Lattice Simulations near the Semimetal-Insulator Phase Transition of Graphene

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Abstract

We present results from Monte Carlo simulations of a three dimensional fermion field theory which can be derived from a model of graphene in which electrons interact via a screened Coulomb potential. For our simulations we employ lattice gauge theory methods used in elementary particle physics. We show that the theory undergoes a second order phase transition and we provide estimates for the critical exponents. The estimated value of the physical critical coupling implies that graphene in vacuum is an insulator. We also present the first results for the quasiparticle dispersion relation.

Key words: graphite, electrical conductivity, simulation

1. Introduction

There has been considerable recent interest in graphene (single layer graphite) sparked by its discovery and subsequent experimental study \cite{1}. The remarkable properties of graphene have been suspected for many years \cite{2}. In brief, for a carbon monolayer having one mobile electron per atom, a simple tight-binding model shows that the spectrum of low-energy excitations exhibits a linear dispersion relation centred on zeros located at the six corners of the first Brillouin zone (see e.g. \cite{3}). Using a linear transformation among the fields at two independent zeros it is possible to recast the Hamiltonian in Dirac form with $N_f = 2$ flavors of four-component spinor $\psi$ - the counting of the massless degrees of freedom coming from two carbon atoms per unit cell times two zeros per zone times two physical spin components per electron. Electron propagation in the graphene layer is thus relativistic, albeit at a Fermi velocity $v_F \approx 10^6 \text{m/s}$. The implications for the high mobility of the resulting charge carriers is the source of the current excitement. The electronic properties of graphene are discussed in detail in a recent review paper \cite{4}.

Although the semimetallic properties of graphene on a substrate are well-known, it remains unclear whether graphene in vacuum undergoes a phase transition from the semimetal phase to an insulating phase. A sufficiently strong Coulomb interaction may lead to a condensation of electron and hole pairs thus turning the conducting phase into a gapped insulator at a critical value of fermion flavors $N_{fc}$. Recent estimates of $N_{fc}$ have been obtained by: self-consistent solutions of...
Schwinger-Dyson equations yielding $N_{fc} = 2.55$ [3]; renormalization group treatment of radiatively induced four-fermion interactions yielding $N_{fc} = 2.03$ [6]; and lattice simulations yielding $N_{fc} = 4.8(2)$ [7]. Furthermore, a lattice simulation of graphene based on a four dimensional gauge invariant action with fermions propagating in two spatial dimensions predicted that freely suspended graphene is an insulator [8, 9]. The results of lattice simulations of a Thirring-like model pertinent to graphene presented in this paper are consistent with this observation.

2. The Model

While the above considerations apply quite generally, a realistic model of graphene must incorporate interactions between charge carriers. One such model, due to Son [10], has $N_f$ massless fermion flavors propagating in the plane, but interacting via an instantaneous 3$d$ Coulomb interaction. In Euclidean metric and static gauge $\partial_0 A_0 = 0$ the action reads

$$S_1 = \sum_{a=1}^{N_f} \int dx_0 d^2 x (\bar{\psi}_a \gamma_0 \partial_0 \psi_a + \nu_F \bar{\psi}_a \vec{\nabla} \psi_a + iV \bar{\psi}_a \gamma_0 \psi_a) + \frac{1}{2e^2} \int dx_0 d^3 x (\partial_0 V)^2,$$

where $e$ is the electron charge, $V \equiv A_0$ is the electrostatic potential, and the $4 \times 4$ Dirac matrices satisfy $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \mu = 0, \ldots, 3$. In our notation $\vec{x}$ is a vector in the 2$d$ plane while the index $i$ runs over all three spatial directions. In the large-$N_f$ limit the resummed $V$ propagator becomes [10]

$$D_1(p) = (D_0^{-1}(p) - \Pi(p))^{-1} = \left(\frac{2|\bar{p}|}{e^2} + \frac{N_f}{8} \frac{|\bar{p}|^2}{(p^2)^2}\right)^{-1},$$

where $p^2 = p_0^2 + \nu_F^2 |\bar{p}|^2$. $D_0$ corresponds to the classical propagation of $V$ and $\Pi$ comes from a vacuum polarisation fermion-antifermion loop. In either the strong coupling or large-$N_f$ limits $D_1(p)$ is thus dominated by quantum corrections - the relative importance of the original Coulomb interaction being governed by a parameter $\lambda \equiv |\Pi/D_0|_{p_0=0}$. Chiral symmetry breaking due to the spontaneous condensation of particle - hole pairs is signalled by an order parameter $\langle \bar{\psi} \psi \rangle \neq 0$. Physically the most important outcome is the generation of a gap in the fermion spectrum, implying the model is an insulator.

The physics of eq. (1) is very reminiscent of the three dimensional Thirring model, which is analytically tractable at large-$N_f$, but exhibits spontaneous chiral symmetry breaking at small $N_f$ and strong coupling [11, 12]. Arguably the Thirring model is the simplest field theory of fermions requiring a computational solution. The location of the phase transition at $N_f = N_{fc}$ in the strong coupling limit has recently been determined by lattice simulations to be $N_{fc} = 6.6(1)$ [13]. The apparent similarity of the two systems has led us to propose a Thirring-like model pertinent to graphene [7], with Lagrangian

$$S_2 = \sum_{a=1}^{N_f} \int dx_0 d^2 x \left[\bar{\psi}_a \gamma_\mu \partial_\mu \psi_a + iV \bar{\psi}_a \gamma_0 \psi_a + \frac{1}{2g^2} V^2\right].$$

As for eq. (1) we assume a large-$N_f$ limit to estimate the dominant vacuum polarisation correction; the resultant propagator for $V$ is

$$D_2(p) = \left(\frac{1}{g^2} + \frac{N_f}{8} \frac{|\bar{p}|^2}{(p^2)^2}\right)^{-1}.$$
In the strong-coupling or large-$N_f$ limits, $D_2$ coincides with $D_1$, implying that the fermion interactions are equivalent. We thus expect predictions made with the model eq. (3), and in particular critical behavior such as the value of $N_{fc} = 4.8(2)$ \cite{7}, to be generally valid for Son’s model eq. (1) in the limit of large $\lambda$.

3. Lattice Simulation Results

In this section we present results from simulations with $N_f = 2$ which corresponds to real graphene. Details for the lattice action and the algorithm employed for our simulations can be found in \cite{7}. The anisotropic nature of the model dynamics results in the systematic effects due to finite temporal extend $L_t$ being more important than those due to finite spatial extend $L_s$. By comparing the values of the chiral condensate from simulations on different lattice sizes we found that the finite size effects on $24^2 \times 48$ are within statistical errors for the parameter ranges $m_0 = 0.005, 0.525 \leq g^{-2} \leq 0.65$ and $m_0 = 0.010, ..., 0.025, 0.525 \leq g^{-2} \leq 0.70$ (where $m_0$ is the fermion bare mass). The chiral condensate as a function of $m_0$ and $(g_{c}^{-2} - g^{-2})$ near a continuous phase transition scales according to an equation of state given by

$$m_0 = A(g^{-2} - g_{c}^{-2})(\bar{\psi}\psi)^{\delta - 1/2} + B(\bar{\psi}\psi)^{\delta}$$ \hspace{1cm} (5)

We used eq. (5) to curve-fit our data and extracted $g_{c}^{-2} = 0.607(5), \delta = 2.72(7)$, and $\beta = 0.68(2)$. The data and the fitting curves including the $m_0 = 0$ curve are shown in Fig. 1. Our estimates of the critical exponents are clearly distinct from their strong coupling values $\delta = 5.5(3)$ and $\beta = 0.22(2)$ \cite{7}. We also note that the exponent $\delta$ is larger than the estimate $\delta = 2.26(6)$ of Drut and Lähde \cite{9}.

The fermion dynamical mass $m_f$ is an inverse time-like correlation length of the system. At the critical coupling, $\langle \bar{\psi}\psi \rangle$ and $m_f$ obey the following scaling relations for $m_0 \neq 0$:

$$\langle \bar{\psi}\psi \rangle = a_1 m_0^{1/\delta}, \quad m_f = a_2 m_0^{\nu/\beta \delta}.$$ \hspace{1cm} (6)
By fitting our data at $\beta = 0.60$ (which is close to the critical coupling $g^{-2} = 0.607(5)$) to eq. (6) we obtain $\delta = 2.81(2)$ and $\nu_t = 0.80(6)$. This value of $\delta$ is consistent with $\delta = 2.72(7)$ obtained from the equation of state. In Fig. 2 we present the data and the fitting functions.

For systems with anisotropic interactions the correlation lengths in the time and space directions may scale with different exponents $\nu_t$ and $\nu_s$ respectively. The dynamic critical exponent $z \equiv \nu_t/\nu_s$ describes relative scaling of time and space length scales and governs the quasiparticle dispersion relation $E \sim p^z$ for $p \rightarrow 0$. In $d$ spacetime dimensions the exponents $\nu_t$ and $\nu_s$ are related to $\beta$ and $\delta$ via a generalized hyperscaling relation [14]:

$$\nu_t + (d - 1)\nu_s = \beta(\delta + 1)$$  \hspace{1cm} (7)

From eq. (7) we obtain $\nu_s = 0.90(5)$ and $z = 0.89(8)$. This value of $z$ is close to the strong coupling and large-$N_f$ $z \approx 0.8$ estimate of Son [10]. A value of $z < 1$ implies that the quasiparticle excitations are stable, because energy momentum conservation forbids their decay into two or more quasiparticles.

Before we decide whether our model predicts that graphene in vacuum is a conductor or an insulator we need an estimate of the physical critical coupling $\lambda_c$. First we calculate the renormalized critical coupling $g_{cR}^2$. We must note however, that the vacuum polarisation calculation leading to eqs. (2) and (4) does not go through in quite the same way for the lattice regularised model; rather, there is an additive correction which is momentum independent and ultraviolet-divergent:

$$\Pi^{\text{lat}}(p) = \Pi^{\text{cont}}(p) + g^2 J(m),$$  \hspace{1cm} (8)

where $J(m)$ comes from incomplete cancellation of a lattice tadpole diagram [11]. This extra divergence not present in the continuum treatments can be absorbed by a wavefunction renormalisation of $V$ and a coupling constant renormalisation

$$g_R^2 = \frac{g^2}{1 - g^2 J(m)}. \hspace{1cm} (9)$$

In the large-$N_f$ limit we thus expect to find the strong coupling limit of the lattice model at $g_R^2 \rightarrow \infty$ implying $g^2 \rightarrow g_{\text{lim}}^2 = J^{-1}(m)$. For $g^2 > g_{\text{lim}}^2$ $D^{\text{lat}}(p)$ becomes negative, and $S_{\text{lat}}$ no
longer describes a unitary theory. For small-$N_f$ we identify $g_{\text{lim}}^2$ with the value of the coupling where the chiral condensate has its maximum value [7]. For $N_f = 2$, $g_{\text{lim}}^2 = 0.30$ [7] and from eq. (9) we obtain $g_{cR} = 3.23(4)$. Next, we match $D_2^{\text{latt}}(p)$ to $D_1(p)$ at a reference momentum $p_0 = 0$, $|\vec{p}| = \frac{\pi}{2}$, so that the propagators are equal at a distance of roughly one lattice spacing (for shorter distances $D_2^{\text{latt}} > D_1$ and vice-versa) yielding the condition

$$\lambda_c = \frac{\pi g_{cR}^2}{4} = 2.54(2).$$

(10)

This value of $\lambda_c$ is larger than the value $\lambda_c \approx 1.25$ calculated for graphene on an SiO$_2$ substrate [10], but smaller than the value $\lambda_0 \approx 3.4$ based on a substrate with unit dielectric constant. Our result thus suggests freely-suspended graphene is an insulator. Drut and Lähde obtained from simulations of a gauge invariant action of graphene $\lambda_c = 1.67(2)$, which also implies that graphene in vacuum is an insulator [8].

A major advantage of our formulation is that it permits a relatively straight-forward analysis of the quasiparticle dispersion relation. Here we present our first results from simulations on $32^2 \times 48$ and $48^3$ lattices. We fitted the fermion energy as a function of momentum $p$ in the $x$ direction to the following discretized free field dispersion relation which assumes $z = 1$:  

$$E(p) = A \sinh^{-1} \left( \sqrt{\sin^2 p + M^2} \right),$$

(11)

where $AM$ is the quasiparticle dynamical mass $m_f$ and $A \sim \lim_{p \to 0} \frac{dE}{dp}$ is the Fermi velocity. Equation (11) fitted the data relatively well, providing no evidence for $z \neq 1$. An example of fits to data generated with $g^{-2} = 0.8, 0.9$ and $m_0 = 0.005$ on a $48^3$ lattice is shown in Fig. 3. In Fig. 4 we show that within the accuracy of our analysis the parameter $A$ is independent of both $m_0$ and $g^{-2}$ with a value roughly $A \approx 0.7$ suggesting that the free field value of $v_F$ is renormalized.
4. Summary and Conclusions

In this paper we studied a (2 + 1)d Thirring-like model pertinent to graphene based on eq. (3). We performed Monte Carlo simulations using lattice gauge theory techniques and showed that the model undergoes a second order phase transition with critical exponents $\delta = 2.72(7)$, $\beta = 0.68(2)$, and $\nu_s = 0.80(6)$. Using a generalized hyperscaling relation valid for theories with anisotropic interactions we obtained $\nu_s = 0.90(5)$ and $z = 0.89(8)$. Our preliminary $z < 1$ estimate implies that the quasiparticles are stable based on energy-momentum conservation. The value of the physical critical coupling $\lambda_c = 2.54(2)$ implies that freely-suspended graphene is an insulator in agreement with [8]. We also presented the first results for the quasiparticle dispersion relation and within the accuracy of our simulations we showed that the free field Fermi velocity is renormalized. Simulations with higher resolution in momentum on larger spatial lattices are currently in progress for a more accurate study of the dispersion relation.

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