Emerging Zero Modes for Graphene in a Periodic Potential

L. Brey
Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco 28049, Spain

H. A. Fertig
Department of Physics, Indiana University, Bloomington, Indiana 47405, USA
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We investigate the effect of a periodic potential on the electronic states and conductance of graphene. It is demonstrated that for a cosine potential $V(x) = V_0 \cos(G_0 x)$, new zero energy states emerge whenever $J_0(\frac{2V_0}{\hbar v_F G_0}) = 0$. The phase of the wave functions of these states is shown to be related to periodic solutions of the equation of motion of an overdamped particle in a periodic potential, subject to a periodic force. Numerical solutions of the Dirac equation confirm the existence of these states, and demonstrate the chirality of states in their vicinity. Conductance resonances are shown to accompany the emergence of these induced Dirac points.

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The laboratory realization of graphene [1–3], a two-dimensional honeycomb lattice of carbon atoms, has motivated intense theoretical and experimental investigations of, among many other things, its transport properties [4]. Graphene differs from conventional two-dimensional electron systems in that it supports two inequivalent Dirac points, through which the Fermi energy passes when the system is nominally undoped. The chirality of the electron wave functions near the Dirac points severely limits electron backscattering, enhancing the conductivity of the system [5]. The unusual transport properties associated with the Dirac points may in principle be explored and exploited if the edge structure can be controlled [6,7], or by application of nonuniform potentials, such as in a *p-n* junction [8–12]. Periodic potentials may be induced by interaction with a substrate [13–15] or controlled adatom deposition [16]. Recently, the existence of periodic ripples in suspended graphene has been demonstrated [17]; in a perpendicular electric field this would also induce a periodic potential [18,19].

In this Letter we discuss the effects of a one-dimensional superlattice potential on the transport properties of graphene. Previously it has been noted that such a potential may create a strong anisotropy in the electron velocity around the Dirac point [20,21]. In fact this behavior is a precursor to the formation of further Dirac points in the band structure of the system. We will show that such new zero energy states of the Dirac equation are associated with how the phase of the wave function varies with position along the superlattice direction, and is connected with the dynamics of a highly overdamped particle subject to periodic potentials both in space and time. From an analysis of this problem we demonstrate that the emergence of new Dirac points is controlled by the parameter V_0/G_0, where V_0 is the potential amplitude (assumed to be a cosine) and $L_0 = 2\pi/G_0$ is the period. New Dirac points emerge whenever $J_0(\frac{2V_0}{\hbar v_F G_0}) = 0$, where J_0 is a Bessel function and v_F the speed of the Dirac fermions in the absence of the potential. The total number of Dirac points (associated with a single valley and spin) is thus $2N + 1$, with N the number of zeros of $J_0(x)$, with $|x| < \frac{2V_0}{\hbar v_F G_0}$. We verify the existence of these new zero energy points numerically, and demonstrate the chirality of the wave functions in their vicinity.

We find that, when stabilized, the new Dirac points associated with the superlattice potential have dramatic consequences for transport along the superlattice axis. For undoped graphene, the conductivity σ along this direction depends only on the ratio V_0/G_0, and supports strong resonances at the values of V_0/G_0 where the new zero energy states appear. This is illustrated in Fig. 1. Also illustrated [Fig. 1(b)] is the Fano factor [22], a measure of the degree of correlation in current noise due to the discreteness of the electron charge, which typically has the value 1/3 for diffusive transport, and vanishes when the transport is ballistic. Despite the absence of disorder in this system, both the Fano factor and the scaling of the conductivity with system length L_x suggest that the transport has a diffusive character for most values of V_0/G_0, which becomes ballistic in the vicinity of the resonances. The periodic appearance of the conductance resonances as a function of V_0/G_0 provides a clear signature of the new zero energy states as they emerge.

Zero energy states.—We consider an external potential of the form $V(x) = V_0 \cos G_0 x$, where the period of the perturbation is much larger than the graphene lattice parameter, a, and the amplitude V_0 is much smaller than the energy bandwidth of the graphene π orbitals. In this situation the low energy properties for electrons in a single valley and a given spin are well described by the massless Dirac Hamiltonian with a potential,

$$H = \hbar v_F(-i\sigma_x \partial_x - i\sigma_y \partial_y) + V(x)I \tag{1}$$

where $\sigma_{x,y}$ are the Pauli matrices, and I is the identity

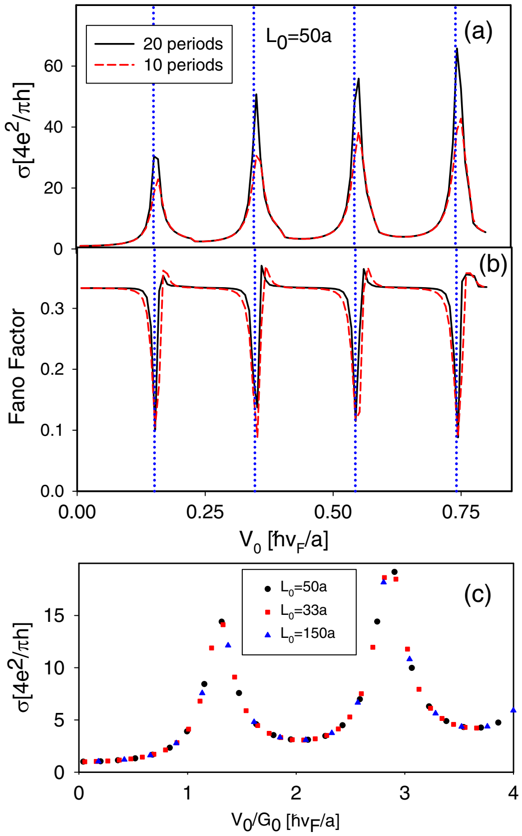

FIG. 1 (color online). (a) Conductivity and (b) Fano factor, as function of V_0 and for $L_0 = 50a$, for two different graphene sample lengths containing 10 and 20 periods of the periodic potential $V_0 \cos G_0 x$. Panel (c) shows the conductivity as a function of V_0/G_0 as obtained from different superlattices' potentials. This result indicates that the conductivity only depends on V_0/G_0. Vertical lines indicate the position of the zeros of $J_0(\frac{2V_0}{\hbar v_F G_0})$.

matrix. The wave functions which this may multiply have two components, $\Phi_{A,B}$, corresponding to the two triangular sublattices that make up a honeycomb lattice.

To demonstrate the emergence of zero energy states, it is convenient to implement a unitary transformation [23–25] of the Hamiltonian, $H' = U_1^\dagger H U_1$, with

$$U_1 = \begin{pmatrix} e^{-i(\alpha(x)/2)} & -e^{i(\alpha(x)/2)} \\ e^{-i(\alpha(x)/2)} & e^{i(\alpha(x)/2)} \end{pmatrix}$$
$$\text{and} \quad \alpha(x) = \frac{2}{\hbar v_F}\int_0^x V(x')dx', \tag{2}$$

so that, for $\Phi_{A,B}(\mathbf{r}) = e^{ik_y y}\phi_{A,B}(x)$, the Hamiltonian acting on the transformed wave functions $U^\dagger \vec{\phi}$ is

$$H' = \hbar v_F \begin{pmatrix} -i\partial_x & -ik_y e^{i\alpha(x)} \\ ik_y e^{-i\alpha(x)} & i\partial_x \end{pmatrix}. \tag{3}$$

For the cosine potential, $e^{i\alpha(x)} = \sum_{l=-\infty}^{l=\infty} J_\ell(\frac{2V_0}{\hbar v_F G_0})e^{ilG_0 x}$, where J_n is the nth Bessel function of the first kind.

For zero energy states, we search for solutions of $H'\vec{\phi} = \vec{0}$. Such solutions have the property $\phi_A = \phi_B^*$. For a single valley system this would mean the two components are related by time reversal; this is not quite the case here because time reversal in graphene also involves interchanging valleys. Writing $\phi_A = |\phi_A|e^{i\chi}$, we obtain a single component equation

$$\partial_x|\phi_A| + k_y e^{i\alpha - 2i\chi}|\phi_A| + i(\partial\chi)|\phi_A| = 0. \tag{4}$$

An analogous manipulation for the zero modes of the Bogoliubov-de Gennes equation of states in a vortex of a p-wave superconductor [26] yields a very simple value for the phase χ, and the resulting state is a Majorana fermion due to the time-reversal relation between components. In our case, we need to find solutions for χ that are consistent with the symmetries of the problem; when they exist the resulting state is that of a real fermion, since the two magnitudes $\phi_{A,B}$ are not truly related by time reversal. The equation governing χ is obtained by taking the imaginary part of Eq. (4),

$$k_y \sin(\alpha - 2\chi) + \partial_x \chi = 0. \tag{5}$$

The real part yields $\partial_x|\phi_A| + k_y\cos(\alpha - 2\chi)|\phi_A| = 0$, with the formal solution

$$|\phi_A| \propto \exp\left\{-k_y \int_{x_0}^x \cos[\alpha(x') - 2\chi(x')]dx'\right\}. \tag{6}$$

Since $\vec{\phi}$ is a Bloch state of the superlattice, it must obey the Bloch relation $\phi_{A,B}(x + L_0) = e^{ik_x L_0}\phi_{A,B}(x)$, with k_x the crystal momentum. For a zero energy state only $k_x = 0$ is possible. We then require (i) $\chi(x + L_0) = \chi(x) + 2\pi m$ with m an integer, and (ii) $\int_0^{L_0}\cos[\alpha(x) - 2\chi(x)] = 0$. To see whether χ can satisfy these relations, it is helpful to recast Eq. (5) by writing $\tilde{\chi} = 2\chi - \alpha$, and $x \to t$, so that

$$-\partial_t\tilde{\chi} - \partial_t\alpha + 2k_y\sin\tilde{\chi} = 0. \tag{7}$$

This is the equation of motion for the position $\tilde{\chi}$ of an overdamped particle (with unit viscosity), subject to a periodic time-dependent force $\partial_t\alpha$ and a spatially periodic force $2k_y\sin\tilde{\chi}$. Despite the periodicity of the forces involved, the generic solution to this equation is not periodic. However, for certain parameters periodic solutions can be found, which correspond to allowed zero energy solutions of the Dirac equation in a periodic potential.

To see this, we solve Eq. (5) perturbatively in k_y. Writing $\chi = k_y\chi^{(1)} + k_y^2\chi^{(2)} + O(k_y^3)$, one finds

$$\chi^{(1)} = -\int^x dx'\sin\alpha(x') + C^{(1)}$$

$$\text{and} \quad \chi^{(2)} = 2C^{(1)}\int^x dx_1\cos\alpha(x_1) - \int^x dx_1\int^{x_1} dx_2\sin\alpha(x_2) + C^{(2)},$$

where $C^{(1,2)}$ are constants of integration. Explicitly performing the integrations for the above two equations, one finds that condition (i) can be satisfied if

$$k_y^2\left[2C^{(1)}J_0L_0 - \sum_{\ell\,\mathrm{odd}}\frac{J_\ell}{\ell G_0}L_0\right] = 2\pi m. \tag{8}$$

Here J_0 and J_ℓ are Bessel functions evaluated at $2V_0/\hbar v_F G_0$. Since we have employed a small k_y expansion, the only consistent solution is for $m = 0$. In this case Eq. (8) fixes $C^{(1)}$, and the resulting χ (and the associated $\tilde{\chi}$) is periodic. Condition (ii) may then be implemented to fix the value of k_y at which a zero mode appears,

$$\left(\frac{k_y}{G_0}\right)^2 = -\frac{J_0}{2\sum_{\ell_1,\ell_2\mathrm{odd}} J_{\ell_1}J_{\ell_2}J_{-\ell_1-\ell_2}/\ell_1\ell_2}. \tag{9}$$

Equation (9) predicts the presence of a zero mode whenever the right-hand side is positive. This turns out to occur when $x = \frac{2V_0}{\hbar v_F G_0}$ is just above the values for which $J_0(x) = 0$; we have confirmed numerically that the sign of the denominator on the right-hand side of Eq. (9) always works out such that $k_y^2 > 0$ in this situation. With increasing x, the solution moves to larger $|k_y|$ until it diverges where the three Bessel function sum vanishes, which is always prior the next zero of $J_0(x)$. We note that since our approximation is only valid for small k_y, Eq. (9) cannot accurately predict the location of the zero energy states well away from $k_y = 0$. However, since zero energy states can only annihilate in pairs [27], we expect that once they emerge from the origin, they should persist. We now show that a numerical solution of the Dirac equation supports this expectation.

Numerical studies.—Our expectations about the new zero energy states can be confirmed by numerically solving the Dirac equation in a periodic potential. To accomplish this we represent the Hamiltonian $H = H_0 + V_0\cos G_0 x$ in a plane wave basis and diagonalize the resulting matrix for momenta (k_x, k_y), with $-G_0/2 < k_x < G_0/2$. We have checked that our results converge with respect to the number of plane wave states used.

Because of the chiral nature of the Dirac quasiparticles the effect of the periodic potential is highly anisotropic: at the $k_x = 0$, $k_y = 0$ Dirac point the group velocity is unchanged in the direction of the superlattice but is strongly reduced, even to zero in some cases, in the perpendicular direction [20,28,29]. In Fig. 2 we plot, for different values of V_0, the lowest few energy eigenvalues as a function of k_y for $k_x = 0$ and $L_0 = 50a$. As V_0 increases the group velocity at the Dirac point decreases to zero [20,28,29], and thereafter two zero energy states emerge from $k_y = 0$ as the group velocity of the $k_y = 0$ Dirac point becomes finite again. These are the new zero energy states discussed above; we find that they emerge precisely when $J_0(\frac{2V_0}{\hbar v_F G_0}) = 0$. Upon further increase of V_0, the group velocity along k_x at $k_y = 0$ becomes zero again and a new pair of zero energy states emerge from $k_y = 0$, again

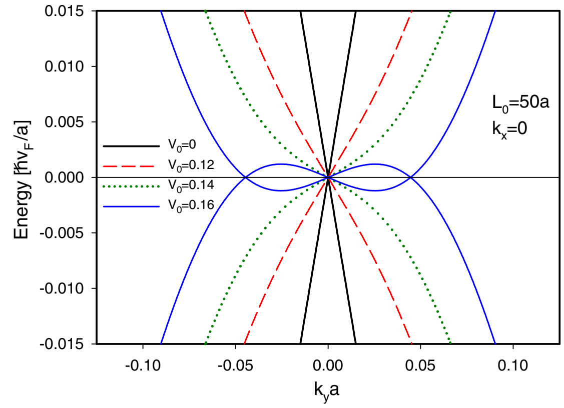

FIG. 2 (color online). Energy bands of graphene in the presence of a superlattice potential $V_0\cos G_0 x$, as a function of k_y with $k_x = 0$, for several values of V_0, in units $\hbar v_F/a$, and $L_0 = 50a$.

precisely at the next zero of $J_0(\frac{2V_0}{\hbar v_F G_0}) = 0$. This pattern continues to repeat itself with increasing V_0. Further studies for different periodicities confirms the prediction that the emergence of these points depends only on the ratio V_0/G_0, precisely as predicted in the analysis of the previous section.

These zero energy points in fact represent new Dirac points, as can be demonstrated by studying the chirality of the wave functions in their vicinity. In Fig. 3 we plot the expectation value of the pseudospin $(\langle\sigma_x\rangle, \langle\sigma_y\rangle)$ for the lowest positive energy eigenvalue as a function of crystal momentum. One may see that this vector undergoes a 2π rotation for any path enclosing one of the zero energy states. The nonvanishing winding of this vector for such paths is a clear signal of the Dirac-like nature of the spectrum in the vicinity of a zero energy state.

Conductivity.—Using the transfer matrix method we have computed the transmission probability through a graphene strip of length L_x, containing N_p periods of the superlattice potential. We assume metallic contacts connected to the strip may be modeled by heavily doped graphene [30]. Boundary conditions are taken to be periodic in the transverse direction, leading to transverse wave functions which can be labeled by a momentum k_y; this is justified when the width of the strip, L_y, is much larger than its length. From the transmission probability of each mode, T_{k_y}, we obtain the conductance G and the Fano factor (ratio of noise power and mean current) F,

$$G = 4\frac{e^2}{h}\sum_{k_y} T_{k_y} \qquad F = \frac{\sum_{k_y} T_{k_y}(1 - T_{k_y})}{\sum_{k_y} T_{k_y}} \tag{10}$$

where the factor 4 accounts for the spin and valley degeneracy. The conductivity is related to the conductance via geometrical factors, $\sigma = G \times L_y/L_x$. In what follows we work in the limit $L_y \gg L_x$.

For pristine graphene, $V_0 = 0$, the conductivity is independent of L_x and takes the value $\sigma_0 = 4e^2/\pi h$, and the

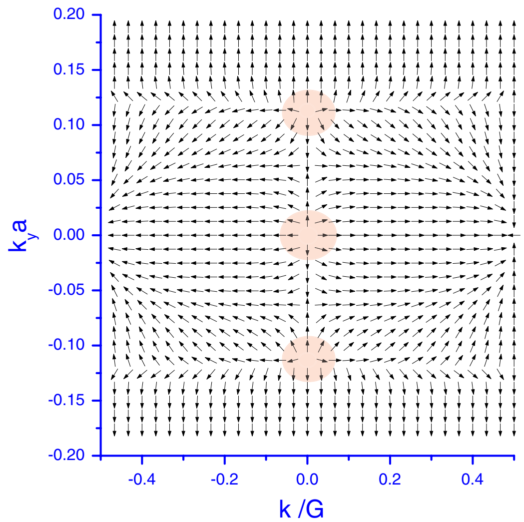

FIG. 3 (color online). Expectation value of the vector field (σ_x, σ_y) of the lowest energy positive subband for a superlattice of period $50a$ and $V_0 = 0.1\hbar v_F/a$. The zero energy Dirac points at $k_x = 0$ are highlighted. High energy Dirac points with opposite chirality also appear between the $k_y = 0$ Dirac point and the superlattice induced Dirac points.

Fano factor takes on the universal value $1/3$. In the absence of disorder one might expect the conductivity of graphene to be zero or infinity and the electrical current to be noiseless. The deviation from these naive expectations, consistent with diffusive transport, is a unique property of the Dirac points, which has been interpreted in terms of the spontaneous creation of virtual electron-hole pairs [30].

Figure 1 shows the conductivity and the Fano factor, as a function of V_0, for two graphene strips, respectively, containing 10 and 20 periods of a potential of the form $V_0 \cos G_0 x$. For finite values of V_0, apart from some resonances which we discuss momentarily, the system behaves diffusively ($F = 1/3$) and the conductivity is well defined. Interestingly, between the peaks the overall scale increases with V_0, showing that the periodic potential tends to enhance the conductivity.

At certain values of V_0 one observes peaks in the conductance, for which the conductivity is not well defined and the Fano factor tends to zero. These resonances occur precisely whenever new zero energy states emerge from the origin in k space, and represent a direct experimental signature of their presence. We believe the resonances occur because the group velocity vanishes when a zero energy state emerges, leading to a strong enhancement of the density of states. A further check that the resonances are associated with the zero energy states is to see that they depend on the ratio V_0/G_0; Fig. 1(c) demonstrates that this is the case not just for the resonances but for the entire conductance curve.

In summary, we have shown that a search for zero energy states in graphene in a periodic potential shows that they may be stabilized for large enough V_0/G_0, and that their presence may be detected in the conductance of the system. The generation of new Dirac points is reported in Ref. [31], which focuses on different properties than the ones described above.

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