Numerical simulation of graphene in external magnetic field

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Published in Phys. Rev. B 89, 245404

Abstract

The results of numerical simulation of monolayer graphene in external magnetic field are presented. The numerical simulation is performed in the effective lattice field theory with noncompact $1+1$ dimensional Abelian lattice gauge fields and $2+1$ dimensional staggered lattice fermions. The dependences of fermion condensate and graphene conductivity on the dielectric permittivity of substrate for different values of external magnetic field are calculated. It is found that magnetic field shifts insulator-semimetal phase transition to larger values of the dielectric permittivity of substrate. The phase diagram of graphene in external magnetic field is drawn.

1. Introduction

Graphene is a two dimensional crystal composed of carbon atoms packed in a honeycomb lattice. It is interesting to study the phase diagram of graphene in the presence of the external magnetic field.

2. Effective theory

The partition function of graphene can be written in the following form

$$Z = \int D\psi D\bar{\psi} \exp \left( -\frac{i}{\hbar} \int d^3x \left( \bar{\psi} \frac{\partial}{\partial t} \psi - \frac{1}{2} \sum_{j=1}^2 \left( \bar{\psi} \gamma_j \partial_j \psi \right)^2 - \frac{1}{2} \sum_{i,\mu} \left( \bar{\psi} \gamma_i \partial_\mu \gamma_i \psi \right)^2 \right) \right).$$

where $A_i$ is the zero component of the vector potential of the $1+1$ electromagnetic field, $\gamma_i$ are Euclidean gamma-matrices and $\psi_j (j=1,2)$ are two flavours of Dirac fermions which correspond to two spin components of the non-relativistic electrons in graphene. Effective coupling constant is $g^2 = 2\pi \alpha / (\sqrt{3} + 1)$ ($\hbar = \epsilon = 1$ assumed). It is worth to note that partition function (1) doesn’t contain dynamical vector part of the potential $A_i$, since the inclusion of this part leads to the corrections which are suppressed by the factor $v_F / c \sim 1/300$.

3. Simulation Algorithm

In order to discretize the fermionic part of the action in (1) the staggered fermions are used:

$$S_f [\bar{\psi}, \psi] = \frac{\beta}{2} \sum_{x,\mu} \left( \bar{\psi} \gamma_\mu \psi \delta_{x,\mu} + \delta_{x,\mu} \bar{\psi} \gamma_\mu \psi \right),$$

where the lattice coordinate $\delta_{x,\mu}$ is restricted to $x^2 = 0$. One flavor of staggered fermions in $2+1$ dimensions corresponds to two flavors of continuum Dirac fermions. To discretize the electromagnetic part of partition function (1) noncompact action is used

$$S_{EM} [\psi, \bar{\psi}] = \frac{1}{2} \sum_{x,\mu} \left( \bar{\psi} \gamma_\mu \psi \right)^2,$$

where

$$\beta = \frac{\lambda}{\Delta_0} = \frac{\epsilon}{\epsilon + 1}.$$

The introduction of nonzero homogeneous magnetic field $B$ perpendicular to graphene plane can be done in a standard way through the modification of the link variable $\theta_{x,\mu, i}$, i = 1, 2, $\gamma_\mu \theta_{x,\mu, i} = \theta_{x,\mu, i} = \theta_{x,\mu, i = 2}$, which corresponds to the vector potential $A_i = B(x_2, x_0)$. The resulting phase diagram for graphene in the presence of the external magnetic field is drawn.

4. Observables

The goal is to measure the phase diagram. So, one need the electric conductivity of graphene in external magnetic field. By virtue of the Green-Kubo dispersion relations, the Euclidean current-current correlators

$$G(r) = \frac{1}{2} \sum_{x,\mu} \int dx_2 dx_0 \left( J_{\mu} (0) J_{\mu} (x) \right)$$

can be expressed in terms of the conductivity $\sigma$ as

$$G(r) = \int 0 \to \infty d\omega \left( \frac{\omega}{\hbar} \right) C (\omega) \sigma (\omega).$$

Note that the conductivity $\sigma$ is dimensionless. Moreover, the DC conductivity $\sigma (0)$ is a universal quantity which does not depend on the lattice spacing or on the ratio of lattice spacings in temporal and spatial directions. For conversion to the SI system of units, it should be multiplied by $e^2/\hbar$. We use middle point of Euclidean current-current correlator to measure the conductivity at low frequencies:

$$\lim_{t \to 0} \left( G (\frac{1}{2} t) \right) \approx e^2 \sigma (0).$$

To study insulator-semimetal phase transition it is useful to consider the fermion condensate $\langle \bar{\psi} \psi \rangle$. In the insulator phase $\langle \bar{\psi} \psi \rangle \neq 0$, and in the semimetal phase $\langle \bar{\psi} \psi \rangle = 0$. So, the fermion condensate $\langle \bar{\psi} \psi \rangle$ at dielectric permittivity $\epsilon = 1$ as a function of the fermion mass $m$ for the fields $H = 0.5, 2.5, 4.0$ K.T. Solid lines are the linear extrapolations to the massless limit.

From the study of the fermion condensate $\langle \bar{\psi} \psi \rangle$ one can state that external magnetic field shifts the insulator-semimetal phase transition in graphene to the direction of larger values of $\epsilon$.

5. Results

The conductivity $\sigma$ as a function of the $\epsilon$ for the fields $H = 0.5, 1$ K.T. One can clearly see that magnetic field shifts point of phase transition to the larger values of $\epsilon$ and makes transition broader.

References