Charge localization around disclinations in monolayer graphite

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Abstract

Using a continuum model, we obtain qualitative results that imply charge localization around negative curvature disclinations (i.e. rings with more than 6 Carbon atoms) in a graphite sheet. Conversely, it is found that positive curvature disclinations repel charge, independent of its sign.
1 Introduction

Although the electronic properties of elastic materials containing topological defects have been widely studied since the early 50’s [1, 2] in the context of deformation potential theory, there has been a recent revival of interest in such problems using both gauge field theory [3, 4, 5] and Riemann-Cartan geometry [6, 7, 8]. In this work we use the latter approach to study the effects of the curvature associated with disclinations in a monolayer of graphite.

Disclinations have a fundamental role in the formation of non-flat low-dimensional carbon structures such as fullerenes and graphene tubules among others. They are responsible for the local curvature that bends those structures into their various shapes. This is easily seen by incorporating disclinations to a graphite sheet. Graphite is the honeycomb-like, flat, two-dimensional carbon network made solely of 6-membered rings. Rings made of a number of carbon atoms other than 6 correspond to disclinations. They are formed, at least conceptually, by a “cut and glue” process characteristic of topological defects [9]. For instance, to create a single 5-membered ring in an infinite graphite sheet cut out a wedge of angle $2\pi/6$ from the center of any hexagon (so that one of the edges of the hexagon is removed) and identify the lose ends. The result is a conical graphitic structure with a pentagonal ring at its (truncated) apex. Conversely, a 7-membered ring may be introduced by inserting a wedge of angle $2\pi/6$, adding an extra edge to one of the hexagons. Here, the result is a saddle-like structure with the heptagonal ring at the center.

The $n$-membered rings, with $n < 6$, are an essential part of the closed, positively curved, fullerenes that are topologically equivalent to spheres [10] and of graphene tubules [11]. The rings with $n > 6$ are indispensable to the open, negatively curved, carbon networks [12]. Toroidal [13] and helical [14] forms of carbon require both.

The electronic states of disclinated monolayer graphite were studied by
Tamura and Tsukada [20] based on the connectivity of the atoms in the network, leaving out the effects of curvature. It is our aim here, to point out some of the curvature effects relevant for their discussion.

2 The self-interaction

In this section we obtain the self-energy and self-force of a point charge in a graphite sheet with a single disclination. We work in the continuum space limit, where Riemannian geometry makes sense. Although a discrete geometrical approach is also possible, along the lines of Regge calculus [15], the properties we want to describe are easier to deduce this way. The “cut and glue” process, in the two-dimensional continuum, produces a disclination which is associated with a point with singular curvature. The interaction of a charged particle with the defect, the deformation potential, results from the non-Euclidean metric of the defected medium and the modified topology which contribute with a self-energy to the charged particle [7]. The corresponding two-dimensional space metric is given by [6]

\[ ds^2 = dr^2 + \frac{r^2}{p^2} d\theta^2, \quad 0 \leq \theta \leq 2\pi, \]  

where \( p \) measures the angular excess or deficit due to the disclination (since the total angle is \( 2\pi/p \) an angular excess or deficit of \( \pm \lambda \) makes \( 2\pi/p = 2\pi\pm\lambda \)). The curvature tensor corresponding to this metric is zero everywhere except at the origin (where the defect is located) where it has a \( \delta \)-function singularity [16]. For \( p > 1 \) the curvature is positive and for \( 0 < p < 1 \) it is negative. \( p = 1 \), zero curvature, corresponds to the absence of the defect.

In Reference [7] we studied a charged particle in a disclinated three-dimensional medium. The self-energy can be visualized as the energy associated with the distortion in the spacial distribution of the field lines of a charge due to the defected background. This is similar to what happens to a
charge near a conducting plane: the field lines are distorted due to the boundary condition on the plane and the charge is subjected to a force (which is minus the gradient of its self-energy due to the distortion). We must be careful here since, although the charge is confined to a two-dimensional surface, its field lines are distributed in three-dimensional space (three-dimensional electrodynamics: the Coulomb potential proportional to the inverse of the distance). So, only the field lines contained in the surface are affected by the defect. In what follows we take as the material medium (i.e. the graphite sheet) the surface $z = 0$ and position the defect at the origin ($r = 0$).

We basically follow the procedure used by Smith [17] in order to compute the self-force on a point charge in a background space of non-trivial topology. It goes as follows: we first solve Poisson’s equation for a single charge in the chosen background in order to find its Green function. The Green function is then renormalized by the extraction of its divergent part, namely the Green function in the absence of the defect. The self-energy is obtained from the coincidence limit of the renormalized Green function. Notice that, because we are dealing with three-dimensional electrodynamics (even though restricted to a two-dimensional surface) we need to work with the three-dimensional Green function.

We start then with Poisson’s equation

$$\nabla^2 G_p(\vec{x}, \vec{x}') = -4\pi \delta^{(3)}(\vec{x} - \vec{x}').$$

(2)

In the defectless medium, $\nabla^2$ is the usual three-dimensional Laplacian operator whereas in the disclinated medium it is given by

$$\nabla^2 = \frac{\partial^2}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{p^2}{r^2} \frac{\partial^2}{\partial \theta^2},$$

(3)

in cylindrical coordinates $z, r, \theta$, with $p \neq 1$ in the surface $z = 0$ and 1 otherwise. That is, for $z \neq 0$ we still have the usual Laplacian but in the disclinated surface ($z = 0$) it is modified by $p$. 

\"\)
Defining
\[ f(z) = 1 - [\Theta(z) + \Theta(-z)], \] (4)
where \( \Theta(z) \) is the Heaviside step function such that \( f(z) = 1 \) if \( z = 0 \) and \( f(z) = 0 \) if \( z \neq 0 \), we write the Green function as a sum of two parts
\[ G_p(\vec{x}, \vec{x}') = f(z)G_p(\vec{x}, \vec{x}') + [1 - f(z)]G_p(\vec{x}, \vec{x}'). \] (5)
The first term corresponds to the Green function in the \( z = 0 \) surface while the second term corresponds to the Green function in the three-dimensional space minus this surface. Since the defect affects only the \( z = 0 \) surface, \( p = 1 \) in the second term.

Now we need to regularize the Green function by subtraction of its defectless counterpart \( G_1 \), i.e.
\[ G_p(\vec{x}, \vec{x}')_{\text{ren}} = G_p(\vec{x}, \vec{x}') - G_1(\vec{x}, \vec{x}') = f(z)[G_p(\vec{x}, \vec{x}') - G_1(\vec{x}, \vec{x}')]. \] (6)
which is the three-dimensional renormalized Green function restricted to the \( z = 0 \) surface. Since the next step is to take the coincidence limit, we can therefore use Smith’s result for the three-dimensional renormalized Green function \[17\]:
\[ G_p(\vec{x}, \vec{x})_{\text{ren}} = \lim_{\vec{x}' \to \vec{x}} [G_p(\vec{x}, \vec{x}') - G_1(\vec{x}, \vec{x}')] = \frac{1}{2\pi} \frac{\kappa(p)}{r}, \] (7)
where the numerical coefficient \( \kappa(p) \) is given (here we use the notation of Reference \[7\] which differs from Reference \[17\] by a factor of \( 2/\pi \))
\[ \kappa(p) = 2 \int_0^\infty \frac{p \coth(px) - \coth(x)}{\sinh(x)}. \] (8)
Since this result is independent of \( z \) it already satisfies the restriction to the \( z = 0 \) surface.

The self-energy of a point charge \( q \) positioned at \( \vec{x} \) is given by \[18\]
\[ U(\vec{x}) = \frac{1}{2} \int [\rho(\vec{x} - \vec{x}')\Phi(\vec{x}')] d^3x'. \] (9)
Table 1: Numerical values for $\kappa(p)$ for selected $n$-membered rings.

| $n$ | $p$   | $\kappa(p)$ |
|-----|-------|-------------|
| 4   | $6/4$ | 1.418       |
| 5   | $6/5$ | 0.5249      |
| 6   | 1     | 0           |
| 7   | $6/7$ | -0.3351     |
| 8   | $6/8$ | -0.5622     |

where

$$\rho(\vec{x} - \vec{x'}) = q\delta^3(\vec{x} - \vec{x'}) = \frac{q}{r}\delta(r - r')\delta(\theta - \theta')\delta(z), \quad (10)$$

and $\Phi(\vec{x'}) = \frac{q}{\epsilon}G(\vec{x}, \vec{x'})$ is the electrostatic potential at $\vec{x'}$ of the charge $q$ located at $\vec{x}$. Here $\epsilon$ is the dielectric constant.

It follows that

$$U(\vec{x}) = \frac{q^2}{2\epsilon}G(\vec{x}, \vec{x'})_{ren} = \frac{q^2}{4\pi\epsilon}\frac{\kappa(p)}{r} \quad (11)$$

and

$$\vec{F}(\vec{x}) = -\nabla U(\vec{x}) = -\frac{\kappa(p)q^2}{4\pi\epsilon r^2}. \quad (12)$$

It is interesting to notice here that this result is identical to the one of a point charge in the presence of a line disclination in three-dimensional medium. In other words, the problem of a point charge embedded in a two-dimensional surface with a point defect is the same as the charge in a three-dimensional medium with a line defect (except for the translational invariance along the $z$ direction).

Notice that $\kappa(1) = 0$, meaning that the self-energy and self-force vanish in the absence of the defect. As mentioned in the Introduction, a five-membered Carbon ring corresponds to a disclination of deficit angle $2\pi/6$, whereas a 7-membered ring corresponds to an excess angle of the same value, and so on. In Table 1 we list numerical values of $\kappa(p)$ for the different rings relevant
to graphite. It is clear that for \( p < 1 \) the coefficient \( \kappa(p) < 0 \) implying an attractive self-force; i.e., charge of any sign will be attracted by rings with less than 6 Carbon atoms. For \( p > 1 \), we have that \( \kappa(p) < 0 \) meaning that rings with more than 6 Carbon atoms repel charge.

### 3 Localization

We study here the case \( p < 1 \) which corresponds to a classical attractive self-force and which leads to quantum bound states. It was shown in the previous section that we have the same situation of a charge in a three-dimensional medium with a line defect except that the translational invariance along the \( z \) direction is broken. This enables us to use our previous results on the binding of charged particles to line disclinations. The two-dimensional Hamiltonian for a quasiparticle of charge \( q = \pm e \) and effective mass \( m^* \), moving in the strain field of a \( p < 1 \) disclination is obtained from the Laplacian, Equation (3), and the self-energy, Equation (11):

\[
-\frac{\hbar^2}{2m^*}[\frac{1}{r} \frac{\partial}{\partial r}(r \frac{\partial}{\partial r}) + \frac{p^2}{r^2} \frac{\partial^2}{\partial \theta^2}] - \frac{e^2}{4\pi\varepsilon} \frac{|\kappa(p)|}{r}
\]

with \( 0 < p < 1 \).

Schrödinger’s equation for this Hamiltonian is easily solvable. Writing the wavefunction as \( R(r) e^{il\theta} \), where \( l \) is an integer, the remaining radial equation,

\[
r^2 R'' + r R' - (p^2 l^2 + \gamma r + \beta r^2) R = 0,
\]

where \( \beta^2 = -2m^*E/\hbar^2 \), \( \gamma = -(m^*e^2/2\pi\varepsilon\hbar^2)|\kappa(p)| \) and \( E \) is the energy, is a special case of the hypergeometric equation. We find then the spacially localized eigenfunctions

\[
R_{n,l} = C_{n,l} e^{-\beta r} (\beta r)^{|l|/\alpha} \, _1F_1(-n, 2p|l| + 1, \beta r),
\]

and the eigenenergies

\[
E = -\frac{m^*e^4 \kappa^2(p)}{32\pi^2\hbar^2\varepsilon^2} \frac{1}{(n + \frac{1}{2} + p|l|)^2},
\]
where $C_{n,l}$ is a normalization constant, $\text{}_1F_1$ is the confluent hypergeometric function, $n = 0, 1, 2, \ldots$ and $l = 0, \pm 1, \pm 2, \ldots$.

## 4 Concluding remarks

In this work we obtained qualitative data on the dynamics of point charges near disclinations in a graphite sheet in a continuum model. We found that disclinations corresponding to rings with more than 6 Carbon atoms function as attractors to point charges. On the other hand, disclinations corresponding to rings with fewer than 6 Carbon atoms will repel the point charges. This is in sharp contrast with the topological analysis done by Tamura and Tsukada [20] who found that the five-membered ring is attractive and the seven-membered ring is repulsive to electrons. In their work they take into account only how atoms are connected to each other, and the effect of the curvature of the surface is not considered. In the approach of the present work we do the opposite, we are concerned exclusively with the curvature effect, not taking into account the connectivity. It is clear that some kind of interpolation between the two approaches is needed. Although our results are qualitative, and therefore not suitable for a numeric comparison, they strongly point out the importance of taking the curvature effects into account in calculations of the electronic structure of graphite sheets with disclinations.

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**References**

[1] J. Bardeen and W. Shockley, Phys. Rev. 80, 72 (1950).
[2] R. Landauer, Phys. Rev. 82, 520 (1951).

[3] H. Teichler, Phys. Lett. A 87, 113 (1981).

[4] V. A. Osipov and S. E. Krasavin, J. Phys. C 7, L95 (1995).

[5] Y. T. Rebane, Phys. Rev. B 52, 1590 (1995).

[6] M. O. Katanaev and I. V. Volovich, Ann. Phys. (N.Y.) 216, 1 (1992).

[7] Claudio Furtado and Fernando Moraes, Phys. Lett. A 188, 394 (1994).

[8] C. Furtado, B. G. C. da Cunha, F. Moraes, E. R. Bezerra de Mello and V. B. Bezerra, Phys. Lett. A 195, 90 (1994).

[9] W. F. Harris, Scient. Amer. 237(6), 130 (1977).

[10] D. Ugarte, Nature (London) 359, 707 (1992).

[11] M. Fujita, R. Saito, M. S. Dresselhaus, and G. Dresselhaus, Phys. Rev. B 45, 13834 (1992).

[12] Mitsutaka Fujita and Takahide Umeda, Phys. Rev. B 51, 13778 (1995).

[13] J. K. Johnson et al., Phys. Rev. B 50, 17575 (1994).

[14] B. I. Dunlap, Phys. Rev. B 50, 8134 (1994).

[15] C. W. Misner, K. S. Thorne and J. A. Wheeler, Gravitation (Freeman, San Francisco, 1973).

[16] D.D. Sokolov and A.A. Starobinskii, Sov. Phys. Dokl. 22, 312 (1977).

[17] A. G. Smith, in: The formation and evolution of cosmic strings, eds. G. W. Gibbons, S. W. Hawking and T. Vachaspati (Cambridge Univ. Press, Cambridge, 1990) pp. 263-292.
[18] J. D. Jackson, Classical Electrodynamics (John Wiley, New York, 1975).

[19] James B. Seaborn, Hypergeometric Functions and their applications (Springer-Verlag, New York 1991).

[20] Ryo Tamura and Masaru Tsukada, Phys. Rev. B 49, 7697 (1994).