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Chiral Model of Graphene

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The chiral model of graphene based on the $SU(2)$ order parameter is suggested in the long-wave approximation, the ideal graphene plane being determined by the kink-like solution. Corrugation of the graphene surface is described in the form of ripple and rings. The approximate solution corresponding to an infinite carbon nanotube is found.

Key words and phrases: graphene, order parameter, C-nanotube, chiral model.

1. Introduction. Structure of the Model

Since the very discovery of mono-atomic carbon layers called graphenes this material attracted deep interest of researchers due to its extraordinary properties concerning magnetism and high electric conductivity. The concept behind this research is the following. As is well known, the carbon atom possesses of four valence electrons in the so-called hybridized *sp*-states, the one of them being "free" in graphene lattice and all others forming *sp*-bonds with the neighbours.

It appears natural to introduce scalar a_0 and 3-vector $\mathbf{a}$ 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, the long-wave approximation being adopted, i. e.

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

where τ_0 is the unit 2×2-matrix and τ are the three Pauli matrices, with the $SU(2)$-condition

$$a_0^2 + \mathbf{a}^2 = 1 \tag{2}$$

being imposed. It is convenient to construct via the differentiation of the chiral field (1) the so-called left chiral current

$$l_\mu = U^+\partial_\mu U, \tag{3}$$

the index μ running $0, 1, 2, 3$ and denoting the derivatives with respect to the time $x^0 = ct$ and the space coordinates x^i, $i = 1, 2, 3$. Then the simplest Lagrangian density will be given by

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

and corresponds to the sigma-model approach in the field theory with the mass term. Here the constant model parameters I and λ were introduced. Comparing the Lagrangian density (4) with that of the Landau—Lifshits theory corresponding to the quasiclassical long-wave approximation to the Heisenberg magnetic model [1–4], one can interpret the parameter I in (4) as the exchange energy between the atoms (per spacing).

Inserting (1) into (3) and (4) and taking into account the condition (2), one easily finds the following Lagrangian density:

$$\mathcal{L} = \frac{1}{2}I\,(\partial_\mu a_0\,\partial^\mu a_0 + \partial_\mu\mathbf{a}\cdot\partial^\mu\mathbf{a}) - \frac{1}{2}\lambda^2\mathbf{a}^2. \tag{5}$$

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For the case of small **a**-excitations the equations of motion generated by (5) read as

$$\Box\,\mathbf{a} - (\lambda^2/I)\mathbf{a} = 0$$

and correspond to the dispersion law

$$\omega = k_0 c, \quad k_0^2 = \mathbf{k}^2 + \lambda^2/I,$$

which in the high-frequency approximation has the linear photon-like form.

First we begin with the static $1D$ configuration corresponding to the ideal graphene plane, the normal being oriented along the z-axis. In this case the order parameter has the form

$$U = \exp(\imath\psi\tau_3), \quad \psi = \psi(z),$$

with the Lagrangian density being

$$\mathcal{L} = -\frac{1}{2} I\psi'^2 - \frac{1}{2}\lambda^2 \sin^2\psi. \tag{6}$$

The Lagrangian (6) yields the equations of motion

$$2I\psi'' - \lambda^2 \sin 2\psi = 0. \tag{7}$$

The solution to (7) satisfying the natural boundary conditions

$$\psi(-\infty) = 0, \quad \psi(+\infty) = \pi$$

has the well-known kink-like form

$$\psi_0(z) = 2\arctan\,\exp(z/\ell) \tag{8}$$

with the characteristic thickness (length parameter)

$$\ell = \sqrt{I}/\lambda \tag{9}$$

and the energy per unit area

$$E = \frac{1}{2}\int \mathrm{d}z\,\left(I\psi_0'^2 + \lambda^2 \sin^2\,\psi_0\right) = 2\lambda\sqrt{I}.$$

2. Ripple on graphene surface

Let us now consider small static perturbations to the solution (8) in the vicinity of the ideal graphene plane, i. e. for small z. Since $\psi_0(0) = \pi/2$, one finds for the perturbations $\xi = \delta a_3$ and $a_+ = a_1 + \imath\, a_2$ the following equations:

$$\triangle\xi = 0, \quad (\triangle - \ell^{-2})a_+ = 0. \tag{10}$$

The Descartes coordinates x, y being the coordinates of the ideal graphene plane $z = 0$, one easily finds the excitations of the periodic form:

$$\xi = \xi_0 e^{kz}\cos\,kx, \quad a_+ = A_+\, e^{\bar{k}z}\cos\,Kx, \quad K^2 = \bar{k}^2 - \lambda^2/I, \tag{11}$$

where $\bar{k}\ell > 1$. The exponential increasing in z of the solution (11) signifies the instability of the ideal graphene plane first mentioned by N.D. Mermin and H. Wagner in 1966 for the case of magnetics.

There exist also the ring excitations of the axially-symmetric form:

$$\xi = \xi_0 e^{kz}\, J_0(k\rho), \quad a_+ = A_+\, e^{\imath m\varphi} e^{\bar{k}z}\, J_m(K\rho), \tag{12}$$

where J_m is the Bessel function of the m-th order, $m = 0, 1, 2, \ldots$, and ρ, φ are the polar coordinates in the graphene plane. Thus, one concludes that the graphene plane has the tendency of bending. The corrugation of the graphene plane was observed experimentally [5–7].

In view of (10) it should also be underlined that the dispersion curve reveals the anisotropic character and has the two branches. The first one concerns the transverse a_3-perturbations and has the photon-like behaviour. The second one concerns the longitudinal a_1- and a_2-perturbations and has the "massive" behaviour mentioned above.

3. C-nanotubes

Let us now search for the static axially-symmetric configuration of the form

$$U = \exp(\imath\psi\sigma), \tag{13}$$

where

$$\psi = \psi(\rho), \quad \sigma = \tau_1 \cos\,\varphi + \tau_2 \sin\,\varphi, \quad \varphi = n\varphi, \quad n = 1, 2, \ldots.$$

The configuration (13) describes the infinite C-nanotube with the hedgehog structure in the transverse section. Substituting (13) into (4), one gets

$$\mathcal{L} = -\frac{1}{2} I \left(\psi'^2 + \frac{n^2}{\rho^2} \sin^2\,\psi \right) - \frac{1}{2}\lambda^2 \sin^2\,\psi. \tag{14}$$

The corresponding equations of motion for the chiral angle $\psi(\rho)$ read

$$2\,\rho(\rho\psi')' = (n^2 + \rho^2/\ell^2)\,\sin 2\,\psi. \tag{15}$$

After changing the variable $\eta = \log(\rho/\ell)$ one finds in the limit $n \gg \rho/\ell$ the solution to the equation (15) of the kink-like type:

$$\psi(\eta) = 2\arctan[\exp(n\eta_0 - n\eta)] \tag{16}$$

satisfying the boundary conditions

$$\psi(+\infty) = 0, \quad \psi(-\infty) = \pi,$$

where the parameter $R = \ell \exp\eta_0$ plays the role of the tube radius. Inserting (16) into (14), it is possible to calculate the energy of the C-nanotube per unit length:

$$E = 2\pi I n^2 \int \mathrm{d}\eta\, \sin^2\,\psi = 4\pi I n. \tag{17}$$

It is worthwhile to remark that the integer number n in (17) is the so-called topological charge of the degree type (the winding number)

$$Q = \frac{1}{4\pi} \int\limits_{S^2} \mathrm{d}\varphi \mathrm{d}\psi\, \sin\,\psi = n. \tag{18}$$

As follows from (17) and (18), the energy of the tube per unit length is proportional to the topological charge $Q = n$.

4. Discussion

The proposed chiral model of the graphene permits one to describe the ripple structure of the real graphene surface illustrating the Mermin–Wagner instability of the $2D$ configurations. It also contains very simple graphene and tube solutions, the latter one confirming the existence of carbon nanotubes. In future it is desirable to include in the model the interaction with the electromagnetic field for the description of conductivity and magnetic properties.

References

1. *Kosevich A. M., Ivanov B. A., Kovalev A. S.* Nonlinear Magnetization Waves. Dynamical and Topological Solitons. — Kiev: Naukova Dumka, 1988. — 190 p.
2. *Rybakov Yu. P., Jimenez R. Ochoa.* Topological Excitations in Non-Heisenberg Ferromagnetic with Biquadratic Spin Exchange Interaction // Applied Nonlinear Dynamics. — 2001. — Vol. 9, No 4/5. — Pp. 155–161.
3. *Izyumov Yu. A., Katsnelson M. I., Skryabin Yu. N.* Itinerant Electron Magnetism. — M.: Nauka, 1994. — 368 p.
4. *Tyablikov S. V.* Methods of Quantum Theory of Magnetism. — M.: Nauka, 1975. — 528 p.
5. *Fasolino A., Los J. H., Katsnelson M. I.* Intrinsic Ripples in Graphene // Nature Materials. — 2007. — Vol. 6. — Pp. 858–861.
6. Controlled Ripple Texturing of Suspended Graphene and Ultra Thin Graphite Membranes / W. Bao, F. Miao, Z. Chen et al. // Nature Nanotechnology. — 2009. — Vol. 4. — Pp. 562–566.
7. The Structure of Suspended Graphene Sheets / J. C. Meyer, A. K. Geim, M. I. Katsnelson et al. // Nature. — 2007. — Vol. 446. — Pp. 60–63.

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Киральная модель графена

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В длинноволновом приближении предложена киральная модель графена, построенная на основе матричного параметра порядка из группы $SU(2)$. При этом идеальная графеновая плоскость определяется кинковым решением. Описывается возмущение графеновой поверхности в виде ряби и колец. Находится приближённое решение, соответствующее бесконечной углеродной нанотрубке.

Ключевые слова: графен, параметр порядка, C-нанотрубка, киральная модель.