Scientific
Research

Ferroelectric Phase Transition in Graphene with Anderson Interaction

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ABSTRACT

The normal transverse electric field which appears in impurity graphene spontaneously in the presence of a high applied electric field was calculated. The given effect can be associated with non-equilibrium of electron subsystem in graphene. The characteristics of spontaneous field on the parameters of the problem were investigated.

1. Introduction

A study of phase transitions is the one of the famous paradigm in modern fundamental physics. It should be noted that phase transition (in wide extend) means a substance's transition from one phase to another at the change of external conditions-temperature, pressure, magnetic field and electric field, and so on. And phase transition, in restricted sense, is saltatory variation of physical properties at the continuous changing of the external parameters. So, in particularly, non-equilibrium phase transition takes place one of the main in variety of phase transitions. This kind of transition arises at the presence of external fields with the different characters.

In [1,2] it was shown theoretically that under the action of a high electric field non-equilibrium phase transitions are possible in the electron gas in conductors with a body-centered cubic lattice. The effect consists in spontaneous appearance of a transverse field E_y playing the role of order parameter. The applied electric field E_x, directed along one of the crystal symmetry axis, is the controlling parameter. A necessary condition for the appearance of a transverse field is the non-additivity of the electron energy spectrum when the electron energy: $\varepsilon(\vec{p}) \neq \varepsilon(p_x) + \varepsilon(p_y) + \varepsilon(p_z)$, where $\vec{p}$ is the quasi-momentum of electrons (e.g., when using a tight-binding approximation the electron spectrum in the body-centered cubic lattice becomes non-additive: $\varepsilon(\vec{p}) \approx \cos(p_x a / 2\hbar)$ $\cos(p_y a / 2\hbar) \cos(p_z a / 2\hbar)$, where a is the lattice constant. Besides, the spectrum must be bounded.

All these conditions are carried out for the impurity gra- phene, and one can investigate an existence possibility of phase transitions in impurity graphene, which is considered in the frameworks of the Anderson model. It can be expect the appearance of transverse component E_x when a filed E_y is applied (which plays the role of order parameter). Graphene is a structure which consists of one layer of carbon atoms, located in the units of hexagonal lattice. A great attention is paid to large electron mobility in the graphene and to its unique properties which are an alternative of silicic base in the modern microelectronics [3-6]. We note that electromagnetic waves in the carbon structures become strongly nonlinear even in the weak fields that gives rise to spread possibility of solitary electromagnetic waves in the graphene and carbon nanotubes. These properties of carbon nanostructures have theoretical interest and attempts of applying in the nonlinear optics [7]. Nonlinearity is caused by change of classical function of electron distribution and by non-parabolic dispersion law of electrons.

Summarizing, one can draw a conclusion, that the problem of graphene response in the magnetic field with taking into account Anderson interaction between the impurity and graphene electrons, is very important and actual.

2. Basic Equations

Let us consider the response of graphene on external electric field along axis x in geometry is given in **Figure 1**.

Then the Anderson Hamiltonian of the electron system can be written in the Formula (1) [8,9].

where $a_{j\sigma}^+, a_{j\sigma}, b_{j\sigma}^+, b_{j\sigma}$ are the creation and annihila- tion operators of electrons in a graphene unit with spin σ, t_A is the overlap integral between adjacent grapheme units determined by overlapping of the wave functions of the
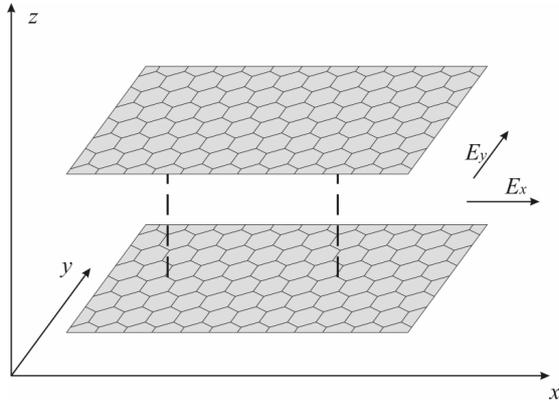
Figure 1. Geometry of a problem

grapheme electrons, U is the constant of Coulomb repulsion of the electros at the same unit; $d_{j\sigma}^+, d_{j\sigma}$ are the creation and annihilation operators of impurity electrons in a graphene spin; ε is the energy of impurity electrons; U_1 is the energy of Coulomb repulsion of impurity electrons only. V is the hybridization parameter.

The following parameters were estimated by MNDO method [10]: $t_\Delta \approx 2$ eV, $U \approx 12$ eV, $U_1 \approx 12$ eV, $V \approx 2$ eV. Since the properties of the model described by the Anderson Hamiltonian is sufficiently complex, further we will use the approximation: $U \rightarrow \infty$ and consider, all mean value is to be spatially homogenous. Note that the approximation $U \rightarrow \infty$ is well supported by quantum chemical calculations for graphene-like. In this approxima-

tion the Hamiltonian (1) can be written as [11,12].

$$H = \sum_{k\sigma} Eps(k) C_{k\sigma}^+ C_{k\sigma} \tag{2}$$

where $C_{k\sigma}^+, C_{k\sigma}$ are the creation and annihilation operators of elementary excitations (with momentum k and spin σ), and $Eps(k)$ is the spectrum which, according to [11,12], can be presented as:

$$Eps(k) = \frac{1}{2}\Big[\varepsilon(k) + \varepsilon - n^\sigma + \\ + \sqrt{(-\varepsilon(k) + \varepsilon - n^\sigma)^2 + 4(1 - n_\sigma^{im})|V|^2}\Big] \tag{3}$$

where V is the hybridization parameter, $\varepsilon(k)$ is the spectrum of graphene electrons determined by the Hamiltonian H_h, a n^σ and n_σ^{im} are parameters determined from the self-consistency conditions of the problem.

Note, that dispersion law, which describes graphene properties without taking into account Coulomb repulsion at the same unit, has a following form [13].

$$\varepsilon(k) = \gamma \sqrt{1 + 4\cos(ap_x)\cos(\frac{ap_y}{\sqrt{3}}) + 4\cos^2(\frac{ap_y}{\sqrt{3}})} \tag{4}$$

where $\gamma \approx 2.7$ eV, $a = 3b/2\hbar$, $b = 0.142$ nm is the distance between adjacent carbon atoms in graphene, and $k = (p_x, p_y)$. According to [11,12], the self-consistency conditions are:

We use the average electron method with taking into

$$H = H_h + H_{im} + H_{hyb}$$
$$H_h = -\sum_{j\Delta\sigma} t_\Delta (a_{j\sigma}^+ b_{j+\Delta\sigma} + b_{j+\Delta\sigma}^+ a_{j\sigma}) + U\sum_j (a_{j\sigma}^+ a_{j\sigma} a_{j-\sigma}^+ a_{j-\sigma} + b_{j\sigma}^+ b_{j\sigma} b_{j-\sigma}^+ b_{j-\sigma})$$
$$H_{im} = \sum_j (\varepsilon d_{j\sigma}^+ d_{j\sigma} + \varepsilon d_{j-\sigma}^+ d_{j-\sigma} + U_1 d_{j\sigma}^+ d_{j\sigma} d_{j-\sigma}^+ d_{j-\sigma}) \tag{1}$$
$$H_{hyb} = V\sum_{j\sigma} (a_{j\sigma}^+ d_{j\sigma} + d_{j\sigma}^+ a_{j\sigma})$$

$$n^\sigma = \sum_{k,v} A_v^{-\sigma} F(E_{-\sigma v}(k)),$$
$$n_\sigma^{im} = \sum_{k,v} B_v^\sigma F(E_{\sigma v}(k)),$$
$$A_v^\sigma = (-1)^v \frac{|V|^2}{2Q_\sigma(k)},$$
$$B = (-1)^v \frac{E_{\sigma v} - \varepsilon(k)}{2Q_\sigma(k)}, \tag{5}$$
$$E_{\sigma v} = \frac{1}{2}\Big[\varepsilon(k) + \varepsilon - n^\sigma + (-1)^v \sqrt{(-\varepsilon(k) + \varepsilon - n^\sigma)^2 + 4(1 - n_\sigma^{im})|V|^2}\Big],$$
$$Q_\sigma(k) = \frac{1}{2}\sqrt{(-\varepsilon(k) + \varepsilon - n^\sigma)^2 + 4(1 - n_\sigma^{im})|V|^2}$$

account the motion equation can be written as [14].

$$\frac{d\overline{p}}{dt} = \overline{E} \qquad (6)$$

one can apply: $\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$, and for low-temperaturecase it is possible to obtain:

$$p_x = p_{0x} + E_x t$$
$$p_y = p_{0y} + E_y t$$

It should be noted:

$$\upsilon(p_x) = \frac{\partial Eps(p_x, p_y)}{\partial p_x}, \quad \upsilon(p_y) = \frac{\partial Eps(p_x, p_y)}{\partial p_y}$$

Further, we use the average electron method, according to which the current can be expressed as [15].

$$j = \int_0^{¥} \upsilon(\overline{p}(t))\exp(-t)dt \qquad (7)$$

where j is the density of current, $\overline{p}(t)$ is the solution of (6) with some initial conditions, which correspond to the energy minimum. In our case, it is necessary to consider the solutions of (8) for four initial conditions (correspond to minimum of $E(p)$):

$$ap_x = 0; ap_x = \pi; ap_y = \pi / 3; ap_y = 2\pi / 3 .$$

Then we should sum up all values for current.

It is convenient to represent the dispersion law of graphene in the following form:

$$\varepsilon(p_x, p_y) = \sum_{m,n} A_{mn}\cos(mp_x)\cos(np_y),$$

$$A_{mn} = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\varepsilon(p_x, p_y)\cos(mp_x)\cos(np_y)dp_x dp_y$$

Finally, in this case:

$$j_x = \sum_{m,n} A_{mn}\left(\cos(2\pi\frac{m}{3}) + \cos(\pi\frac{k}{3})\times(-1)^i\right)\times$$
$$\times\frac{m^2 E_x(n^2 E_y^2 - 1 - m^2 E_x^2)}{(1+(nE_y + mE_x)^2)(1+(nE_y - mE_x)^2)} \qquad (8)$$

The transverse field E_x is defined by boundary conditions for the given applied filed E_y . Let us assume that a circuit is opened in the x-direction:

$$j_x = 0 \qquad (9)$$

This condition corresponds to some solve for the transverse field: $E_x = E_x(E_y)$. Equation (9) has two solves:

$$E_x = 0$$

$$\sum_{m,n} A_{mn}\frac{m^2(n^2 E_y^2 - 1 - m^2 E_x^2)}{(1+(nE_y + mE_x)^2)(1+(nE_y - mE_x)^2)} = 0 \qquad (10)$$

The transverse field spontaneously appears in one of two mutually opposite directions at the some values of parameters in the second equation of (10). In this case, we deal with non-equilibrium one-order phase transition. The appearance of the transverse field component represents perhaps the simplest example of self-organization in the impurity graphene.

3. Calculation Results

A typical dependence of j_x on E_x, which described by (8), is represented in **Figure 2**. Dependence of the transverse field E_x on the applied field E_y, which determined as non-zero solve of (10) is given in **Figure 3** and **Figure 4**.

It worth to note that analogous dependence on the parameter V is weak, and existence of two non-zero solves is more important. One of this solve (smaller in module) is thermodynamically unstable. As might be expected, according to the numerator of expression (10) increase in the field E_y leads to an increase in the field E_x, due to the non-additivity of the electron dispersion. Note the fact that the dependence of the field E_x on E_y is mainly associated with the view of the electron spectrum without interaction (4), and the effects of the interaction of electrons with impurities contribute only relatively small corrections. This can also be attributed to the effect is due to non-additivity of the dispersion and less sensitive to the particular type of spectrum. It should be noted that it follows from (10) and **Figures 3** and **4** at large E_y can be written: $E_x \propto E_y$ that may be useful in evaluating the field intensities in the experiment. Dependence of a minimal value of the field E_y, at which the transverse field appears, on the n_σ^{im} at the different n^σ is given in **Figure 5**.

Note, that the minimal value of E_y is more strongly depends on impurity concentration. It can be associated with reconstruction of the graphene electron spectrum in the presence of impurities.

The transverse field E_x, which is emergent spontaneously, can be thermodinamically unstable, as opposite to always stable solve for open circuit in the x-direction $E_x = 0$.

We also investigate the stability using the method proposed in [1]. We introduce the following function:

$$\Phi(E_x) = \int_0^{E_x} j_x(E_x')dE_x' + cons\tan t \qquad (11)$$
$$E_y = fixed$$

The given function is usually called with synergetic potential and it is the analogue of a thermodynamic potential for non-equilibrium tasks. According to [1], the
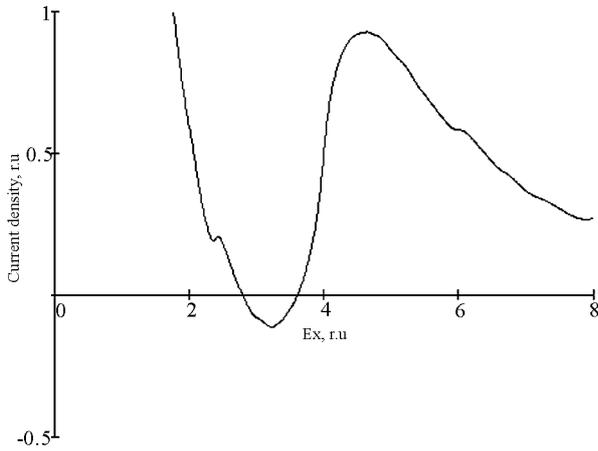
Figure 2. Dependence of current density on the field E_x, when the field E_y is fixed ($E_y = 4.0$). All magnitudes are in the non-dimensionless units
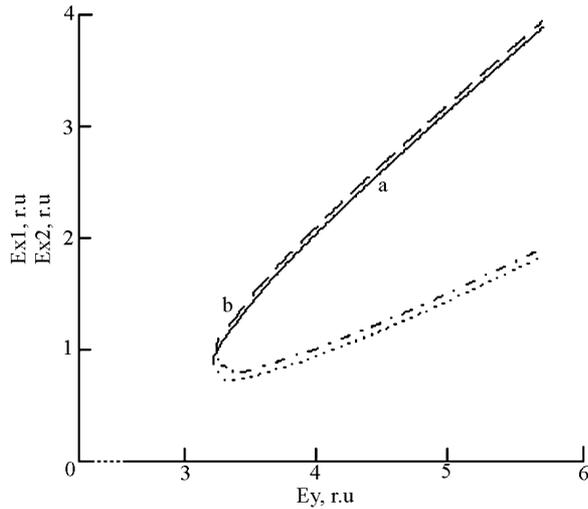

Figure 3. Dependence of the field E_x on the field E_y:(a) $n_\sigma^{im} = 0.1, n^\sigma = 0.25$; (b) $n_\sigma^{im} = 0.5, n^\sigma = 0.25$. All magnitudes are in the non-dimensionless units

stable conditions are:

$$\frac{d\Phi}{dE_x} = 0 \qquad \frac{d^2\Phi}{dE_x^2} > 0 \qquad (12)$$

These formulas mean that in given non-equilibrium situation the function (11) attains its minimum in the stationary state. Thus the function Φ may be regarded as the analogue of a thermodynamic potential for equilibrium systems. Dependence of the "potential" Φ on the field E_x for some values of the E_y is presented in **Figure 6**. It can be seen that the function Φ has the minimum and the maximum. It should be noted, maximum corresponds to a smaller in module solve of Equation (10), and minimum corresponds to a larger in module solve. It means the
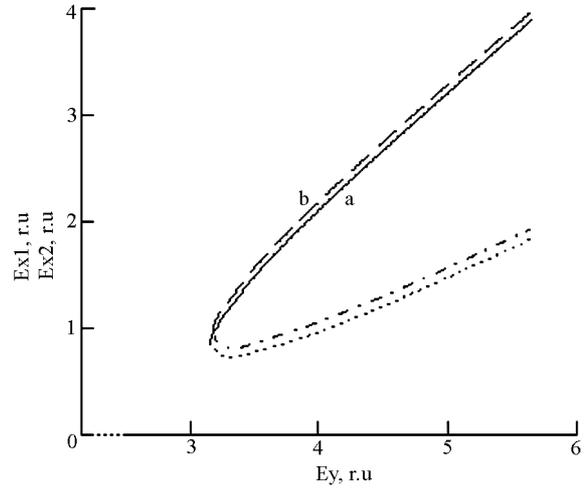

Figure 4. Dependence of the field E_x on the field E_y:(a) $n_\sigma^{im} = 0.1, n^\sigma = 0.25$; (b) $n_\sigma^{im} = 0.1, n^\sigma = 0.75$. All magnitudes are in the non-dimensionless units
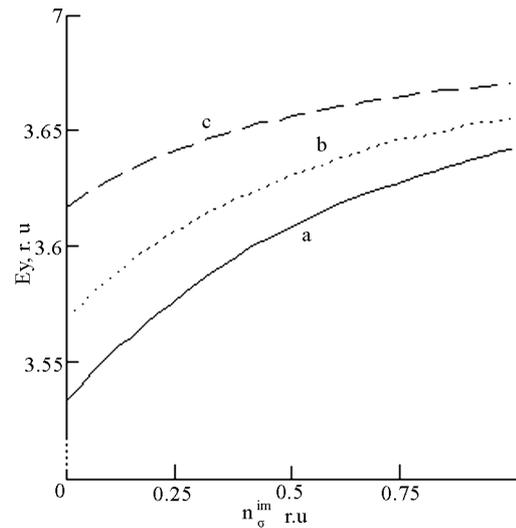

Figure 5. Dependence of the minimum E_y on the n_σ^{im} : (a) $n^\sigma = 0.25$; (b) $n^\sigma = 0.50$; (c) $n^\sigma = 0.75$. All magnitudes are in the non-dimensionless units

larger in module solve is stable. Note that dotted branhes in **Figure 3** and **Figure 4**. correspond to the maximum of function Φ (unstable solve), but solid curve and dashed curve correspond to minimum (stable solve).

This transition, in which the electric field appears spontaneously, is concerned to ferroelectric type. Though, the transverse field E_x plays the role of the order parameter, and the field E_y is the analogue of temperature (controlling parameter).

The transverse field occurred spontaneously, obviously, can be found by measuring the charge on the capacitor,
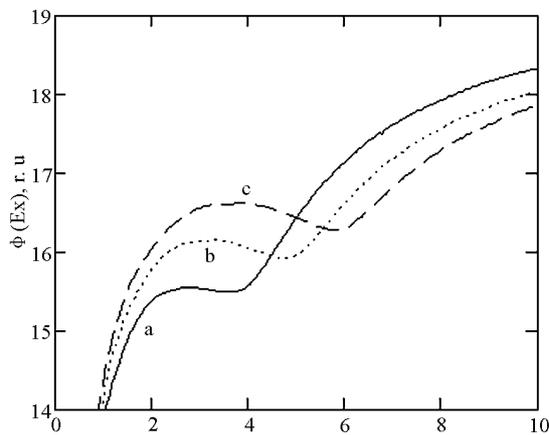
Figure 6. Dependence of the function Φ on the field E_x, when the field E_y is fixed: (a) $E_y = 3.5$; (b) $E_y = 4.5$; (c) $E_y = 5.5$. All magnitudes are in the non-dimensionless units

which is must be attached to the ends of graphene sheets, oriented in the x direction. A transverse field will contribute to accumulation of charge on the capacitor plates, and the total charge will be clearly defined potential difference, which creates an electric field necessary to compensate for a transverse electric field.

4. Conclusions

In conclusion we formulate our main results:

1) The appearance of the electric field, which is perpendicular to the external applied field, in impurity The 1. The appearance of the electric field, which is perpendicular to the external applied field, in impurity graphene with the Anderson interaction was obtained.

2) The minimal value of the applied field is strong defined by electron concentration in the impurity.

3) The analysis of the synergetic potential has shsown that the emergent state with the spontaneous transverse field is stable.

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