Persistence of zero modes in a gauged Dirac model for bilayer graphene

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A recently constructed model for low-lying excitations in bilayer graphene exhibits midgap, zero-energy modes in its Dirac-type spectrum when a scalar order parameter takes a vortex profile. We show that these modes persist when the dynamics is extended by a gauge field interaction, which also renders finite the vortex energy. The effect of the gauge field on the zero-energy wave function is to shift the phase of the (damped) oscillatory component of the wave function in the absence of the gauge field.

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The old subject of Dirac zero modes and fractional charge[1] revived recently, owing to the emergence of graphene as an experimentally realized planar substance,[2] whose low-energy excitations can be described by a Dirac equation in two spatial dimensions.[3] If the material exhibits various dimerization patterns, the effective Dirac fields also interact with a homogenous scalar field (order parameter), and this gives rise to a gap in the Dirac spectrum. When the scalar field acquires a topologically interesting profile (e.g., a vortex in which the phase of the scalar field winds around the vortex position), a zero-energy, midgap state can occur with fractional (fermion) charge.[1]

An early instance of planar Dirac zero modes was found in Ref. 4, but no actual experimental setting was given. Today graphene and graphene-like substances offer the possibility of a physical realization.

Monolayer graphene consists of a hexagonal honeycomb lattice, which may be presented as a superposition of two triangular sublattices A and B. In the tight-binding approximation, there are two Dirac points. If a particular dimerization—called Kekulé distortion—occurs, the effective Dirac Hamiltonian also possesses an interaction with a scalar field φ,[5]

$$h_1 = \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta|\varphi|e^{-i\gamma_5\chi}. \tag{1}$$

Here,

$$\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}, \quad \beta = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

$$\boldsymbol{p} = \frac{1}{i}\boldsymbol{\nabla}, \quad \varphi = |\varphi|e^{i\chi}.$$

The 4×4 Dirac Hamiltonian h_1 acts on a four-spinor Ψ,

$$\Psi = \begin{pmatrix} \psi_+^B \\ \psi_+^A \\ \psi_-^A \\ \psi_-^B \end{pmatrix}, \tag{2}$$

where $(\pm)$ refer to the two Dirac points and (A,B) label the sublattices. The vector quantities $\boldsymbol{p}$, $\boldsymbol{\alpha}$, and $\boldsymbol{\sigma}$ are two dimensional. The kinetic term $\boldsymbol{\alpha}\cdot\boldsymbol{p}$ does not mix the Dirac points; mixing arises through φ as a consequence of the Kekulé distortion. Homogenous $\varphi=m$ produces a mass gap, while an n-vortex profile for $\varphi(\mathbf{r})$ produces zero modes. The Hamiltonian [Eq. (1)] anticommutes with $\alpha_3=\left(\begin{smallmatrix}\sigma_3 & 0\\ 0 & -\sigma_3\end{smallmatrix}\right)$,

$$\alpha_3 h_1 \alpha_3 = -h_1. \tag{3}$$

Therefore α_3 maps positive energy solutions onto negative energy solutions, and zero modes can be chosen to be eigenmodes of α_3. This "energy reflection symmetry" is a manifestation of the sublattice symmetry found in the honeycomb graphene lattice.

The above model was extended by including an interaction with a gauge field, $\mathbf{A}$, whose purpose is to unpin the vortices.[6] [The energy density of the vortex is not included in Eq. (4), below. Were one to consider it without a gauge field contribution, one would encounter an infrared divergence, arising from the gradients of the scalar field. This divergence is screened by the vector potential.] Here,

$$h_1^{\mathbf{A}} = \boldsymbol{\alpha}\cdot(\boldsymbol{p} - \gamma_5\mathbf{A}) + \beta|\varphi|e^{-i\gamma_5\chi}. \tag{4}$$

The gauged model possesses a local chiral gauge symmetry

$$\Psi \to e^{i\omega\gamma_5}\Psi, \quad \varphi \to e^{2i\omega}\varphi \Rightarrow \chi \to \chi + 2\omega,$$

$$\mathbf{A} \to \mathbf{A} + \boldsymbol{\nabla}\omega, \tag{5}$$

and one readily verifies the identity

$$h_1^{\mathbf{A}} = \exp\left(\alpha_3\frac{1}{\nabla^2}b\right) h_1 \exp\left(\alpha_3\frac{1}{\nabla^2}b\right), \tag{6}$$

$$b = \varepsilon^{ij}\partial_i A^j. \tag{7}$$

Thus the extended model still retains the energy reflection symmetry, and possesses zero-energy eigenmodes, whose wave functions differ from those with just a scalar vortex by the factor $e^{-\alpha_3 1/\nabla^2 b}$.

However, it may be difficult to achieve experimentally the Kekulé distortion. Recently a model that is physically different but mathematically similar to Eq. (1) has been put forward, with the suggestion that the excitation condensate—needed for topological effects, fractional charge etc.—can

"be produced in the laboratory in the near future."[7] The physical system consists of a graphene bilayer, separated by a dielectric barrier, and biased by an external, constant voltage V. In a mean-field approximation, the Hamiltonian for the above bilayer system is given by

$$h_2 = \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta|\varphi|e^{-i\gamma_5\chi} + \gamma_5 V, \tag{8}$$

which acts on the four-spinor Ψ,

$$\Psi = \begin{pmatrix} \psi_1^B \\ -\psi_1^A \\ \psi_2^B \\ \psi_2^A \end{pmatrix}. \tag{9}$$

As before (A,B) refer to the sublattices, but (1, 2) label the two layers, which are nested, one directly above the other. There are no Dirac point labels because the above description refers to a single Dirac point in each lattice of the two stacked lattices. Here φ describes the condensate arising from states bound by interlayer Coulomb forces between particles in one layer and holes in the other. This dynamics is modeled by a four-Fermi interaction of strength U. A gap equation is solved in the Hartee-Fock approximation, leading to

$$|\varphi| \approx \sqrt{\Lambda V}e^{-\sqrt{3}\pi t^2/UV}. \tag{10}$$

Here t is the hopping amplitude between sites on each of the two monolayers; there is no interlayer hopping within this model's approximations. Equation (10) holds in the limit $\Lambda \gg V \gg |\varphi|$, where Λ is an energy cutoff.[7] It is striking that this order parameter enters the bilayer theory in a way identical to the Kekulé distortion of the monolayer model h_1 in Eq. (1).

The presence of $\gamma_5 V$ in h_2, which has no analog in h_1, spoils the energy reflection symmetry [Eq. (3)]. But another property of h_2 ensures similar behavior. One verifies that h_2 satisfies

$$\beta\alpha_2 h_2^* \beta\alpha_2 = h_2. \tag{11}$$

Thus energy reflection works as

$$\Psi_{-E} = \beta\alpha_2\Psi_E^*, \tag{12}$$

and h_2 possesses zero-energy eigenstates, satisfying[7]

$$\alpha_2\beta\Psi_0 = \Psi_0^*. \tag{13}$$

In view of our earlier work on gauging the monolayer graphene model,[6] we are led to study the gauged version of h_2,

$$h_2^{\mathbf{A}} = \boldsymbol{\alpha}\cdot(\boldsymbol{p} - \gamma_5\mathbf{A}) + \beta|\varphi|e^{-i\gamma_5\chi} + \gamma_5 V. \tag{14}$$

Gauge transformations follow Eq. (5) and V is gauge invariant. The new energy reflection property [Eqs. (11) and (12)] is maintained. Consequently we expect to find zero modes, which we now exhibit.

The four-spinor equation [Eq. (9)] is presented in terms of two spinors,

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}, \quad \Psi_1 = \begin{pmatrix} \psi_1^B \\ -\psi_1^A \end{pmatrix}, \quad \Psi_2 = \begin{pmatrix} \psi_2^B \\ \psi_2^A \end{pmatrix}. \tag{15}$$

With our Dirac matrices, the zero-energy spinors satisfy according to Eq. (13) $\Psi_2 = \sigma_2\Psi_1^*$, and the eigenvalue equation reads

$$[\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \mathbf{A}) + V]\Psi_1 + \varphi\sigma_2\Psi_1^* = 0, \tag{16a}$$

$$\varphi^*\Psi_1 - [\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \mathbf{A}) + V]\sigma_2\Psi_1^* = 0. \tag{16b}$$

In fact, the second equation is a consequence of the first, and needs not be considered separately. Continuing with the matrix reduction, we set $\Psi_1(\mathbf{r}) = \binom{F(\mathbf{r})}{G(\mathbf{r})}$, and Eq. (16) now reads

$$VG - ie^{i\theta}\left[\partial_+ + \frac{n}{r}A\right]F + ime^{in\theta}F^* = 0, \tag{17a}$$

$$VF - ie^{-i\theta}\left[\partial_- - \frac{n}{r}A\right]G - ime^{in\theta}G^* = 0, \tag{17b}$$

$$\partial_\pm \equiv \frac{\partial}{\partial r} \pm i\frac{i}{r}\frac{\partial}{\partial\theta},$$

where we have taken $A^i = -n\varepsilon^{ij}\frac{r^j}{r^2}A(r)$, with $A(0)=0$, $A(\infty)=\frac{1}{2}$, and $\varphi = m(r)e^{in\theta}$, with $m(0)=0$ and $m(\infty)=m$.

To separate the angular dependence, to make the equations real, and to simplify them, we posit the *Ansatz*

$$F(\mathbf{r}) = -i\frac{f(r)}{\sqrt{r}}e^{-[M(r)-il_1\theta]}, \tag{18a}$$

$$G(\mathbf{r}) = \frac{g(r)}{\sqrt{r}}e^{-[M(r)-il_2\theta]}, \tag{18b}$$

$l_1 = \frac{n-1}{2}$, $l_2 = \frac{n+1}{2}$, $M'(r) = m(r)$, and f, g are real. Single valuedness requires that n be an odd integer. The final equations read

$$\left[\partial_r - \frac{n}{r}\left(\frac{1}{2} - A\right)\right]f - Vg = 0, \tag{19a}$$

$$\left[\partial_r + \frac{n}{r}\left(\frac{1}{2} - A\right)\right]g + Vf = 0. \tag{19b}$$

When A remains unspecified (apart from its asymptotes) Eq. (19) does not appear explicitly integrable and A cannot be removed, as in the monolayer case [Eq. (6) and (7)]. However, one can show that a normalizable solution exists.

For $r\to\infty$, $A\to\frac{1}{2}$ and Eq. (19) reduce to

$$f' - Vg = 0, \tag{20a}$$

$$g' + Vf = 0, \tag{20b}$$

with solution that involves two constants, (c,d),

$$f(r) = c\cos Vr + d\sin Vr, \tag{21a}$$

$$g(r) = -c \sin Vr + d \cos Vr. \tag{21b}$$

Evidently owing to the $r^{-1/2}e^{-M(r)}$ factor both F and G are always damped at large r. Thus the wave function will be acceptable and normalizable if a solution that is regular at the origin can be constructed.

At the origin A vanishes and the Eq. (19) reduces to

$$\left(\frac{\partial}{\partial r} - \frac{n}{2r}\right) f - Vg = 0, \tag{22a}$$

$$\left(\frac{\partial}{\partial r} + \frac{n}{2r}\right) g + Vf = 0. \tag{22b}$$

Of course these are the same equations, which hold for all r in the absence of **A**, as with the Hamiltonian h_2 in Eq. (8). Their solution is given in terms of Bessel functions,[7]

$$f = r^{1/2} J_{n/2-1/2}(Vr), \quad g = -r^{1/2} J_{n/2+1/2}(Vr). \tag{23}$$

Note that the large r asymptote of Eq. (23) is of the form (21) with specific values for $c = \sqrt{\frac{2}{\pi}} \cos\frac{n\pi}{4}$ and $d = \sqrt{\frac{2}{\pi}} \sin\frac{n\pi}{4}$. Thus the effect of the gauge field is to move c and d from the above values; i.e., **A** causes a phase shift in the profiles without gauge field.

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