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On the semimetal-insulator transition and Lifshitz transition in simulations of mono-layer graphene

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We report on the status of ongoing Hybrid-Monte-Carlo simulations of the tight-binding model of mono-layer graphene. We present results concerning the semimetal-insulator phase transition, whereby two-body interactions are modeled by a partially screened Coulomb potential which takes into account screening by electrons in the lower σ-orbitals. We obtain evidence that finite-size effects may still be present in the current estimate of the critical coupling strength α_C, which was previously extracted from simulations on lattice-sizes up to $N_x = N_y = 18$. We also present preliminary results concerning the Neck-disrupting Lifshitz transition which occurs at finite Fermion-density in the limit of vanishing two-body interactions. A sign-problem is circumvented by using a spin-dependent chemical potential in our simulations.

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1. Introduction

In recent years, much interest has arisen in graphene, a two-dimensional sheet of carbon atoms arranged on a hexagonal lattice, due to its many unusual properties which make it an interesting candidate for a number of technological applications [1]. From a theoretical perspective, graphene is interesting because its electronic properties are governed by a massless Dirac equation in the limit of low energies and because the small Fermi velocity $v_F \approx c/300$ leads to strong electromagnetic interactions with an effective fine-structure constant of $\alpha_{\text{eff}} = e^2/(\hbar v_F) \approx 2.2$ [2]. Thus, graphene provides an example of the physics of strongly coupled relativistic field theory, realized in a condensed matter system. Furthermore, the coupling-constant in graphene can be directly manipulated by affixing the sheet to a substrate, which leads to di-electric rescaling $\alpha_{\text{eff}} \to \alpha_{\text{eff}}/\varepsilon$.

Early on, the lattice community took an interest in graphene since it seemed obvious that the well-developed machinery for simulating field theories should be applicable. Several works were published which focused on electronic properties in the low-energy limit (see e.g. Refs. [3]). Later it was shown how the full microscopic theory with hexagonal symmetry can be formulated as a lattice theory [4]. This was henceforth adopted as the de-facto standard and a number of works were published presenting simulations based on this derivation [5, 6, 7, 8].

In this work we report on our ongoing efforts to simulate the electronic properties of graphene via Hybrid-Monte-Carlo. We implement a fully hexagonal lattice theory based on the derivations presented in Ref. [4].

The aim of this paper is two-fold: After summarizing the methodology, we first present a follow-up discussion of our investigation of the semimetal-insulator phase-transition which was published in Ref. [8]. Therein simulations of the interacting tight-binding theory of graphene were presented in which electronic two-body interactions were modeled by a partially screened Coulomb potential, which accounts for screening by electrons in the lower σ-orbits at short distances and crosses over smoothly to an unscreened Coulomb potential at long distances. We contrasted these results to a similar study presented in Ref. [6], which instead assumed that at long distances the potential is screened by a constant di-electric screening factor. We found that for a lattice of dimensions $N_x = N_y = 18$ the exact form of the long-range tail doesn't seem to affect the precise location of the critical coupling strength α_C for gap-formation much. In this work we present results obtained on $N_x = N_y = 36$ which may indicate that for larger systems the transition is shifted to smaller α_C. This would mean that previous simulations are affected by finite-size effects and that an extrapolation to infinite surface area is in order to conclusively decide whether the long-range part of the potential is of relevance.

Second we present preliminary results concerning the Neck-disrupting Lifshitz transition, which is known to occur in the limit of vanishing two-body interactions at finite Fermion-density and which is characterized by a change of the topology of the Fermi surface and a logarithmic divergence of the density of states [9]. To avoid a Fermion sign-problem we implement the "isospin" chemical potential, the sign of which differs for the two spin-orientations of electrons. The results presented here concern the non-interacting limit only. Our long-term goal is to investigate how a small interaction term affects the Lifshitz transition.

2. The setup

The setup of our simulations has been described in great detail in Ref. [8], where a step-by-step derivation of every component of the Hybrid-Monte-Carlo algorithm for the interacting tight-binding theory based on the concepts worked out in Ref. [4] is presented. We will only summarize the basic principles here. Our goal is to simulate the thermodynamics of the interacting tight-binding theory of graphene

$$H = \sum_{\langle x,y \rangle} (-\kappa)(a_x^\dagger a_y - b_x^\dagger b_y + \text{h.c.}) + \sum_{x,y} q_x V_{xy} q_y + \sum_x m_s (a_x^\dagger a_x + b_x^\dagger b_x) \,, \tag{2.1}$$

where $a_x, a_x^\dagger, b_x, b_x^\dagger$ are ladder operators for particles with spin $+1/2$ and anti-particles ("holes") with spin $-1/2$ respectively. The sums run over all pairs of nearest neighbors, pairs of coordinates and all coordinates of the hexagonal lattice respectively. $q_x = a_x^\dagger a_x - b_x^\dagger b_x$ is the charge operator, $\kappa \approx 2.7$ the hopping parameter and m_s a "staggered" mass-term, the sign of which alternates on the triangular sub-lattices of the hexagonal lattice. The mass term is added to remove zero-modes from the Hamiltonian and the limit $m_s \to 0$ is later taken. The matrix V, which describes two-body interactions, must be positive-definite but otherwise may be chosen arbitrarily. We use the "partially screened Coulomb potential" in our simulations as described below.

A lattice path-integral representation for the grand-canonical partition function $Z = \text{Tr} e^{-\beta H}$, in which the operators $a_x, a_x^\dagger, b_x, b_x^\dagger$ are replaced by Grassmann-valued field variables, can be derived by factorizing $e^{-\beta H}$ into N_t terms (implying a discretization error $\mathcal{O}(\delta^2)$ where $\delta = \beta / N_t$) and inserting complete sets of of *Fermionic coherent states*. The interaction term $\sim q_x V_{xy} q_y$ at first prevents the usual procedure of integrating out Grassmann-fields via Gaussian integration, since it contains fourth-powers of latter operators. These can be eliminated through *Hubbard-Stratonovich* transformation

$$\exp\Big\{ -\frac{\delta}{2} \sum_{x,y} q_x V_{xy} q_y \Big\} \propto \int \Big[\prod_x \phi_x \Big] \exp\Big\{ -\frac{\delta}{2} \sum_{x,y} \phi_x V_{xy}^{-1} \phi_y - i\,\delta \sum_x \phi_x q_x \Big\} \,, \tag{2.2}$$

at the expense of introducing a dynamical scalar auxiliary field ϕ ("Hubbard field"), which plays the role of a gauge field. In fact, ϕ can be understood as representing the scalar electric potential. A magnetic vector-potential does not appear since interactions are taken to be instantaneous (which is a valid approximation since $v_F \ll c$). The final result is the functional integral

$$Z = \int \mathscr{D}\phi \, \det\big[M(\phi) M^\dagger(\phi) \big] \exp\Big\{ -\frac{\delta}{2} \sum_{t=0}^{N_t - 1} \sum_{x,y} \phi_{x,t} V_{xy}^{-1} \phi_{y,t} \Big\} \,, \tag{2.3}$$

which is of a form that can be dealt with, using a standard Hybrid-Monte-Carlo algorithm to generate representative configurations of the Hubbard field ϕ. The Fermion-operator is given by

$$M_{(x,t)(y,t')} \;=\; \delta_{xy} (\delta_{tt'} - e^{-i \frac{\beta}{N_t} \phi_{x,t}} \delta_{t-1,t'}) - \kappa \frac{\beta}{N_t} \sum_{\vec{n}} \delta_{y,x+\vec{n}} \delta_{t-1,t'} + m_s \frac{\beta}{N_t} \delta_{xy} \delta_{t-1,t'} \,. \tag{2.4}$$

We choose to simulate rectangular graphene sheets with periodic boundary conditions. The dimensions N_x and N_y refer to the rhombic coordinate system which spans the triangular sub-lattices.

3. Semimetal-insulator transition

A question which is of immediate significance to technological applications (since electronic devices require a gate-voltage) is whether two-body interactions generate a band-gap for some effective coupling constant α_{eff} which is smaller than the upper bound given by suspended graphene ($\alpha_{\text{eff}} \approx 2.2$). This corresponds to electronic quasi-particles acquiring a dynamical mass and at a microscopic level implies a spontaneous breaking of the symmetry under exchange of the two triangular sub-lattices by formation of some condensate. Both charge-density-wave (CDW) and spin-density-wave (SDW) formation are mechanisms which have been discussed in literature. As a result of studies which directly assumed or indirectly implied that the two-body interactions in graphene were essentially unmodified Coulomb-type interactions (see e.g. Refs. [3, 5] and references therein) it was predicted that the transition to a gapped phase happens for $\alpha_{\text{eff}} \gtrsim 1.0$, well within the physically accessible region. This contradicted experiments which found graphene in vacuum to be a conductor [10].

In Ref. [6] a Monte-Carlo study of the formation of an anti-ferromagnetic condensate was conducted which suggested screening of interactions by electrons in the lower σ-orbitals as a mechanism which moves the transition to $\alpha_{\text{eff}} \approx 3.14$ (to the unphysical region) and thus reconciles theory with experiment. Therein explicit values for the on-site (V_{00}), nearest-neighbor (V_{01}), next-nearest-neighbor (V_{02}) and third-nearest-neighbor (V_{03}) potentials from calculations within a constrained random phase approximation (cRPA) conducted in Ref. [11] were used. At long distances, it was assumed that the potential falls off as $\sim 1/(\varepsilon_\sigma r)$, where the constant $\varepsilon_\sigma \approx 1.41$ was adjusted to match the V_{03} term. A single lattice-size ($N_x = N_y = 18, N_t = 20$) and temperature ($\beta = 2\text{eV}^{-1}$) were considered.

Our work (Ref. [8]) aimed at eliminating residual doubts concerning the long range tail. At long-distances we thus instead used a phenomenological model

$$\varepsilon_\sigma^{-1}(\vec{k}) = \frac{1}{\varepsilon_1} \frac{\varepsilon_1 + 1 + (\varepsilon_1 - 1)e^{-kd}}{\varepsilon_1 + 1 - (\varepsilon_1 - 1)e^{-kd}} \,, \tag{3.1}$$

proposed in Ref. [11] that describes a thin film of thickness $d = 2.8$ Å ($\approx 1.41 \cdot 10^{-3}\,\text{eV}^{-1}$) with a dielectric screening constant $\varepsilon_1 = 2.4$ and computed a *partially screened Coulomb potential* via Fourier back-transformation

$$V(\vec{r}) = \frac{1}{(2\pi)^2} \int_{\mathbb{K}^2} d^2k \widetilde{V}_0(\vec{k})\, \varepsilon_\sigma^{-1}(\vec{k})\, e^{-i\vec{k}\vec{r}} \,, \qquad \widetilde{V}_0(\vec{k}) = (2\pi e^2)/k \,, \tag{3.2}$$

which smoothly goes over to an unscreened potential as $r \to \infty$ (see Fig. 1, left). Simulations using this potential were carried out, and the α_{eff} dependence of the anti-ferromagnetic condensate

$$\Delta_N = \frac{1}{N_x N_y} \Big\{ \sum_{x \in X_A} (a_x^\dagger a_x + b_x^\dagger b_x) - \sum_{x \in X_B} (a_x^\dagger a_x + b_x^\dagger b_x) \Big\}, \tag{3.3}$$

was investigated for $N_x = N_y = 18, N_t = 20$ and $\beta = 2\text{eV}^{-1}$ (the sums in Eq. (3.3) run over coordinates in the two sub-lattices). We found no substantial difference to the results of Ref. [6] and thus concluded that the gap-transition is insensitive to the long-range tail of the potential for this

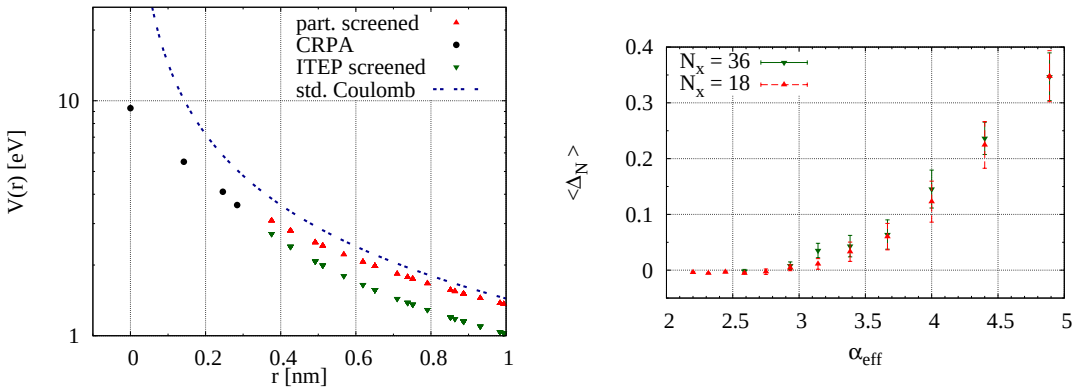

Figure 1: Left: Comparison of standard Coulomb potential, partially screened potential and potential used in Ref. [6] ("ITEP screened"). Right: Order-parameter for gap-transition in the limit $m_s \to 0$.

lattice-size.

Fig. 1, right, shows recent results for $\Delta_N(\alpha_{\text{eff}})$ which were obtained on several hundreds of independent configurations of a $N_x = N_y = 36, N_t = 20$ lattice (for a range of m_s which allowed the limit $m_s \to 0$ to be taken) and compares them with our published results obtained from $N_x = N_y = 18$. A slight systematic effect is visible which may indicate a small shift of the transition to a smaller value of α_{eff}. We take this result as evidence that finite-volume effects may still be present on $N_x = N_y = 18$ and that an infinite volume extrapolation is thus in order. It is conceivable that the precise form of the long-range tail becomes more relevant for larger system-size.

4. Neck-disrupting Lifshitz transition

In the non-interacting limit the band structure of the tight-binding Hamiltonian can be computed exactly [2]. It is known that the valence and conduction bands possess within the first Brillouin zone, (following the convention to count points which are shared by cells fractionally) three saddle-points, the so-called M-points. These points separate the low-energy region, where the dispersion relation is approximately linear, from a region in which electronic excitations are described by the non-relativistic Schroedinger equation. By introducing a chemical potential ($H \to H + \mu \sum_{x,s} n_{x,s}$) it is possible to shift the Fermi-energy across these points, which leads to a change of the topology of iso-energy lines (see Fig. 2). This is known as a *Neck-disrupting Lifshitz transition* and is accompanied by a logarithmic divergence of the density of states [9] ("Van-Hove singularity").

To date, little is known about the effect of two-body interactions on the Lifshitz transition. Our goal is to clarify this issue through Monte-Carlo simulation. In particular, it will be interesting to see how a small interaction term affects the logarithmic scaling behavior. Adding a chemical potential leads to a Fermion sign-problem however, since the Fermion operators are modified as

$$M_{(x,t)(y,t')} \to M_{(x,t)(y,t')} + \mu \frac{\beta}{N_t} \delta_{xy} \delta_{t-1,t'} \ , \qquad M^\dagger_{(x,t)(y,t')} \to M^\dagger_{(x,t)(y,t')} - \mu \frac{\beta}{N_t} \delta_{xy} \delta_{t+1,t'} \ , \tag{4.1}$$

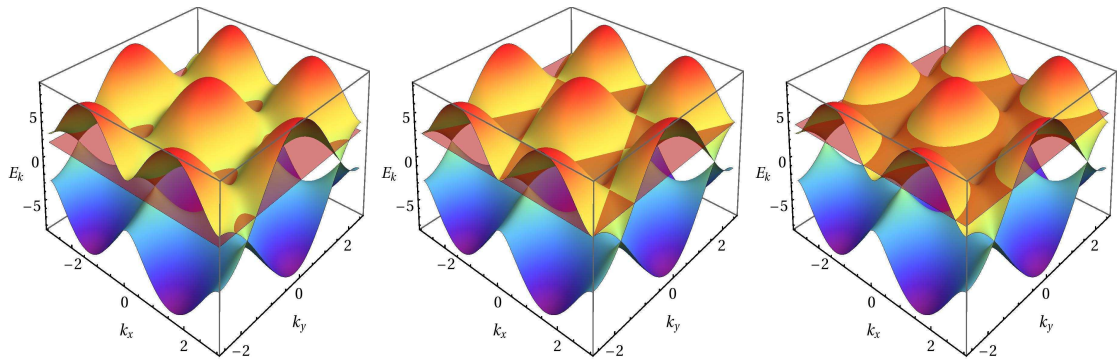

Figure 2: Band structure of tight-binding model, with Fermi-energy below (left), exactly crossing (middle) and above (right) the M-points (saddle points). Topology of the intersecting lines ("Fermi surface") are different in each case.

which implies that the phases in Eq. (2.3) no longer cancel. As a first step it is reasonable to consider an *isospin chemical potential* $\mu_S \equiv s\mu$ (the sign of μ_S depends on the direction of electron spin). In the non-interacting limit it is clear that the Lifshitz transition is blind to the sign of the spin. For μ_S there is no sign-problem since positive terms are added to both M and $M^\dagger$.

We have so-far obtained preliminary results concerning the *particle-number-susceptibility* associated with μ_S

$$\chi(\mu_S) = \frac{1}{V\beta}\frac{d^2 \ln Z}{d\mu_S^2}\,, \tag{4.2}$$

which is related to the density of states $\rho(\mu)$ (for $T = 0$ they are exactly proportional) and displays the characteristic scaling behavior of the Lifshitz transition. Hereby we restricted ourselves to the the non-interacting limit, where $\chi(\mu_S)$ can be computed directly from inversions of the Fermion matrix on Gaussian noise vectors and no HMC updates are necessary (since the Hubbard field is taken to zero). Furthermore, $\chi(\mu_S)$ can in fact be computed exactly in this limit (by numerical integration) from the retarded particle-hole polarization (Lindhard) function (see Ref. [9]). For a given temperature T it is (in infinite volume) given by

$$\chi(\mu_S) = \frac{1}{2T}\int_{BZ}\frac{d^2k}{4\pi^2}\left[\mathrm{sech}^2\left(\frac{\mu_S - E(\vec{k})}{2T}\right) + \mathrm{sech}^2\left(\frac{\mu_S + E(\vec{k})}{2T}\right)\right]\,, \tag{4.3}$$

where $E(\vec{k})$ is the dispersion-relation of the tight-binding theory and the integral runs over the first Brillouin zone. These results are important, since they allow us to compare lattice results to direct calculations and serve as a validation of our method. Simulations at non-zero coupling are currently in progress.

Fig. 3 shows the susceptibility for two different temperatures ($\beta = 2; 4\,\mathrm{eV}^{-1}$) obtained from a $N_x = N_y = 24$ lattice with $m_s = 0.5\mathrm{eV}$. We obtained data for different lattice-spacings and extrapolated to the limit $\delta \to 0$. The results are compared to solutions of Eq. (4.3) (for finite volumes the integral is replaced by a sum over discrete momenta). We find exact agreement within errors. Furthermore, we have confirmed that the peak-height scales logarithmically with temperature as Eq. (4.3) also predicts.

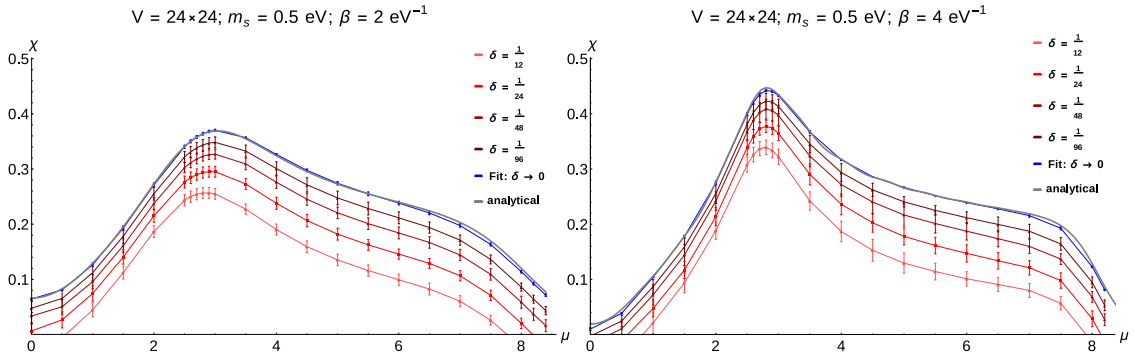

Figure 3: $\chi(\mu_S)$ in the non-interacting limit for $N_x = N_y = 24$ and $m_s = 0.5$eV. Results are obtained with different discretizations and the limit $\delta \to 0$ is extrapolated. Two temperatures ($\beta = 2; 4\,\mathrm{eV}^{-1}$) are displayed. The solid line represents the exact results, obtained from Eq. (4.3).

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