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ZERO MODES FOR DIRAC FERMIONS ON A SPHERE WITH FRACTIONAL VORTEX

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Normalized zero-energy states are shown to emerge for massless Dirac fermions in an external gauge field that gives rise to non-quantized vortices on a sphere. A field-theory model is used to describe electronic states of a fullerene-like molecule. In particular, we predict an existence of exactly one zero-energy mode due to a disclination. For 60° disclination the normalized electron density at zero energy is found to behave as $R^{-5/3}$ with R being the fullerene radius.

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In [1] the 3D space-time Dirac equation

$$i\gamma^{\mu}(\partial_{\mu} + ieA_{\mu})\psi = 0 \tag{1}$$

for massless fermions in the presence of the magnetic field was found to yield $N-1$ zero modes in the N-vortex background field. Zero modes for fermions in topologically nontrivial manifolds have been of current interest both in the field theory and condensed matter physics. In particular, they play a major role in getting some insight into understanding anomalies [2] and charge fractionalization that results in unconventional charge-spin relations (e.g. the paramagnetism of charged fermions) [3] with some important implications for physics of superfluid helium (see, e.g., review [4]). More recently, an importance of the fermion zero modes was discussed in the context of the high-temperature chiral superconductors [5 – 7] and the fullerene molecules [8]. The last example is of our main concern in this paper. As we show below, the problem of the local electronic structure of fullerene is closely related to Jackiw's consideration [1]. Indeed, it was shown within the effective-mass-approximation [9] that the electronic spectrum of a graphite plane linearized around the corners of the hexagonal Brillouin zone coincides with that of (1) for $A_{\mu} = 0$. As a consequence, the field-theory models for Dirac fermions on a plane and sphere [10, 8] were invoked to describe the variously shaped carbon materials.

What is important, disclinations appear as generic defects in closed carbon structures, fullerenes and nanotubes. Actually, in accordance with Euler's theorem these microcrystals can only be formed by having a total disclination of 4π. According to the geometry of the hexagonal network this means the presence of twelve pentagons (60° disclinations) on the closed hexatic surface. In an attempt to describe the electronic spectrum of fullerenes in the presence of disclinations, in [10, 8] the Dirac equation on the surface of a sphere was studied where the lattice curving due to insertion of pentagons was mimicked by introducing an effective gauge field. Indeed, since fivefold rings being inserted in the honeycomb lattice induce frustration, Dirac spinors acquire a nontrivial phase when rotated

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around a pentagon. It was demonstrated in [8] that the rotation can be implemented by inserting a line of magnetic flux at each of the pentagons. The flux is selected in a form needed to satisfy the transformation properties. It was assumed that the flux has to be nonabelian with the only nonvanishing component, A_ϕ, around each puncture so that the correct value of a phase $\exp(i \oint 2)$ is achieved at $\Phi = \pi/2$. Thus, this picture implies the existence of a fictitious magnetic monopole inside the surface with a charge $g = (1/4\pi) \sum \Phi_i = N/8$ where N is a number of conical singularities on the surface. In continuum approximation the effect of magnetic field is smoothed over the sphere by considering a monopole sitting at its center. This phenomenological model was then used for the description of the low-lying electronic levels of the fullerene molecule. In particular, the model predicts the existence of two zero modes with the monopole charges $g = 1/2$ and $g = 3/2$. Notice that a similar problem for an electron in a monopole field was used in studying anyons and the fractional quantum Hall effect on a sphere [11] in the non-relativistic formulation.

In the present paper we suggest a more adequate continuum model to describe electronic spectrum of a fullerene molecule. The distinctive feature of our approach is that both electrons and disclinations are considered to be located on the *surface* of a sphere. In other words, we deal with vortices on a sphere instead of the monopole inside a sphere. In this case, the flux due to a disclination is abelian. Actually, we extend a self-consistent gauge model formulated recently for the description of disclinations on fluctuating elastic surfaces [12] to include fermionic fields.

The basic field equation for the $U(1)$ gauge field in a curved background reads

$$D_a F^{ab} = 0, \quad F^{ab} = \partial^a W^b - \partial^b W^a, \tag{2}$$

where covariant derivative $D_a := \partial_a + \Gamma_a$ includes the Levi – Civita (torsion-free, metric compatibale) connection

$$\Gamma^b_{ac} := (\Gamma_a)^b_c = \frac{1}{2} g^{bd} \left(\frac{\partial g_{dc}}{\partial x^a} + \frac{\partial g_{ad}}{\partial x^c} - \frac{\partial g_{ac}}{\partial x^d} \right), \tag{3}$$

g_{ab} being the metric tensor on a certain Riemannian surface Σ. For a single disclination on arbitrary elastic surface a singular solution to (2) is found to be [12]

$$W^b = -\nu \varepsilon^{bc} D_c G(x, y), \tag{4}$$

where

$$D_a D^a G(x, y) = 2\pi \delta^2(x, y)/\sqrt{g}, \tag{5}$$

with $\varepsilon_{ab} = \sqrt{g}\epsilon_{ab}$ being the fully antisymmetric tensor on Σ, $\epsilon_{12} = -\epsilon_{21} = 1$. It should be mentioned that eqs. (2) and (5) self-consistently describe a defect located on an arbitrary surface [12].

Metric tensor $g_{\mu\nu} = e^\alpha{}_\mu e^\beta{}_\nu \delta_{\alpha\beta}$ where e_α^μ is the zweibein, $\alpha, \beta = \{1, 2\}$, and coordinate indices $\mu, \nu = \{x, y\}$. We employ the real projective coordinates on a sphere. Explicitly,

$$e^1{}_x = e^2{}_x = e^1{}_y = -e^2{}_y = \sqrt{2}R^2/(R^2 + x^2 + y^2),$$

where R is a radius of the sphere. Notice that e_α^μ is the inverse of $e^\alpha{}_\mu$. In this case,

$$g_{xx} = g_{yy} = 4R^4/(R^2 + x^2 + y^2)^2, \qquad g_{xy} = g_{yx} = 0. \tag{6}$$

From eqs. (4) and (5) the following solution can be easily read off

$$W_x = -\nu\partial_y G, \qquad W_y = \nu\partial_x G, \qquad G = \log r, \quad r = \sqrt{x^2+y^2}. \tag{7}$$

Locally, it corresponds to the topological vortex on an Euclidean plane, which confirms an observation that disclinations can be viewed as vortices in elastic media.

An elastic flow through a surface on a sphere is given by a circular integral

$$\frac{1}{2\pi}\oint \mathbf{W} d\mathbf{r} = \nu. \tag{8}$$

Generally there are no restrictions on a value of the winding number ν apart from $\nu > -1$ for topological reasons. However, if we take into account the symmetry group of the underlying crystal lattice the possible values of ν become "quantized" in accordance with the group structure (e.g., $\nu = 1/6, 1/4, 1/3, ...$ for hexagonal lattice). Note that the elastic flux is characterized by the Frank vector $\boldsymbol{\omega}$, $|\boldsymbol{\omega}| = 2\pi\nu$ with ν being the Frank index. Thus, the elastic flux is 'classical' in its origin, i.e. there is no quantization as opposed to the magnetic vortex. In some physically interesting applications, however, vortices with the fractional winding number have already been considered (see, e.g., discussion in [5]). Note also that a detailed theory of magnetic vortices on a sphere has been presented in [13].

The Dirac equation on a sphere takes the form

$$i\gamma^\alpha e_\alpha^{\ \mu}(\nabla_\mu + iW_\mu)\psi = E\psi, \tag{9}$$

where $\nabla_\mu = \partial_\mu + \Omega_\mu$ with Ω_μ being the spin connection which is generally defined as

$$\Omega_\mu = -\frac{1}{8}\Gamma^\alpha{}_\mu{}^\beta[\gamma_\alpha, \gamma_\beta]$$

where $\Gamma^\alpha{}_\mu{}^\beta = e^\alpha{}_\nu D_\mu e^{\beta\nu}$. One can check that $\Omega_x = \Omega_y = 0$, so that the spin connection does not enter (9). In general spin connection Ω_μ vanishes if $\dim\Sigma = 2$ [14].

In 2D the Dirac matrices can be chosen to be the Pauli matrices: $\gamma^1 = -\sigma^2$, $\gamma^2 = \sigma^1$. For massless fermions σ^3 serves as a conjugation matrix, and the energy eigenmodes are symmetric about $E = 0$ ($\sigma^3\psi_E = \psi_{-E}$). We are interested in the zero-energy modes. Let us write down the wave function as $\psi_0 = \binom{u}{v}$. Then (9) reduces to the pair

$$\begin{aligned}(\partial_x + i\partial_y)v - \nu[(\partial_x + i\partial_y)G]v = 0,\\ (\partial_x - i\partial_y)u + \nu[(\partial_x - i\partial_y)G]u = 0.\end{aligned} \tag{10}$$

The solution is obvious

$$u = \exp(-\nu G)g(x - iy), \qquad v = \exp(\nu G)f(x + iy), \tag{11}$$

where $f(x + iy)$ and $g(x - iy)$ are arbitrary entire functions. One can construct self-conjugate solutions $\binom{u}{0}$ and $\binom{0}{v}$. For non-vanishing flux either u or v are normalizable. In particular, for planar systems in a vortex magnetic field f and g are considered to be any polynomial functions of the form $r^n e^{in\theta}$ with $n = 0, 1, ..., [\nu - 1]$ where the brackets indicate integer part. In this case, there are exactly $[\nu - 1]$ normalized zero energy states because of the fact that the $\nu \leq 1$ mode can not be normalized on a plane. As was mentioned by Jackiw [1], a mismatch between the value of the quantized flux and the number of zero modes may be removed, provided R^2 is compactified to a two-sphere, S^2. Another possible solution is to consider a sort of extended model to include coupling of fermions to a scalar field [15]. It is clear that on a sphere for $0 < |\nu| < 1$, which is of our interest in this paper, one can expect only one isolated zero-energy bound state with $n = 0$.

In the nontrivial geometry, the measure factor $\sqrt{g}$ should be taken into account, which on a sphere yields

$$\int |\psi_0|^2 \sqrt{g} dx dy = \int_0^\infty \int_0^{2\pi} r^{-2|\nu|} \frac{2R^2}{R^2 + r^2} r dr d\theta = \frac{2\pi^2}{\sin \pi(1 - |\nu|)} R^{2(1-|\nu|)}, \quad 0 < |\nu| < 1. \tag{12}$$

As is seen from (12), the zero-energy mode cannot be normalized on a plane. Indeed, the planar case corresponds to the limit $R \to \infty$ so that (12) diverges as $R^{2(1-|\nu|)}$. As a consequence, there are no localized zero-energy electronic states on disclinations in monolayer graphite. It should be emphasized that this conclusion agrees with the results of numerical calculations [16] where the local density of states at the Fermi level ($E = 0$) was found to be zero for the case of five- and seven-membered rings which correspond to single disclinations of the 2D graphite. Notice that though the eigenvalue equation (9) acquires a weight for nonzero eigenvalues, the zero eigenvalues remain unchanged. This finding agrees with Jackiw's conjecture [1]. The measure, however, affects the condition (12) resulting in normalizable zero-energy wave function for fractional vortex on a sphere.

For a fullerene molecule we thus predict an existence of only one zero-energy mode due to a disclination since it has been possible to normalize only one of two self-conjugate solutions for any elastic flux with $0 < |\nu| < 1$. In accordance with (12) the expected electron density at zero energy behaves like $R^{-2(1-|\nu|)}$. In particular, for $\nu = 1/6$ the normalized electron density behaves as $R^{-5/3}$. It would be interesting to verify our conclusions in experiments with the fullerene molecules.

To conclude, we have formulated the field theory model to describe electronic states of a fullerene-like molecule. The key point of our approach is to consider disclinations located directly on a sphere, rather than describe the system in a mean-field approach by placing a fictitious monopole in the centre of the sphere. The latter case [8, 10] is essentially the 3D one, which implies that a nonvanishing spin connection is to be added to the covariant derivative in the Dirac equation (9) and, as a consequence, two normalizable zero modes appear in contrast to our result.

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