Numerical simulation of graphene in external magnetic field

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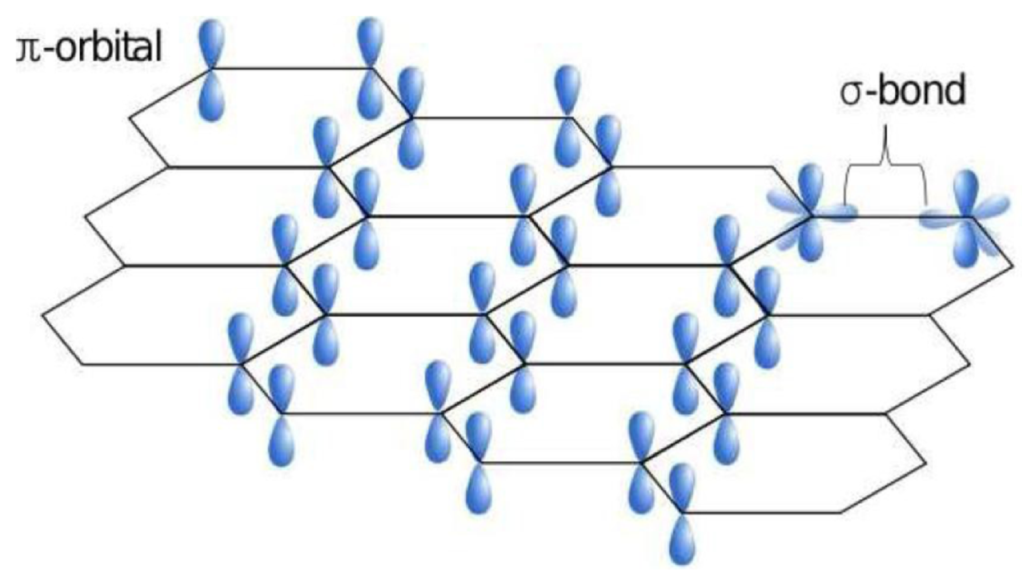
Abstract

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 $3+1$-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

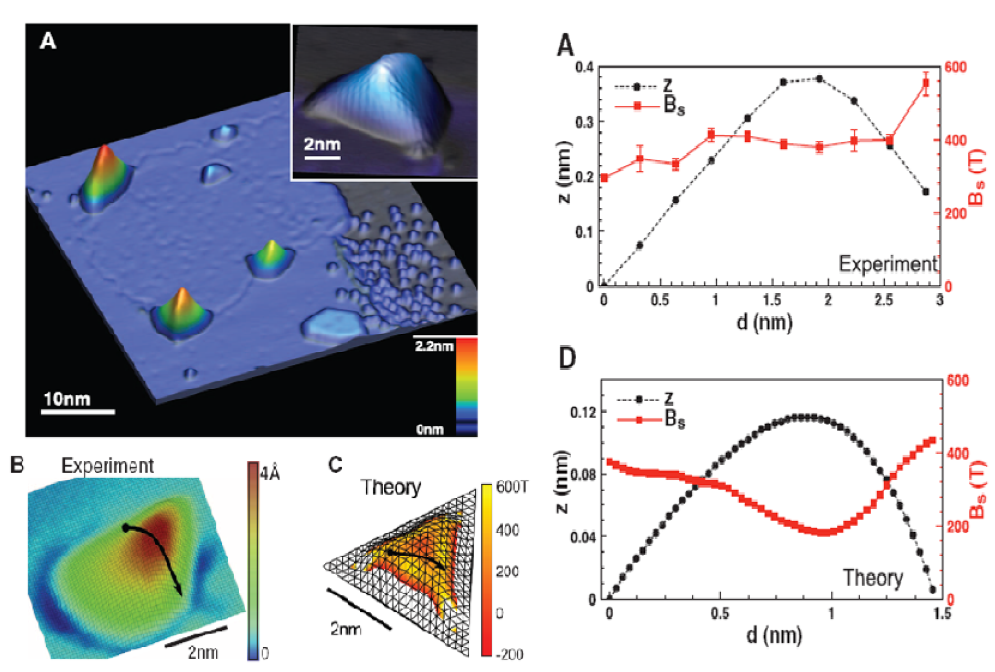
Graphene is a two dimensional crystal composed of carbon atoms packed in a honeycomb lattice.



This material is well known due to its low energy electronic spectrum which can be described by an effective theory with two massless Dirac fermions living in two dimensions with sufficiently large coupling constant $\alpha_{eff} \sim \alpha_{em} c/v_F \sim 300/137 \sim 2$.

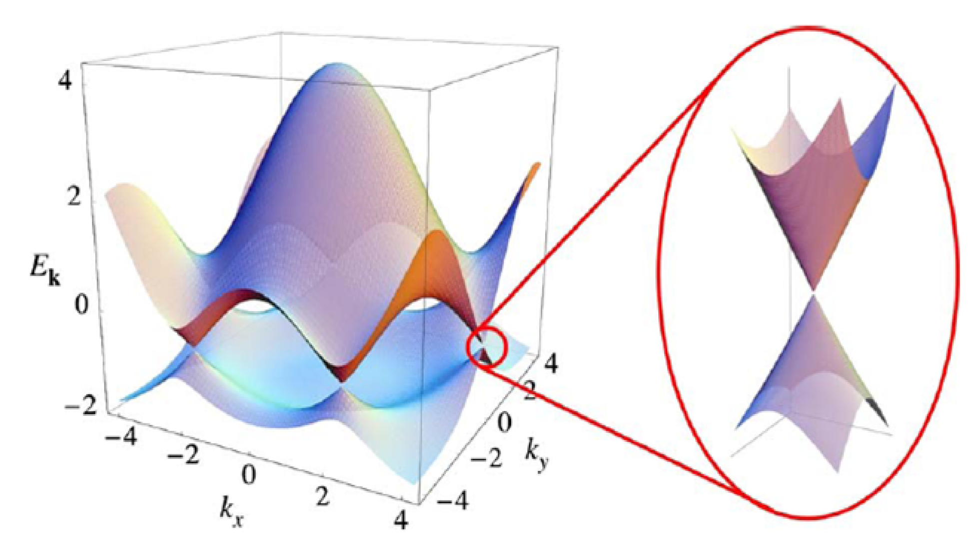
Due to technological limitations graphene is usually placed on some substrate which effectively screens interactions in graphene. This screening is characterized by dielectric permittivity ϵ.

Graphene sheet in real life is not plain and may contain many defects. One of them are so called "ripples" (see pic. A). It is known that "artificial" magnetic field may appear due to stretching of graphene sheet. This magnetic field will lead to the emergence of Landau levels and it can be observed in experiment [1].



It is interesting to study the phase diagram of graphene in the presence of the external magnetic field.

2. Effective theory



Dispersion relation of electronic excitations in graphene.

Fermi velocity $v_F/c \sim 1/300$ plays the role of the speed of light for the fermionic fields.

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

$$\mathcal{Z}=\int \mathcal{D}\bar\psi\mathcal{D}\psi\mathcal{D}A_0 \exp\left(-\frac{1}{2}\int d^4x\,(\partial_i A_0)^2 - \right.$$
$$\left. -\int d^3x\,\bar\psi_f\left(\Gamma_0\,(\partial_0 - igA_0) - \sum_{i=1,2}\Gamma_i\partial_i\right)\psi_f\right), \quad (1)$$

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 flavours of Dirac fermions which correspond to two spin components of the non-relativistic electrons in graphene. Effective coupling constant is $g^2 = 2\alpha_{em}/(v_F(\epsilon+1))$ ($\hbar = c = 1$ is 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:

$$S_\Psi\left[\bar\Psi_x, \Psi_x, \theta_{x,\mu}\right] = \sum_{x,y}\bar\Psi_x\, D_{x,y}\left[\theta_{x,\mu}\right]\,\Psi_y =$$
$$=\frac{1}{2}\sum_x \delta_{x_3,0}\left(\sum_{\mu=0,1,2}\bar\Psi_x\alpha_{x,\mu}e^{i\theta_{x,\mu}}\Psi_{x+\hat\mu} - \right.$$
$$\left. - \sum_{\mu=0,1,2}\bar\Psi_x\alpha_{x,\mu}e^{-i\theta_{x,\mu}}\Psi_{x-\hat\mu} + m\bar\Psi_x\Psi_x\right), \quad (2)$$

where the lattice coordinate x^3 is restricted to $x^3=0$. 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

$$S_g\left[\theta_{x,\mu}\right] = \frac{\beta}{2}\sum_x\sum_{i=1}^{3}\left(\theta_{x,0}-\theta_{x+\hat i,0}\right)^2, \quad (3)$$

where

$$\beta \equiv \frac{1}{g^2} = \frac{v_F}{4\pi e^2}\frac{\epsilon+1}{2}. \quad (4)$$

The introduction of nonzero homogeneous magnetic field H perpendicular to graphene plane can be done in a standard way through the modification of the link variable $\theta_{x,i}, i=1,2$, which corresponds to the vector potential $A_i = H(x_2\delta_{i1} - x_1\delta_{i2})/2$ and quantized magnetic field

$$H = \frac{2\pi}{eL_s^2}n, \quad (5)$$

where L_s is the size of the lattice.

Since action (2) is bilinear in fermionic fields, they can be integrated out and one gets the following effective action

$$S_{eff}\left[\theta_{x,0}\right] = S_g\left[\theta_{x,0}\right] - \ln\det\left(D\left[\theta_{x,0}\right]\right). \quad (6)$$

To generate configurations of the field $\theta_{x,0}$ with the statistical weight $\exp\left(-S_{eff}\left[\theta_{x,0}\right]\right)$ the standard Hybrid Monte-Carlo Method is used.

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

$$G(\tau) = \frac{1}{2}\sum_{i=1,2}\int dx^1\,dx^2\,\langle J_i(0)\;J_i(x)\rangle \quad (7)$$

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

$$G(\tau) = \int_0^\infty \frac{dw}{2\pi}K(w,\tau)\;\sigma(w). \quad (8)$$

Note that the conductivity $\sigma(w)$ 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 $e^2/(2\pi\hbar)$. We use middle point of Euclidean current-current correlator to measure the conductivity at low frequencies:

$$G\left(\frac{1}{2T}\right) \approx \pi T^2\sigma(w). \quad (9)$$

To study insulator-semimetal phase transition it is useful to consider the fermion condensate $\langle\bar\psi\psi\rangle$. In the insulator phase

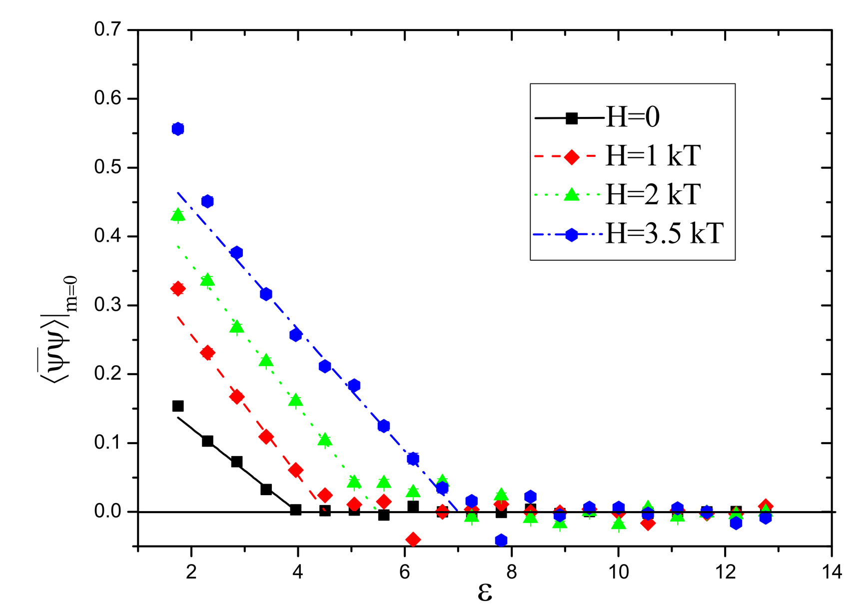
$$\langle\bar\psi\psi\rangle \neq 0 \quad (10)$$

and in the semimetal phase

$$\langle\bar\psi\psi\rangle = 0. \quad (11)$$

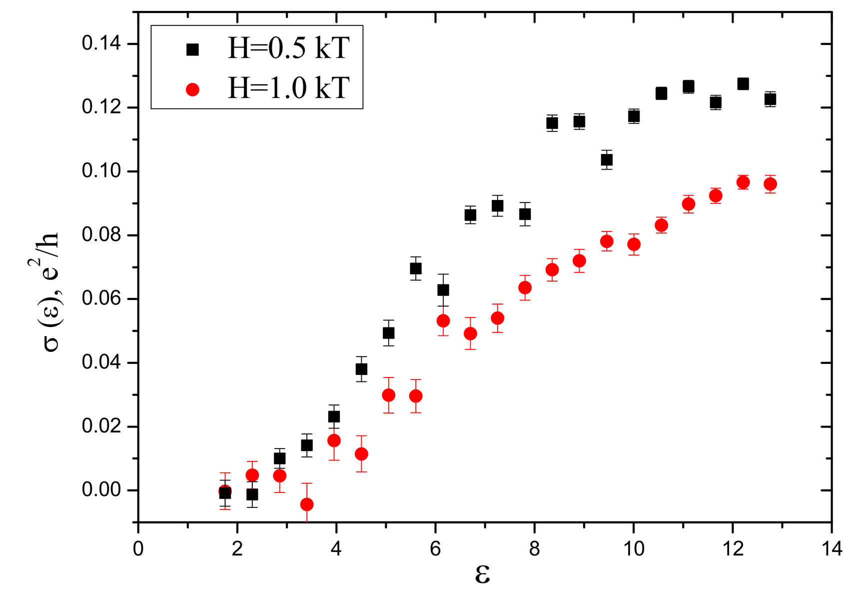
So, the fermion condensate $\langle\bar\psi\psi\rangle$ is the order parameter for the insulator-semimetal phase transition.

5. Results



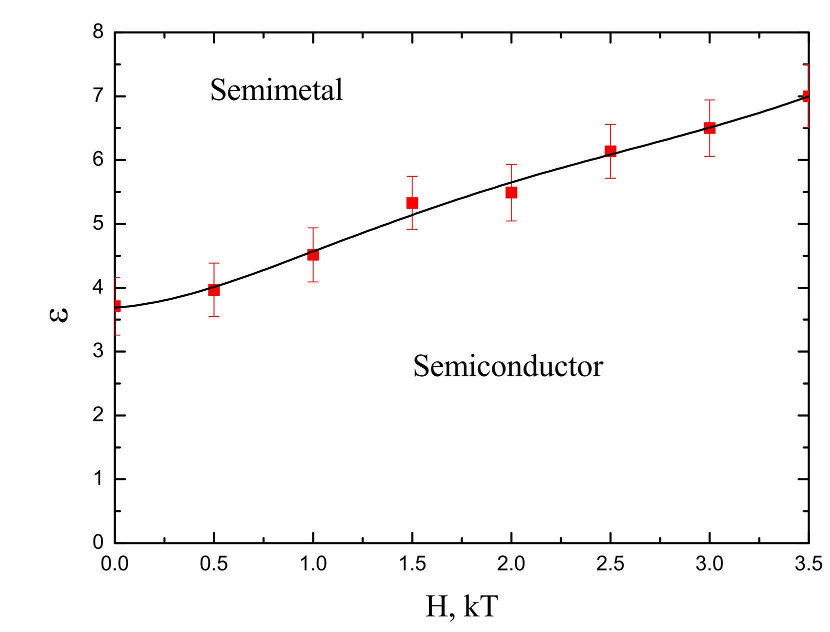
The fermion condensate $\langle\bar\psi\psi\rangle$ at dielectric permittivity $\epsilon = 15$ as a function of the fermion mass m for the fields $H = 0.5, 2.5, 4.5$ kT. Solid lines are the linear extrapolations to the massless limit.

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 the ϵ.



The conductivity σ as a function of the ϵ for the fields $H = 0.5,\ 1$ kT.

One can clearly see that magnetic field shifts point of phase transition to the larger values of ϵ and makes transition broader.



The resulting phase diagram for graphene in the (H, ϵ) plane.

References

[1] N. Levy et. al., Science **329**, 544, (2010)

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