Interaction of static charges in graphene

V V Braguta, S N Valgushev, A A Nikolaev, M I Polikarpov and M V Ulybyshev

1 Institute for High Energy Physics, Protvino, 142281 Russia
2 Institute of Theoretical and Experimental Physics, Moscow, 117218 Russia
3 Moscow Institute for Physics and Technology, Dolgoprudny, 141700 Russia
4 School of Biomedicine, Far Eastern Federal University, Vladivostok, 690950 Russia
5 Institute for Theoretical Problems of Microphysics, Moscow State University, Moscow, 119899 Russia

E-mail: victor.v.braguta@gmail.com

Abstract. 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 \( \epsilon_R \). The dependence of \( \epsilon_R \) 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.

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 \( v_F \approx c/300 \). Since the Fermi velocity is much smaller than the speed of light, magnetic effects and effects of delay 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 \( g^2 = e^2/v_F \approx 2 \) is large, and this material may be considered as a strongly interacting system. For graphene on substrate with the dielectric permittivity \( \epsilon \) the effective coupling constant is reduced by a factor \( 2/(\epsilon + 1) \). The variation of the dielectric permittivity \( \epsilon \) 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, 7] and insulator-semimetal phase transition was found. In the weak coupling regime (\( \epsilon > 5, g^2 < 0.7 \)) graphene is in the semimetal phase. In this phase the conductivity is \( \sigma \approx e^2/h \) and there is no gap in the spectrum of fermionic excitations. The chiral symmetry of graphene is not broken. In the strong coupling regime (\( \epsilon < 3, g^2 > 1 \)) graphene is in the insulator
phase. In this phase the conductivity is considerably suppressed and fermionic excitations acquire dynamical mass \([8]\). The phase transition between the weak and the strong coupling regimes takes place at the value of the dielectric permittivity of substrate \(\epsilon \approx 4 [3, 4, 6]\).

2. Lattice simulation of graphene

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 \([9]\) (see also references therein).

The partition function of the effective field theory of graphene can be written as \([2, 10, 11, 12]\):

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

(1)

where \(A_0\) is the zero component of the vector potential of the 3 + 1 D electromagnetic field, \(\gamma_\mu\) are Euclidean gamma-matrices, \(\psi_f\) \((f = 1, 2)\) are two flavors of Dirac fermions which correspond to the two spin components of the non-relativistic electrons in graphene and effective coupling constant \(g^2 = 2e^2/(v_F(\epsilon + 1))\) \((\hbar = c = 1\) is assumed). The following notations will be used below:

\[
a_0 = e^2 2 \epsilon / (\epsilon + 1), \quad a_R = \alpha_0 / \epsilon_R,
\]

(2)

where \(\alpha_0\) is the bare effective squared charge, \(\alpha_R\) is the effective squared charge, renormalized due to interaction and \(\epsilon_R\) is the effective dielectric permittivity of graphene.

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

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

(3)

where \(\vec{r}\) is restricted to the graphene plane, \(a\) parameterizes the self-energy part of the correlator and the Polyakov line \(P(\vec{r})\) is

\[
P(\vec{r}) = \exp \left( -ie \int_0^{1/T} dt A_0(t, \vec{r}) \right) = \prod_{t=0}^{L_s-1} \exp \left( -i\theta(t, \vec{r}, 0) \right).
\]

(4)

To suppress statistical errors, we measure the rational power of the correlator of Polyakov lines. 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 \(\gamma = 0.1\) was used. Technical details of the lattice regularization scheme and simulation algorithm may be found in \([13]\).

The results of the numerical simulations of \(V(\vec{r})\) in the correlator (3) is fitted by the lattice potential with screening

\[
V(\vec{r}) = \frac{1}{\epsilon_R} V_{fhl}(\vec{r}) + c
\]

(5)

As a result the value of \(\epsilon_R\) is determined. The constant \(c\) in formula (5) parameterizes the self-energy contribution to the potential. Two different potentials \(V_{fhl}(\vec{r})\) were used for fitting: Coulomb potential

\[
V_C(\vec{r}) = \frac{\pi \gamma^2}{L_s^3 a_s} \sum_{n_1,n_2,n_3} \sum_{l=1}^3 \sin^2(p_l a_s/2) e^{i p_l \vec{r}}
\]

(6)
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 (8). The insulator-semimetal phase transition takes place at $\alpha_0/v_F \sim 0.9$.

Figure 2. The dependence of the ratio $r = (m_D e^2)/(T\alpha_R)$ on the $\epsilon$ at different temperatures. The line parallel to the $\epsilon$-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.

and Debye potential

$$V_D(\vec{r}) = 4\pi\alpha_0 \gamma^2 \sum_{n_1,n_2} \frac{f(p_1,p_2)}{1 + 2m_D(L_s a_s)^2 f(p_1,p_2)} e^{i\vec{p}\vec{r}}, \quad f(p_1,p_2) = \frac{1}{4L_s^2 a_s} \sum_{n_3} \frac{1}{\sum_i \sin^2(p_i a_s/2)}, \quad (7)$$

where in both formulae $p_i = (2\pi n_i)/(L_s a_s)$ and the integers $n_1, n_2, n_3$ run over the values 0, 1, ..., $L_s - 1$ (the point $n_1 = n_2 = n_3 = 0$ is excluded). Debye potential without explicit expression for the screening mass can be thought of as a modification of the Coulomb potential with unknown parameter $m_D$ (at $m_D = 0$ formula (7) evolves into (6)).

3. Numerical results and discussion

First, let us consider the dependence of $\epsilon_R$ on $\epsilon$ 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. In the one loop approximation the dependence of $\alpha_R$ on the $\alpha_0$ for graphene is given by the following expression [14]:

$$\frac{\alpha_R}{\alpha_0} = \frac{1}{1 + \frac{\pi \alpha_0}{2 v_F}} = \frac{1}{1 + 3.4 \frac{2}{\epsilon + 1}}. \quad (8)$$

Fig. 1 shows that at small $\alpha_0$ we have a good agreement with perturbation theory.

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 from the term proportional to $\alpha_R$, which determines the strength of the interaction. The second property of the $m_D$ is its disappearance in the case of zero quasiparticles density $n$. One concludes that $m_D \sim (\alpha_R n)/T$. In Fig. 2 we present the observable $r = (m_D e^2)/(T\alpha_R)$, which is proportional to $n/T^2$. This observable allows to study the density of quasiparticles in graphene. If the interaction between the quasiparticles is weak, the ratio $(m_D e^2)/(T\alpha_R)$ is equal to $r = 8 \log 2 \frac{\epsilon_F^2}{v_F^2} \simeq 3600$ [13].
One can see from Fig. 2 that at low temperature Debye mass \(m_D\) plays the role of order parameter for the insulator-semimetal phase transition. At small values of the dielectric permittivity of substrate \(m_D\) is equal to zero within the accuracy of the calculation, this means that the interaction potential is the ordinary Coulomb potential. At \(\epsilon \sim 4 - 5\) Debye mass becomes nonzero, abruptly reaching the regime of the two-dimensional plasma. Thus the study of Debye screening mass allows to determine the position of the insulator-semimetal phase transition, which takes place at \(\epsilon \sim 4 - 5\), in accordance with the results of papers [3, 4, 6]. At large temperatures \(m_D\) is nonzero for any values of the \(\epsilon\). This is a smoothly increased function of \(\epsilon\), which is saturated at \(\epsilon \sim 4 - 5\).

Now let us consider the semimetal phase in the region \(\epsilon > 5\). In this region the ratio \((m_D e^2)/(T \alpha_R)\) tends to a certain constant value and this value is \(\sim 1.5 - 2.0\) times smaller than the one given by the theoretical predictions. The possible source of this disagreement is that we used the bare Fermi velocity \(v_F\). The renormalized Fermi velocity \(v'_{F}\) larger than \(v_F\), and taking into account \(v'_{F}\) will push the value into the correct direction. The ratio \(v'_{F}/v_F\) may be estimated as \(\sim 1.2 - 1.4\) according to Fig. 2. This value is in a reasonable agreement with the results obtained within Monte-Carlo simulation of graphene [15] and with experiment [16]. Taking into account the renormalization of Fermi velocity 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 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 Development Program of Far Eastern Federal University. 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**

1. Heyrovská R 2008 Atomic Structures of Graphene, Benzene and Methane with Bond Lengths as Sums of the Single, Double and Resonance Bond Radii of Carbon Preprint arXiv:0804.4086
2. Semenoff G W 1984 Phys. Rev. Lett. 53 2449
3. Drut J E and Lähde T A 2009 Phys. Rev. Lett. 102 026802; 2009 Phys. Rev. B 79 165425; 2009 Phys. Rev. B 79 241405
4. Drut J E, Lähde T A and Tölo E, 2010 Proc. XXVIII Int. Symp. on Lattice Field Theory (Villasimius) PoS(Lattice 2010)006; 2011 Proc. XXIX Int. Symp. on Lattice Field Theory (Squaw Valley) PoS(Lattice 2011)074
5. Hands S and Strouthos C 2008 Phys. Rev. B 78 165423; Armour W, Hands S and Strouthos C 2010 Phys. Rev. B 81 125105; 2011 Phys. Rev. B 84 075123
6. Buividovich P V, Luschevskaya E V, Pavlovsky O V, Polikarpov M I and Ulybyshev M V 2012 Phys. Rev. B 86 045107
7. Buividovich P V and Polikarpov M I 2012 Phys. Rev. B 86 245117
8. Araki Y 2011 Annals of Physics 326 1408–24
9. M van Schilfgaarde and Katsnelson M I 2011 Phys. Rev. B 83 081409
10. Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666
11. Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109
12. Geim A K and Novoselov K S 2007 Nature Materials 6 183
13. Braguta V V, Valguise S N, Nikolaev A A, Polikarpov M I and Ulybyshev M V 2013 Interaction of static charges in graphene within Monte-Carlo simulation Preprint arXiv:1306.2544
14. Gonzalez J, Guinea F and Vozmediano M A H 1994 Nucl. Phys. B 424 595
15. Drut J E and Lähde T A 2013 Fermi velocity renormalization and the excitonic insulator in graphene Preprint arXiv:1304.1711
16. Yu G L et al 2013 Proc. National Academy of Sciences of the USA 110(9) 3282-86