Superconducting properties of bi-layer graphene in chiral model

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Abstract. Within the scope of the graphene chiral model we suggest a description of superconducting properties of the bi-layer graphene with some twisting angle $\alpha$ between the layers. The interaction with an external magnetic field is included through the gauge invariance principle, the field being oriented along the graphene plane. The expression for the optimal twisting angle generating superconductivity is obtained, the latter being equivalent to the vanishing magnetic field between the graphene layers (the Meissner effect).

1. Introduction

Since the discovery of mono-atomic carbon layers called graphenes [1, 2] this material attracted deep interest of researchers due to its extraordinary properties concerning magnetism, stiffness and high electrical and thermal conductivity [3, 4]. The interesting connection was revealed with other graphene-based materials: Fullerenes [5] and carbon nano-tubes [6]. A very simple explanation of these unusual properties of graphene was suggested in [7], where the idea of massless Dirac-like excitations of honeycomb carbon lattice was discussed, the latter one being considered as a superposition of two triangular sub-lattices. Some phenomenological development of this idea was realized in [8] and [9].

It is worth-while to stress that a new stage in the graphene physics began since studying the properties of twisted bi-layer graphene (TBG) created by stacking two sheets of graphene that are twisted relative to each other by a small angle of about 1.1°- the so-called first “magic” angle. This specific angle was predicted by Alan MacDonald [10] who calculated the amount of energy which was necessary for a free electron in a cell to tunnel between the two graphene sheets. It was found that the tunneling energy would disappear at exactly 1.1°. However, the physics of this phenomenon was not clear. One might only suppose that for this specific TBG configuration the electrons in the sheets would slow down and become strongly correlated with one another. Therefore, they could pair up and form a superfluid like that in the standard superconductivity model by J. Bardeen, L. Cooper, J. Schrieffer and N. Bogolyubov [11]. Recent fascinating discovery of unconventional superconductivity in the TBG [12] opens a new field of research that has already garnered its own name – “twisttronics”.

2. Scalar chiral model of graphene

The concept behind this research is the following. As is well known, the carbon atom possesses four valence electrons in the so-called hybridized $sp^2$ – states, the one of them being “free” in graphene lattice and all others forming strong covalent bonds with the neighbors. It appears natural to introduce
scalar $a_0$ and 3-vector $\vec{a}$ fields corresponding to the $s$–orbital and the $p$–orbital states of the “free” electron, respectively. These two fields can be combined into the unitary matrix $U \in SU(2)$ considered as the order parameter of the model in question:

$$U = a_0 \tau_0 + i \vec{a} \cdot \vec{\tau},$$

(1)

where $\tau_0$ is the unit $2 \times 2$–matrix and $\vec{\tau}$ are the three Pauli matrices, with the $SU(2)$–condition

$$a_0^2 + \vec{a}^2 = 1$$

(2)

being imposed. It is convenient to construct via differentiating the chiral field $U$ the so-called left chiral current

$$I_\mu = U^* \partial_\mu U, \quad \mu = 0, 1, 2, 3,$$

(3)

the index $\mu$ denoting the derivatives with respect to the time $x^0 = ct$ and the space coordinates $x^i, \quad i = 1, 2, 3$. The Lagrangian density reads

$$L = -\frac{1}{4} \text{tr} \left( I_\mu I_\nu - \frac{\lambda^2}{2} \vec{a}^2 \right),$$

(4)

and corresponds to the sigma-model approach in the field theory with a small mass term. Here the constant model parameters $I$ and $\lambda$ are introduced. Comparing the Lagrangian density (4) with that of the Landau – Lifshits theory corresponding to the quasi-classical long-wave approximation to the Heisenberg magnetic model, one can interpret the parameter $I$ in (4) as the exchange energy between the atoms (per spacing). As was shown in [8], the model (4) admits the kink-like or the domain-wall configuration

$$U = \exp \left( i \vec{n} \Theta \right), \quad \Theta = \Theta(z), \quad \vec{n} = \vec{n} \cdot \vec{\tau},$$

(5)

corresponding to the ideal graphene plane with the normal oriented along the $z$–axis. In this case

$$\Theta(z) = 2 \arctan \left( -z/l_0 \right),$$

(6)

where the characteristic length appears: $l_0 = 1^{1/2}/\lambda$, which can be identified with the diameter of the carbon atom $l_0 = 0.26$ nm.

To describe the multi-layer graphene system we suggest to use the so-called product ansatz:

$$U = U_1 U_2 \cdots U_n,$$

(7)

with $U_k, k = 1, 2, \ldots, n$, having the standard form

$$U_k = \exp \left( i \vec{n}_k \Theta_k \right), \quad \Theta_k = \Theta_k (z), \quad \vec{n}_k = \vec{n}_k \cdot \vec{\tau},$$

(8)

where the unit vector $\vec{n}_k$ determines the orientation of the corresponding graphene sheet.

3. Electromagnetic interaction for bi-layer graphene

The interaction with the electromagnetic field can be introduced into the chiral model through the gauge invariance principle. To this aim, we consider the following gauge transform:

$$U' = V U V^{-1}, \quad V = \exp \left( i \zeta \Gamma_e \right), \quad A'_\mu = A_\mu + \partial_\mu \Lambda,$$

(9)

combined with extending the derivative:

$$D'_\mu U = \partial_\mu U - i e_0 A_\mu [\Gamma_e, U],$$

(10)

where $e_0$ and $\Gamma_e$ stand for the electromagnetic coupling constant and the charge operator, respectively. Then the gauge invariance principle implies that

$$L'_\mu = V L_\mu V^{-1}, \quad L_\mu = U' D'_\mu U.$$

(11)

For the natural choice $\Gamma_e = \tau_3$, this amounts to requiring $\zeta = e_0 \Lambda$. It should be noticed that the coupling constant $e_0 = e / hc = \pi / \phi_0$ appears to be connected with the magnetic flux quantum $\phi_0$, where $e$ stands for the electron charge. Therefore, in view of (10), the extended left chiral current $L_\mu$ takes the form:
\[ L_\mu = l_\mu - e_\alpha A_\mu (U^* \tau_3 U - \tau_3), \quad (12) \]

and the Lagrangian density (4) should be replaced with the following one:

\[ L = \frac{1}{4} \text{tr} (L_\mu L^\mu) - \frac{\lambda^2}{2} \alpha + \frac{1}{16\pi} F_{\mu \nu} F^{\mu \nu}, \quad F_{\mu \nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \quad (13) \]

where the proper electromagnetic part was added.

Let us now consider the TGB configuration \( U = U_1 U_2 \) in the constant longitudinal external magnetic field \( \vec{B}_0 = (0, B_0, 0) \), with the vectors \( \vec{n}_1, \vec{n}_2 \) in (8) being chosen as follows:

\[ \vec{n}_1 = (\cos \alpha / 2, \sin \alpha / 2, 0), \quad \vec{n}_2 = (\cos \alpha / 2, -\sin \alpha / 2, 0). \quad (14) \]

Using the covariant components of the vector potential \( A_\mu = A(z) \delta_\mu \), one finds the magnetic intensity \( B = A'(z) \) and the following nontrivial components of \( L_\mu \):

\[ L_\alpha = -i e_\alpha A (U^* \tau_3 U - \tau_3), \quad L_\beta = i \Theta_1 U_2 \vec{n}_1 U_2 + i \Theta_2 \vec{n}_2. \quad (15) \]

Inserting (14) into (15), one gets:

\[ \text{tr} L_1^2 = -4e_\alpha^2 A^2 (1 - \cos 2\Theta_1 \cos 2\Theta_2 + \cos \alpha \sin 2\Theta_1 \sin 2\Theta_2), \quad \text{tr} L_2^2 = -2(\Theta_1^2 + \Theta_1^2 + 2 \cos \alpha \Theta_1 \Theta_2 \Theta_2). \]

Also it is necessary to calculate the vector \( \vec{a} \) in (13):

\[ \vec{a} = -(i / 2) \text{tr} (\vec{U} U_2) = \cos \Theta_2 \sin \Theta_1 \vec{n}_1 + \cos \Theta_1 \sin \Theta_2 \vec{n}_2 - \sin \Theta_1 \sin \Theta_2 \vec{n}_1 \times \vec{n}_2. \]

Finally, the Lagrangian density for the TGB configuration takes the form:

\[ -L = \frac{1}{2} (\Theta_1^2 + \Theta_2^2 + 2 \cos \alpha \Theta_1 \Theta_2) + 4e_\alpha^2 A^2 (1 - \cos 2\Theta_1 \cos 2\Theta_2 + \cos \alpha \sin 2\Theta_1 \sin 2\Theta_2) + \alpha^2 + \frac{1}{8\pi} \left( \cos^2 \Theta_2 \sin^2 \Theta_1 + \cos^2 \Theta_1 \sin^2 \Theta_2 + \sin^2 \alpha \sin^2 \Theta_1 \sin^2 \Theta_2 + \frac{1}{2} \cos \alpha \sin 2\Theta_1 \sin 2\Theta_2 \right). \quad (16) \]

4. Analysis of solutions to equations of motion

Let us first fix the distance \( 2l \) between the sheets and write down the boundary conditions:

\[ \Theta_i (-\infty) = \pi, \quad \Theta_i (+\infty) = 0, \quad i = 1, 2, \quad \Theta_i (-l) = \Theta_1 (l) = \pi / 2. \quad (17) \]

In view of (17), it is convenient to make the substitution

\[ \tan \Theta_i = u_i = (\sinh w_i)^{-1}. \quad (18) \]

Taking into account that \( u_i (\pm \infty) = 0 \), let us first study the behavior of solutions at \( z \to \infty \), where one can put \( A \approx B_0 z \) and \( u_i'' = 4e_\alpha^2 B_0^2 z^2 u_i \), with the asymptotic solution being

\[ u_i = u_0 \exp (-4e_\alpha B_0^2 z^2). \quad (19) \]

In view of (17), (18) and (19), this is equivalent to the following good approximation for \( w_i \), which proves to be valid both at small and large \( z \):

\[ w_1 = (z + l)(k + e_\alpha B_0 z), \quad w_2 = (z - l)(k + e_\alpha B_0 z) \quad (20) \]

and \( u_0 = 2 \) in (19). In the light of the fact that at large \( z \): \( A(z) = B_0 z + a(z) \), where \( a' (\infty) = 0 \), one derives, due to (19), the following equation for \( a(z) \):

\[ a'' = 128\pi I e_\alpha^2 B_0^2 z (1 + \cos \alpha) \exp (-2e_\alpha B_0^2 z^2), \]

with the evident solutions for \( B(z), A(z) \):

\[ B = B_0 - 32\pi I e_\alpha^2 (1 + \cos \alpha) \exp (-2e_\alpha B_0^2 z^2), \quad A = B_0 z - 32\pi I e_\alpha^2 (1 + \cos \alpha) \int_0^z \exp (-2e_\alpha B_0^2 t^2) dt. \quad (21) \]

As can be seen from (20), at small \( z \) the symmetry transform \( w_1 (z) = -w_2 (z) \) implies the antisymmetry of \( A(-z) = -A(z) \), which is compatible with (21) and the structure of the equation:

\[ A'' = 16\pi I e_\alpha^2 A (\sinh^2 w_1 + \sinh^2 w_2 + 2 \cos \alpha \sinh w_1 \sinh w_2) \cosh^2 w_1 \cosh^2 w_2. \quad (22) \]
Thus, approximately for small $z$, one can put
\[ A = \beta z + \gamma z^3, \]  
with $\beta, \gamma$ being some constants. Inserting (23) into (22) and equating the linear terms, one finds the relation between $\beta$ and $\gamma$, which yields the magnetic intensity at $z \to 0$:
\[ B = \beta [1 + 16\pi I e_0^2 M (1 - \cos \alpha) z^2], \quad M = \tanh^2 k l (1 - \tanh^2 k l). \]  
Let us perform a smooth matching of the corresponding functions (21) and (23), (24), equating them at some intermediate point $z = \tilde{l}$ and introducing the appropriate denotations:
\[ x^2 = 2e_0 B_0 \tilde{l}^2; \quad y = \beta / B_0; \quad \Gamma = 8\pi I e_0 / B_0; \quad C(\alpha) = \Gamma (1 - \cos \alpha); \quad D(\alpha) = \Gamma (1 + \cos \alpha). \]  
We also explore the special representation for the error function [13]:
\[ \frac{\pi^{1/2}}{2x} \text{erf} (x) = \exp (-x^2) [1 + g(x^2)], \quad g = \sum_{n=1}^{\infty} \frac{2^n x^{2n}}{(2n+1)!}. \]

Finally, we obtain the expression for the relative magnetic intensity $y$ inside the material and also the relation determining the value of the angle $\alpha$:
\[ y = \left[ 1 + (x^2 + h^{-1}) C(\alpha) \right], \quad 4D(\alpha) \exp (-x^2) [h + C(\alpha) (1 + h x^2) ] = C(\alpha), \]  
where $h = 3g / (2x^2)$.

It is worth-while to notice that, in accordance with the Meissner effect [11], the superconductivity of the TBG is equivalent to vanishing magnetic intensity within the material, that is $B \to 0$ as $z \to 0$. As follows from (25), it means that $y \ll 1$, or
\[ 4h \exp (-x^2) D(\alpha) \ll C(\alpha), \]
where $1 + \cos \alpha \approx \xi \ll 1$. However, in accordance with (25), the parameter $\xi$ satisfies the quadratic equation
\[ \xi^2 \Gamma - \xi (2\Gamma + 1 + M / 4) + M / 2 = 0, \]  
with the roots being
\[ \xi_{\pm} = \frac{1}{2\Gamma} \left( 2\Gamma + 1 + M / 4 \pm \Delta^{1/2} \right), \quad \Delta = (2\Gamma + 1 - M / 4)^2 + M, \]  
where it was taken into account that $x^2 \sim 10^{-6}$ and $h = 1$ for the typical values of $\tilde{l} = 2l = 0.34 \text{nm}$ and $B_0 = 10 \text{mT}$. As can be seen from (27), the small root reads
\[ \xi = \xi_{-} \approx y M / 2; \quad y = (1 + 2 \Gamma M)^{-1}. \]  
As for the second root to the equation (26), it appears to be nonphysical and should be deleted, since $\xi_{+} > 2$, in accordance with (27).

For numerical estimations we should specify the parameters in our model [14]: the spacing $a = 0.287 \text{nm}$; $k l = 1$, $M = 0.2436$ and the exchange energy between carbon atoms $E_0 = 2.9 \text{eV}$; $I = E_0 / a = 1.619 \text{nN}$; $I e_0 = 0.246T$; $2\Gamma = 16\pi I e_0 / B_0 = 12.3653 / B_0$; with $B_0$ being measured in Tesla. The results of calculating the relative intensity $y$ and the twisting angle $\delta = \pi - \alpha$ according to (28) are represented in the Table 1 below for some typical values of $B_0$. Here it was taken into account that $\xi \approx \delta^2 / 2$.

5. Conclusion
We studied superconducting properties of the TBG configuration within the framework of the scalar chiral model of graphene suggested earlier in [8]. This model is a variant of the sigma-model approach and exploits the $sp^3$-hybridization effect for valence electrons in carbon atoms through employing the $SU(2)$ matrix as an order parameter. This fact permits us to describe the single-layer graphene configuration, in the long-wave approximation, via the kink-like solution and that of the TBG via the
corresponding product ansatz. Due to economy of the model in question, we confine our attention to the orbital motion of the fourth valence electron, with spin effects being neglected. The interaction with an external magnetic field being included through the gauge invariance principle, we use the appropriate trial functions to approximate the behaviour of the vector potential at small and large distances, respectively. Matching these functions, in a smooth way, at some intermediate point, we derive a pair of equations for the parameters of the magnetic field configuration and also for the twisting angle $\alpha$. The analysis of these equations yields the important information about the dependence of $\alpha$ on the magnetic intensity $B_0$. This functional dependence is illustrated through corresponding numerical data.

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| $B_0$ (mT) | $\gamma \times 10^3$ | $\xi \times 10^4$ | $\delta$ (rad) | $\delta$ (deg) |
|----------|----------------------|------------------|----------------|---------------|
| 3        | 0.995                | 1.212            | 0.015          | 0.89          |
| 4        | 1.326                | 1.615            | 0.018          | 1.03          |
| 5        | 1.657                | 2.018            | 0.020          | 1.15          |
| 10       | 3.309                | 4.030            | 0.028          | 1.63          |

Table 1. The relative magnetic intensity $\gamma = \beta / B_0$ inside the TBG and the twisting angle $\delta = \pi - \alpha$ as functions of $B_0$.

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