Existence and topological stability of Fermi points in multilayered graphene

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We study the existence and topological stability of Fermi points in a graphene layer and stacks with many layers. We show that the discrete symmetries (spacetime inversion) stabilize the Fermi points in monolayer, bilayer and multilayer graphene with orthorhombic stacking. The bands near \( k = 0 \) and \( \epsilon = 0 \) in multilayers with the Bernal stacking depend on the parity of the number of layers, and Fermi points are unstable when the number of layers is odd. The low energy changes in the electronic structure induced by commensurate perturbations which mix the two Dirac points are also investigated.

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I. INTRODUCTION.

The recent synthesis of monolayer graphite [1, 2] (graphene), the experimental ability to manipulate few layer samples [3, 4, 5] and the observations of quasi two dimensional behavior in graphene [6, 7] have awaken an enormous interest in these systems. The conduction band of graphene is well described by a tight binding model which includes the \( \pi \) orbitals which are perpendicular to the plane at each C atom [7, 8]. This model describes a semimetal, with zero density of states at the Fermi energy, and where the Fermi surface is reduced to two inequivalent K-points located at the corners of the hexagonal Brillouin Zone. The low-energy excitations with momenta in the vicinity of any of the Fermi points have a linear dispersion and can be described by a continuum model which reduces to the Dirac equation in two dimensions [9, 10].

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II. ELECTRONIC STRUCTURE AND STABILITY IN GRAPHENE.

The Fermi surface (FS) is a central concept in condensed matter that controls the low-energy physics of the systems. In a Landau Fermi liquid at \( T = 0 \), J. Luttinger [25] defined the FS of an interacting Fermi system in terms of the single-particle Green’s function \( G(\vec{k}, \omega) \), as the solution of the equation \( G^{-1}(\vec{k}, 0) = 0 \) and showed that it encloses the same volume, equal to the fermion density \( n \), as in the noninteracting system. The robustness of the Fermi liquid idea has been understood recently in the context of the renormalization group where the Fermi and Luttinger liquids are seen as infrared fixed points [26, 27]. In recent works [28, 29] Volovik has emphasized the idea of the topological stability of the Fermi surface as the origin of the robustness of the Fermi liquid and has suggested a classification of general fermionic systems in universality classes dictated by momentum space topology. A more recent proposal relates the stability of Fermi surfaces with K-theory, a tool used to classify D-brane charges in string theory [30]. The idea behind the topological stability is to study the zeroes of the matrix \( G_0^{-1}(\vec{k}, \omega) \) (free inverse propagator) that can not be lifted by small perturbations. Here we will analyze the stability of the Fermi points of single and multilayer
electronic excitations behave like massless Dirac fermions with relativistic spectrum $E = \pm |k|$.

Under a $k$-independent, translationally invariant perturbation

$$H(\vec{K}_1 + \vec{\kappa}) \to \begin{pmatrix} a_x & k^* + a^* \\ k & -a_z \end{pmatrix}$$

where $a \equiv a_x + ia_y$, the spectrum becomes $E = \pm \sqrt{a_x^2 + |k + a|^2}$ and a gap $2|a_z|$ is generated. This is consistent with Horava’s general arguments [30], which show that Fermi points for Dirac fermions in two dimensions are unstable. However, this is not the end of the story, since the existence of discrete symmetries can sometimes stabilize the Fermi loci. In the case of the graphene, this role is played by time-reversal $T : t \to -t$ and spatial inversion $I : (x, y) \to (-x, -y)$. The reality of the $\pi$ orbitals implies that time reversal merely reverses $\vec{K}$

$$T \Phi_1(\vec{K}) = \Phi_1^*(\vec{K}) = \Phi_1(-\vec{K})$$

whereas the spatial inversion also exchanges the two types of atoms

$$I \Phi_A(\vec{K}) = \Phi_B(-\vec{K}), \quad I \Phi_B(\vec{K}) = \Phi_A(-\vec{K})$$

Invariance under these symmetries imposes the following constraints on the Hamiltonian

$$T : H(\vec{K}) = H^*(-\vec{K})$$
$$I : H(\vec{K}) = \sigma_x H(-\vec{K}) \sigma_x$$

Although these are useful properties that relate the Hamiltonians at opposite values of $\vec{K}$, what we need is a constraint on the form of $H(\vec{K})$. This is obtained by combining time reversal with the spatial inversion

$$TI : H(\vec{K}) = \sigma_x H^*(-\vec{K}) \sigma_x$$

implying $H_{11}(\vec{K}) = H_{22}(\vec{K})$. This enforces $a_x = 0$ in (3) and we see that no gap opens if the perturbation preserves the space-time inversion $TI$.

This has an interesting topological interpretation, which extends the previous arguments to $k$-dependent—but translationally invariant—perturbations. The low energy Hamiltonian $H(\vec{K}_1 + \vec{\kappa})$ in (2) defines a map from the circle $k_x^2 + k_y^2 = R^2$ to the space of $2 \times 2$ Hamiltonians $H = \vec{h} \cdot \vec{\sigma}$:

$$k = Re^{i\theta} \to (h_x, h_y, h_z) = R(\cos \theta, \sin \theta, 0)$$

Since Fermi points correspond to zeroes of the determinant $-Det(H) = h_x^2 + h_y^2 + h_z^2$, a perturbation will be able to create a gap only if the loop represented by the map (5) is contractible in the space Hamiltonians with non-vanishing determinants, which is just $R^2 - \{0\}$. This is clearly the case, since $\pi_1(R^2 - \{0\}) = \pi_1(S^2) = 0$. On

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**FIG. 1:** (Color online) Direct lattice and unit cell for monolayer graphene.

**FIG. 2:** (Color online) First Brillouin zone and Fermi points. The vectors $\vec{K}_1, \vec{K}_2$ ($\vec{K}_2, \vec{K}_3$) are equivalent to $\vec{K}_1$ ($\vec{K}_2$).
the other hand, hamiltonians invariant under $TI$ are represented by points in $R^2$, and we have

$$\pi_1(R^2 - \{0\}) = \pi_1(S^1) = Z$$

(9)

This means that non-trivial maps such as the ones implied by (2) can only be extended to the interior of the circle by going through the origin, i.e., by having at least one zero. This precludes the creation of a gap.

Note also the maps defined by the low energy hamiltonian in the proximity of the two Fermi points

$$H(\pm \vec{K}_1 + \vec{k}) : k = Re^{i\theta} \rightarrow h_x + ih_y = \pm Re^{\pm i\theta}$$

(10)

have opposite winding numbers $N = \pm 1$, which can be computed by the formula

$$N = \frac{1}{4\pi i} \int_0^{2\pi} d\theta \text{Tr}(\sigma_z H^{-1} \partial_\theta H)$$

(11)

The fact that the two Dirac points carry opposite charges suggests that they could annihilate mutually if brought together by a perturbation. Any external potential commensurate with the honeycomb lattice, which has a finite Fourier component at the wavevector $\vec{G} = \vec{K}_1 - \vec{K}_2$, induces terms which hybridize the two Dirac points and it will lead to the possibility of a gap. We can compute all the possible perturbations which are compatible with the symmetries of the lattice. The most general $(4 \times 4)$ hamiltonian including perturbations at $\vec{G} = 0$ and $\vec{G} = \vec{K}_1 - \vec{K}_2 = -\vec{K}_1$ is:

$$\mathcal{H} = \begin{pmatrix} 0 & k^* + Q_1^* & Q_2 & Q_4 \\ k + Q_1 & 0 & Q_4 & Q_3 \\ Q_2^* & Q_4^* & 0 & -k + Q_1 \\ Q_1^* & Q_3^* & -k^* + Q_1^* & 0 \end{pmatrix}$$

(12)

where $Q_1 = Q_1^* + iQ_1^1$ transforms according to the $E_2$ representation of the $C_{6v}$ symmetry group at the $\Gamma(\vec{K} = 0)$ point. $Q_2$ and $Q_3$ belong to the $E$ representation of the $C_{3v}$ group at $\vec{K}_1$, and $Q_4$ to the $A_1$ representation of the same group (see [33] for notation). At this point it is worth noticing a point on notation. When grouping the hamiltonians attached to the two Dirac points $(K_{1,2})$ into a $4$-dimensional matrix it is a common practice to reverse the order of the sublattices $(A,B)$ in one of the Fermi points in such a way that the $4$-dimensional wavefunctions have the form

$$\psi = (\Phi_{K_1,A} , \Phi_{K_1,B} , \Phi_{K_2,B} , \Phi_{K_2,A})$$

If this is done the topological structure of the hamiltonian is messed up and the computation of charges becomes less clear. For this reason, we follow instead the convention in [21], where

$$\psi = (\Phi_{K_1,A} , \Phi_{K_1,B} , \Phi_{K_2,A} , \Phi_{K_2,B})$$

This is also important if one tries to compare the analysis of the perturbations written in eq. (12) with the ones produced by the different types of disorder [34, 35, 36].

The perturbation given by $Q_1^f$ and $Q_1^o$ shifts the Dirac points, but does not open a gap. In fact, the only parameter which opens a gap is $Q_4$. When only $Q_4$ is different from zero, the spectrum becomes $E = \pm \sqrt{|Q_4|^2 + |k|^2}$ and, for $Q_4$ real, the deformation of the lattice is given in Fig. [3] where one can see that no point symmetry is broken. This shows, in particular, that invariance under space-time inversion is not enough to guarantee the stability of Fermi points — translation invariance plays a crucial role: $TI$ by itself makes de Fermi points individually stable, but they may still annihilate against each other in the presence of a perturbation that breaks translation invariance. A distortion of the type of $Q_4$ can be induced by a substrate with a periodicity commensurate with the lattice, or by the effect of one layer on another when there is a lattice mismatch between them, as in samples grown on a substrate [33]. It can be responsible for the gap observed recently photoemission experiments [38]. It is worth noting that the perturbation denoted here $Q_4$ has been studied in a graphene ribbon in [39].

When only $Q_2$ or $Q_3$ are different from zero, we find:

$$\epsilon_k = \pm \frac{|Q_{2,3}|}{2} \pm \sqrt{\frac{|Q_{2,3}|^2}{4} + |k|^2}$$

(13)

The energy bands are represented in Fig. [4] for the particular case $Q_2 = 0, Q_3 = 1$. We can see that the spectrum is the same as the one obtained in a simple model for a bilayer system [40], which will be discussed later. A complete analysis of the most general perturbation of the form (12) will be given elsewhere [31].

In the absence of time reversal symmetry, other perturbations are possible, such as

$$\delta H = B_1 \sigma_z \tau_z + B_2 \sigma_y \tau_y$$

(14)

where $\sigma$ and $\tau$ are Pauli matrices whose entries are the sublattice and K point indices respectively, and $B_1$ and $B_2$ transform like the $z$ component of a magnetic field and are odd under time inversion. Note that the first term is the orbital part of the intrinsic spin orbit coupling in graphene [21, 22, 23, 24], and it opens a gap. The second term should appear in a general spin orbit hamiltonian which takes into account the coupling between the two $K$ points.
III. ELECTRONIC STRUCTURE AND STABILITY IN MULTILAYERED GRAPHENE.

The case of the multilayer is more interesting. We will concentrate on the ability of the TI invariance to prevent the creation of a gap. For the sake of definiteness, only staggered (ABA) and rhombohedral (ABC) stacking will be considered. The relative orientations of the ABC planes are sketched in Fig. 5. The two inequivalent atoms in layer \( n \) will be denoted \( (A_n,B_n) \). Our conventions are such that the couplings of an \( A_n \) (\( B_n \)) atom to the three in-plane nearest neighbors are shaped as a \( Y \) (inverted \( Y \)), independently of \( n \). Thus, the low energy limit of the “free” hamiltonian obtained by neglecting inter-layer couplings is block-diagonal, with \( 2 \times 2 \) blocks given by (2).

The simplest model introduces interlayer hoppings \( t \) only between nearest neighbors. The resulting hamiltonian for bilayer graphene in the vicinity of the \( K_1 \) Fermi point is

\[
\mathcal{H}(k) = \begin{pmatrix}
0 & k^* & 0 & t \\
0 & k & 0 & 0 \\
0 & 0 & 0 & k^* \\
t & 0 & k & 0 \\
\end{pmatrix}
\]

and the energy bands are given by (13) with the replacement \( Q_{2,3} = \rightarrow t \). In the limit \( E \ll t \), one can obtain an effective hamiltonian \( H_{\text{eff}} \) for the lowest energy bands. To this end, reorder the wavefunctions according

\[
(A_1, B_1, A_2, B_2) \rightarrow (A_2, B_1, A_1, B_2),
\]

so that in the new basis the hamiltonian becomes

\[
\mathcal{H}(k) = \begin{pmatrix}
0 & 0 & 0 & k^* \\
0 & k & 0 & 0 \\
k^* & 0 & t & 0 \\
t & k & 0 & 0 \\
\end{pmatrix}
= \begin{pmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22} \\
\end{pmatrix}
\]

where \( H_{ij} \) is a \( 2 \times 2 \) block. The identity

\[
\text{Det}(\mathcal{H} - E) = \text{Det}\left( H_{11} - H_{12}(H_{22} - E)^{-1}H_{21} - E \right) \text{Det}(H_{22} - E)
\]

shows that, for \( E \ll t \), the substitution \( H_{22} - E \rightarrow H_{22} \) reduces the computation of the lowest energy bands to the diagonalization of the \( 2 \times 2 \) effective hamiltonian

\[
\mathcal{H}_{\text{eff}} \equiv H_{11} - H_{12}H_{22}^{-1}H_{21} = -\frac{1}{t} \begin{pmatrix}
0 & k^{*2} \\
k^2 & 0 \\
\end{pmatrix}
\]

This effective hamiltonian involves only the atoms \( (A_2,B_1) \), which are not linked by \( t \) and give rise to bands with zero energy at the Fermi points. Since \( (A_2,B_1) \) are interchanged under spatial inversion \( \vec{r} \rightarrow -\vec{r} \), the combined TI-invariance imposes a constraint \( \mathcal{H}_{\text{eff}}(k) = \sigma_x \mathcal{H}_{\text{eff}}^*(k) \sigma_x \) identical to (7). This implies \( H_{11}^{\text{eff}}(k) = H_{22}^{\text{eff}}(k) \), which shows that no gap can open. According to (11) the topological charge for the \( K_1 \) Fermi point is +2 and, by time reversal invariance, the charge for \( -\vec{K}_1 \) is −2. Thus, as in the case of monolayer graphene, the Fermi points are stable under perturbations that preserve TI and translation invariance. For instance, a perturbation like trigonal warping \( \varepsilon \) changes the off diagonal elements in eq. (13), \( k^2 \rightarrow k^2 + \varepsilon k^* \) and splits the Fermi point of charge \( Q = +2 \) into three Dirac points away from the \( K \) point, and charge \( Q = +1 \), and another Dirac point at the \( K \) point and \( Q = -1 \), but the total charge is conserved and no gap opens. However, a perturbation hybridizing \( \vec{K}_1 \) and \( -\vec{K}_1 \) or one breaking TI might lead to a gapped system with no Fermi points at all. A physical example is provided by the experiment described in [15] where a gap is controlled by changing the carrier concentration in each layer.

This analysis can be easily generalized to multilayer graphene with rhombohedral stacking. This type of stacking includes the links \( (B_1-A_2,B_2-A_3,\ldots,B_{N-1}-A_N) \) and the effective hamiltonian, which involves only the unlinked atoms \( (A_1,B_N) \), is given by

\[
\mathcal{H}_{\text{eff}} = -\frac{1}{t^{N-1}} \begin{pmatrix}
0 & k^{*N} \\
k^{N} & 0 \\
\end{pmatrix}
\]

The topological charge for the \( \vec{K}_1 \) (\( -\vec{K}_1 \)) Fermi point is +\( N \) (−\( N \)). As the point group for multilayer graphene with rhombohedral stacking is \( D_{3d} \), which contains the inversion \( I \), the system is invariant under TI, which interchanges \( (A_1,B_N) \), and the whole argument goes through as before. Thus we conclude that the Fermi points for
multilayer graphene with rhombohedral stacking are stable against perturbations that respect $TI$ and translation invariance.

The situation is very different for $ABA$ stacking. An $N$-layer graphene stack is invariant under the spatial inversion $I$ only for even $N$, where the point group is $D_{3d}$, while it is $D_{3h}$ for odd $N$.

The $2N$ eigenstates in a stack with $N$ layers at $k = 0$ can be divided into two sets: $N$ states at the orbitals connected by the interlayer hopping $t$, and $N$ states in the other sublattice sites of each layer. If we only consider the hopping $t$, the first $N$ states acquire a dispersion [91], lying in the range $-2t \leq \epsilon \leq 2t$. The other $N$ states are degenerate with $\epsilon = 0$. A perturbation compatible with all the symmetries of the stack is a layer dependent shift of the onsite energies. This shift can be arbitrary, except for the twofold degeneracy related with the equivalence between layers which are symmetrically placed around the center, $\epsilon_n = \epsilon_{N-n+1}$. This is illustrated in Fig. 6.

The results in Fig. 6 show a gap at half filling in the stack with four layers, and overlapping bands at all energies for the stack with eight and nine layers. Note that the gap in the stack with four layers does not require the existence of an external electric field, which will break the equivalence of the layers at opposite sides of the stack. In all stacks with an even number of layers, the two bands which start at the onsite energy of layers $n$ and $N - n + 1$ are degenerate at $k = 0$. The effective $2 \times 2$ Hamiltonian describing the bands near these degeneracy points have off-diagonal elements with a non-trivial phase as in eq. [18]. Hence, the degeneracy has topological charge $Q = 2$, and it cannot removed by perturbations compatible with the symmetries of the stack. For even $n$, an explicit computation shows that these two bands will have curvatures with the same sign near $k = 0$. Thus, the corresponding degeneracy points do not represent Fermi points. For odd numbered layers, the two bands disperse in opposite directions away from $k = 0$, and the degeneracy points become stable Fermi points at the appropriate doping.

Note that the symmetries of the system allow for a direct trigonal-like coupling between the two layers, which will split this Fermi point and give rise to four Fermi points showing linear dispersion, as in the bilayer. On physical grounds, this coupling will be negligible, unless the two layers are contiguous.

The low energy bands in a stack with an odd number of layers also contain doubly degenerate states at $k = 0$, associated to the equivalence between layers at opposite sides of the stack. But in this case the inversion $I$ is not part of the symmetry group $D_{3h}$ of the stack, no invariance under $TI$ can be imposed and, as a consequence, the first homotopy group $\pi_1$ is trivial. This means that no conserved topological charge exists. Hence, a gap may open at $k = 0$ when other perturbations consistent with the symmetries of the stack are included. Concretely, a direct coupling between orbitals in the same sublattice in layers separated by an odd number of other layers will open a gap. Such a coupling, between layers which are second nearest neighbors, has been proposed in graphite [12].

![Fig. 6: (Color online) Energy bands close to $\epsilon = 0$ for a stack with 4 layers (left), 8 layers (center), and 9 layers (right). All stacks have the Bernal stacking. The Fermi velocity is $v_F = 1$, $t = 0.1$ and a layer dependent shift has been included: $\epsilon_n \equiv \{0.02, 0.01\} \ (left)$, $\epsilon_n \equiv \{0.02, 0.01, 0.005, 0.002\} \ (center)$, and $\epsilon_n \equiv \{0.02, 0.01, 0.005, 0.002, 0\} \ (right)$.](image)

IV. CONCLUSIONS.

We have presented a classification of the bands at low momenta and low energy of graphene layers and stacks with many layers.

Each Fermi point in single layer graphene is stable against perturbations which preserve the discrete $TI$ symmetry, and which do not mix the two Fermi points. A magnetic field, for instance, induces a gap in the spectrum, see eq. [17]. This term arises from the discreteness of the lattice, and it should be of higher order than the minimal coupling which leads to the formation of Landau levels. Combining this and dimensional arguments, we expect it to be $B_1 \propto v_F / l_B \times (a / l_B)$, where $a$ is the lattice constant, and $l_B = \sqrt{(eB)/(c\Phi_0)}$ is the cyclotron radius. Thus, for $B \sim 10^4$, we have $B_1 \approx 0.1\text{meV}$.

We have also classified the long wavelength perturbations commensurate with the graphene lattice, which can hybridize the two $K$ points. Some of these perturbations open a gap in the spectrum, while others shift the position of the Dirac points. We expect that their strength will decay like a power law with the wavelength of the distortion.

The low energy and low momentum spectrum of stacks with many graphene layers depend on the stacking order and the number of layers. For the most common case of the Bernal stacking, we find that layer dependent onsite energies lead to Fermi points with double degeneracy, topological charge $Q = \pm 2$, and a parabolic dispersion in $k$. This situation will be stable in stacks with a large...
with a large topological charge, Stacks with rhombohedral order lead to degenerate states. This degeneracy will be broken by additional interactions. The most likely origin of the inequivalence between layers is the charge accumulation at the layers close to the surface. An induced doping of $10^{10} - 10^{12}$ cm$^{-2}$ gives rise to shifts in the local potential of 0.01 – 0.1 eV, so that the splittings associated to this effect can be easily measurable. We find that a true gap opens, in the absence of an external field which breaks spatial inversion, only in a stack with four layers and Bernal stacking. Finally, stacking defects, which break the equivalence between pairs of layers, will also break the degeneracy of all bands at $k = 0$.

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