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Interaction of static charges in graphene within Monte-Carlo simulation

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The study of the interaction potential between static charges within Monte-Carlo simulation of graphene is carried out. The numerical simulations are performed in the effective lattice field theory with noncompact 3 + 1-dimensional Abelian lattice gauge fields and 2 + 1-dimensional staggered lattice fermions. At low temperature the interaction can be described by the Coulomb potential reduced by some dielectric permittivity ε_R. The dependence of the ε_R on the dielectric permittivity of substrate is determined. In addition, the renormalization of the quasiparticle charge is studied. At large temperatures the interaction potential can be described by the two dimensional Debye screening. The dependence of Debye screening mass on the dielectric permittivity of substrate allows to determine the position of the insulator-semimetal phase transition. It is shown that graphene reveals in the semimetal phase the properties of the two-dimensional plasma of fermions excitations.

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1. Introduction

Graphene is an allotrope of carbon, in which atoms form a two-dimensional honeycomb lattice. Carbon atoms in graphene are bonded by sp^3-bonds and the bond length is about 0.142 nm [1].

The charge carriers in graphene at low energies behave as massless Dirac fermions [2]. The Fermi velocity of charge carriers $v_F \approx \frac{c}{300}$. Since the Fermi velocity is much smaller than the speed of light, magnetic and retardation effects in the interactions between charge carriers in graphene may be neglected, thus electron-electron interaction in graphene is described by the instantaneous Coulomb potential. The effective coupling constant for the Coulomb interaction in suspended graphene

$$g^2 = \frac{e^2}{v_F} \approx 2 \tag{1.1}$$

is large, so this material may be considered as a strongly interacting system.

In real experiments graphene is put on a substrate. The effective coupling constant for graphene on substrate with the dielectric permittivity ε is reduced by a factor $2/(\varepsilon+1)$. The variation of the dielectric permittivity ε of substrate changes effective coupling constant and thus allows to study the properties of graphene in both strong and weak coupling regime.

There exists a number of papers where graphene was studied by Monte-Carlo method [3, 4, 5, 6] and insulator-semimetal transition was found. At weak coupling regime ($\varepsilon > 5$, $g^2 < 0.7$) graphene is in the semimetal phase. In this phase the conductivity is $\sigma \approx \frac{e^2}{h}$ and there is no gap in the spectrum of fermionic excitations. The chiral symmetry of graphene is not broken. At strong coupling regime ($\varepsilon < 3$, $g^2 > 1$) graphene is in the insulator phase. In this phase the conductivity is considerably suppressed and fermionic excitations acquire dynamical mass [7]. The phase transition from weak to strong coupling regime takes place at the dielectric permittivity of substrate $\varepsilon \approx 4$.

2. Lattice simulation of graphene

2.1 Effective field theory Lagrangian

We present the results of MC simulations of graphene in the framework of effective field model. Potential between static charges in graphene plane was measured. The non-MC calculations of the potential were performed in [8] (see also references therein). The partition function of graphene effective field theory can be written as [2, 9, 10, 11]:

$$\mathscr{Z} = \int \mathscr{D}\bar{\psi}\mathscr{D}\psi\mathscr{D}A_0 \exp\left(-\frac{1}{2}\int d^4x\,(\partial_i A_0)^2 - \right.$$
$$\left. - \int d^3x\,\bar{\psi}_f\left(\gamma_0\,(\partial_0 - igA_0) - \sum_{i=1,2}\gamma_i\partial_i\right)\psi_f\right), \tag{2.1}$$

where A_0 is the zero component of the vector potential of the $3+1$ electromagnetic field, γ_μ are Euclidean gamma-matrices and ψ_f ($f = 1,2$) are two flavors of Dirac fermions which correspond to the two spin components of the non-relativistic electrons in graphene, effective coupling constant $g^2 = 2e^2/(v_F(\varepsilon+1))$ ($\hbar = c = 1$ is assumed).

The simulation of partition function (2.1) is carried out within the approach developed in [5]. In order to discretize the fermionic part of the action in (2.1) the staggered fermions [12, 13] are used. One flavor of staggered fermions in $2+1$ dimensions corresponds to two flavors of continuum Dirac fermions [12, 13, 14], which makes them especially suitable for simulations of the graphene effective field theory. Noncompact lattice electric field is used for the electromagnetic part of the action in (2.1). Technical details of the lattice regularization scheme and simulation algorithm may be found in [15].

2.2 Physical observables on the lattice

To measure the potential, $V(\vec{r})$, between static charges in graphene, we calculate the correlator of two Polyakov lines $\langle P^\gamma(0)(P^\gamma(\vec{r}))^+\rangle$:

$$\langle P^\gamma(0)(P^\gamma(\vec{r}))^+\rangle = a\exp\left(-\frac{V(\vec{r})}{T}\right), \tag{2.2}$$

where T[1] is the temperature of graphene sample, $\vec{r}$ is restricted to the graphene plane, a parameterizes the self-energy part of the correlator, the Polyakov line $P(\vec{r})$ is

$$P(\vec{r}) = \exp\left(-ie\int_0^{1/T} dtA_0(t,\vec{r})\right) = \prod_{t=0}^{L_t-1}\exp\left(-i\theta_{(t,\vec{r}),0}\right). \tag{2.3}$$

To suppress statistical errors, we measure the correlator of Polyakov lines in some rational power. Physically this means that the interaction potential between static charges $\pm e\cdot\gamma$ is considered. We have found that for $\gamma\sim 0.1$ the uncertainty of the calculation is much smaller than for $\gamma = 1$ (usual Polyakov line). In the calculations the value $\gamma = 0.1$ is used.

Below we use the following notations:

$$\alpha_0 = e^2\frac{2}{\varepsilon+1} \tag{2.4}$$

is the bare effective squared charge and

$$\alpha_r = \frac{\alpha_0}{\varepsilon_R} \tag{2.5}$$

is the effective squared charge, renormalized due to interaction, ε_R is the effective dielectric permittivity of graphene.

To get the potential between static charges, we measure the correlator of Polaykov lines and fit $V(\vec{r})$ by lattice screened Coulomb potential:

$$V(\vec{r}) = \frac{1}{\varepsilon_R}V_C(\vec{r}) + c, \tag{2.6}$$

$$V_C(\vec{r}) = -\alpha_0\frac{\pi\gamma^2}{L_s^3 a_s}\sum_{n_1,n_2,n_3}\frac{1}{\sum_i\sin^2(p_i a_s/2)}e^{i\vec{p}\vec{r}}, \tag{2.7}$$

$$p_i = \frac{2\pi}{L_s a_s}n_i. \tag{2.8}$$

[1] $T = v_F/(L_t a_t)$ in terms of lattice regularization (L_t and a_t denote lattice size and lattice spacing in temporal direction respectively).

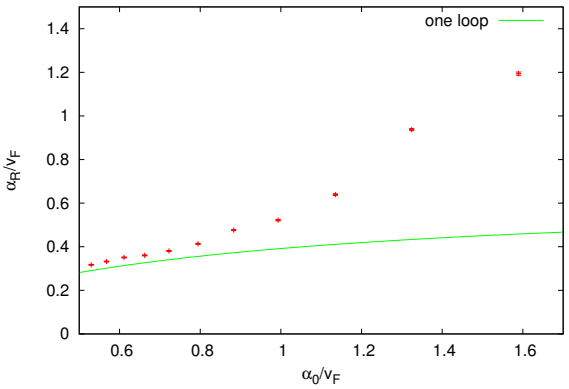

Figure 1: The renormalized squared charge α_R as a function of the bare squared charge α_0 (rescaled by the v_F) and the plot of one loop renormalization formula (3.1). The insulator-semimetal phase transition takes place at $\alpha_0/v_F \sim 0.9$.

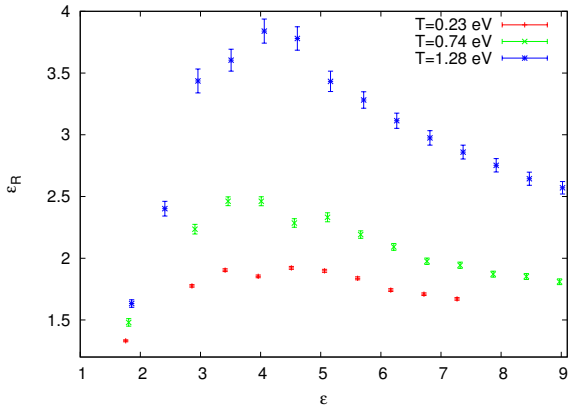

Figure 2: The dependence of the ε_R on the ε at different temperatures obtained from the fitting with Coulomb potential $V_C(\vec{r})$ (2.7).

and determine ε_R. The constant c in formula (2.6) parameterizes self-energy contribution to the potential, $V_C(\vec{r})$ is the lattice Couloumb potential, which takes into account spatial discretization and finite volume effects, n_i are integers which run in the interval $(0, L_s - 1)$ (the point $n_1 = n_2 = n_3 = 0$ is excluded).

3. Numerical results and discussion

To study the dependence of the dielectric permittivity ε_R on ε and on the temperature, we generated 100 statistically independent gauge field configurations at the lattices $20^3 \times L_t, L_t$ =120, 56, 50, 38, 28, 26, 22, 18 for a set of values of the dielectric permittivity of substrate $\varepsilon \in (1,8)$. These lattices correspond to the temperatures $T = 0.23$ eV, 0.50 eV, 0.56 eV, 0.74 eV, 1.00 eV, 1.08 eV, 1.28 eV, 1.56 eV respectively[2]. The calculations were performed with $a_s/a_t = 6$ and $m =$ 0.01, because these values of temporal lattice spacing and excitation mass reproduce continuum limit rather well (see [15] for details). We have found an excellent agreement between our data and expression (2.7) ($\chi^2/dof \sim 1$ for all ε). Thus this result confirms that *static charges at low temperature in graphene interact via Coulomb potential.*

At first let us consider the dependence of ε_R on ε at low temperature. In Fig. 1 we show how α_R is renormalized due to the interaction ($T = 0.23$ eV). In the semimetal phase the effective coupling constant is not large $\alpha_0/v_F < 1$ and one can try to apply perturbation theory to desribe our data. At one loop approximation the dependence of α_R on the α_0 for graphene is given by the following expression [16]:

$$\frac{\alpha_R}{\alpha_0} = \frac{1}{1 + \frac{\pi}{2}\frac{\alpha_0}{v_F}} = \frac{1}{1 + 3.4\frac{2}{\varepsilon+1}}. \tag{3.1}$$

[2]It is important to note that we discuss phenomena related to electron degrees of freedom and neglect the thermal vibration of the graphene honeycomb lattice. Thus we can consider the temperatures $T \sim 10^3 - 10^4$ K, at which the real graphene is melted.

Fig. 1 shows that at small α_0 we have a good agreement with perturbation theory.

The dependence of ε_R on ε at different temperatures is shown in Fig. 2. Formula (2.7) fits data satisfactory ($\chi^2/dof \sim 1-3$) for all temperatures, but it is clear that the form of the $\varepsilon_R = f(\varepsilon)$ curve depends heavily on temperature. Moreover, the larger the temperature the larger χ^2/dof. One can assume that the worsening of the fitting model can be assigned to the following fact. At sufficiently large temperature graphene contains equal number of electrons and holes. If one puts electric charge into such media, a nonzero charge density will be created. This charge density leads to some sort of Debye screening in graphene which is not accounted in (2.7).

To carry out the study of the temperature dependence of the interaction potential we replace the lattice Coulomb potential $V_C(\vec{r})$ in model (2.6) by the lattice version of Debye screening potential:

$$V_D(\vec{r}) = 4\pi\alpha_0\gamma^2 \sum_{n_1,n_2} \frac{f(p_1,p_2)}{1+2m_D(L_s a_s)^2 f(p_1,p_2)} e^{i\vec{p}\vec{r}}, \qquad (3.2)$$
$$f(p_1,p_2) = \frac{1}{4L_s^3 a_s} \sum_{n_3} \frac{1}{\sum_i \sin^2(p_i a_s/2)}, \quad p_i = \frac{2\pi}{L_s a_s} n_i,$$

where the integers n_1, n_2, n_3 run over the values $0,1,..,L_s-1$, except the case $n_1=n_2=n_3=0$. The derivation of the formula (3.2) is given in appendix A of [15]. It is assumed that the interaction between quasiparticles is weak (this condition is satisfied only for sufficienty large ε). Debye potential without explicit expression for the screening mass can be thought of as a modification of the Coulomb potential with unknown parameter m_D. In this sense formula (3.2) can be applied for all values of ε and temperature.

The description of the available data became more precise ($\chi^2/dof > 1-3$ vs $\chi^2/dof < 1$) for all temperatures and ε after the modification of the potential. In Fig. 3 we plot the values of ε_R as a function of ε for different temperatures. One can see that the ε_R obtained from the potential with Debye screening is almost temperature independent contrary to the fitting procedure with ordinary Coulomb potential. So, the fitting with Debye screening potential cancels the temperature dependence of the dielectric permittivity ε_R and encodes it into Debye mass m_D. This confirms that in some region the temperature dependence of the interaction potential results from the Debye screening.

Now let us turn to Debye screening mass. Evidently, m_D is equal to zero if there is no interaction between quasiparticles. This means that the expansion of m_D starts for the term proportional to the α_R, which determines the strength of the interaction. The second property of the m_D is its disappearance in case of zero quasiparticles density n. So, one concludes that $m_D \sim \alpha_R \frac{n}{T}$, where temperature appeares in the denominator for the dimensional reasons[3]. In Fig. 4 we present the following observable $r = (m_D e^2)/(T\alpha_R)$ which is proportional to the n/T^2. This observable allows to study the density of quasiparticles in graphene. If the interaction between quasiparticles is weak, the ratio $(m_D e^2)/(T\alpha_R)$ equals to [15]

$$r = \frac{m_D e^2}{T\alpha_R} = 8\log 2 \frac{e^2}{v_F^2} \simeq 3600. \qquad (3.3)$$

[3]The density n in graphene has dimension $\sim$(energy)^2.

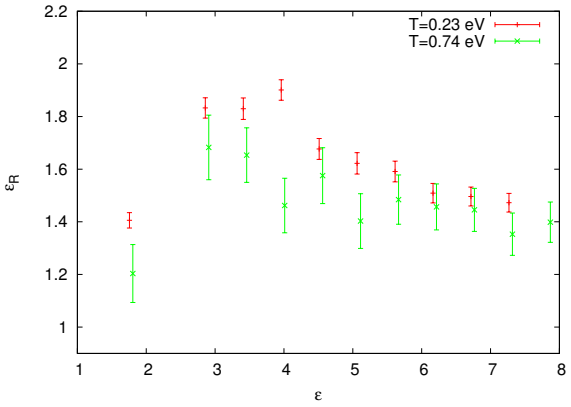

Figure 3: The dependence of the ε_R on the ε at different temperatures obtained from the fitting with Debye screening potential $V_D(\vec{r})$ (3.2).

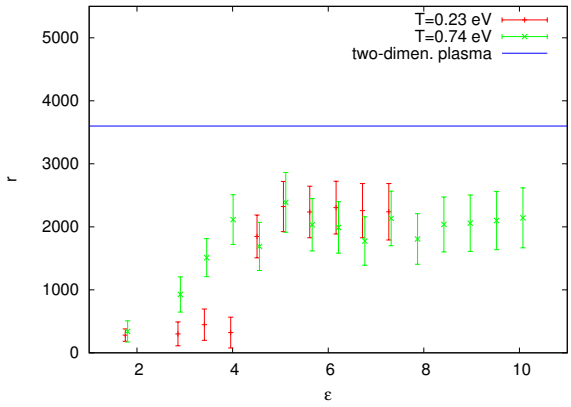

Figure 4: The dependence of the ratio $r = (m_D e^2)/(T\alpha_R)$ on the ε at different temperatures. The line parallel to the ε-axis is the value of the ratio $(m_D e^2)/(T\alpha_R)$ at the approximation of weakly interacting two-dimensional plasma of quasiparticles.

One can see from Fig. 4 that *at low temperature Debye mass m_D plays a role of order parameter of the insulator-semimetal phase transition.* At small dielectric permittivity of substrate, m_D is equal to zero within the accuracy of the calculation, it means that the interaction potential is ordinary Coulomb. At $\varepsilon \sim 4-5$ Debye mass becomes nonzero, abruptly reaching the regime of two-dimesional plasma. Thus the study of Debye screening mass allows to determine the position of the insulator-semimetal phase transition, which takes place at $\varepsilon \sim 4-5$, in accordance with the results of papers [3, 5]. At large temperatures m_D is nonzero for any values of the ε. It is a smoothly rising function of ε which is saturated at $\varepsilon \sim 4-5$.

Now let us consider the semimetal phase in the region $\varepsilon > 5$. In this region the introduced ratio $(m_D e^2)/(T\alpha_R)$ tends to some constant value and this value is by a factor $\sim 1.5-2.0$ smaller than the one given by the formula (3.3). The possible source of this disagreement is that we used the bare Fermi velocity v_F in formula (3.3). Possibly one should use the renormalized Fermi velocity v_F^R, but this study is beyond the scope of this paper. The v_F^R is larger than the v_F, so the inclusion of Fermi velocity renormalization will push the constant (3.3) to the correct direction. The ratio v_F^R/v_F may be estimated as $\sim 1.2-1.4$ according to Fig. 4. This value is in a reasonable agreement with the results obtained within Monte-Carlo simulation of graphene [17] and with experiment [18]. Accounting the fact of Fermi velocity renormalization one can conclude that *in the semimetal phase electron excitations in graphene form a weakly interacting two-dimensional plasma.*

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