Superconductivity of twisted double bi-layer graphene in chiral model

Yu P Rybakov¹, M Umar¹

¹Peoples’ Friendship University of Russia (RUDN University), Moscow, 117198, Russia

e-mail: soliton4@mail.ru, rybakov-yup@rudn.ru

Abstract. Taking into account the \( sp \) – hybridization effect for valence electrons in carbon atoms, a very simple chiral model of graphene was suggested some years ago [1]. This model used as a special order parameter the unitary \( SU(2) \) matrix \( U \) with the kink-like (or domain wall) structure for the description of electrons in a mono-atomic graphene sheet. However, later the new graphene physics began since studying twisted multilayer configurations revealing unconventional superconducting properties (twistronics) [2]. Within the scope of the chiral model these twisted configurations can be described by the so-called “product ansatz” \( U = U_1U_2 \cdots U_n \). As an example, the special case of twisted double bi-layer graphene (TDBG) configuration is studied and the corresponding twist angles, for which the superconductivity takes place, are found.

1. Introduction. Structure of the chiral model

Mono-atomic carbon lattices called graphenes attracted a deep interest of researchers due to their extraordinary electronic and mechanical properties [3], which can be effectively described within the scope of the chiral model based on the \( sp \) – hybridization effect. As is well known, the strong coupling between carbon atoms forming hexagon lattices is created by three covalent bonds with the neighbors, the fourth valence electron being “free” for each atom. Therefore, it seems natural to combine scalar \( a_0 \) and vector \( \vec{a} \) fields corresponding to the \( s \) – orbital and the \( p \) – orbital states of the “free” electron, respectively, into the unitary matrix \( U \in SU(2) \) serving as the order parameter in our model:

\[
U = a_0 \tau_0 + i \vec{a} \cdot \vec{\tau}.
\]

(1)

Here \( \tau_0 \) is the unit \( 2 \times 2 \) – matrix and \( \vec{\tau} \) stands for the three Pauli matrices with the subsidiary \( SU(2) \) – condition being imposed: \( a_0^2 + \vec{a}^2 = 1 \).

The Lagrangian density of the model can be constructed through the left chiral currents

\[
I_\mu = U^+ \partial_\mu U, \quad \mu = 0, 1, 2, 3,
\]

(2)
involving the coordinate \( x^1, x^2, x^3 \) and the time \( x^0 = ct \) derivatives:

\[
 L = -\frac{I}{4} \text{tr} (L_\mu L^\mu) - \frac{\lambda^2}{2} \bar{a}^2. \tag{3}
\]

The parameter \( I \) in (3) can be interpreted as the exchange energy between carbon atoms (per spacing). The equations of motion corresponding to (3) admit the kink-like solution [1]:

\[
 U = \exp (i \hat{n} \Theta), \quad \hat{n} = \bar{n} \cdot \bar{r}, \quad \Theta = \Theta(z) = 2 \arctan (-z/l_0), \tag{4}
\]

describing the electrons distribution in an ideal graphene plane oriented along the unit vector \( \bar{n} \) and orthogonal to the \( z \)-axis. The configuration (4) contains the characteristic length \( l_0 = l^{1/2} / \lambda \), which can be identified with the diameter of the carbon atom.

It is worth-while to underline that the interaction with an external electromagnetic field can be included via extending the derivatives in accordance with the gauge invariance principle:

\[
 \partial_\mu U \Rightarrow D_\mu U = \partial_\mu U - i e_0 A_\mu [\tau, U], \tag{5}
\]

where \( e_0, \tau, A_\mu \) denote the electromagnetic coupling constant, the charge operator and the 4-potential, respectively. In particular case of the interaction with the uniform magnetic field oriented along the \( y \)-axis the Lagrangian density reads:

\[
 L = -\frac{I}{4} \text{tr} (L_\mu L^\mu) - \frac{\lambda^2}{2} \bar{a}^2 - \frac{\bar{B}^2}{8\pi}, \tag{6}
\]

where

\[
 L_\mu = U^* D_\mu U, \quad \bar{B} = (0, B, 0), \quad B = A'(z), \quad A(z) = A_1, \quad B(\pm \infty) = B_0 = \text{const.}
\]

2. **Strongly correlated states in multi-layer graphene and the Meissner effect**

The main concept behind this research concerns the ample justification of the connection between the formation of twisted graphene configurations and the emergence of the orbital superconductivity confirmed by the Meissner effect, that is vanishing magnetic intensity within the sample. Our approach builds on estimating the internal magnetic field for the TDBG configuration interacting with the uniform magnetic field parallel to the graphene sheets.

To this end, let us consider the product ansatz \( U = U_{-2} U_{-1} U_1 U_2 \) with the fixed positions of the sheets along the \( z \)-axis:

\[
 z_{-2} = -3l, \quad z_{-1} = -l, \quad z_1 = l, \quad z_2 = 3l,
\]

where \( 2l \) stands for the distance between the sheets and the matrices \( U_\kappa = \exp (i \hat{n}_\kappa \Theta_\kappa) \) contain the following unit vectors:

\[
 \hat{n}_{-2} = (\cos \beta / 2, \sin \beta / 2, 0), \quad \hat{n}_{-1} = (\cos \alpha / 2, \sin \alpha / 2, 0), \quad \hat{n}_1 = \hat{n}_{-1} (-\alpha), \quad \hat{n}_2 = \hat{n}_{-2} (-\beta)
\]
and the unknown phases $\Theta_i(z - z_k)$. In this case the Lagrangian density (6) includes only two components of the chiral current:

$$L_\alpha = -i e_\alpha A (U^+ \tau_j U - \tau_j), \quad L_\alpha = U^+ \partial_\psi U$$

and the vector $\vec{a} = -(i/2) \text{tr}(\overline{\tau} U)$. The corresponding calculations appear to be drastically simplified through using the formula:

$$\exp (i \hat{m} \Theta) \hat{n} \exp (-i \hat{m} \Theta) = \hat{n} \cos 2\Theta + (1 - \cos 2\Theta) \hat{m} \cdot \hat{n} - \sin 2\Theta \hat{m} \cdot \hat{n} \cdot \overline{\tau}.$$

The resulting Lagrangian density takes the form:

$$L = \frac{1}{4} \left( \text{tr} L^2_\alpha + \text{tr} L^2_\alpha \right) - \frac{\lambda^2}{2} \vec{a}^2 - \frac{A^2}{8\pi}.$$ (7)

Using the denotations $4X_\alpha = -\text{tr} L^2_\alpha$, the corresponding terms read:

$$X_\alpha = \frac{1}{2} \sum_i \Theta_i^2 + \cos \frac{\beta - \alpha}{2} (\Theta_{i-1} \Theta_i + \Theta_i \Theta_{i+1}) + \cos \alpha \Theta_{i-1} \Theta_i +$$

$$\Theta_{i-1} \Theta_i \left( \cos \frac{\beta + \alpha}{2} + 2 \sin^2 \Theta_i \sin \alpha \sin \frac{\beta - \alpha}{2} \right) + \Theta_{i-1} \Theta_i \left( \cos \frac{\beta + \alpha}{2} + 2 \sin^2 \Theta_i \sin \alpha \sin \frac{\beta - \alpha}{2} \right) +$$

$$\Theta_{i-1} \Theta_i \cos^2 \frac{\beta - \alpha}{2} \left[ \cos \alpha - \sin \tan \frac{\beta - \alpha}{2} (\cos 2\Theta_i + \cos 2\Theta_i) + \tan \frac{\beta - \alpha}{2} (\sin 2\Theta_i \cos 2\Theta_i - \cos \alpha \cos 2\Theta_i \cos 2\Theta_i) \right];$$

$$X_1 = e_\alpha^2 A^2 \left[ 1 - \prod_i \cos 2\Theta_i \left[ 1 - \prod_i \tan 2\Theta_i - \cos \alpha \tan 2\Theta_i \tan 2\Theta_i - \cos \beta \tan 2\Theta_i \tan 2\Theta_i \right] +$$

$$- \cos \frac{\beta + \alpha}{2} (\tan 2\Theta_i \tan 2\Theta_i + \tan 2\Theta_i \tan 2\Theta_i) \cos \frac{\beta - \alpha}{2} (\tan 2\Theta_i \tan 2\Theta_i + \tan 2\Theta_i \tan 2\Theta_i) \right] +$$

$$\prod_i \sin 2\Theta_i \cos \frac{\beta - \alpha}{2} \left[ \sin \frac{\beta + \alpha}{2} (\tan 1 \Theta_i \tan 1 \Theta_i + \tan 1 \Theta_i \tan 1 \Theta_i) + \cos \alpha \sin \frac{\beta - \alpha}{2} \tan 1 \Theta_i \tan 1 \Theta_i + \sin \alpha (\tan 1 \Theta_i \tan 1 \Theta_i + \tan 1 \Theta_i \tan 1 \Theta_i) \right] \right] \equiv e_\alpha^2 A^2 V_0;$$

$$\vec{a}^2 = M_{\alpha}^2 \left[ \cos^2 \Theta_{i-1} \cos^2 \Theta_i - M_{\beta}^2 + \frac{1}{2} (\sin^2 \Theta_{i-1} + \sin^2 \Theta_i) \right] + 2 \sin \alpha \sin \beta \prod_i \sin \Theta_i \left( M_{\alpha}^2 - M_{\beta}^2 \right) + 2 M_{\alpha} \sin \Theta_i \left( \sin^2 \Theta_{i-1} - \sin^2 \Theta_i \right) \left( \sin^2 \Theta_i - \cos \Theta_i \right) +$$

$$\frac{1}{16} (1 - P_i) [4(1 + P_i) - 2 S_i (\cos \alpha + \cos \beta) + (1 - P_i)(1 - \cos \alpha \cos \beta)].$$

Here the following denotations were introduced:
First, to study the behaviour of solutions at large $\pi$. Introducing the denotations:

\[ M_{\alpha \beta} = \prod_k \cos \Theta_k \tan \Theta_k \left( \tan \Theta_{-2} \cos \frac{\beta - \alpha}{2} + \tan \Theta_{2} \cos \frac{\beta + \alpha}{2} \right) ; \]

\[ P_1 = \cos 2\Theta_{-1} \cos 2\Theta_2 ; \quad P_2 = \cos 2\Theta_{-2} \cos 2\Theta_3 ; \quad S_2 = \sin 2\Theta_{-2} \sin 2\Theta_2 . \]

3. Structure of solutions to the equations of motion

Let us now fix the boundary conditions for our problem:

\[ \Theta_i(-\infty) = \pi ; \quad \Theta_i(\infty) = 0 ; \quad \Theta_i(0) = \pi / 2 \]  

and make the substitution $\tan \Theta_j = u_j = \sinh^{-1} w_j$. First, to study the behaviour of solutions at large $z \to \infty$, it is convenient to consider the asymptotic limit of the Lagrangian as $u_j \to 0$:

\[ L = -\int \left[ \sum_i u_i^2 + \cos \alpha u_{-1} u_1 + \cos \beta u_{-2} u_2 + \cos \frac{\beta - \alpha}{2} (u_{-1} u_2 + u_2 u_{-1}) + \cos \frac{\beta + \alpha}{2} (u_{-2} u_1 + u_1 u_{-2}) \right] - 4a e_0^2 A^2 \int \left[ \sum_i u_i^2 + \cos \alpha u_1 u_i + \cos \beta u_{-2} u_i + \cos \frac{\beta - \alpha}{2} (u_{-2} u_i + u_i u_{-2}) + \cos \frac{\beta + \alpha}{2} (u_{-2} u_i + u_i u_{-2}) \right] - \frac{A^2}{8\pi}, \]

where it was taken into account that $A = B_0 z + (2 \alpha / 2 + \cos \alpha / 2)^2$. Therefore, the equations for $u_j$ admit the symmetric solution of the form:

\[ u_j = 2 \exp (-e_0 B_0 z^2). \]  

As follows from (9), the equation for the magnetic field reads:

\[ B' = a'' = 256 \pi \gamma I e_0^2 B_0 z \exp (-2e_0 B_0 z^2); \quad \gamma = (\cos \beta / 2 + \cos \alpha / 2)^2, \]  

and admits the evident solution:

\[ B = B_0 - 64 \pi \gamma I e_0 \exp (-2e_0 B_0 z^2); \quad A = B_0 z - 64 \pi \gamma I e_0 \int \exp (-2e_0 B_0 t^2) \, dt. \]

Let us now consider the central part of the sample, where the reflection symmetry holds:

\[ z \Rightarrow -z: \quad w_{-1}(-z) = k(l - z) = -w_1(z); \quad w_{-2}(-z) = k(3l - z) = -w_2(z); \quad A(-z) = -A(z), \]

and the vector potential satisfies in the first approximation the equation:

\[ A'' = 8\pi I e_0^2 V_0 A, \quad V_0 = \text{const}, \]

with the following approximate solution:

\[ B = C(1 + z^2 4\pi I e_0^2 V_0); \quad A = Cz \left[ 1 + z^2 (4\pi / 3) I e_0^2 V_0 \right]; \quad C = \text{const}. \]

A global behavior of the magnetic field can be obtained by matching the asymptotic configurations at some intermediate point $z = \bar{l}$. Introducing the denotations:
\[ x^2 = 2e_o B \partial^2, \quad y = C / B_o, \quad \Gamma = 8\pi le_o / B_o, \quad \gamma = (\cos \beta/2 + \cos \alpha/2)^2 \]

and using the special representation for the error function [4]:

\[
\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x ds \exp(-s^2) = \frac{2x}{\sqrt{\pi}} [1 + g(x^2)] \exp(-x^2); \quad g = \sum_{n=1}^{\infty} \frac{2^n x^{2n}}{(2n+1)!} = \frac{2}{3} x^2; \quad h(0) = 1,
\]

one finds the following matching conditions:

\[
y(1 + x^2 \Gamma V_o / 12) = 1 - 8\Gamma \gamma (1 + g) \exp(-x^2); \quad y(1 + x^2 \Gamma V_o / 4) = 1 - 8\Gamma \gamma \exp(-x^2).
\]

(11)

It should be underlined that the system (11) determines the conditions under which our sample reveals superconducting properties. It means that the magnetic intensity in the central part \((z \rightarrow 0)\) of the TDBG configuration should be vanishing (the Meissner effect), i.e. \(y << 1\). Taking into account that for realistic magnetic fields \(\Gamma \gg 1\), \(x^2 << 1\), \(h \approx 1\), one gets from (11) the value

\[
y \approx (1 + \Gamma V_o / 4)^{-1} << 1.
\]

(12)

Eliminating the variable \(y\) between the equations (11), one derives the constraint on \(\alpha, \beta\):

\[
\left(\cos \frac{\beta}{2} + \cos \frac{\alpha}{2}\right)^2 \approx \frac{V_o}{8(\Gamma V_o + 4)}.
\]

(13)

In view of the restriction (12) caused by the Meissner effect, this amounts to searching the maximal value of \(V_o(\alpha, \beta)\) under the condition (13). Due to the Lagrangian structure (7), one finds

\[
V_o = 4 \sinh^2 w_1 \sinh^2 w_2 \left[ 4 \sinh^2 w_1 \sinh^2 w_2 \left\{ \cos \frac{\alpha}{2} \cos \frac{\beta}{2} (\sinh^2 w_1 - 1) - \sin \alpha \sin \beta - \alpha \right\} + 2(1 + \cos(\beta - \alpha) - 2 \cos \alpha) + \sinh^2 w_1(1 + \cos \beta) + \sinh^2 w_1(1 + \cos(2\alpha - \beta)) + (\sinh^2 w_2 + \sinh^2 w_2)(1 + \cos \alpha) \right],
\]

\[
2 \sinh w_1 \sinh w_2 \left[ \cos \frac{\alpha}{2} \cos \frac{\beta}{2} (\sinh^2 w_1 - 1) - \sin \alpha \sin \beta - \alpha \right] + (\sinh^2 w_2 + \sinh^2 w_2)(1 + \cos \alpha),
\]

(14)

where in accordance with the kink structure [1] \(w_1 = kl \approx 1, \quad w_2 = 3kl \approx 3\). As follows from (14), the maximal value of \(V_o\) corresponds to the choice \(\beta = \alpha = \pi - \mu\), \(\mu << 1\), that implies the structure:

\[
V_o(\mu) = M(1 + N\mu^2); \quad M \approx 0.0761; \quad N \approx 6.511.
\]

(15)

Solving equations (13) and (15) with respect to \(\mu^2\), one derives the dependence of the “magic” angle on the external magnetic field:

\[
\mu^2 = [8(\Gamma + \rho)]^{-1}; \quad \rho = 4 / M - N / 8 \approx 51.715.
\]

(16)

For numerical illustration of the twist effect one can use the following parameters of the chiral model [5]: the spacing \(a = 0.287\) nm, the exchange energy between atoms \(E_o = 2.9\) eV with the value
\( I = E_o / a = 1.619 \text{ nN}, \) the coupling constant \( e_o = e / (\hbar c) \) with the value \( le_o = 0.246 \text{ T}, \) the distance between the sheets \( 2l = 0.34 \text{ nm}. \) The dependence of the relative magnetic intensity \( (12) \) and the “magic” angle \( (16) \) on the intensity of the external magnetic field is represented in the Table 1.

**Table 1.** The relative magnetic intensity \( y \) inside the TDBG and the twisting angle \( \mu \) as functions of \( B_o. \)

| \( B_o \) (mT) | \( \Gamma \times 10^{-3} \) | \( y \times 10^{-3} \) | \( \mu \) (deg) |
|----------|-----------------|-----------------|---------|
| 5        | 1.2364          | 4.08            | ± 0.56  |
| 10       | 0.6182          | 7.85            | ± 0.78  |
| 15       | 0.4121          | 11.3            | ± 0.94  |

4. **Conclusion**

To sum up, notice that within the scope of the chiral graphene model the special TDBG sample was studied and proved to reveal superconducting properties for some critical “magic” twisting angles [6, 7]. This fact confirms the idea of forming strongly correlated electronic states as a result of twisting graphene sheets. Another consequence of this twist effect appears to be a creation of giant hexagon super-lattices, so-called moiré patterns [8], that facilitates the transitions of electrons between the sheets due to flat bands in dispersion curves of the model (3).

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