

EXTERNAL MAGNETIC FIELD IN CHIRAL MODEL OF GRAPHENE

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ABSTRACT

The simplest scalar chiral model of graphene suggested earlier and based on the $SU(2)$ order parameter is generalized by including 8-spinor field as an additional order parameter for the description of spin (magnetic) excitation in graphene. As an illustration the interaction of the graphene layer with the external magnetic field was studied and the result showed the weakening of the field inside the graphene.

Keywords: Graphene, spin excitation, chiral model, 8-spinor

INTRODUCTION

Quantum mechanics had many clear understandings of phenomena from astrophysics. It also gives rise to analogies with particle physics, including an exotic type of tunneling which was predicted by the Swedish physicist Oscar Klein. Graphene has attracted increasing interest due to its remarkable properties both physical and chemical. Graphene, an allotrope of carbon, was discovered lately due to the reason that: graphene was expected to be unstable in the free state before its discovery, no experimental tool existed to detect the one-atom thin material (graphene).

The Nobel Prize in Physics 2010 honours two scientists, who have made the decisive contribution to this development. They are Andre K. Geim and Konstantin S. Novoselov, both at the University of Manchester, UK. They have succeeded in producing, isolating, identifying and characterizing graphene (K.S. Novoselov &

A.K. Geim, 2005). However, the zero band gap of monolayer graphene limits its further electronic and optoelectronic applications (Zhang & S.S. Lin, 2016).

Graphene, made of carbon atoms arranged on a honeycomb lattice with lattice constant $a = 1.42 \text{ \AA}$. These graphitic materials (Fig. 1) are classified as the allotropes of graphene (allotropes are different structural modifications of an element in the same phase of matter, e.g., different solid form).

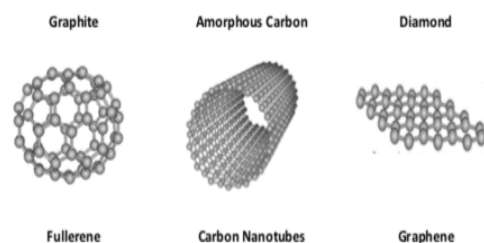


Figure 1: Allotropes of carbon (Karthik Paneer Selvam & Surya Prakash Sing, 2014).

The fact that graphene is a gapless semiconductor it cannot be used in its pristine form for Nano-electronic application

(Sivabrata Sahu & G.C.Roout, 2017). The origin of the band structure is simply related to the fact that un-hybridized Pz overlap with nearest neighbors to form π – orbitals spread out in energy and give rise to band states extending over a range of energies (R.Saito, et al., 1998). Every carbon atom of the graphene lattice uses three of its four electrons in covalent bonding to three other carbon atoms, while the fourth electron is free to move through the lattice by tunnelling effects. In summary, graphene is harder than diamond but flexible like a piece of iron sheet and a much better conductor of electricity than other materials. With such properties, graphene could revolutionize the whole micro- and computer-technology

The in cooperation of magnetism to the long list of graphene capabilities has been pursued since its first isolation in 2004 (A.B.Ahmed, et al., 2017) and also in the case of quantum dots (Yuanyuan Sun, et al., 2017) and artificial magnetic fields (Jose Tedeu Arantes, 2018)(Milan Orlita, et al., 2013)It is also well known that local magnetic moment may persist in condensed-matter systems, giving raise to many different ordered configurations. Graphene, as a metal-free material, contains no magnetic atoms. Its honeycomb structure contains a bipartite

The Lagrangian density L of the model,

$$L = \frac{1}{2} \vec{D}_\mu \bar{\Psi} P \vec{D}^\mu \Psi - \frac{\lambda^2}{2} \vec{a}^2 j_\mu j^\mu + i\mu_0 \vec{a}^2 \bar{\Psi} \sigma_{\mu\nu} F^{\mu\nu} \Psi \quad (1)$$

The Lagrangian in (1) Contain the projector $P = \gamma^v j_v$ on the positive energy states, where $j_\mu = \bar{\Psi} \gamma_\mu \Psi$, $\mu=0,1,2,3$, designetes

lattice, formed by two interpenetrating triangular sublattics, (A and B) (ERJUN KAN, et al., 2016). The magnetism discovered in graphene-based systems opens the possibility of their spintronics and other applications

MATERIALS AND METHODS

Mathematical Formulation of the Model

The s- and p- hybridization effect for the valence electrons of carbon atoms appear to the main property of the electron bonding in mono-atomic carbon layers of graphene. For realizing this effect the chiral model (YU.P.Rybakov, 2012) of graphene was suggested, the unitary $SU(2)$ matrix $V = a_0 \tau_0 + i(\vec{a} \vec{\tau})$ being considered as an order parameter.

where τ_0 , $\vec{\tau}$ denote the unit matrix and the Pauli matrices respectively, scalar and vector fields a_0 , \vec{a} ; $a_0^2 + \vec{a}^2 = 1$, describing s- and p- states of the free valence electron. For the description of spin and quasi-spin excitations in graphene, the latter ones corresponding to independent excitation modes of the two triangular sublattices of graphene, we introduce the two Dirac spinors ψ_1, ψ_2 and consider the combined spinor field $\Psi = \xi \otimes (\psi_1 \oplus \psi_2)$, as a new order parameter, where ξ stand for the first column of V .

the Dirac current, $\bar{\Psi} = \Psi^\dagger \gamma_0$ and γ_μ stands for Dirac matrices.

The model contains the two constant parameters: the exchange energy I per

lattice spacing and some characteristic inverse length $\sqrt{\lambda}$.

The interaction with electromagnetic field is realized though the extension of the derivative: $D_\mu = \partial_\mu - ie_0 A_\mu \Gamma_e$, with $e_0 > 0$ being the coupling constant and $\Gamma_e = (1 - \tau_3)/2$ being the charge operator chosen in accordance with the natural boundary condition at infinity: $a_0(\infty) = 1$. However, the additional interaction term of the Pauli type should be added to take into account the proper magnetic moments of the electrons. Here $\sigma_{\mu\nu} = [\gamma_\mu, \gamma_\nu]/4$, $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and $\mu_0 > 0$ denotes the Bohr magneton per lattice spacing cubed.

Let us now consider the case with the orientation of the magnetic field \vec{B}_0 along the z-axis. Using the cylindrical coordinates r, ϕ, z we introduce the vector potential

$$L = -8I \left[R^2 (\partial_\perp \Theta)^2 + \frac{1}{4} (\partial_\perp R)^2 + e_0^2 R^2 A^2 \sin^2 \Theta \right] - 8\lambda^2 R^2 \sin^2 \Theta + 8\mu_0 R \sin^2 \Theta \frac{1}{r} \partial_r (rA) - \frac{1}{8\pi} \left[\frac{1}{r^2} (\partial_r (rA))^2 + (\partial_z A)^2 \right], \quad (2)$$

where the new variable for the spin, chiral field is introduced: $R = u^2$ and ∂_\perp signifies the differentiation with respect to r and z .

$$I \left[\frac{1}{r} \partial_r (r \partial_r R) + \partial_z^2 R - 4R (\partial_\perp \Theta)^2 - 4e_0^2 R A^2 \sin^2 \Theta \right] = 2 \sin^2 \Theta \left[2\lambda^2 R - \mu_0 \frac{1}{r} \partial_r (rA) \right] \quad (3)$$

$$I \left[\frac{2}{r} \partial_r (r R^2 \partial_r \Theta) + 2 \partial_z (R^2 \partial_z \Theta) - e_0^2 R^2 A^2 \sin 2\Theta \right] = R \sin 2\Theta \left[\lambda^2 R - \mu_0 \frac{1}{r} \partial_r (rA) \right] \quad (4)$$

$$\frac{1}{4\pi} \left[\frac{1}{r} \partial_r (r \partial_r A) + \partial_z^2 A - \frac{A}{r^2} \right] = 16I e_0^2 R^2 A \sin^2 \Theta + 8\mu_0 \partial_r (R \sin^2 \Theta) \quad (5)$$

Let us now search for solutions to the equations (3), (4), (5) in the domain $z \rightarrow \infty$, where $\Theta \rightarrow 0$, $R = 1/4 + \zeta$, $A = B_0 r/2 + \alpha$, $\zeta \rightarrow$

$A_\phi = A$, with the intensity of the magnetic field being $B_z = \partial_r (rA)/r$, $B_r = -\partial_z A$ and the natural boundary condition at infinity being imposed: $A(z \rightarrow \infty) = B_0 r/2$. The model in question admits the evident symmetry $\psi_1 \Leftrightarrow \psi_2$, γ_0 -invariance $\Psi \Rightarrow \gamma_0 \Psi$, that permits to introduce 2-spinor φ by putting $\psi_1 = \psi_2 = \text{col}(\varphi, \varphi)$, $\varphi = \text{col}(v, u)$.

RESULTS

Considering the smallness of the radial magnetic field we assumed that: $B_r \ll B_z$. In this approximation the new discrete symmetry holds: $\varphi \Rightarrow -\sigma_3 \varphi$, $v \Rightarrow -v$, $u \Rightarrow u^*$, $a_{2,3} \Rightarrow -a_{2,3}$, that permits to introduce the chiral angle Θ : $a_0 = \cos \Theta$, $a_1 = \sin \Theta$ and consider the axially-symmetric configuration: $u = u(r, z)$, $\Theta = \Theta(r, z)$. As a result, the new Lagrangian density takes the form:

The equations of motion corresponding to (2), become

$0, \alpha \rightarrow 0$. Thus, the equation (4) takes the form:

$$I \left[\frac{1}{r} \partial_r (r \partial_r \Theta) + \partial_z^2 \Theta - \frac{1}{4} e_0^2 B_0^2 r^2 \Theta \right] = \Theta [\lambda^2 - 4\mu_0 B_0] \quad (6)$$

and its solution can be found by separation of variables:

$$\Theta = \Theta_0 \exp(-vr^2 - \kappa z), \Theta_0 = \text{const},$$

with the following constant parameters:

$$v = \frac{e_0 B_0}{4}, \kappa^2 = \frac{B_0}{I} (e_0 I - 4\mu_0) + \frac{\lambda^2}{I} \quad (7)$$

Inserting (6) into (3) and (5), one gets the inhomogeneous equations for ζ and α :

$$\frac{1}{r} \partial_r (r \partial_r \zeta) + \partial_z^2 \zeta = (\partial_\perp \theta)^2 + \left[\frac{1}{4} e_0^2 B_0^2 r^2 + \frac{1}{I} [\lambda^2 - 4\mu_0 B_0] \right] \theta^2 \quad (8)$$

$$\frac{1}{r} \partial_r (r \partial_r \alpha) + \partial_z^2 \alpha - \frac{\alpha}{r^2} = 2\pi e_0 B_0 (e_0 I - 4\mu_0) r \theta^2 \equiv \delta r \theta^2 \quad (9)$$

with the solution of the form:

$$\zeta = \theta_0^2 \exp(-2vr^2 - 2\kappa z) N(r); \alpha = \delta \theta_0^2 \exp(-2vr^2 - 2\kappa z) K(r) \quad (10)$$

where the radial function $N(r)$ and $K(r)$ satisfy the following equations:

$$N'' + N' \left[\frac{1}{r} - 8vr \right] + N \left[2B_0 \left(e_0 - 8\frac{\mu_0}{I} \right) + 4\frac{\lambda^2}{I} + e_0^2 B_0^2 r^2 \right] = \quad (11)$$

$$\frac{1}{2} e_0^2 B_0^2 r^2 + e_0 B_0 + \frac{2}{I} (\lambda^2 - 4\mu_0 B_0)$$

$$K'' + K' \left[\frac{1}{r} - 8vr \right] + K \left[4\kappa^2 - 8v + 16v^2 r^2 - \frac{1}{r^2} \right] = r \quad (12)$$

The magnetic intensity was estimated to be:

$$B_z = B_0 + b_z, b_z = \frac{1}{r} \partial_r (r\alpha), B_r = b_r = -\partial_z \alpha$$

Taking into account from (12) at $r \rightarrow \infty$, $K \approx (e_0^2 B_0^2 r)^{-1}$ one gets from (10) $b_z = -2\pi(e_0 I - 4\mu_0)\theta_0^2 \exp(-2vr^2 - 2\kappa z)$ (13)

$$b_r = \frac{4\pi\kappa}{e_0 B_0 r} (e_0 I - 4\mu_0)\theta_0^2 \exp(-2vr^2 - 2\kappa z) \quad (14)$$

DISCUSSION

In the phenomenological approach to the study of condensed system such as graphene The spin and quasi-spin excitations of graphene layer and the interaction with electromagnetic field is realized though the extension of the derivative and The model in question admits the evident symmetry $\psi_1 \Leftrightarrow \psi_2$, γ_0 - invariance and $\Psi \Rightarrow \gamma_0 \Psi$, that permits us to introduce 2-spinor φ , chiral field and the magnetic field by putting $\psi_1 = \psi_2 = \text{col}(\varphi, \varphi)$, $\varphi = \text{col}(v, u)$.

From equations (13) and (14) our result predicts the diamagnetic or paramagnetic behavior. It means that the parameter $e_0 I - 4\mu_0$ is positive and the weakening of the

magnetic field inside the graphene is predicted in accordance with equations (13) and (14). With the promising results obtained, graphene can become an ideal material for spintronics and other optoelectronic devices. Therefore, it would be interesting in the future to obtain numerical estimates for the parameters of the model.

CONCLUSION

The s- and p- hybridization effect for the valence electrons of carbon atoms appear to the main property of the electron bonding in mono-atomic carbon layers of graphene. From the results obtained in equations (13) and (14) according to the sign of the

multiplier our graphene material reveals diamagnetic or paramagnetic behavior. In view of definitions adopted one has, $e_0 = \frac{e}{\hbar c}$, $\mu_0 = \frac{e\hbar}{2m_e c a^3}$, $I = \frac{E_{exch}}{a}$, where the exchange energy is usually adopted as $E_{exch} = 2,9eV$ and the lattice spacing as $a = 3,56.10^{-8} cm$, with e being the absolute value of the electron charge. Finally the following numerical values were obtained: $e_0 I = 2.10^3 Gauss$, $\mu_0 = 2.10^2 Gauss$.

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