

Symmetry Classification of Energy Bands in Graphene and Silicene

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ABSTRACT

We present the results of the symmetry classification of the electron energy bands in graphene and silicene using group theory algebra and the tight-binding approximation. The analysis is performed both in the absence and in the presence of the spin-orbit coupling. We also discuss the bands merging in the Brillouin zone symmetry points and the conditions for the latter to become Dirac points.

Keywords: Graphene; Silicene; Group Theory; Dirac Points

1. Introduction

Since graphene was first isolated experimentally [1], it is in the focus of attention of both theorists and experimentalists. Obviously, understanding of the symmetries of the electrons dispersion law in graphene is of crucial importance. Actually, the symmetry classification of the energy bands in graphene (or “two-dimensional graphite”) was presented nearly 60 years ago by Lomer in his seminal paper [2]. Later the subject was analyzed by Slonczewski and Weiss [3], Dresselhaus and Dresselhaus [4], Bassani and Parravicini [5]. Recent approaches to the problem are presented in the papers by Malard *et al.* [6], Manes [7] and in our publication [8].

The present work has two aspects: a pragmatic and a pedagogical one. The first aspect is connected with the recent synthesis of silicene, the counterpart of graphene for silicon, with buckled honeycomb geometry. This novel two-dimensional material has attracted recently considerable attention, both theoretically [9,10] and experimentally, due to its exotic electronic structure and promising applications in nanoelectronics as well as its compatibility with current silicon-based electronic technology. So we present the symmetry analysis of the silicene electron bands.

The pedagogical aspect is connected with the fact that different approaches to the symmetry classification, even if giving the same results, are based on different methods of applications of group theory. Thus in our previous paper [8] the labeling of the bands was based on com-

patibility relations and guesses. In the present work we show that in the framework of the tight-binding approximation the representations of the little group in the symmetry points can be rigorously found in the framework of the group theory algebra. Though the idea of using the tight-binding approximation is by no means new (it was used already in the work by Lomer), our mathematical approach is totally different, as one can easily see comparing the present work with [2], and, to our opinion, more convenient for applications. This statement is supported by the analysis of the symmetry of the energy band in silicene.

We also generalize the symmetry classification by taking into account the spin-orbit coupling both for graphene and for silicene. This, to the best of our knowledge, wasn't done before even for graphene. Though in graphene the spin-orbit coupling is very weak, the problem is interesting in principle. One can expect that in silicene the coupling is stronger, and it will become even more so for graphene related materials from heavier elements, provided they can be synthesized.

To remind to a reader a few basic things, important for the symmetry classification of the bands in any crystal, consider a point sub-group R of the space group characterizing the symmetry of a crystal (we restrict ourselves with the consideration of symmorphic space groups). Any operation of the group R (save the unit transformation) takes a general wavevector \mathbf{k} into a distinct one. However, for some special choices of \mathbf{k} some of the operations of the group R will take \mathbf{k} into itself rather than into a distinct wavevector. These particular operations are called the

group of \mathbf{k} ; it is a subgroup of the group R . Points (lines) in the Brillouin zone for which the group of the wavevector contains elements other than the unit element are called symmetry points (lines). We may use a state (states) corresponding to such a special wavevector to generate a representation for the group of \mathbf{k} [11,12]. In this paper we consider crystals with the hexagonal Brillouin zone. In this case the symmetry points are Γ —the center of the Brillouin zone, the points K which are corners of the Brillouin zone and the points M which are the centers of the edges of the Brillouin zone.

2. Tight-Binding Model

We'll deal with the materials with a basis of two atoms per unit cell, and we'll search for the solution of Schrodinger equation as a linear combination of the functions

$$\psi_{\beta,\mathbf{k}}^j = \sum_{\mathbf{R}_j} \psi_{\beta}(\mathbf{r} - \mathbf{R}_j) e^{i\mathbf{k}\cdot\mathbf{R}_j}, \quad (1)$$

where ψ_{β} are atomic orbitals, $j = A, B$ labels the sublattices, and \mathbf{R}_j is the radius vector of an atom in the sublattice j .

A point symmetry transformation of the functions $\psi_{\beta,\mathbf{k}}^j$ is a direct product of two transformations: the transformation of the sub-lattice functions $\phi_k^{A,B}$, where

$$\phi_k^j = \sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j}, \quad (2)$$

and the transformation of the orbitals ψ_{β} . Thus the representations realized by the functions (1) will be the direct product of two representations. Generally, these representations will be reducible. To decompose a reducible representation into the irreducible ones it is convenient to use equation

$$a_{\alpha} = \frac{1}{g} \sum_G \chi(G) \chi_{\alpha}^*(G), \quad (3)$$

which shows how many times a given irreducible representation α is contained in a reducible one [13]. Additional information about the representations can be obtained if we use projection operator [14]

$$O_{\alpha} = \frac{n_{\alpha}}{g} \sum_G \chi_{\alpha}^*(G) P(G), \quad (4)$$

where n_{α} is the dimensionality of the irreducible representation α and $P(G)$ is the operator corresponding to a transformation G . The operator projects a given function to the linear space of the representation α . For a one dimensional representation the operator thus gives basis of the representation.

3. Group Theory Analysis in the Tight-Binding Model without the Spin-Orbit coupling

Our tight-binding model space includes four atomic or-

bitals: $|s, p\rangle$. Notice that we assume only symmetry of the basis functions with respect to rotations and reflections; the question how these functions are connected with the atomic functions of the isolated carbon atom is irrelevant.

3.1. Graphene

The Hamiltonian of graphene being symmetric with respect to reflection in the graphene plane, the bands built from the $|z\rangle$ orbitals decouple from those built from the $|s, x, y\rangle$ orbitals. The former are odd with respect to reflection, the latter are even. In other words, the former form π bands, and the latter form σ bands.

The group of wave vector \mathbf{k} at the point Γ is D_{6h} , at the point K is D_{3h} , at the lines Γ - K is C_{2v} [8,15]. The representations of the groups D_{3h} and D_{6h} can be obtained on the basis of identities

$$D_{3h} = D_3 \times C_s, \quad D_{6h} = C_{6v} \times C_s. \quad (5)$$

the irreducible representations of the group D_3 are presented in the **Table 1**. Each representation of the group, say A_1 , begets two representations of the group D_{3h} : A_1' and A_1'' ; prime means that the representation is even with respect to reflection σ_h , double prime means that it is odd.

The irreducible representations of the group C_{6v} are presented in the **Table 2**. Because the inversion transformation I can be presented as

$$I = C_2 \sigma_h, \quad (6)$$

the representations of the group D_{6h} can be classified as symmetric (g) or antisymmetric (u) with respect to inversion. Thus each representation of the group C_{6v} , say A_1 , begets two representations of the group D_{6h} : A_{1g} and A_{1u} .

Notice that the orbitals $|s\rangle$ (or $|z\rangle$) realize A_1 representation both of the group D_3 and of the group C_{6v} , hence the representations of the groups realized by the functions $\psi_{s,z;\mathbf{k}}^{A,B}$ will be identical to those realized by the sub-lattice functions $\phi_k^{A,B}$.

Let us start from the symmetry analysis at the point Γ . Because the transformations C_2, C_6, σ_v change sublattices, the characters corresponding to these transfer of the group C_{6v} .

Table 1. Characters table for irreducible representations of D_3 point groups.

D_3	E	$2C_3$	$3C_2$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table 2. Characters table for irreducible representations of C_{6v} point group.

C_{6v}	E	C_2	$2C_3$	$2C_6$	$2\sigma_v$	$3\sigma_v'$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	-1	-1
B_2	1	-1	1	-1	1	-1
B_1	1	-1	1	-1	-1	1
E_2	2	2	-1	-1	0	0
E_1	2	-2	-1	1	0	0

Motions are equal to zero. The transformations E, C_3, σ_v' leave the sub-lattices as they were. Hence from **Table 2**, we see that the functions $\phi_0^{A,B}$ realizes reducible representation

$$R_\Gamma = A_1 + B_2 \quad (7)$$

Taking into account the symmetry of the states relative to reflection in the plane of graphene, we obtain that at the point Γ the functions ψ_z (here and further on, when this is not supposed to lead to a misunderstanding, we'll suppress the index \mathbf{k} in $\psi_{\beta,\mathbf{k}}$) realize A_{1u} and B_{2g} representations of the group D_{6h} , characterizing π band; the functions ψ_s realize A_{1g} and B_{2u} representations of the group D_{6h} , characterizing σ band.

Acting by projection operators O_A and O_B on a function ψ^j , we obtain that the irreducible representation A_1 is realized by symmetric combination of the A and B orbitals, and the irreducible representation B_2 by the antisymmetric combination. One can expect that the first case occurs in the hole band, and the second in the electron band.

The orbitals $|x, y\rangle$ realize representation E_1 of the group C_{6v} [13]. Hence, representation of the group realized by the functions $\psi_{x,y}^{A,B}$ can be decomposed as

$$E_1 \times R_\Gamma = E_1 + E_2. \quad (8)$$

Taking into account the symmetry of the states relative to reflection in the plane of graphene, we obtain that at the point Γ the functions $\psi_{x,y}$ realize E_{1u} and E_{2g} representations of the group D_{6h} , characterizing σ bands.

To find wavefunctions, realizing each of the irreducible representations, we apply the projection operators and obtain

$$O_{E_1} \psi_\pm^j \square \psi_\pm^j + \psi_\pm^{\bar{j}}, \quad O_{E_2} \psi_\pm^j \square (\psi_\pm^j - \psi_\pm^{\bar{j}}), \quad (9)$$

where $\bar{j} = B$ if $j = A$, and vice versa. Thus representation $E_1 (E_2)$ is realized by symmetric (antisymmetric) combinations of $|x, y\rangle$ orbitals. One can expect that the first representation is realized at the hole band, and the

second at the valence band.

Now let us perform the symmetry analysis at the point K . The representation of the group realized by the functions $\phi_K^{A,B}$ is determined by the transformation law of the exponentials $e^{i\mathbf{K}\cdot\mathbf{R}_j}$ under the symmetry operations. Rotation of the radius vector by the angle $2\pi/3$ anticlockwise, is equivalent to rotation of the vector \mathbf{K} in the opposite direction, that is to substitution of the three equivalent corners of the Brillouin zone:

$\mathbf{K} \rightarrow \mathbf{K}_2 \rightarrow \mathbf{K}_3 \rightarrow \mathbf{K}$, where

$$\mathbf{K} = (2\pi/3a, 2\pi/3\sqrt{3}a), \quad \mathbf{K}_2 = (0, -4\pi/3\sqrt{3}a) \quad \text{and}$$

$\mathbf{K}_3 = (-2\pi/3a, 2\pi/3\sqrt{3}a)$. The rotation multiplies each basis vector by the factor $e^{2\pi i/3}$. Using Equation (3), we obtain

$$a_E = (1/3)(2 - e^{2\pi i/3} - e^{-2\pi i/3}) = 1. \quad (10)$$

Hence, the functions $\phi_K^{A,B}$ realize irreducible representation E of the group D_3 .

Taking into account the symmetry of the states relative to reflection in the plane of graphene, we obtain representation E'' of the group D_{3h} , realized by the ψ_z functions (merging π bands), and representation E' , realized by the ψ_s functions, characterizing σ bands.

The orbitals $|x, y\rangle$ realize representation E of the group D_3 [13]. Hence, representation of the group realized by the quartet of functions $\psi_{x,y}^{A,B}$ can be decomposed as

$$E \times E = A_1 + A_2 + E. \quad (11)$$

taking into account the symmetry of the states relative to reflection in the plane of graphene, we obtain representations A_1' , A_2' and E' of the group D_{3h} , realized by the $\psi_{x,y}$ functions, characterizing σ bands.

Acting by projection operators, we obtain that the representation A_1 is realized by the vector space with the basis vector $\psi_+^A + \psi_-^B$, and the representation A_2 is realized by the vector space with the basis vector $\psi_-^A - \psi_+^B$. The vector spaces realizing representations A_1 and A_2 being found, the representation E is obviously realized by the vector space spanned by the vectors $\psi_+^A - \psi_-^B, \psi_-^A + \psi_+^B$.

Because the irreducible representation E' is realized both by ψ_s and $\psi_{x,y}$ functions, these representations should be considered together. According to Wigner theorem [16] we still have two E' representations, each of them being realized by two functions from a quartet $\psi_s^A, \psi_s^B, \psi_+^A - \psi_-^B, \psi_-^A + \psi_+^B$. Each E' representation characterizes two σ bands, merging at the point K .

The symmetry of the electron bands at the points Γ and K being determined, the symmetry at the lines $\Gamma-K$ follows unequivocally from the compatibility relations, presented in **Table 3** [8,13]. The table shows

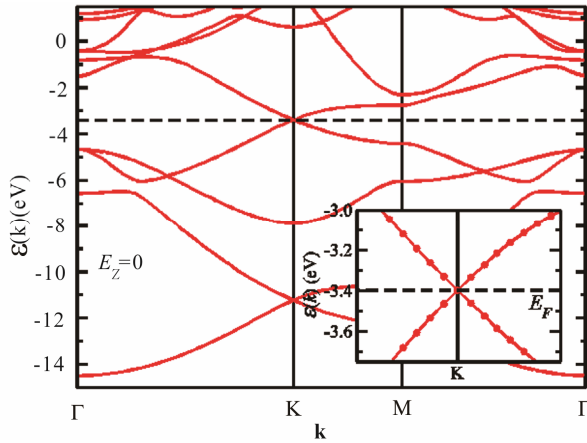


Figure 2. (Color online) DFT-PBE band structures for silicene. The dashed line shows the Fermi energy and the insets show the spectrum near the Fermi level in the vicinity of the K point [reproduced from [10] with permission].

lattice functions (2) remain the same. However, instead of atomic orbitals we should consider atomic terms. So for the case of sp hybridization, β enumerates states from doublets $|s, p\rangle^{(1/2)}$ and quartet $|p\rangle^{(3/2)}$.

Due to the semi-integer value of the angular momentum J we have to consider double-valued representations realized by the atomic terms (and by the crystal wave functions). We remind that in this case it is convenient to introduce the concept of a new element of the group (denoted by Q); this is a rotation through an angle 2π about an arbitrary axis, and is not the unit element, but gives the latter when applied twice: $Q^2 = E$.

The characters of the rotation by angle ϕ applied to the term $|\cdot\rangle^{(j)}$ is

$$\chi^j(\phi) = \sin\left(J + \frac{1}{2}\right)\phi / \sin\frac{1}{2}\phi. \quad (16)$$

With respect to the inversion I the character is

$$\chi^j(I) = \pm(2J+1), \quad (17)$$

where the sign plus corresponds to the s states, and the sign minus to the p states. Finally, the characters corresponding to reflection in a plane σ and rotary reflection through an angle ϕ are found writing these symmetry transformations as

$$\sigma = IC_2, \quad S(\phi) = IC(\phi + \pi). \quad (18)$$

Both in graphene and in silicene we'll restrict ourselves by the symmetry analysis at the point K .

4.1. Graphene

The sub-lattice functions $\phi_K^{A,B}$ realize E_g representation of point group D_{3h} . The electron terms realize two-valued representations of the group, which are presented in **Table 5** [17].

Doublet $|s\rangle^{(1/2)}$ realizes Γ_7 representation of the group; doublet $|p\rangle^{(1/2)}$ realizes Γ_8 representation, quartet $|p\rangle^{(3/2)}$ realizes Γ_7 representation twice (We decided to use chemical notation for the single-valued representation, and BSW notation for double-valued representations [9]). The sub-lattice functions realize representation E_g ; from Equation (3) we obtain

$$\Gamma_7 \times E_g = \Gamma_8 \times E_g = \Gamma_7 + \Gamma_8. \quad (19)$$

Thus at the point K four bands realize representation Γ_7 of the group D'_3 each, and four bands realize representation Γ_8 each. In particular, we obtained the (well known) result that the four-fold degeneracy (including spin) of the bands merging at the point K is partially removed by the spin-orbit coupling, and only two-fold (Kramers) degeneracy is left.

4.2. Silicene

The two-valued representations of D'_3 are presented in **Table 6** [17]. Each of the doublets $|s, p\rangle^{(1/2)}$ realizes Γ_4 representation of the group. Quartet $|p\rangle^{(3/2)}$ realizes this representation twice. The sub-lattice functions realize representation E of the group. From Equation (3) we obtain

$$\Gamma_4 \times E = \Gamma_4 + \Gamma_5 + \Gamma_6. \quad (20)$$

(For the same reasons as for ordinary representations, two complex conjugate two-valued representations $\Gamma_5 + \Gamma_6$ must be regarded as one physically irreducible representation of twice the dimension).

Thus at the point K four bands which realize representation Γ_4 of the group D'_3 each, and four bands realize representation $\Gamma_5 + \Gamma_6$ each.

5. Dirac Points

In this final part of the paper we would like to clarify the relation between the symmetry and the existence of dirac points.

According to the classical approach [18,19], the merging of the bands at a point k_0 is connected with the multi (higher than one)-dimensional representation of the space group G_0 , realized in this point. Looking for a linear dispersion point in the vicinity of the merging point we may use the degenerate $k \cdot p$ perturbation theory. Let a two-dimensional irreducible representation is realized at a point k_0 . Expanding the wavefunction with respect to the basis of the representation

$$\psi(k) = \sum_{i=1}^2 c_i(k) \psi_i(k_0), \quad (21)$$

for the expansion coefficients we obtain equation in the form

Table 3. Characters for two-valued irreducible representations of group D'_{3h} .

D'_{3h}	E	Q	σ_h	C_3	C_3^2	S_3	S_3^2	$3U_2$	$3\sigma_v$
			$\sigma_h Q$	$C_3 Q$	$C_3^2 Q$	$S_3^2 Q$	$S_3 Q$	$3U_2 Q$	$3\sigma_v Q$
Γ_7	2	-2	0	1	-1	$\sqrt{3}$	$-\sqrt{3}$	0	0
Γ_8	2	-2	0	1	-1	$-\sqrt{3}$	$-\sqrt{3}$	0	0
Γ_9	2	-2	0	-2	2	0	0	0	0

Table 4. Characters for two-valued irreducible representations of group D' .

Rep	E	Q	C_3	C_3^2	$3U_2$	$3U_2 Q$
			$C_3^2 Q$	$C_3 Q$		
Γ_5	1	-1	-1	1	i	$-i$
Γ_6	1	-1	-1	1	$-i$	i
Γ_4	2	-2	1	-1	0	0

$$\sum_{j=1}^2 \frac{\mathbf{k} \cdot \mathbf{p}_{ij}}{m} c_j(\mathbf{k}) = \varepsilon(\mathbf{k}) c_i(\mathbf{k}), \quad (22)$$

where $p_{ij} = \langle \psi_i(k_0) | p | \psi_j(k_0) \rangle$ (of course, we need the absence of inversion symmetry at the point, for the matrix elements to be different from zero). The dispersion law is given by the equation

$$\varepsilon(\mathbf{k}) = \sum_{\alpha} a_{\alpha} k_{\alpha} \pm \sqrt{\sum_{\alpha\beta} \gamma_{\alpha\beta} k_{\alpha} k_{\beta}} \quad (23)$$

where α, β are cartesian indexes x, y . Equation (24) should contain only combinations of wavevector components which are invariant with respect to all elements of the group G_0 . In the case when the group G_0 does not have any vector invariants, and the only tensor invariant is the quantity $k_x^2 + k_y^2$, we obtain the dispersion law

$$\varepsilon(\mathbf{k}) = \pm v k, \quad (24)$$

which, like it was shown by Dirac himself in 1928, guarantees that Equation (25) is Dirac equation, in the sense the the matrices p_x and p_y satisfy anticommutation relations

$$p_x^2 = p_y^2 \propto I, \quad \{p_x, p_y\}_+ = 0, \quad (25)$$

where I is the unity matrix.

To be more specific, consider the groups of wavevector at the point Γ ; in graphene it is D_{3h} , and in silicene it is D_3 . In both cases, to find the dispersion law at the point Γ it is enough to study invariants of the group D_3 . And we can easily check up that both conditions, necessary for the existence of the Dirac point, are satisfied. This explains, in particular, why the band calculations show the existence of Dirac points in silicene [9,10], which has a

lower symmetry than graphene.

In general, the role of the tight binding approximation in symmetry classification of the bands in graphene, like its role in symmetry classification of bands in other crystals, is only auxiliary. The approximation greatly helps in the classification and sheds additional light on the nature of the bands. but one must remember that there are more important things that this or that approximation and this is symmetry.

6. Conclusion

This paper presents an applications of group theory to very important cases of graphene and silicene.

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