for "down" components with $\sigma = N/2 + 1, \ldots, N$ accompanied by the exchange of g_a and g_c. The transition is either to $A = \langle \sum_\sigma \sigma \bar{\Psi}_\sigma \Psi_\sigma \rangle \neq 0$, which corresponds to an AF with a finite staggered magnetization, or to a CDW, with the finite staggered density $C = \langle \sum_\sigma \bar{\Psi}_\sigma \Psi_\sigma \rangle \neq 0$. The same, of course, follows from the explicit solution of the model at $N = \infty$. The flow of g_f towards the origin also agrees with the saddle-point equations, which do not show a ferromagnetic critical point at $N = \infty$, whereas the irrelevance of g_d simply means that the chemical potential vanishes.

Equation (14), however, appears to exhibit additional critical points at $\tilde{g}_x = 1/2$. These, however, would occur *within* the AF or the CDW, and are artifacts of our procedure which checks only the stability of the semimetal. It is easy to see from the explicit solution that the existing gap prevents such an additional transition. All $\tilde{g}_x$ are therefore irrelevant.

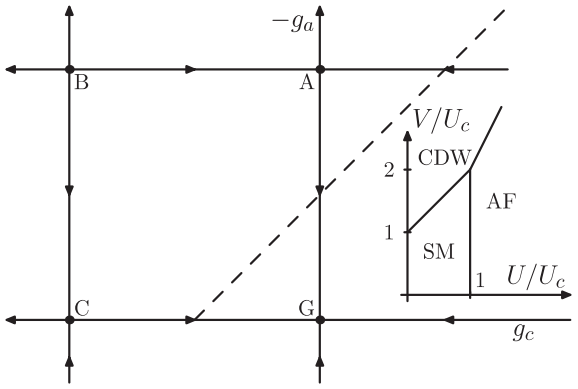

FIG. 1. The large-N flow diagram in the attractive plane $e = g_d = g_f = \tilde{g}_x = 0$. A, B, C, and G are the AF, bicritical, CDW, and the Gaussian fixed points, respectively. A and C are in the Gross-Neveu universality class. The extended Hubbard model in Eq. (2) defines the (dashed) line of initial conditions $g_c = (U - V)/4U_c$ and $g_a = -U/4U_c$, with V as a fixed nearest-neighbor repulsion. Inset: the resulting phase diagram.

The transition in the pure, $e = 0$, repulsive Hubbard model with $g_a < 0$ and $g_c > 0$ in the large-N limit is controlled therefore by the critical point A. Recalling that $g_a = Ua^2\Lambda/(8\pi)$, with $\Lambda \approx 1/a$, and $ta\sqrt{3}/2 = 1$ by our convention, one finds that this corresponds to the critical value of $U_c/t \approx 5.5$, certainly fortuitously close to the values found in numerical calculations [6]. Above the critical interaction the system develops a gap, at the same time becoming insulating and antiferromagnetic. At the critical line $g_c = g_f = g_d = \tilde{g}_x = e^2 = 0$, upon the change of sign of γ matrices for down components the Lagrangian becomes identical to the much studied Gross-Neveu model in $2 + 1$ dimensions [12]. Evidently, the Gross-Neveu critical point has only one unstable direction to the order $1/N$. Since the actual expansion parameter is $4N$, I expect this feature to survive even for $N = 2$. This leads to the conjecture that the SM-AF transition in the Hubbard model is continuous and described by the $N = 2$ Gross-Neveu critical point, at which

$$\langle \bar{\Psi}_\sigma(\vec{q}, \omega)\Psi_\sigma(\vec{q}, \omega)\rangle \sim (q^2 + \omega^2)^{(\eta_\Psi - 1)/2}, \tag{17}$$

with the fermion's anomalous dimension $\eta_\Psi = [2/(3\pi^2 N)] + O(1/N^2)$ [17]. The order parameter's correlation function at the critical point also decays as

$$\langle A(\vec{x}, \tau)A(0,0)\rangle \sim (x^2 + \tau^2)^{-(1+\eta)/2}, \tag{18}$$

where η is the standard anomalous dimension, and $\eta = 1\text{–}16/(3\pi^2 N) + O(1/N^2)$. The correlation length diverges at the critical point with the exponent $\nu = 1 + 8/(3\pi^2 N) + O(1/N^2)$, and the usual scaling laws are

expected to be satisfied. The critical exponents have been computed to the order $1/N^2$ (with η_Ψ known even to the order $1/N^3$) [17], as well as being determined by Monte Carlo calculations, the ϵ expansion [18], and the exact renormalization group [19]. In summary, for $N = 2$ one finds $\eta_\Psi = 0.038 \pm 0.006$, $\nu = 0.97 \pm 0.07$, and $\eta = 0.770 \pm 0.016$ [19].

The presence of gapless fermions on the semimetallic side places the Gross-Neveu phase transition outside the usual Ginzburg-Landau-Wilson paradigm, as evidenced by the large anomalous dimension η, for example. In fact, the Gross-Neveu model probably defines the simplest such a universality class. Its distinct characteristic is the fermion's anomalous dimension η_Ψ, which governs the disappearance of quasiparticles as the transition is approached on the semimetallic side. Scaling dictates that the residue of the quasiparticle pole behaves as

$$Z_\Psi \sim (U_c - U)^{\eta_\Psi}, \tag{19}$$

so that a very small η_Ψ would make it appear discontinuous at $U = U_c$.

In the AF, the eight generators that anticommute with $\sigma_z \otimes \gamma_0$ become broken; these are $(I_2, \sigma_z) \otimes (\gamma_3, \gamma_5)$ and $(\sigma_x, \sigma_y) \otimes (I, \gamma_{35})$. Among these only $(\sigma_x, \sigma_y) \otimes I$, which generate the usual spin rotations, correspond to the exact symmetry at $U = 0$, whereas the rest emerge as generators of approximate symmetries only at low energies. In the insulating phase the Goldstone bosons which correspond to the emerging generators are gapped, due to the irrelevant terms excluded from L [20]. The low-energy spectrum in the insulator consists therefore only of the usual magnons.

The long-range nature of Coulomb interaction is found to be irrelevant at a large N. On the scale of lattice spacing, however, Coulomb interaction leaves its imprint on the initial value of the coupling g_c, as indicated right below Eq. (11), for example [21]. In general, if the nearest-neighbor repulsion V is made sufficiently strong so that the line of initial conditions in Fig. 1 reaches the left of point C, there is an additional semimetal–CDW transition. Identifying V with $\sim e^2/a$ gives an alternative mechanism to that of Ref. [8] for the CDW formation. The two lines of continuous transitions merge above a certain V, when the line of initial conditions comes left of point B. The direct transition between the AF and the CDW is discontinuous.

For graphene, $t \approx 2.5$ eV, $U \approx 5$–12 eV, and $U/V \approx 2$–3 [10], so that the system is probably on the SM side of the transition. The external magnetic field, however, changes the density of states into a series of delta functions, so that the transition can now in principle take place even at an infinitesimal coupling [11]. In the magnetic field the flow of the couplings should be cutoff at $\sim 1/l_B$, where $l_B \gg a$ is the magnetic length. If the large-N picture presented here holds for $N = 2$, in the pure, $e = 0$, Hubbard model, at a sufficiently low field all couplings would become negligible compared to g_a. This would suggest that the magnetic field, at least with the Zeeman term neglected and the long-range component of the interaction screened by a metallic substrate, for example, should "catalyze" the antiferromagnetic order at a weak U.

The author thanks G. Sawatzky for a helpful correspondence. This work has been supported by NSERC of Canada.

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