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Dirac fermions on a disclinated flexible surface

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A self-consisting gauge-theory approach to describe Dirac fermions on flexible surfaces with a disclination is formulated. The elastic surfaces are considered as embeddings into R^3 and a disclination is incorporated through a topologically nontrivial gauge field of the local $SO(3)$ group which generates the metric with conical singularity. A smoothing of the conical singularity on flexible surfaces is naturally accounted for by regarding the upper half of two-sheet hyperboloid as an elasticity-induced embedding. The availability of the zero-mode solution to the Dirac equation is analyzed.

I. Introduction. Is is now generally accepted that the low-lying electronic states in graphene can be accurately described by two-dimensional massless Dirac fermions [1]. In experiment, multiform graphene structures were observed thus stimulating studies of Dirac fermions on curved graphene sheets (see, e.g., [2, 3]). This problem is markedly complicated when the curvature itself is generated by topological defects like disclinations. Indeed, a disclination is known in elasticity theory as a line defect which can be produced by "cut and glue" Volterra process, namely, by inserting or removing a wedge of material with the following gluing of the dihedral sides. This immediately generates additional large elastic strains inside the crystal. For flexible membranes, however, there is a chance to screen out the strain field by buckling into a cone. The problem thus reduces to coupling Dirac spinors to a topologically nontrivial curved background.

According to Volterra process disclination can be considered as a conical singularity like strings in cosmology. The relevant background is the curved spacetime where all the curvature is concentrated at the apex of the cone. The metric of this 2D space in polar coordinates is written as

$$ds^2 = dr^2 + \alpha^2 r^2 d\varphi^2. \tag{1}$$

Here the parameter α is related to the angular sector that is removed or inserted to form the defect. In this case, any attempt to build a closed loop around the disclination line will result in a closure failure. The deficit angle is equal to $2\pi\alpha$ with $\alpha = 1 - \nu$ where ν is the Frank index, the basic topological characteristic of the disclination. The positive sign of ν corresponds to the removing of a sector. In this case the space has positive curvature. Correspondingly, for negative ν one has a cone of negative curvature. Eventually, the problem reduces to a Dirac equation in the curved spacetime.

In spite of the elegant form of this approach, there is yet an important open question concerning the so-called core region of the defect. To the best of our knowledge, for the first time this problem was raised in cosmological models [4, 5] where long-range effects of cosmic string cores were studied. In geometric theory of defects, an influence of a disclination core on the localization of electrons and holes was investigated in [6]. In both cases, the tip of the conical singularity is replaced by a smooth cap while at large distances a typical cone with the deficit angle $2\pi\alpha$ emerges. In cosmological models the curvature of an infinite strait string is confined within a cylinder of a small radius a (the core radius) that possesses a direct physical meaning: it characterizes the interior structure of the string. Accordingly, the relevant metric can be taken in the form

$$ds^2 = dt^2 + dz^2 + P^2(r/a)dr^2 + r^2 d\varphi^2, \tag{2}$$

where the range of the angular coordinate is $\varphi \in [0, 2\pi\alpha)$ and $P(r/a)$ is a smooth monotonic function satisfying the conditions

$$\lim_{r/a\to 0} P(r/a) = \nu, \qquad P(r/a) = 1, \quad r > a. \tag{3}$$

For example, in [6] the so-called flower-pot model was considered when the curvature of the disclinated media is concentrated on a ring of radius a, which results in the formation of a "seam" on the cylinder.

It should be stressed that this approach is of interest in the description of linear defects with a certain interior structure (finite thickness of a string). However, the situation changes drastically for a disclination on an elastic 2D surface. First of all, in this case there is no parameter (similar to a) that fixes a relevant short-range length scale: a disclination is a point defect. Second, the specificity of 2D elastic surfaces lies in that they may change

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both their intrinsic and extrinsic geometries. For example, the creation of a disclination in a nonstretchable membrane by using the "cut and glue" process will result in a true cone. In reality, however, the membranes are flexible and the cone apex will be smoothed due to finite elasticity. Elastic deformations are by definition smooth deformations. A cone cannot be smoothly evolved into a desired surface with a smoothed apex simply because of the fact that a cone is not a manifold. If one ignores this and just try to formally carry over the P-type smearing procedure used for strings to elastisity theory, one will inevitably run into a problem of fixing boundary conditions at $r = a$. In the present case those conditions are purely artificial and possess no direct physical meaning (see also discussion in [7]). In other words, it is not a straightforward matter to incorporate self-consistently the information about the core region within the geometrical approach in 2D elastic theory with defects.

In this paper, we attempt to develop a variant of the self-consistent gauge-theory approach to take into account both the smoothed apex and the topological characteristic of the defect. Actually, a part of our program was already realized in [8]. The model developed there allows us to describe disclinations on arbitrary elastic surfaces. It includes Riemannian surfaces that may change their geometry under deformations. The local gauge field to describe disclinations on an elastic surface emerges as a gauge field of the local $SO(3)$ group of the local rotations of R^3. This ensures the local rotational invariance of the elasticity action. In spite of the fact that we consider 2D manifolds, the group $SO(3)$ appears rather than the $SO(2)$ one because of the fact that we formulate our theory in terms of the embeddings of a 2D surface into R^3. By construction the local gauge field affects the underlying metric. Within the linear scheme the model recovers the von Karman equations for membranes with a disclination-induced source being generated by gauge fields. For a single disclination on an arbitrary surface a covariant generalization of these equations is obtained.

The dynamical variables of our theory are the embeddings $R^i(x^1, x^2)$ and gauge fields W^i_μ to be determined self-consistently (indices $\mu, \nu, .. = 1, 2$ are tangent to the surface, whereas $i, j, .. = 1, 2, 3$ run over the basis of R^3). As the outcome, the induced metric

$$g_{\mu\nu}(W) = \nabla_\mu \mathbf{R} \nabla_\nu \mathbf{R}, \qquad \nabla_\mu = \partial_\mu + [\mathbf{W}_\mu, ...]$$

emerges. Explicitly,

$$g_{\mu\nu}(W) = \partial_\mu \mathbf{R} \cdot \partial_\nu \mathbf{R} + \partial_\mu \mathbf{R}[\mathbf{W}_\nu, \mathbf{R}] + \partial_\nu \mathbf{R}[\mathbf{W}_\mu, \mathbf{R}] + \\ + (\mathbf{W}_\mu \mathbf{W}_\nu)\mathbf{R}^2 - (\mathbf{W}_\mu \mathbf{R})(\mathbf{W}_\nu \mathbf{R}). \qquad (4)$$

In general, the dynamical fields R^i and W^i_a couple to each other. However, in the linear in elastic field approximation the gauge field can be considered as an external field [8].

II. Dirac fermions on a manifold with a dynamically induced metric. The important issue is how a non-trivial gauge potential can explicitly be incorporated into the theory to self-consistently describe disclination defects on an elastic surface with fermions. To incorporate Dirac fermions we observe that the topologically nontrivial gauge field reasserts itself in the Dirac equation as a topologically nontrivial $SO(2)$ piece of the spin connection [9]. That part of the connection carries a topologically nontrivial flux that does not depend on smooth continuous changes of the underlying metric due to small elastic deformations.

To incorporate fermions on the 2D curved background $(\Sigma, g_{\mu\nu}(W))$ we need a set of orthonormal frames $\{e_\alpha(W)\}$ which yield the same metric, $g_{\mu\nu}(W)$, related to each other by the local $SO(2)$ rotation,

$$e_\alpha \to e'_\alpha = \Lambda^\beta_\alpha e_\beta, \quad \Lambda^\beta_\alpha \in SO(2).$$

It then follows that $g_{\mu\nu} = e^\alpha_\mu e^\beta_\nu \delta_{\alpha\beta}$ where e^μ_α is the zweibein, with the orthonormal frame indices being $\alpha, \beta = \{1, 2\}$, and coordinate indices $\mu, \nu = \{1, 2\}$ (from now on we drop an explicit W-dependance of the metric). As usual, to ensure that physical observables be independent of a particular choice of the zweinbein fields, a local $so(2)$–valued gauge field ω_μ is to be introduced. The gauge field of the local $SO(2)$ group is referred to as a spin connection. For the theory to be self-consistent, zweinbein fields must be chosen to be covariantly constant [10]:

$$\partial_\mu e^\alpha_\nu - \Gamma^\lambda_{\mu\nu} e^\alpha_\lambda + (\omega_\mu)^\alpha_\beta e^\beta_\nu = 0,$$

which determines the spin connection coefficients explicitly

$$(\omega_\mu)^{\alpha\beta} = e^\alpha_\nu D_\mu e^{\beta\nu}, \quad D_\mu = \partial_\mu + \Gamma_\mu, \qquad (5)$$

with Γ_μ being the Levi-Civita connection. The Dirac equation on a surface $(\Sigma, g_{\mu\nu}(W))$ is written as

$$i\gamma^\alpha e_\alpha{}^\mu (\partial_\mu + \Omega_\mu)\psi = E\psi, \qquad (6)$$

with

$$\Omega_\mu = \frac{1}{8}\omega^\alpha_\mu{}^\beta [\gamma_\alpha, \gamma_\beta] \qquad (7)$$

being the spin connection in the spinor representation.

Let us consider first a plane which can be bent but can not be stretched. A single disclination can be inserted in this plane by using the "cut and glue" Volterra process. Obviously, the resulting surface is nothing else but a cone. In our description, we start from a 2D flat metric disturbed by a disclination defect.

In the polar coordinates $(r,\varphi) \in R^2$ a plane can be regarded as an embedding

$$(r,\varphi) \to (r\cos\varphi,\ r\sin\varphi, 0), \quad 0 < r < 1, 0 \le \varphi < 2\pi.$$

The disclination defect is placed at the origin and is described by the gauge field $W_\mu^{i=1,2} = 0$ and $W_\mu^{i=3} = W_\mu$, where in the polar coordinates [8]

$$W_r = 0,\ W_\varphi = \nu. \tag{8}$$

Notice that for any counter C encircling the origin one has

$$\oint_C W = 2\pi\nu \neq 0. \tag{9}$$

Since the counter integral in (9) is a gauge invariant quantity, the field W_μ cannot be gauged away to zero due to the topological obstruction. This is why that field is referred to as a topologically non-trivial one. A physically observable quantity associated with that gauge field is a nonzero flux, $\Phi = 2\pi\nu$, through an area bounded by the counter C. It does not depend on small continuous deformations of that area. This flux instead characterizes the gauge potential globally: it determines the first Chern characteristic class the gauge potential W belongs to. An electron encircling the origin naturally acquires a topological phase associated with that nontrivial flux: the Aharonov-Bohm phase which distinguishes the gauge potential W from a trivial one.

The components of the induced metric (4) can be easily read off

$$g_{rr} = 1, \qquad g_{\varphi\varphi} = \alpha^2 r^2, \qquad g_{r\varphi} = g_{\varphi r} = 0, \tag{10}$$

where $\alpha = 1 - \nu$. Evidently, this is a metric of a cone (cf. (1)), which in view of (5) gives

$$\omega_r^{12} = \omega_r^{21} = 0, \quad \omega_\varphi^{12} = -\omega_\varphi^{21} = 1 - \alpha. \tag{11}$$

At $\nu = 0$ it goes over to a flat one. A topologically nontrivial gauge field (8) results in a conical singularity of the spin connection. The flux

$$\oint_C \omega_\varphi^{12} d\varphi = 2\pi\nu \neq 0.$$

represents a "net" effect produced by a disclination on the moving electrons. We thus show that the gauge-field approach within the linear approximation exactly coincides with that provided by the "cut-and-glue" procedure.

III. Flexible surface. As a matter of fact, a cone with a point-like apex is mathematical abstraction since in a real situation the media has a finite stiffness, which would inevitably result in a certain smearing of a conical singularity. Therefore, a proper description of the disclination implies a smooth deformation of the metric and at the same time one has to preserve a conical behavior far away from the origin. Although such a surface can effectively be approximated by a hyperboloid, we show now that one cannot incorporate finite elasticity into the theory by simply replacing a cone by a smooth surface that asymptotically approaches a cone far away from the origin. This would simply kill the defect.

To illustrate this, consider an upper half of a hyperboloid as an embedding

$$(\chi,\varphi) \to (a\sinh\chi\cos\varphi, a\sinh\chi\sin\varphi, c\cosh\chi),$$

$$0 \le \chi < \infty, \quad 0 \le \varphi < 2\pi.$$

The components of the induced metric can be written as

$$\begin{gathered} g_{\chi\chi} = a^2\cosh^2\chi + c^2\sinh^2\chi, \\ g_{\varphi\varphi} = a^2\sinh^2\chi, \quad g_{\varphi\chi} = g_{\chi\varphi} = 0, \end{gathered} \tag{12}$$

which in view of (5) gives for the spin connection coefficients

$$\omega_\chi^{12} = \omega_\chi^{21} = 0,\ \omega_\varphi^{12} = -\omega_\varphi^{21} = \left[1 - \frac{a\cosh\chi}{\sqrt{g_{\chi\chi}}}\right] =: \omega(\chi). \tag{13}$$

The spin connection in the spinor $SO(2)$ representation becomes

$$\Omega_\varphi = i\omega\sigma^3. \tag{14}$$

Since $\omega(\chi)$ goes to zero as $\chi \to 0$ a circulation of that field over a loop encircling the origin gives a flux which tends to zero as the counter shrinks to zero,

$$\lim_{\epsilon\to 0}\oint_{C_\epsilon} \omega^{12} = 0,$$

where C_ϵ stands for a closed counter which encloses a small area $\sim \epsilon^2$ around the origin. This equation implies that there is no a topologically nontrivial part in the flux. It is therefore clear that one should work out some other way to explicitly accomodate elastic deformations in the "cut-and-glue" procedure that would preserve a conical singularity at the origin.

We show now that the gauge-theory appoach provides the necessary framework. Within this theory the nontrivial flux is kept intact and at the same time the elastic deformations are allowed for. Since a plane can smoothly be deformed into a hyperboloid, a hyperboloid-type smearing naturally emerges due to the elastic deformations of the elastic plane. Actually, the proper metric could be obtained from the exact solution of self-consistent equations in the continuum theory of buckled membranes (see (4.10) in [7] and (25) in [8]). However, this very complicated problem is still unsolved. Instead, we suggest to fulfil these requirements by applying restrictions on the parameters of the hyperboloid. Namely, the parameter c must be proportional to ν^{η} while the parameter a should depend on both the Young's modulus K_0 and the bending rigidity κ. In fact, the first condition comes from a trial solution away from the disclination core found in [7] which reads $c \sim \nu^{1/2}$. The parameter $a(K_0, \kappa)$ must meet the condition $a(K_0, \kappa) \to \infty$ at $K_0 \to \infty$. Indeed, the intrinsic curvature of the hyperboloid reads

$$K = \frac{c^2}{(a^2 \cosh^2 \chi + c^2 \sinh^2 \chi)^2}, \qquad (15)$$

which vanishes at $K_0 \to \infty$ as it should be in the inextensional limit. At the same time, a disclination defect sitting at the origin is taken care of by the gauge field (8). In accordance with (4) this field induces the following explicit changes in the geometry of the hyperboloid:

$$g_{\varphi\varphi} = a^2 \alpha^2 \sinh^2 \chi, \qquad (16)$$

and

$$\omega_{\varphi}^{12} = -\omega_{\varphi}^{21} = \left[1 - \frac{a\alpha \cosh \chi}{\sqrt{g_{\chi\chi}}}\right] =: \omega_{\alpha}(\chi). \qquad (17)$$

Here again $\alpha = 1 - \nu$. Since

$$\omega_{\alpha}(\chi) \to 1 - \alpha, \quad \chi \to 0,$$

this spin connection term in contrast with (13) contains a topologically nontrivial part that gives rise to a fixed flux,

$$\lim_{\epsilon \to 0} \oint_{C_{\epsilon}} \omega^{12} = 2\pi\nu.$$

We thus finally get the smoothed apex, the cone-like asymptotic at large distances and the unremovable conical singularity at the disclination line. It is known that in case a spin connection contains an $SO(2)$ piece with nontrivial flux, that field cannot be eliminated under any smooth deformation of the underlying metric (see, e.g., [10]). Within our approach this simply means that a nontrivial contribution to the spin connection which comes from the gauge field W survives any smooth elastic deformations of the media. Notice also that at large distances we expect only small deviations from the cone resulting from the "cut and glue" procedure, so that the physically reasonable restriction is $\lambda = c/a \ll 1$. In other words, we restrict our consideration to materials with high K_0.

In 2D the Dirac matrices can be chosen to be the Pauli matrices: $\gamma^1 = -\sigma^2, \gamma^2 = \sigma^1$. The Dirac operator then reads

$$\widehat{\mathcal{D}} = \begin{bmatrix} 0 & e^{-i\varphi}\left(-\frac{\partial_\chi}{\sqrt{g_{\chi\chi}}} + \frac{1}{a\alpha \sinh \chi}(i\partial_\varphi + \frac{1}{2}\omega_\alpha(\chi))\right) \\ e^{i\varphi}\left(\frac{\partial_\chi}{\sqrt{g_{\chi\chi}}} + \frac{1}{a\alpha \sinh \chi}(i\partial_\varphi - \frac{1}{2}\omega_\alpha(\chi))\right) & 0 \end{bmatrix}. \qquad (18)$$

At $\alpha = 1\,(\nu = 0)$ it reduces to a flat one. For nonzero α and $K_0 \to \infty$, the parameter $\lambda \to 0$ and one obtains the Dirac operator on a cone.

The eigenfunctions to (18) are classified with respect to the eigenvalues of $J_z = j + 1/2$, $j = 0, \pm 1, \pm 2, \ldots$, and are to be taken in the form

$$\psi = \begin{pmatrix} u(r) e^{i\varphi j} \\ v(r) e^{i\varphi(j+1)} \end{pmatrix}. \qquad (19)$$

The substitution

$$\tilde{\psi} = \psi \sqrt{\sinh \chi}$$

reduces the eigenvalue problem (18) to

$$\begin{aligned} \partial_\chi \tilde{u} - \tilde{j}\sqrt{\coth^2 \chi + \lambda^2}\, \tilde{u} &= \tilde{E} \tilde{v}, \\ -\partial_\chi \tilde{v} - \tilde{j}\sqrt{\coth^2 \chi + \lambda^2}\, \tilde{v} &= \tilde{E} \tilde{u}, \end{aligned} \qquad (20)$$

where $\tilde{E} = \sqrt{g_{\chi\chi}}\, E$ and $\tilde{j} = (j + 1/2)/\alpha$.

One of the most interesting problems associated with Dirac fermions in disclinated elastic media is the manifestation of the topological effects. For various graphene surfaces these issues were discussed in [11 – 20]. Let us study the influence of the smoothed cap on the emergence of the zero-mode states in flexible disclinated materials. A general solution to (20) at $E = 0$ is found to be

$$\tilde{u}_0(\chi) = A\left[(k\cosh\chi+\Delta)^{2k}\,\frac{\Delta-\cosh\chi}{\Delta+\cosh\chi}\right]^{\tilde{j}/2},$$
$$\tilde{v}_0(\chi) = A\left[(k\cosh\chi+\Delta)^{2k}\,\frac{\Delta-\cosh\chi}{\Delta+\cosh\chi}\right]^{-\tilde{j}/2}, \tag{21}$$

where $k=\sqrt{1+\lambda^2}$, $\Delta=\sqrt{1+k^2\sinh^2\chi}$. The normalization conditions read as follows: $-1/2<\tilde{j}<-1/2k$ for $u_0(\chi)$ and $1/2k<\tilde{j}<1/2$ for $v_0(\chi)$ (see [9]). As a result, at small λ, which is of interest here, there are no normalized solutions. This means that in stiff materials smoothing has no marked effect on the existence of zero modes. The situation drastically changes in the presence of the uniform magnetic field directed along the z-axis. In this case, one of the modes (either $\tilde{u}(\chi)$ or $\tilde{v}(\chi)$) becomes normalizable and there exists a true zero-energy state. Therefore, one can expect "switching-like" effects governed by the magnetic field. Studies of this problem are now in progress. Notice that when $\lambda\to 0$ the wave functions $u_0(\chi)$ and $v_0(\chi)$ vanish and we arrive at another class of solutions typical for a true cone (see, e.g., [13]).

IV. Conclusion. In conclusion, we have presented a general approach based on the gauge-theory and geometrical consideration which allows us to describe Dirac fermions on flexible surfaces in the presence of a disclination. Our model takes into account a 'seamless' smearing of the conical singularity in the curvature thus avoiding the evident problem at the core radius in (2). The elasticity of the surface affects the embedding which is chosen to be a plane in the inextentional limit and a hyperboloid-type surface for a flexible material. Within our approach both the elastic deformations and the topologically nontrivial gauge field contribute to the induced metric, which in turn affects the spin connection. It is in this way that Dirac fermions are affected by the topological disclination defects. This approach provides a new insight into disclination theory in a curved 2D background in the presence of electrons and may therefore reveal some novel physical phenomena. In order to apply our consideration to the graphene-based curved materials, one has to take into account an additional non-Abelian gauge field which is responsible for coupling of two Fermi points. This study is now in progress and the results will be published elsewhere.

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