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# Superconductivity and special symmetry of twisted tri-layer graphene in chiral model

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**Abstract.** Superconducting properties of twisted tri-layer graphene (TTG) are studied within the scope of the chiral model based on using the unitary matrix $U \in SU(2)$ as an order parameter. To check the superconductor behavior of this system, the interaction with the external magnetic field $B_0$ oriented along the graphene sheets is switched on and the internal magnetic intensity in the center is calculated as the function of the twisting angle. Vanishing of this function, due to the Meissner effect, being the important feature of the superconductivity, the corresponding dependence of the magic twisting angle on $B_0$ is calculated. The unusual effect of re-entrant superconductivity for large values of $B_0$ is discussed.

**Key words and phrases:** tri-layer graphene, chiral model, superconductivity

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## 1. Introduction

It should be noticed that since the discovery of mono-atomic carbon layers called graphenes [1, 2] this material attracted high attention of researchers due to its extraordinary properties concerning magnetism, stiffness and considerable electric and thermal conductivity [3, 4]. The important connection was revealed with other graphene-based materials: Fullerenes [5] and carbon nanotubes [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 sublattices. The further development of this idea was realized in [8, 9].

The unprecedented raise of interest has emerged to graphene-based materials and especially to moiré super-lattice patterns, this fact being motivated by their unconventional characteristics. In particular, specific magic-angle systems constructed by stacking two or three graphene layers twisted relative to each other have shown superconducting behavior [10–18]. However, these systems exhibit superconducting properties also for the very strong external magnetic fields (up to 10 T) [19], and therefore the standard superconductivity model by J. Bardeen, L. Cooper, J. Schrieffer and N. Bogoliubov [20] appears to be non suitable for the explanation of this fact. Thus, the superconductivity in TTG is likely to be driven by a mechanism that results in non-spin-singlet Cooper pairs. Nevertheless, it can be shown that the phenomenological approach based on the Landau theory of phase transitions [21] and on the corresponding chiral model of graphene suggested earlier [8] seems to be well suitable for the description of TTG.

## 2. Lagrangian density for the chiral model of graphene

In accordance with the hexagonal structure of the graphene mono-atomic carbon lattice, the three valence electrons of the atom form strong covalent bonds with the neighbours, but the forth electron belongs to the so-called hybridized state and appears to be "free". Thus, let us combine scalar $a_0$ and 3-vector $\mathbf{a}$ 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:

$$U = a_0\,\tau_0 + \imath\,\mathbf{a}\cdot\boldsymbol{\tau}. \tag{1}$$

Here $\tau_0$ is the unit $2\times 2$-matrix and $\boldsymbol{\tau}$ stands for the three Pauli matrices, with the subsidiary $SU(2)$-condition being imposed: $a_0^2 + \mathbf{a}^2 = 1$ . To describe a single graphene sheet, one can use the Lagrangian density of the sigma-model form:

$$\mathcal{L} = -\frac{1}{4} I\,\mathrm{Sp}(l_\mu l^\mu) - \frac{1}{2}\lambda^2\mathbf{a}^2, \tag{2}$$

involving the so-called left chiral current $l_\mu = U^+\partial_\mu U$ and the coordinates $x^i$, $i = 1,2,3$ and the time $x^0 = ct$ derivatives. Comparing the Lagrangian density (2) with that of the Landau–Lifshitz theory [22] corresponding to the quasi-classical long-wave approximation to the Heisenberg ferromagnetic model, one can interpret the parameter $I$ in (2) as the exchange energy between carbon atoms (per spacing). The equations of motion corresponding to (2) admit the kink-like or the domain-wall solution [8]:

$$U = \exp(\imath\hat{n}\Theta), \quad \hat{n} = \mathbf{n}\cdot\boldsymbol{\tau}, \quad \Theta = 2\arctan\exp(-z/\ell_0); \tag{3}$$

describing the electrons distribution in an ideal graphene plane oriented along the unit vector $\mathbf{n}$ and orthogonal to the $z$-axis. The configuration 3 contains the characteristic length $\ell_0 = I^{1/2}/\lambda$, which can be identified with the diameter of the carbon atom $\ell_0 = 0.26$ nm.

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:

$$\partial_\mu \Rightarrow D_\mu - \imath e_0 A_\mu[\tau_3,\, U],$$

where $e_0, \tau_3, A_\mu$ 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:

$$\mathcal{L} = -\frac{1}{4} I\,\mathrm{Sp}(l_\mu l^\mu) - \frac{1}{2}\lambda^2\mathbf{a}^2 - \frac{\mathbf{B}^2}{8\pi}, \tag{4}$$

where

$$L_\mu = U^+ D_\mu U, \quad \mathbf{B} = (0,\ B,\ 0), \quad B = A'(z), \quad A(z) = A_1, \quad B(\pm\infty) = B_0 = const.$$

The unitary matrix $U$ for the TTG configuration has the form:

$$U = U_1 U_0 U_2, \quad U_1 = \exp\big(\imath\hat{n}_j\Theta_j\big), \quad \Theta_j = \Theta_j(z), \quad \hat{n}_j = \mathbf{n}_j\cdot\boldsymbol{\tau}; \tag{5}$$

$$\mathbf{n}_1 = \big(\cos(\alpha/2),\ \sin(\alpha/2),\ 0\big), \quad \mathbf{n}_2 = \big(\cos(\alpha/2),\ -\sin(\alpha/2),\ 0\big), \quad \mathbf{n}_0 = (1,\ 0,\ 0), \tag{6}$$

with the vector $\mathbf{a}$ being defined as follows:

$$\mathbf{a} = -(\imath/2)tr(\boldsymbol{\tau}U).$$

Here $j = 0, 1, 2$ is the number of the correspondent sheet.

In accordance with (4), (5) and (6) the Lagrangian density takes the form:

$$\mathcal{L} = -I\Big[S + \cos(\alpha/2)\Theta_0'(\Theta_1' + \Theta_2') + \Theta_1'\Theta_2'(\sin^2\Theta_0 + \cos\alpha\cos^2\Theta_0)\Big] - Ie_0^2A^2(1 - P - Q + R) - (\lambda)^2/2(X + Y + Z) - A'^2/(8\pi);$$

where the following denotations are used:

$$S = (\Theta_1'^2 + \Theta_2'^2 + \Theta_0'^2)/2,$$
$$P = 2\sin^2(\alpha/2)\sin^2\Theta_0\sin 2\Theta_1\sin 2\Theta_2,$$
$$Q = \cos 2\Theta_0\cos 2(\Theta_1 - \Theta_2),$$
$$R = \cos(\alpha/2)\sin 2\Theta_0\sin 2(\Theta_1 + \Theta_2),$$
$$X = \cos^2\Theta_0\Big[\sin^2(\Theta_1 + \Theta_2) - \sin^2(\alpha/2)\sin 2\Theta_1\sin 2\Theta_2 + \sin^2\alpha\sin^2\Theta_1\sin^2\Theta_2\Big],$$
$$Y = \sin^2\Theta_0\Big[\sin^2(\alpha/2) + \cos^2(\alpha/2)\cos^2(\Theta_1 + \Theta_2)\Big],$$
$$Z = \cos(\alpha/2)\sin 2\Theta_0\sin(\Theta_1 + \Theta_2)[\cos\Theta_1\cos\Theta_2 - \cos\alpha\sin\Theta_1\sin\Theta_2].$$

The boundary conditions read:

$$\Theta_j(-\infty) = \pi, \qquad \Theta_j(+\infty) = 0, \tag{7}$$

and central phases are chosen equal: $\Theta_0(0) = \Theta_1(-2l) = \Theta_2(2l) = \pi/2$, where $2l$ stands for the distance between the sheets.

## 3. Asymptotic structure of solutions to the equations of motion

At large $z \to \pm\infty$ one can put $\tan\Theta_j = u_j \to 0$ with the discrete symmetry being $u_1 = u_2 = u$. The asymptotic Lagrangian density

$$\mathcal{L} = -(I/2)[u_0' + 2\cos(\alpha/2)u']^2 - [u_0 + 2\cos(\alpha/2)u]^2\,(2Ie_0^2A^2 + \lambda^2/2),$$

where $A \approx B_0 z$, admits the symmetry $u_0 \leftrightarrow 2u\cos(\alpha/2)$, with the solution being derived through the substitution $u^{-1} = \sinh w$, $u_0 = u\cos(\alpha/2)$. The asymptotic estimation reads:

$$u = 2\exp\big(-e_0B_0z^2\big). \tag{8}$$

As a result, for the vector potential $A = B_0z + a(z)$, where $a'(\infty) = 0$, one finds the equation:

$$\frac{a''}{4\pi} = 128\,I\,e_0^2B_0z(1 + \cos\alpha)\exp\big(-2e_0B_0z^2\big)$$

with the evident solution:

$$A' = B_0 - 128\pi I\,e_0(1 + \cos\alpha)\exp\big(-2e_0B_0z^2\big),$$
$$A = B_0z - 128\pi I\,e_0(1 + \cos\alpha)\int_0^z \exp\big(-2e_0B_0z^2\big)\,dz, \tag{9}$$

where the anti-symmetric property of the vector potential found later was taken into account.

Now let us investigate the behavior of our system at small $z$, where one can put due to (7) the Lagrangian density for the vector potential taking the form:

$$\mathcal{L} = -2I\,e_0^2 A^2 - A'^2/(8\pi).$$

The corresponding equation of motion reads:

$$A'' - 16\pi I\,e_0^2 A = 0$$

and admits the evident solution:

$$A = C\sinh(k\,z), \tag{10}$$

where $C$ is an arbitrary constant and $k^2 = 16\pi I\,e_0^2$. Taking the derivative, it is not difficult to find the magnetic intensity $B = A' = k\,C\cosh(k\,z)$.

Now, to fix the value of the constant $C$ in (10), let us perform the smooth matching of the expressions (3), (9) and (10) at some intermediate point $z = \bar{l}$. However, to simplify this operation, let us introduce some denotations:

$$y = k\,C/B_0, \qquad x^2 = 2\,e_0 B_0 \bar{l}^2, \qquad \Lambda = 16(1+\cos\alpha)\exp\left(-x^2\right);$$

$$\Gamma = 8\pi I\,e_0/B_0, \qquad \xi = \frac{\sinh\left(x\sqrt{2\Gamma}\right)}{x\sqrt{2\Gamma}}, \qquad \eta = \cosh\left(x\sqrt{2\Gamma}\right).$$

Also the special representation for the error function is used [23]:

$$\frac{1}{x}\int_0^x \exp\left(-s^2\right)d\,s = \frac{\pi^{1/2}}{2x}\,\mathrm{erf}(x) = (1+g)\exp\left(-x^2\right); \qquad g = \sum_{n=1}^{i\infty}\frac{2^n\,x^{2n}}{(2n+1)!!}.$$

As a result, one obtains the following system of equations

$$\xi\,y = 1 - \Gamma\Lambda(1+g), \tag{11}$$

$$\eta\,y = 1 - \Gamma\Lambda.$$

Now it is worth while to stress that, in accordance with the Meissner effect [20], our system reveals superconducting properties if the relative magnetic field $y$ vanishes in the central domain. Let us first recall some information about graphene properties [24]. For numerical illustration of the twist effect one can use the following parameters of the chiral model: the spacing $a = 0.287$ nm, the exchange energy between atoms $E_0 = 2.9$ eV with the value $I = E_0/a = 1.619$ nN, the coupling constant $e_0 = e/(\hbar c)$, with $-e$ being the electron charge, the value $I\,e_0 = 0.246$ T being known as the effective (internal) “magnetic” intensity in graphene, the distance between the sheets $2l = 0.34$ nm. Taking into account that for standard graphene experiments

$$x^2 \ll 1, \quad g \ll 1, \quad \Gamma = (8\pi)246/B_0(m\,T) \gg 1, \quad \alpha \approx \pi - \zeta, \quad \zeta \ll 1, \quad \Lambda \approx 8\zeta^2;$$

one concludes that small values of $y$ can be provided by so-called “magic” values of twisting angle:

$$\zeta(rad) \approx (8\Gamma)^{-1/2}.$$

It should be noted that the other possible magic twisting angle can be obtained through the reflection $\alpha \Rightarrow \pi - \alpha$, which leaves the moiré super-lattice invariant.

Let us now discuss, in view of (11), the case of strong magnetic fields, when the quantity $\Gamma(1+g)$ retains large values. This fact implies the so-called re-entrant superconductivity. Experimental verification of this effect can be found in [19], the peculiar symmetry properties of TTG system being underlined earlier in connection with the boundary conditions (7).

## 4. Results and Discussions

In our paper the Landau phase transitions method is applied to the twisted tri-layer graphene model, the order parameter being the unitary matrix, depending on the twisting angle $\alpha$. The superconductivity property of the TTG model is proven for the special "magic" twisting angle, the cases of small and large external magnetic fields being considered.

## 5. Conclusions

The superconducting properties of the TTG configuration were studied within the framework of the chiral graphene model suggested in [8]. The product-ansatz being used for the description of the TTG system, the Lagrangian density and the asymptotic solutions to the equations of motion at small and large distances were found. Using the anti-symmetric behavior of the vector potential and matching these solutions at some intermediate point, a pair of algebraic equations for the magnetic field in the central domain and the twisting angle were obtained. Finally, in view of the Meissner effect, the correlation between the magic angle and the external magnetic intensity was established. The important effect of the re-entrant superconductivity was mentioned for the case of strong magnetic fields.

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## References

1. Novoselov, K. S. *et al.* Electric field effect in atomically thin carbon films. *Science* **306,** 666–669 (2004).
2. Geim, A. K. Graphine: status and prospects. *Science* **324,** 1530–1534 (2009).
3. Lee, C. *et al.* Measurement of elastic properties and intrinsic strength of monolayer graphene. *Science* **321,** 385–388 (2008).
4. Bolotin, K. I. *et al.* Ultrahigh electron mobility in suspended graphene. *Solid State Comm.* **146,** 351–355 (2008).
5. Lu, X. & Chen, Z. Curved $\pi$-conjugation aromaticity, and the related chemistry of small Fullerenes ($C_60$) and single-walled carbon nanotubes. *Chem. Rev.* **105,** 3643–3696 (2005).
6. Terrones, M. Science and Technology of the twenty-first century: synthesis, properties, and applications of carbon nanotubes. *Ann. Rev. Mat. Res.* **33,** 419–501 (2003).
7. Semenoff, G. W. Condensed-matter simulation of a three-dimensional anomaly. *Phys. Rev. Lett.* **53,** 2449–2452 (1984).
8. Rybakov, Y. P. On chiral model of graphene. *Solid State Phenomena* **190,** 59–62 (2012).
9. Rybakov, Y. P. Spin excitations in chiral model of graphene. *Solid State Phenomena* **233–234,** 16–19 (2015).
10. Cao, Y. *et al.* Unconventional superconductivity in magic-angle graphene superlattices. *Nature* **556,** 43–50 (2018).

11. Park, J. M. *et al.* Tunable strongly coupled superconductivity in magic-angle twisted tri-layer graphene. *Nature* **590,** 249–255 (2021).
12. Hao, Z. *et al.* Elastic field-tunable superconductivity in alternating-twist magic-angle tri-layer graphene. *Science* **371,** 1133–1138 (2021).
13. Yankowicz, M. *et al.* Tuning superconductivity in twisted bilayer graphene. *Science* **363,** 1059–1064 (2019).
14. Lu, X. *et al.* Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene. *Nature* **574,** 653–657 (2019).
15. Zondiner, U. *et al.* Cascade of phase transitions and Dirac revivals in magic-angle graphene. *Nature* **582,** 203–208 (2020).
16. Wong, D. *et al.* Cascade of electronic transitions in magic-angle twisted bi-layer gtaphene. *Nature* **582,** 198–202 (2020).
17. Xu, C. & Balents, L. Topological superconductivity in twisted multi-layer graphene. *Phys. Rev. Lett.* **121,** 087001 (2018).
18. Scheurer, M. S. & Samajdar, R. Pairing in graphene-based moiré superlattices. *Phys. Rev. Lett.* **2,** 033062 (2020).
19. Cao, Y. *et al.* Pauli limit violation and re-entrant superconductivity in moiré graphene. *Nature* **595,** 526–531 (2021).
20. Kittel, C. *Quantum theory of solids* (John Wiley & Sons, New York, London, 1963).
21. Landau, L. D. & Lifshitz, E. M. *Statistical Physics, volume 5, Course of theoretical physics* (Butterwert–Heinemann, Oxford, Boston, Johannesburgh, Melburn, New Delhi, Singapore, 1990).
22. Ter Haar, D. *Collected papers of L. D. Landau* (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1965).
23. Abramowitz, M. & Stegun, I. A. *Handbook of mathematical functions* (National Bureau of Standards, Washington, 1964).
24. Sheka, E. *Spin chemical physics of graphene* (Pan Stanford Publishing, Singapore, 2018).

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# Сверхпроводимость и особая симметрия скрученного трехслойного графена в киральной модели

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**Аннотация.** Сверхпроводящие свойства скрученного трёхслойного графена изучаются в рамках киральной модели, основанной на использовании унитарной матрицы $U \in SU(2)$ в качестве параметра порядка. Для проверки сверхпроводящего поведения этой системы включается взаимодействие с внешним магнитным полем $B_0$, ориентированным вдоль листа графена, и вычисляется внутренняя магнитная напряжённость в центре как функция угла закручивания. Обращение этой функции в нуль, вследствие эффекта Мейсснера, являющегося важной особенностью сверхпроводимости, вычисляется соответствующая зависимость магического угла закручивания от $B_0$. Обсуждается необычный эффект возвратной сверхпроводимости при больших значениях $B_0$.

**Ключевые слова:** трёхслойный графен, киральная модель, сверхпроводимость