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Graphene with geometrically induced vorticity

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At half filling, the electronic structure of graphene can be modelled by a pair of free two-dimensional Dirac fermions. We explicitly demonstrate that in the presence of a geometrically induced gauge field, an everywhere-real Kekulé modulation of the hopping matrix elements can correspond to a non-real Higgs field with non-trivial vorticity. This provides a natural setting for fractionally charged vortices with localized zero modes. For fullerene-like molecules we employ the index theorem to demonstrate the existence of six low-lying states that do not depend strongly on the Kekulé-induced mass gap.

Planar graphene and its geometrically related variants offer a rich environment for exploring interesting physics [1]. The electronic properties of graphene are well modelled by a simple Hückel model of nearest-neighbor hopping on a two-dimensional honeycomb lattice [2, 3]. The low energy sector of the resulting band theory may be described by a pair of two-dimensional Dirac equations. As a consequence, graphene is expected to exhibit phenomena more familiar in relativistic quantum theory, such as the Klein Paradox [4]. Recently, Hou *et al.* [5] demonstrated a relation between graphene and p-wave superconductors, where fractionally charged vortices can appear. Energetic considerations guided Jackiw and Pi [6] to extend this model by inserting a gauge potential. Systematic study, including the demonstration of the fractional statistics of these vortices, was given in [7]. Nevertheless, the question of physically realizing these systems remained open.

Spherical configurations of graphene are known as fullerenes. The altered topology requires defects where twelve of the regular carbon hexagons are replaced by pentagons. The resulting frustration and curvature are accounted for in the Dirac equation by introducing a chiral gauge field and a spin connection [8–15]. The gauge-field flux (but not the spin-connection curvature) enters into an index theorem where it is responsible for the six anomalously low-lying states seen in the spectrum of C₆₀ and related molecules [16, 17]. Chemists have long surmised that in fullerenes not all the nearest-neighbor hopping elements are equal. In numerical calculations with the Hückel model it is found that the molecules can lower their electronic energy by undergoing a small Peierls distortion — usually called in this context a Kekulé distortion. This change in the bond lengths introduces a scalar “Higgs” field into the Dirac equation. It has recently been observed, however, that vortices in a complex-valued Higgs field can bind zero-energy mid-gap modes [5–7, 18–20].

Here we demonstrate that the Kekulé distortion Higgs field is not a simple scalar field, but is a section of the non-trivial gauge bundle. This means that a real-valued modulation of the hopping strengths in a fullerene will give rise to a complex-valued Higgs field that automatically contains vortices similar to those of Abrikosov or Nielsen and Olesen. Thus, fullerenes provide a physical setting where vortices with fractionalized charge appear naturally. The number of zero modes bound by these vortices is equal to the number of zero modes required by the index theorem [21, 22]. Indeed, they are the *same* modes.

We begin with the description of a flat sheet of graphene. In the electronic tight binding (Hückel) approximation [8] electrons hop on a two-dimensional honeycomb lattice with lattice constant α . This bipartite lattice can be decomposed into two triangular Bravais sub-lattices Λ_A and Λ_B . The hamiltonian can be written

$$\hat{H} = - \sum_{\mathbf{r} \in \Lambda_A} \sum_{k=1}^3 (t + \delta t_{\mathbf{r}k}) a_{\mathbf{r}}^\dagger b_{\mathbf{r}+\mathbf{s}_k} + \text{H.c.}, \quad (1)$$

where the vector \mathbf{r} gives the position of the vertices of the Λ_A lattice and the vectors \mathbf{s}_k , $k = 1, 2, 3$ connect each site of the Λ_A lattice to the three adjacent sites of Λ_B . The fermionic operators $a_{\mathbf{r}}$ and $b_{\mathbf{r}+\mathbf{s}_k}$ annihilate electrons in the sub-lattices Λ_A and Λ_B , respectively. At half-filling, graphene possesses two independent Fermi points at $\mathbf{K}_\pm = \left(\pm \frac{4}{3\sqrt{3}\alpha}, 0 \right)$ where the positive and negative energy bands touch in conical singularities. For momenta near these Fermi points we can replace the full hamiltonian with a Dirac approximation

$$\hat{H} = \int \Psi^\dagger(\mathbf{r}) H \Psi(\mathbf{r}) d^2r \quad (2)$$

where H is the corresponding one-particle Dirac hamiltonian and the spinor is given by $\Psi(\mathbf{r})^T = (u_a, u_b, v_a, v_b)$ with the a, b indices correspond to the Λ_A and Λ_B sub-lattices and u, v , correspond to the two Fermi points. For the particular case of the Kekulé distortion given by

$$\delta t_{\mathbf{r},k} = \frac{1}{3} \Phi(\mathbf{r}) e^{i\mathbf{K}_+ \cdot \mathbf{s}_k} e^{i(\mathbf{K}_+ - \mathbf{K}_-) \cdot \mathbf{r}} + \text{c.c.}, \quad (3)$$

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the Dirac hamiltonian takes the form [5]

$$H = \begin{pmatrix} \boldsymbol{\sigma}^* \cdot \mathbf{p} & \sigma_1 \Phi \\ \sigma_1 \Phi^* & -\boldsymbol{\sigma} \cdot \mathbf{p} \end{pmatrix} \quad (4)$$

where $\mathbf{p} = -i\boldsymbol{\partial}$, and we have taken an overall constant to unity. Here, $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ are the two-by-two Pauli matrices. Transformations of the form $\sigma_i \otimes \mathbb{1}$ act on the Fermi point components (u, v) , while transformations of the form $\mathbb{1} \otimes \sigma_j$ act on the sublattice indices (a, b) . Here we take Φ to be initially real everywhere.

We wish to compactify the Kekulé distorted graphene sheet into a surface with the topology of a sphere. To do this it helps to make a change of basis. We exchange the role of A and B at the \mathbf{K}_+ Fermi point and rotate the reference frame at the \mathbf{K}_- point by π angle so that it coincides with the frame at \mathbf{K}_+ . These two transformations are effected by conjugating with the $SU(4)$ matrix $\sigma_1 \oplus \sigma_3$. To introduce curvature, we observe that the Kekulé distortion leaves every third hexagon with no double bonds. We select one of these hexagons and, starting from its geometrical center, excise a wedge of opening angle $\pi/3$, the cuts passing through the centers of two lines of bonds. We then reconnect the dangling bonds to form a seam. This operation leaves us with a conical curvature singularity centered on a pentagon, but does not cause a dislocation in the pattern of double bonds. It does, however, introduce frustration in the electron wave functions. This is because the identity of the A and B lattices is interchanged across the seam, and because an electron with wavefunction located near one Dirac point sees itself across the seam as a wavefunction belonging to the other Dirac point. To make the spinors continuous across the cut we therefore introduce a gauge-twist transformation

$$\Psi \rightarrow U\Psi, \quad \text{with } U = \exp \left[-i \int (\mathbf{e}\mathbf{a} + \mathbf{q}) \cdot d\mathbf{r} \right] \quad (5)$$

when the spinor is transported around the apex of the cone. Here $\mathbf{a} = \mathbf{A}(\sigma_2 \otimes \mathbb{1})$ is the non-abelian field with circulation around the pentagonal plaquette $e \oint \mathbf{a} \cdot d\mathbf{r} = \pi/2(\sigma_2 \otimes \mathbb{1})$ and \mathbf{q} is the spin connection with circulation $\oint \mathbf{q} \cdot d\mathbf{r} = -\pi/6(\mathbb{1} \otimes \sigma_3)$. Taking into account that $U^\dagger \partial_i U = -ieA_i(\sigma_2 \otimes \mathbb{1}) - iq_i$ we have that the momentum operator becomes $\mathbf{p} \rightarrow -i(\boldsymbol{\nabla} - ie\mathbf{A})$ with $\boldsymbol{\nabla} = \boldsymbol{\partial} - i\mathbf{q}$. We can diagonalize the gauge field and simplify the Dirac matrices by the rotation $(e^{-i\sigma_1\pi/4} \otimes \mathbb{1})(\mathbb{1} \oplus \sigma_3)$ giving finally

$$H_A = \begin{pmatrix} -ie_\mu^i \sigma_i (\boldsymbol{\nabla} - ie\mathbf{A}) & \Phi \\ \Phi^* & ie_\mu^i \sigma_i (\boldsymbol{\nabla} + ie\mathbf{A}) \end{pmatrix} \quad (6)$$

where the zweibeins, e_μ^i are introduced to make the Hamiltonian covariant in the induced curved space with metric $g_{\mu\nu} = e_\mu^i e_\nu^j \eta_{ij}$, where η_{ij} is the flat metric. Note that, due to the geometric distortion, the initially real Φ has now acquired a phase factor of the form $\exp(i2e \int A)$.

Hamiltonian (6) corresponds to a spinor field defined on a curved manifold coupled to a chiral gauge potential. We observe that the gauge invariant Dirac operator, H_A , that we have derived coincides with the one recently written down by Jackiw and Pi [6]. In our case the pentagon is threaded by a *quarter unit* of gauge flux, and that the phase of the scalar field Φ winds through only π as we circle the defect. Each pentagon is therefore a rather singular ‘‘half-vortex’’. To make the Higgs field smooth, we would need to join pairs of vortices and switch off the Kekulé distortion along a line joining them (see Figure 1(a,b)). We will discuss the significance of this issue later.

We constructed our hamiltonian (4) for the case of a single conical deformation. In order to make a surface with the topology of a sphere we formally need to introduce twelve pentagonal defects. Can we extend our surgical construction globally? It is known that we obtain a consistent assignment of double and single bonds composing a dislocation-free Kekulé structure (a *Fries* structure) if and only if the fullerene belongs to the family C_{60+6k} , $k = 0, 1, \dots$ that is obtained from a parent C_{20+2k} molecule by ‘‘leapfrog’’ inflation [23]. This is exactly the family of molecules we obtain by the previous process, where each of the twelve pentagonal deformations is surrounded by hexagons each possessing three double bonds. The total gauge flux through the twelve pentagons is $3 \cdot 2\pi$, and the total winding number of the Higgs field is six, composed of twelve half-vortices. This can be equivalently described by a monopole sitting inside the molecule providing the net vortex flux [8, 9].

At this point it is convenient to study the transformation properties of the one-particle Dirac hamiltonian H_A . First, note that the different chiralities in the Dirac hamiltonian correspond to normalized solutions, which have their support on the different triangular sublattices of the honeycomb lattice. By comparison with H we deduce that the Dirac hamiltonian H_A acts on the vector (u_b, u_a, v_a, v_b) . For convenience we change basis so that the spinor is given by (u_a, v_a, u_b, v_b) . Then one has $\Gamma_5 H_A \Gamma_5 = -H_A$ where $\Gamma_5 = \sigma_3 \otimes \mathbb{1}$. This transformation maps positive energy eigenvectors of H_A to negative ones, i.e. $\Gamma_5 \Psi_E(\mathbf{r}) = \Psi_{-E}(\mathbf{r})$, while zero energy modes are left unpaired. This property is known as *sublattice symmetry* and it gives rise to charge fractionalization and the emergence of zero modes when the scalar field has non-trivial vorticity [5]. Furthermore, by defining the operator $\Sigma_1 = \mathbb{1} \otimes \sigma_1$ we can show that $\Sigma_1 H_A \Sigma_1 = H_A^*$. As a consequence [24] the eigenfunctions of H_A satisfy $\Sigma_1 \Psi = \Psi^*$ and in spinor components $u_a^* = v_a$ and $u_b^* = v_b$. This symmetry is known as the *time reversal symmetry* and it is present due to the choice of real hopping elements in hamiltonian (1).

We wish to apply the index theorem of Jackiw and Rossi [21], and E. Weinberg [22] to our problem. This theorem was first introduced to study zero modes in a

relativistic analogue of superconducting vortices which is exactly the case here. As we shall see the number of zero modes provided from the index theorem can be computed by *either* counting the number of gauge field flux-units *or* by counting the net winding number of the Higgs field — the two numbers necessarily being equal because of the topology of the gauge bundle.

The sublattice symmetry dictates that the non-zero energy eigenfunctions come in $\pm E$ pairs, whilst zero-energy eigenfunctions (zero modes) can be chosen to be eigenvectors of Γ_5 . Thus, we can arrange the zero modes in terms of their chirality. Suppose that there are n_+ zero modes with Γ_5 eigenvalue $+1$ and n_- with eigenvalue -1 . Weinberg shows [22] that the $\text{Index}(H_{\text{Dirac}}) \stackrel{\text{def}}{=} n_+ - n_-$ is given by

$$\begin{aligned} \text{Index}(H_{\text{Dirac}}) &= \\ &= \frac{e}{\pi} \int_{\Omega} F d^2r + \frac{1}{4\pi i} \oint_{\partial\Omega} d\mathbf{r} \cdot \frac{\Phi^* \mathbf{D}\Phi - \Phi \mathbf{D}\Phi^*}{|\Phi|^2} \\ &= \frac{1}{2\pi} \oint_{\partial\Omega} d\mathbf{r} \cdot \partial \text{Arg} \Phi. \end{aligned} \quad (7)$$

Here

$$\mathbf{D}\Phi = (\partial - 2ie\mathbf{A})\Phi, \quad \mathbf{D}\Phi^* = (\partial + 2ie\mathbf{A})\Phi^*,$$

and the $\partial\Omega$ integral is to be taken over a contour surrounding all the vortices. It is possible to use the consistency equation, $(\partial - 2ie\mathbf{A})\Phi = 0$, of the scalar field that follows from $A_i(\mathbf{r}) = \partial_i\phi(\mathbf{r})$. Then, it is easy to see that the index can be written in terms of the gauge field

$$\text{Index}(H_{\text{Dirac}}) = \frac{e}{\pi} \int_{\Omega} F d^2r. \quad (8)$$

From this form of the index of H_{Dirac} we deduce that one can take the scalar field continuously to zero, $\Phi \rightarrow 0$, without changing the number of zero modes.

As derived by Weinberg, the index theorem applies to the case of open boundary conditions. To apply the theorem to a spherical fullerene with hamiltonian H_A requires the following step. We recognize that there is a net gauge-field flux through the sphere, and so the gauge and associated Higgs bundle are non-trivially twisted. We must therefore introduce two hemispherical patches and sew them together with a gauge-transformation that identifies $\partial - ie\mathbf{A}$ in the upper hemisphere with $e^{ie\chi}(\partial - ie\mathbf{A})e^{-ie\chi}$ in the lower, and similarly identifies Φ in the upper hemisphere with $e^{2ie\chi}\Phi$ in the lower. The phase $e\chi$ in the $U(1)$ group element $e^{ie\chi}$ will wind through $\int_{S^2} eF = 6\pi$ as we encircle the common boundary of the hemispheres. It is the twisting of the Higgs field that allows us to have a net number (six) of Higgs field vortices. If the field Φ were an ordinary scalar instead of a section of a twisted bundle the net vortex number would necessarily be zero. Thus, the index theorem demonstrates that the mass term appearing due to the Kekulé distortion does not actually destroy the zero modes.

We have seen that the introduction of curvature through pentagonal defects automatically turns Kekulé distorted planar graphene into a gauge theory of the form introduced by Jackiw and Pi. The defects form half-vortices in the Higgs field corresponding to the Kekulé distortion. We can apply the Jackiw-Rossi-Weinberg index theorem to find a lower bound on the number of low energy states on the curved surface. When applied to the leapfrog fullerenes C_{60+6k} we find that there should be six low-lying modes that are insensitive to the magnitude of the Kekulé distortion. The singular nature of the vortices is a problem however, and numerical investigation of the leapfrogs C_{3n-60} with a uniform distortion shows six low lying modes that *do* depend on the distortion (Figures 2(a) and 3(a)). This is not surprising as in this form the Higgs field is discontinuous due to its half vorticity at each pentagon. To rectify it one must allow the vortices to pair up by joining them with cuts, that is regions with $\Phi = 0$. Moreover, the energy contribution from the scalar field Φ is given by $\int d^2r \{|\mathbf{D}\Phi|^2 + V(\Phi^*\Phi)\}$, where V is a function with a minimum at Φ_0 with $V'(\Phi_0^*\Phi_0) = 0$ that enforces Ψ to acquire mass. To avoid divergences of the energy the scalar field [6] has to vanish polynomially as $r \rightarrow 0$. This forces us to consider vortices with enlarged size. As we shall see in the following these modifications in the configuration of the Kekulé distortion of a fullerene molecule provide a spectrum that is in agreement with the prediction of the index theorem.

Figures 2 and 3 depict the spectrum of C60 and C180 molecules with Kekulé distortion for the various cases of uniform and smoothed Higgs fields. The coupling of the single bond has been set to 1 and that of the double bonds is denoted by h . The case of uniform Kekulé distortion, presented in Figure 1(a), has been modified in order to ensure smoothness of the effective Higgs field. For that we first introduced cuts among the vortices, i.e. we removed double bonds along paths that connect pairs of vertices, as seen in Figure 1(b). Moreover, we enlarged the size of the vortices by removing double bonds from the links attached to the pentagons, as seen in Figure 1(c). When the last process is performed on the C60 molecule it removes all double bonds due to its small size.

As expected from the index theorem there are six modes with near zero energy when the coupling h is varied. While for the case of uniform Kekulé distortion these modes seem to be sensitive to variations of h (see Figures 2(a) and 3(a)) this is rectified by introducing cuts and by enlarging the vortices. These processes make the Higgs field continuous and the energy of the low-lying modes becomes even closer to zero with an energy that is insensitive to variations of h . Indeed, in Figures 2(c) and 3(c) there are six low-lying modes which are to a good degree insensitive to variations of h . The difference of their energy from being exactly zero is due to the small size of the system and it is expected to converge to zero when larger molecules are employed [8].

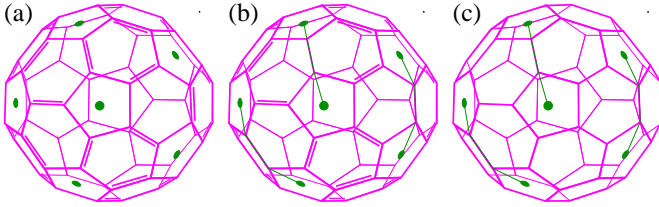


FIG. 1: The coupling configuration of the C60 molecule, where vortices reside on the pentagons. (a) The Kekulé distortion. (b) Cuts between vortices are introduced by replacing a double bond with single ones. (c) An enlargement of the vortices is introduced by removing all double bonds connected to the pentagons. For C60 this removes all double bonds.

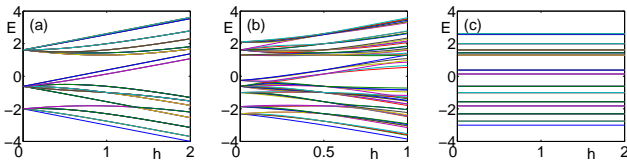


FIG. 2: The spectrum of the C60 molecule as a function of the double bond coupling, h , with single bond coupling equal to 1. There are six modes (two triplets) that are near zero energy. (a) With Kekulé distortion. (b) With cuts between pairs of vortices. (c) With enlarged vortices, where all double bonds are removed.

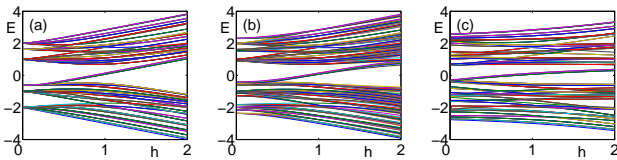


FIG. 3: The spectrum of the C180 molecule. (a) With Kekulé distortion. (b) With cuts between pairs of vortices. (c) With enlarged vortices.

To summarize, we explicitly demonstrated that the effective gauge field induced in a graphene sheet, when it is geometrically deformed, couples non-trivially to the Higgs field induced from a distortion in the tunnelling couplings. As a result, the fullerene-like molecules have six half vortices that are *fractionally charged* [5] giving a natural setting where this topological effect appears. By employing the index theorem we demonstrated that there should be one zero mode for each pair of such vortices. While the effective gauge field is responsible for the presence of the zero modes the scalar field assures that

the corresponding degenerate states are not locally distinguishable implying their topological robustness (topological degeneracy). In the case of fullerene-like molecules a study of the corresponding low-lying states showed that a Kekulé distortion is energetically favorable actually reducing the overall energy of the electrons.

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