Interaction of static charges in graphene within Monte-Carlo simulation

Victor Braguta
Institute for High Energy Physics, Protvino, 142281 Russia
Institute of Theoretical and Experimental Physics, Moscow, 117218 Russia
E-mail: braguta@mail.ru

Semen Valgushev
Institute of Theoretical and Experimental Physics, Moscow, 117218 Russia
Moscow Institute for Physics and Technology, Dolgoprudny, 141700 Russia
E-mail: valgushev@itep.ru

Alexander Nikolaev
School of Biomedicine, Far Eastern Federal University, Vladivostok, 690950 Russia
E-mail: nikolaev.aa@dvfu.ru

Mikhail Polikarpov
Institute of Theoretical and Experimental Physics, Moscow, 117218 Russia
Moscow Institute for Physics and Technology, Dolgoprudny, 141700 Russia
E-mail: polykarp@itep.ru

Maxim Ulybyshev
Institute of Theoretical and Experimental Physics, Moscow, 117218 Russia
Institute for Theoretical Problems of Microphysics, Moscow State University, Moscow, 119899 Russia
E-mail: ulybyshev@goa.bog.msu.ru

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 \( \varepsilon_R \). The dependence of the \( \varepsilon_R \) 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.

31st International Symposium on Lattice Field Theory - LATTICE 2013
July 29 - August 3, 2013
Mainz, Germany
Interaction of static charges in graphene within Monte-Carlo simulation

Victor Braguta

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

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

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 $\varepsilon$ is reduced by a factor $2/(\varepsilon + 1)$. The variation of the dielectric permittivity $\varepsilon$ 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 $\sigma \approx \frac{e^2}{\hbar}$ 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]:

$$Z = \int D\bar{\psi} D\psi DA_0 \exp \left( -\frac{1}{2} \int d^4x (\partial_\alpha A_0)^2 - \int d^3x \bar{\psi}_f \left( \gamma_0 (\partial_0 - igA_0) - \sum_{i=1,2} \gamma_i \partial_i \right) \psi_f \right),$$

where $A_0$ is the zero component of the vector potential of the $3+1$ electromagnetic field, $\gamma_\mu$ are Euclidean gamma-matrices and $\psi_f$ ($f = 1, 2$) 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 \( \langle P^{\gamma}(0)(P^{\gamma}(\vec{r}))^+ \rangle \):

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

where \( T \) 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

\[
P(\vec{r}) = \exp(-i e \int_0^{1/T} dt A_0(t, \vec{r})) = \prod_{t=0}^{L_t-1} \exp(-i \theta(t, \vec{r}, 0)),
\]

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:

\[
\alpha_0 = e^2 \frac{2}{\varepsilon + 1}
\]

(2.4)

is the bare effective squared charge and

\[
\alpha_r = \frac{\alpha_0}{\varepsilon_R}
\]

(2.5)

is the effective squared charge, renormalized due to interaction, \( \varepsilon_R \) is the effective dielectric permittivity of graphene.

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

\[
V(\vec{r}) = \frac{1}{\varepsilon_R} V_C(\vec{r}) + c, 
\]

(2.6)

\[
V_C(\vec{r}) = -\alpha_0 \frac{\pi \gamma^2}{L_s^2 a_s} \sum_{n_1,n_2,n_3} \frac{1}{\sin^2(p_i a_s/2)} e^{i \vec{p_i} \vec{r}},
\]

(2.7)

\[
p_i = \frac{2 \pi}{L_s a_s n_i}.
\]

(2.8)

\( T = v_F / (L_t a_t) \) in terms of lattice regularization (\( L_t \) and \( a_t \) denote lattice size and lattice spacing in temporal direction respectively).
Interaction of static charges in graphene within Monte-Carlo simulation

Victor Braguta

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

and determine $\varepsilon_R$. The constant $c$ in formula (2.6) parameterizes self-energy contribution to the potential, $V_C(\vec{r})$ is the lattice Coulomb 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 $\varepsilon_R$ on $\varepsilon$ 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. 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) ($\chi^2/\text{dof} \sim 1$ for all $\varepsilon$). Thus this result confirms that static charges at low temperature in graphene interact via Coulomb potential.

At first let us consider the dependence of $\varepsilon_R$ on $\varepsilon$ at low temperature. In Fig. 1 we show how $\alpha_R$ 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 describe our data. At one loop approximation the dependence of $\alpha_R$ on the $\alpha_0$ for graphene is given by the following expression [16]:

$$\frac{\alpha_R}{\alpha_0} = \frac{1}{1 + \frac{c}{2} \frac{\alpha_0}{v_F}} = \frac{1}{1 + 3.4 \frac{2}{\varepsilon + 1}}. \quad (3.1)$$

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.

2.5
3
3.5
4
1 2 3 4 5 6 7 8 9
$\alpha_0/v_F$
$\varepsilon_R$
$\varepsilon$

Figure 2: The dependence of the $\varepsilon_R$ on the $\varepsilon$ at different temperatures obtained from the fitting with Coulomb potential $V_C(\vec{r})$ (2.7).
Fig. 1 shows that at small \( \alpha_0 \) we have a good agreement with perturbation theory.

The dependence of \( \epsilon R \) on \( \epsilon \) at different temperatures is shown in Fig. 2. Formula (2.7) fits data satisfactorily \((\chi^2/dof \sim 1 - 3)\) for all temperatures, but it is clear that the form of the \( \epsilon_R = f(\epsilon) \) curve depends heavily on temperature. Moreover, the larger the temperature the larger \( \chi^2/dof \). 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:

\[
V_D(\vec{r}) = 4\pi\alpha_0\gamma^2 \sum_{n_1,n_2} \frac{f(p_1,p_2)}{1 + 2m_D(L_s a_s)^2 f(p_1,p_2)} e^{ip\vec{r}},
\]

(3.2)

\[
f(p_1,p_2) = \frac{1}{4L_s^3 a_s} \sum_{n_3} \frac{1}{\sum \sin^2(p_i a_s/2)}, \quad p_i = \frac{2\pi}{L_s a_s} n_i,
\]

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 sufficiently large \( \epsilon \)). 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 \( \epsilon \) 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 \( \epsilon \) after the modification of the potential. In Fig. 3 we plot the values of \( \epsilon_R \) as a function of \( \epsilon \) for different temperatures. One can see that the \( \epsilon_R \) 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 \( \epsilon_R \) 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 \( \alpha_R \), 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 \( m_D \sim \alpha_R \frac{1}{T} \), where temperature appears 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]

\[
r = \frac{m_D e^2}{T \alpha_R} = 8 \log 2 \frac{e^2}{v_F^2} \simeq 3600.
\]

(3.3)

\(^3\)The density \( n \) in graphene has dimension \( \sim (\text{energy})^2 \).
Interaction of static charges in graphene within Monte-Carlo simulation

Victor Braguta

Figure 3: The dependence of the $\varepsilon_R$ on the $\varepsilon$ at different temperatures obtained from the fitting with Debye screening potential $V_D(r)$ (3.2).

Figure 4: The dependence of the ratio $r = (m_D e^2)/(T \alpha_R)$ on the $\varepsilon$ at different temperatures. The line parallel to the $\varepsilon$-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 $\varepsilon$. It is a smoothly rising function of $\varepsilon$ 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 $v_{RF}$, but this study is beyond the scope of this paper. The $v_{RF}$ 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 $v_{RF}/v_F$ 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.

Acknowledgments

The authors are grateful to Prof. Mikhail Zubkov for interesting and useful discussions. The work was supported by Grant RFBR-11-02-01227-a, by the Russian Ministry of Science and Education, under contract No. 07.514.12.4028 and by Far Eastern Federal University, under contract No. 12-02-13000-m-02/13. Numerical calculations were performed at the ITEP system Stakan (authors are much obliged to A.V. Barylov, A.A. Golubev, V.A. Kolosov, I.E. Korolko, M.M. Sokolov...
for the help), the MVS 100K at Moscow Joint Supercomputer Center and at Supercomputing Center of the Moscow State University.

References


