Fullerenes as solitons in chiral model of graphene

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Abstract. Taking into account the \( sp^2 \)-hybridization effect for valence electrons in carbon atoms, we introduce a unitary matrix \( U \) as an order parameter and suggest a scalar chiral model of graphene for the description of graphene-like configurations. Using the well-known hedgehog ansatz for modeling Fullerene \( C_{60} \), we estimate the polarizability of a single Fullerene specie in a uniform external electric field. Finally, we use this result for calculating the parameters of the van der Waals potential for the two interacting Fullerene species.

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 electric 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]. In the first paper [8] the simplest scalar chiral model of graphene excitations was considered, spin and magnetic excitations being studied in [9].

The objective of the current study was to show the applicability of the scalar chiral model for the description of electromagnetic properties of Fullerene configurations. In particular, we calculated the electric polarizability of a single Fullerene specie and also estimated the parameters of the interaction potential for the two Fullerene species at large distance between them.

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 \( sp^2 \)-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:

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

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

\[
a_0^2 + \vec{a}^2 = 1
\]

being imposed. It is convenient to construct, via differentiating the chiral field \( U \), the so-called left chiral current

\[
I_\mu = U^+ \partial_\mu U, \quad \mu = 0, 1, 2, 3,
\]
the index \( \mu \) denoting the derivatives with respect to the time \( x^0 = ct \) and the space coordinates \( x^i, \ i = 1, 2, 3 \). The Lagrangian density reads

\[
L = -\frac{I}{4} \text{tr} (l^\mu l^\mu) - \frac{\lambda^2}{2} \vec{a}^2
\]

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

\[
U = \exp (i \tau_1 \Theta), \quad \Theta = \Theta(z),
\]

(5)

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

\[
\Theta(z) = 2 \arctan \exp (-z/\ell),
\]

where the characteristic length appears:

\[
\ell = \frac{\sqrt{I}}{\lambda}.
\]

(6)

The model (4) admits also the two-dimensional hedgehog configuration [10]

\[
U = \exp (i \sigma \Theta), \quad \Theta = \Theta(\rho),
\]

(7)

where

\[
\sigma = (\tau_1 x + \tau_2 y)/\rho, \quad \rho^2 = x^2 + y^2.
\]

The configuration (7) corresponds to the infinite carbon nano-tube oriented along the \( z \)–axis. In the sequel we consider the three-dimensional hedgehog configurations describing Fullerene species.

### 2 Materials and Methods

As a material we consider Fullerene species described by spherically-symmetric soliton-like configurations. For approximating these configurations we use trial functions found via the variational method.

#### 2.1 Fullerene configurations

It is worth-while to stress that three-dimensional configurations should meet the scale-invariance Hobart – Derrick requirements [11, 12]. To this end, the Lagrangian density (4) should be modified through including the Skyrme – Faddeev term [13, 14]:

\[
L = -\frac{I}{4} \text{tr} (l^\mu l^\mu) - \frac{\lambda^2}{2} \vec{a}^2 + \frac{\varepsilon^2}{16} (l^\mu l^\nu [l^\mu l^\nu]),
\]

(8)
with \( \varepsilon \) being some new dimensionless coupling constant. For the description of \( C_{60} \) Fullerenes we suggest to use the well-known hedgehog ansatz

\[
U = \exp[i \tau \Theta(r)], \quad \tau = (\vec{\tau} \vec{n}), \quad \vec{n} = \vec{r} / r,
\]

(9)
corresponding to the nucleon structure in the Skyrme model [13], where the baryon charge was identified with the unit topological invariant of the degree type:

\[
Q = \text{deg} (S^3 \to S^3) = 1, \quad \Theta(0) = \pi, \quad \Theta(\infty) = 0.
\]

(10)

Inserting (9) into (3), one finds the space components of the left chiral current:

\[
l_j = i \frac{\tau_j}{r} \Theta' + i \frac{r}{2r} \sin 2\Theta \left( \frac{\tau_j}{r} \right) + i \sin^2 \Theta \frac{\tau_k}{r^2} \delta_{kj} \tau_l,
\]

(11)

Using (11), one can reduce the Lagrangian density (8) to the following form:

\[
L = \frac{-I}{2} \left( \Theta'^2 + \frac{2}{r^2} \sin^2 \Theta \right) - \frac{\Lambda^2}{2} \sin^2 \Theta - \varepsilon^2 \frac{\sin^2 \Theta}{r^2} \left( \frac{\sin^2 \Theta}{r^2} + 2\Theta'^2 \right).
\]

(12)

The configuration with the unit topological charge satisfying boundary conditions (10), can be approximated by the trial function

\[
\tan (\Theta/2) = \exp \left(-\eta - k (1 + e^\eta)\right), \quad \eta = \ln (r/r_0), \quad k = r_0 / \ell .
\]

(13)

Identifying this configuration with that of \( C_{60} \) Fullerene [15], one finds \( r_0 = 3.55 \) Å.

3 Results

3.1 Electromagnetic properties of Fullerenes

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

\[
U' = VUV^{-1}, \quad V = \exp(i \gamma \tau_3), \quad A'_\mu = A_\mu + \partial_\mu \Lambda, \quad L'_\mu = VL_\mu V^{-1},
\]

(14)

combined with extending the derivative:

\[
D_\mu U = \partial_\mu U - i e_0 A_\mu [\Gamma_\gamma, U], \quad L_\mu = U^+ D_\mu U,
\]

(15)

where \( e_0 \) and \( \Gamma_\gamma \) stand for the electromagnetic coupling constant and the charge operator respectively. Finally, the gauge invariance holds, if \( \Gamma_\gamma = \tau_3, \quad \gamma = e_0 \Lambda \).

Let us now estimate the electric polarizability \( \alpha \) of a single Fullerene specie in a uniform electric field with the intensity \( E_0 \). In the simplest dipole approximation one can put:
\[ A_0 = -E_0 r \cos \vartheta + \frac{p_0 r \cos \vartheta}{r^3 + r_0^3}, \]  

(16)

where \( p_0 = \alpha E_0 \) is the induced dipole moment of the Fullerene specie and the spherical coordinates \( r, \vartheta \) are used. Exploiting (16), one can calculate the part of the electromagnetic energy depending on \( p_0 \):

\[ W_{em} = -\frac{p_0}{3} E_0 + \frac{p_0^2}{3r_0^3}. \]  

(17)

Minimizing (17) with respect to \( p_0 \), one easily obtains

\[ p_0 = \frac{1}{2} r_0^3 E_0 = \alpha E_0, \quad \alpha = \frac{1}{2} r_0^3. \]  

(18)

### 3.2 Interaction of two Fullerene species

Let us now consider the two Fullerene species with the centers \( O_1, O_2, \ O_1O_2 = R \), where \( R \gg r_0 \). Our goal will be the calculation of the induced dipole moments and the van der Waals interaction potential. In this case one can put in the first approximation

\[ U = U_1 U_2, \quad U_j = \cos \Theta_j + i \sin \Theta_j (\tilde{r} \cdot \tilde{R}_j) / R_j, \quad \Theta_j = \Theta(R_j), \]  

(19)

where \( \tilde{R}_1 = \tilde{r} + \tilde{e} R_j / 2 \), \( \tilde{R}_2 = \tilde{r} - \tilde{e} R_j / 2 \) and \( \Theta(R_j) \) corresponds to (13). In the static case the electromagnetic part of the Lagrangian reads:

\[ L_{em} = -\frac{I}{4} tr L_0^2 + \frac{1}{8 \pi} (\nabla A_0)^2 - j_0 A_0 - \frac{\nu_0}{4} A_0^2, \]  

(20)

where

\[ j_0 = \frac{1}{4 \pi} \text{div} (\tilde{E}_1 + \tilde{E}_2) \]

and the nonlinear term of the Mie type is added, with \( \nu_0 \) being some new coupling constant. Inserting (19) into (15), one gets

\[ -\frac{1}{2} tr \rho^2 = e_0^2 A_0^2 \rho \left[ 1 - (U_1^+ \tau_2 \tau_3 U_1)(U_2^+ \tau_3 \tau_5 U_2^+) \right] \approx e_0^2 A_0^2 \rho^2 \left( \frac{\sin^2 \Theta_1}{R_1^2} + \frac{\sin^2 \Theta_2}{R_2^2} \right). \]  

(21)

Let us estimate the electromagnetic energy \( W_{em} \) of the system. To this end, we use the dipole deformation of the Fullerene species:

\[ A_0 = p \frac{(z + R/2)R_1^3}{(R_1^2 + r_0^2)^3} + p \frac{(z - R/2)R_2^3}{(R_2^2 + r_0^2)^3} = A_0^{(1)} + A_0^{(2)}. \]  

(22)
It should be underlined that the proper electrostatic part of $W_{\text{em}}$ is small due to the Maxwell equations and therefore

$$W_{\text{em}} = 2\pi \int_{0}^{\infty} \rho \, d\rho \int_{-\infty}^{\infty} dz L_{\text{em}} \approx W_{1} + W_{2}, \quad (23)$$

where the following main contributions are separated:

$$W_{1} = 8\pi I_{e}\int \rho \, d\rho \int \left[\frac{e^{2}}{\rho^{2}} \sin^{2} \Theta_{1} R_{1} \right] \rho^{2} \, d\rho \, dz \left(\frac{1}{\rho} \right)^{2}, \quad W_{2} = -\pi v_{0} \int \rho \, d\rho \, dz \, e_{0}^{2} \left(\frac{1}{\rho} \right)^{4}. \quad (24)$$

Inserting (22) into (24), one finds

$$W_{1} + W_{2} \approx \frac{\pi p^{2} I_{e}^{2}}{15(1+k)r_{0}} - 0.17 \frac{\pi v_{0} \rho^{4}}{r_{0}^{3}}. \quad (25)$$

Minimizing the energy (25) with respect to $p^{2}$, one gets

$$p^{2} \approx \frac{I_{e}^{2} \rho^{4}}{5v_{0}(1+k)}. \quad (26)$$

Now we are in a position to estimate the interaction potential between the two Fullerene species. To this end, in view of (18), we can calculate the interaction force between two effective dipoles:

$$\vec{F}_{12} = (\hat{\rho}_{1} \nabla_{2}) \vec{E}_{2} \approx \rho_{0}^{3} (\vec{E}_{2} \nabla_{2}) \vec{E}_{2} / 2 = -\nabla_{2} V, \quad (27)$$

where the potential $V$ coincides with that of van der Waals:

$$V = -\frac{r_{0}^{3}}{4} E_{2}^{2} = -\frac{r_{0}^{3} p^{2}}{R^{6}}. \quad (28)$$

Here it was taken into account that

$$E_{2} = E_{z} = \frac{2p}{R^{3}}.$$  

Finally, inserting (26) into (28), one finds

$$V = -\frac{I_{e}^{2} \rho_{0}^{7}}{5v_{0}(1+k)R^{6}}. \quad (29)$$

Identifying the potential (29) with that of Girifalco [16, 17, 18, 19]:

$$V = -\frac{\sigma}{R^{6}}, \quad \sigma = 2^{9} \rho_{0}^{6} 7.5 \times 10^{-21} J,$$
one can estimate the value of the constant $\nu_0$:

$$\nu_0 = \frac{Ie_0^2r_0^7}{5(1 + k)\sigma} = 1.7 \times 10^{11} (Jm)^{-1},$$

where it was taken into account that $I = 1.3 nN$, $k = 2.67$, $e_0 = e/(hc)$.

4 Discussion
For the description of Fullerene electromagnetic properties we used the method of consecutive approximations. First, we estimated the electric dipole moment

$$p_0 = \frac{1}{2} r_0^3 E_0 = \alpha E_0$$

induced in a single Fullerene specie under the influence of the external electric field $E_0$. As a result, we found the electric polarizability $\alpha$, which proved to be proportional to the volume of the Fullerene specie. This fact was taken into account for estimating the interaction potential $V$ between the two separated Fullerene species. This potential proved to coincide with that of van der Waals [cf. (27) and (28)].

It is worth-while to stress that this result follows from minimizing the electric energy of the two interacting Fullerene species in supposition that the special nonlinear term of the Mie type was added to the Lagrangian [cf. (20)]. Comparing the form of the interaction potential $V$ with that of Girifalco [16], it was possible to estimate the Mie constant $\nu_0$ in (20).

Conclusions
1. Within the scope of the suggested earlier scalar chiral model of graphene we constructed trial spherically-symmetric Fullerene configurations corresponding to the “hedgehog” ansatz or the Skyrmions in nuclear physics.
2. Using the gauge invariance principle, we included in the model the interaction with the electromagnetic field via extending the derivatives.
3. Using the trial Fullerene configurations, we estimated the electric polarizability of a single Fullerene specie in a uniform electrostatic field.
4. Minimizing the electromagnetic part of the energy for the case of the two Fullerene species at large distance between them, we confirmed the validity of the van der Waals interaction potential.

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