

Symmetry classification of energy bands in graphene

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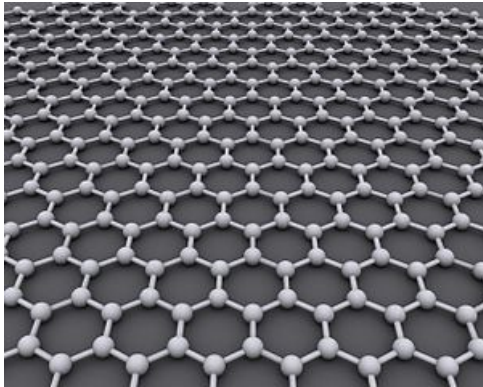
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E. Kogan and V. U. Nazarov,
SYMMETRY CLASSIFICATION OF ENERGY BANDS IN GRAPHENE,
Phys. Rev. B **85**, 115418 (2012).

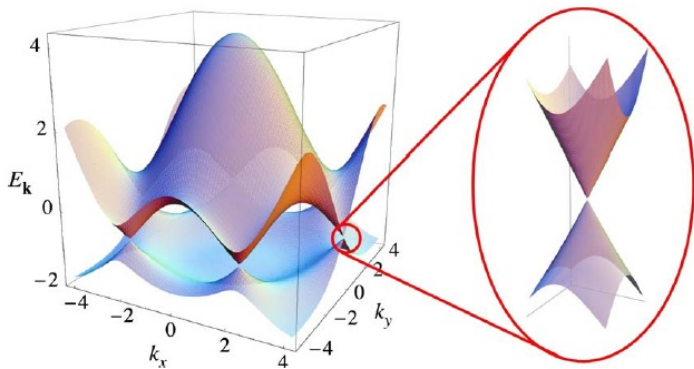
E. Kogan,
SYMMETRY CLASSIFICATION OF ENERGY BANDS IN GRAPHENE: TIGHT-BINDING MODEL AND SPLITTING OF DEGENERACIES BY SPIN-ORBIT COUPLING,
arXiv:1203.4492.

INTRODUCTION
GROUP THEORY
LCAO
BANDS MERGING FOREVER
Dirac Hamiltonian
SPIN-ORBIT COUPLING
CONCLUSIONS

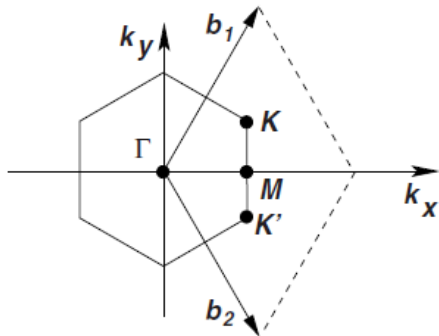
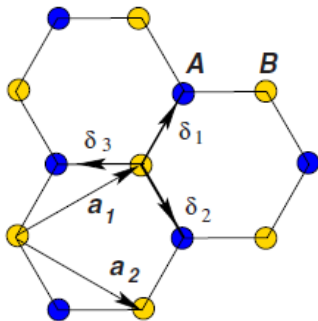
Graphene 2004



Electronic dispersion in the honeycomb lattice

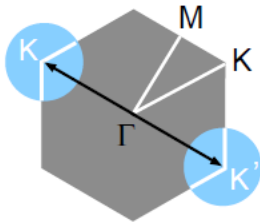


Graphene sublattices and Brillouin zone



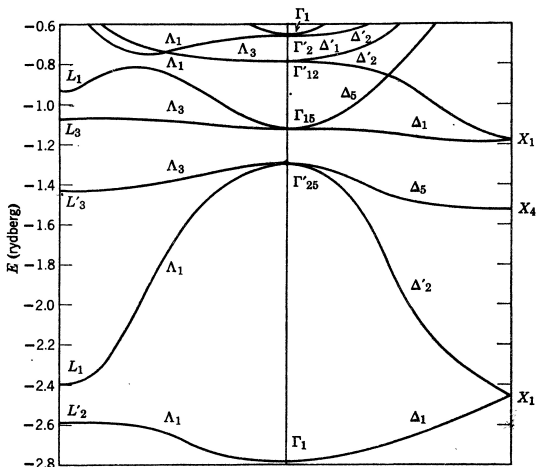
Bands merging

The merging π and π^* bands at the point K was explained using a lot of different approaches.

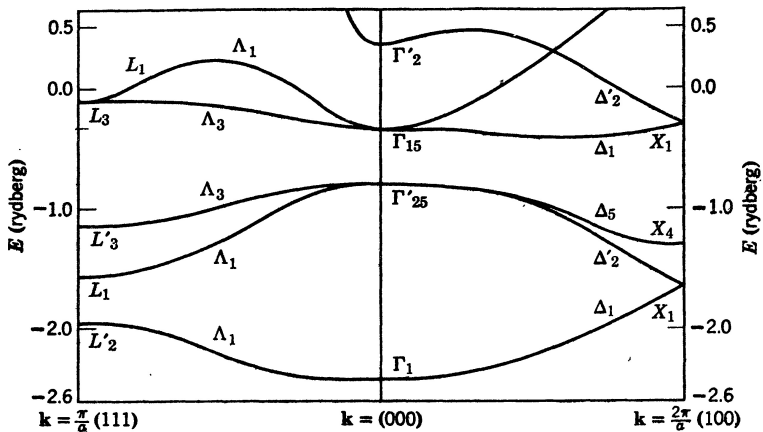


However, the merging at the point K of the σ bands somehow was not paid enough attention to.

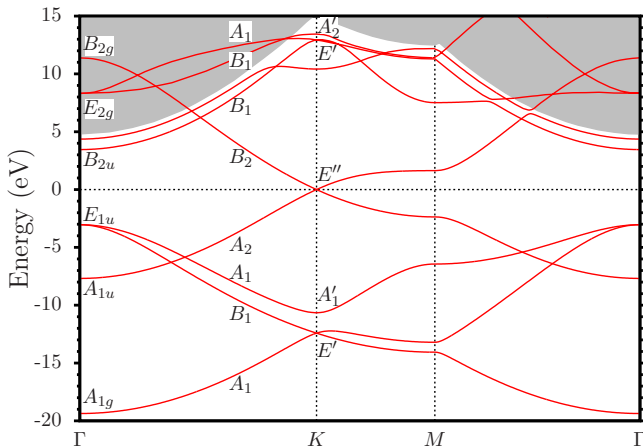
Energy bands of silicon



Energy bands of diamond



Energy bands of graphene



Symmetry types at the point Γ of cubic lattice

SYMMETRY TYPES AT POINTS Γ , R , H OF CUBIC LATTICES

Notation

BSW	LB	Chem	Basis Functions
Γ_1	α	A_{1g}	1
Γ_2	β'	A_{2g}	$x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2)$
Γ_{12}	γ	E_g	$\{z^2 - \frac{1}{2}(x^2 + y^2), (x^2 - y^2)\}$
Γ_{15}'	δ'	T_{1g}	$\{xy(x^2 - y^2), yz(y^2 - z^2), zx(z^2 - x^2)\}$
Γ_{25}'	ϵ	T_{2g}	$\{xy, yz, zx\}$
Γ_1'	α'	A_{1u}	$xyz[x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2)]$
Γ_2'	β	A_{2u}	xyz
Γ_{12}'	γ'	E_u	$\{xyz[z^2 - \frac{1}{2}(x^2 + y^2)], xyz(x^2 - y^2)\}$
Γ_{15}	δ	T_{1u}	$\{x, y, z\}$
Γ_{25}	ϵ'	T_{2u}	$\{z(x^2 - y^2), x(y^2 - z^2), y(z^2 - x^2)\}$

Note: BSW \equiv Bouckaert, Smoluchowski, and Wigner, *Phys. Rev.* **50**, 58(1936).

LB \equiv Von der Lage and Bethe, *Phys. Rev.* **71**, 612(1947).

Chem \equiv used by most chemists; also in the text by Heine,

Little group (group of the wavevector)

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 crystal symmetry group 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).

Small representation

Suppose that the states $\phi_{\mathbf{k}\mu}$ of a given \mathbf{k} are degenerate in energy: the operations of the group of \mathbf{k} transform $\phi_{\mathbf{k}\mu}$ into a $\phi_{\mathbf{k}\lambda}$ with the same \mathbf{k} , and the ϕ 's are said to form a representation of the group of \mathbf{k} . The representation is known as the small representation.

Point groups

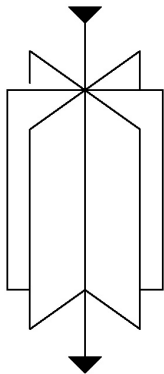
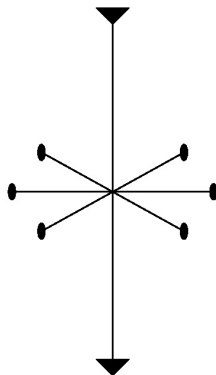
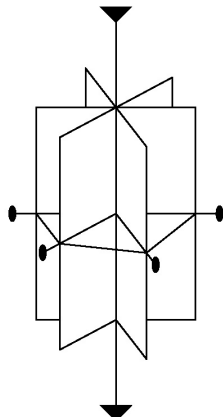
The group C_{nv} contains $2n$ elements: n rotations about an axis of the n th order and n reflections σ_v in the vertical planes.

The group C_i (S_2) contains only two elements: E and I .

The group C_s (C_{1h}) contains only two elements: E and σ_h .

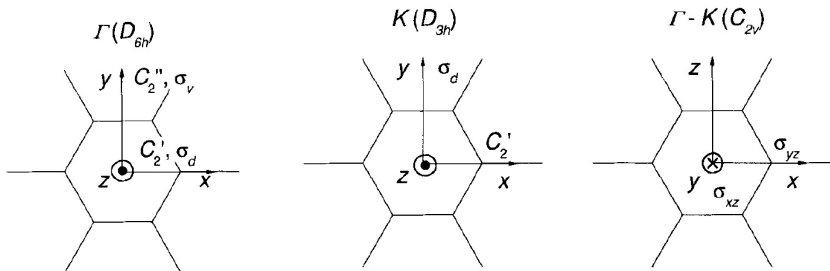
The group D_n contains $2n$ elements: n rotations about an axis of the n th order and n rotations through an angle π about horizontal axes.

The group D_{nh} contains $4n$ elements: besides the $2n$ elements of the group D_n it contains also n reflections σ_v and n rotary-reflection transformations $C_n^k \sigma_h$.

 C_{3v}  D_3  D_{3h}

Little groups in graphene

The group of vector \mathbf{k} at the point Γ – the center of the Brillouine zone – is D_{6h} . The group of vector \mathbf{k} at the point $K(K')$ –corner of the Brillouine zone – is D_{3h} . The group of vector \mathbf{k} at the lines $\Gamma - K$ is C_{2v} .



Irreducible representations of D_{3h}

The representations of the group D_{3h} we can obtain on the basis of identity

$$D_{3h} = C_{3v} \times C_s.$$

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Each representation of the group C_{3v} , 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.

Irreducible representations of D_{6h}

Classification of irreducible representations of the group D_{6h} can be based on each of the following identities

$$D_{6h} = C_{6v} \times C_s, \quad D_{6h} = D_6 \times C_i.$$

D_6	C_{6v}	D_{3h}	E	C_2	$2C_3$	$2C_6$	$3U_2$	$3U'_2$
			E	C_2	$2C_3$	$2C_6$	$3\sigma_v$	$3\sigma'_v$
			E	σ_h	$2C_3$	$2S_3$	$3U_2$	$3\sigma_v$
A_1	A_1	A'_1	1	1	1	1	1	1
A_2	A_2	A'_2	1	1	1	1	-1	-1
B_1	B_2	A''_1	1	-1	1	-1	1	-1
B_2	B_1	A''_2	1	-1	1	-1	-1	1
E_2	E_2	E'	2	2	-1	-1	0	0
E_1	E_1	E''	2	-2	-1	1	0	0

Irreducible representations of D_{6h}

Each representation of the group D_6 , say A_1 , begets two representations of the group D_{6h} : A_{1g} and A_{1u} , where the letters g and u in the notation mean that the representation is even or odd with respect to inversion respectively. One should keep in mind that even representations having positive character of the transformation C_2 and odd representations having negative character of the transformation C_2 are even with respect to reflection σ_h ; odd representations having positive character of the transformation C_2 and even representations having negative character of the transformation C_2 are odd with respect to reflection σ_h .

Representation decomposition

Equation

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

shows how many times a given irreducible representation is contained in a reducible one.

Atomic orbitals

The tight-binding Hamiltonian includes four orbitals per atom: $\psi_s, \psi_{p_z}, \psi_{p_{\pm}}$. The structure of graphene can be seen as a triangular lattice with a basis of two atoms per unit cell, and we search for the solution of Schrodinger equation as a linear combination of the functions

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

where $j = A$ or B labels the atoms on the two sublattices A and B and \mathbf{R}_j is the radius vector of an arbitrary carbon atom in sublattice j .

π and σ bands

The Hamiltonian being symmetric with respect to reflection in the graphene plane, the bands built from the ψ_{2p_z} orbitals decouple from those built from the other three 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.

Representation of the group C_{6v} realized by p_z and s orbitals

The transformations C_2 , C_6 , σ_v change sublattices, the characters corresponding to these transformations are equal to zero.

The transformations E , C_3 , $\sigma_{v'}$ are the identity transformations for the functions $\psi_{m=0}^j$. Hence, the representation of the group C_{6v} realized by these functions can be decomposed as

$$R = A_1 + B_2.$$

Projection operator

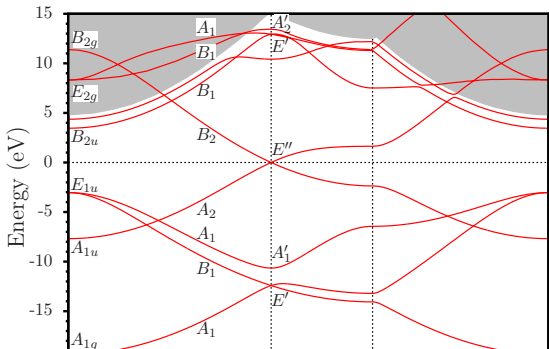
The operator

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

where n_α is the dimensionality of the irreducible representation α and P is the operator corresponding to a given symmetry G , 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. Acting by projection operators O_A and O_B on a function $\psi_{m=0}^j$, we obtain that the irreducible representation A has symmetric combination of the A and B orbitals as the basis function, and the irreducible representation B –the antisymmetric combination. The first representation is realized at the hole band, and the second – at the electron band.

Small representations at Γ by p_z and s orbitals

Representations A_{1u} and B_{2g} of the group D_{6h} are realized by ψ_{p_z} orbitals and representations A_{1g} and B_{2u} – by ψ_s orbitals. A and B representations label hole and electron band respectively.



Representation of the group C_{6v} realized by $p_{x,y}$ orbitals

If C_3 is the anticlockwise rotation, then

$$C_3 \psi_{\pm}^j = e^{\pm 2\pi i/3} \psi_{\pm}^j.$$

Hence the representation generated by the quartet can be decomposed as

$$R = E_1 + E_2$$

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

$$O_{E_1} \psi_{\pm}^j \sim 2\psi_{\pm}^j - e^{2\pi i/3} \psi_{\pm}^j - e^{-2\pi i/3} \psi_{\pm}^j \\
+ e^{2\pi i/6} \psi_{\pm}^{\bar{j}} + e^{-2\pi i/6} \psi_{\pm}^{\bar{j}} + 2\psi_{\pm}^{\bar{j}} \sim \psi_{\pm}^j + \psi_{\pm}^{\bar{j}}.$$

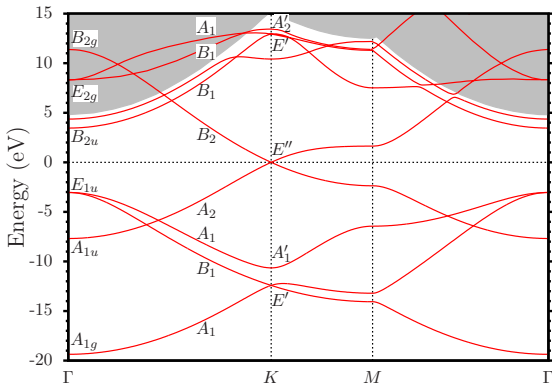
where $\bar{j} = B$ if $j = A$, and vice versa. Similarly we obtain

$$O_{E_2} \psi_{\pm}^j \sim \psi_{\pm}^j - \psi_{\pm}^{\bar{j}}.$$

Thus representation E_1 is realized by the vector space of sublattice symmetric combinations of p_{\pm} orbitals, with the basis vectors $\psi_{+}^A + \psi_{+}^B$, $\psi_{-}^A + \psi_{-}^B$, and representation E_2 is realized by the vector space of sublattice antisymmetric combination of the orbitals $\psi_{+}^A - \psi_{+}^B$, $\psi_{-}^A - \psi_{-}^B$.

Small representations at Γ by $p_{x,y}$ orbitals

Representations E_{1u} and E_{2g} of the group D_{6h} label hole and electron bands respectively.



Representation of the group C_{3v} realized by p_z and s orbitals

The nature of the representation generated by the functions $\psi_{0;\mathbf{K}}^j$ follows from the transformation law of the exponentials $e^{i\mathbf{K}\cdot\mathbf{R}_j}$ under the group 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:

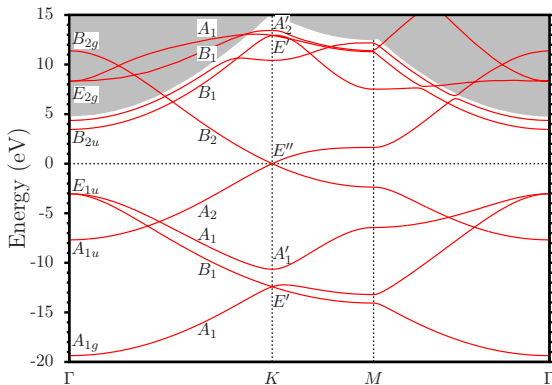
$\mathbf{K} \rightarrow \mathbf{K}_2 \rightarrow \mathbf{K}_3 \rightarrow \mathbf{K}$. Hence, rotation multiplies each function by the factor $e^{2\pi i/3}$, and

$$a_E = \frac{1}{3} \left(2 - e^{2\pi i/3} - e^{-2\pi i/3} \right) = 1; \quad (2)$$

the functions $\psi_{0;\mathbf{K}}^j$ realize representation E of the group C_{3v} .

Small representation at K by p_z orbitals

Representation E'' of the group D_{3h} describes merging of π and π^* bands.



Representation of the group C_{3v} realized by $p_{x,y}$ orbitals

Combining law of transformations of the functions $\psi_{\pm;\mathbf{K}}^j$ with the law of transformation of the exponents, we obtain that the representation generated by the quartet can be decomposed as

$$R = A_1 + A_2 + E. \quad (3)$$

Acting by projection operators we obtain that for $\mathbf{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a} \right)$ the representation A_1 is realized by the vector space with the basis vector $\psi_{+,\mathbf{K}}^A + \psi_{-,\mathbf{K}}^B$, and the representation A_2 is realized by the vector space with the basis vector $\psi_{-,\mathbf{K}}^A - \psi_{+,\mathbf{K}}^B$. The vector spaces realizing representations A_1 and A_2 being found, the representation E is obviously realized by the vector space, with the basis vectors $\psi_{+,\mathbf{K}}^A - \psi_{-,\mathbf{K}}^B$, $\psi_{-,\mathbf{K}}^A + \psi_{+,\mathbf{K}}^B$.

Representation of the group C_{3v} realized by s and $p_{x,y}$ orbitals

Because the irreducible representation E is realized both by ψ_s orbitals and by $\psi_{p\pm}$ orbitals, representations realized by all these orbitals should be considered together. The matrix representing an arbitrary element of such a representation has the form

$$D(g) = \begin{pmatrix} D^{(A_1)}(g) & & & \\ & D^{(A_2)}(g) & & \\ & & D^{(E)}(g) & \\ & & & D^{(E)}(g) \end{pmatrix}.$$

Wigner theorem

$$H = \begin{pmatrix} H^{(A_1)} & & & & \\ & H^{(A_2)} & & & \\ & & H_{11}^{(E)} & & H_{12}^{(E)} \\ & & & H_{11}^{(E)} & H_{12}^{(E)} \\ & & H_{21}^{(E)} & & H_{21}^{(E)} \\ & & & H_{21}^{(E)} & H_{22}^{(E)} \end{pmatrix}.$$

For complete digitalization of the Hamiltonian matrix one needs additional transformation in the space of basis vectors, corresponding to the same irreducible representation (E).

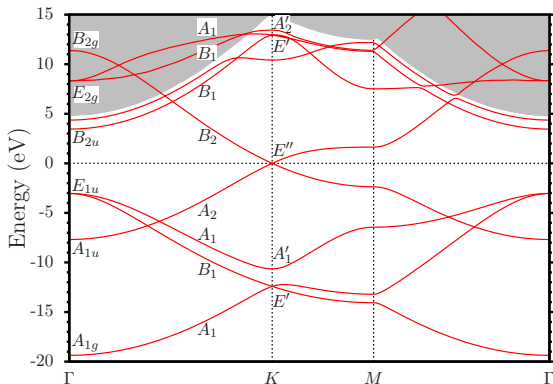
Additional diagonalization

After diagonalizing the matrix $\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$ we get

$$H = \begin{pmatrix} H^{(A_1)} & & & \\ & H^{(A_2)} & & \\ & & H_1^{(E)} & \\ & & & H_2^{(E)} \end{pmatrix}.$$

Small representations at K by s and $p_{x,y}$ orbitals

Representations A'_1 and A'_2 of the group D_{3h} label hole and electron band. Representations E'' describe merging of σ bands.

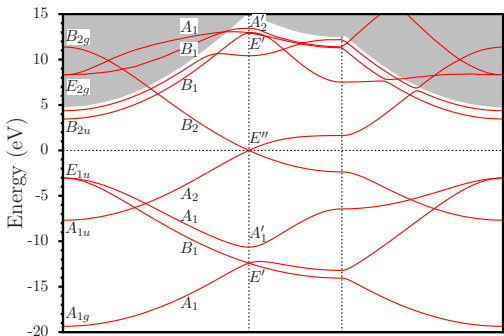


Compatibility relations

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.

C_{2v}	D_{6h}	D_{3h}
Rep	Compatible with	
A_1	$A_{1g}, B_{2u}, E_{1u}, E_{2g}$	A'_1, E'
A_2	$A_{1u}, B_{2g}, E_{1g}, E_{2u}$	A''_1, E''
B_1	$B_{1u}, A_{2g}, E_{1u}, E_{2g}$	A'_2, E'
B_2	$A_{2u}, B_{1g}, E_{1g}, E_{2u}$	A''_2, E''

C_{2v}	E	C_2	σ_v^{xy}	σ_v^{xz}
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1



The structure of graphene can be seen as a triangular lattice with a basis of two atoms per unit cell, displaced from each other by any one (fixed) vector connecting two sites of different sub-lattices, say $\delta = -a(1, 0)$.

Tight binding, nearest and next-nearest neighbor hopping

$$H = -t \sum_{\langle ij \rangle, \sigma} \left(a_{\sigma, i}^\dagger b_{\sigma, j} + H.c. \right) - t' \sum_{\langle\langle ij \rangle\rangle, \sigma} \left(a_{\sigma, i}^\dagger a_{\sigma, j} + b_{\sigma, i}^\dagger b_{\sigma, j} + H.c. \right)$$

The general Hamiltonian for the π bands is

$$H = - \begin{pmatrix} \sum_{\mathbf{a}} t'(\mathbf{a}) e^{i\mathbf{k} \cdot \mathbf{a}} & \sum_{\mathbf{a}} t(\mathbf{a} + \delta) e^{i\mathbf{k} \cdot (\mathbf{a} + \delta)} \\ \sum_{\mathbf{a}} t^*(\mathbf{a} + \delta) e^{-i\mathbf{k} \cdot (\mathbf{a} + \delta)} & \sum_{\mathbf{a}} t'(\mathbf{a}) e^{i\mathbf{k} \cdot \mathbf{a}} \end{pmatrix}$$

Tight binding hamiltonian for σ bands

$\hat{H}(\mathbf{k})$ is a 2×2 Hermitian matrix. The dispersion law is

$$\varepsilon_{\pm} = \frac{H_{11} + H_{22} \pm \sqrt{(H_{11} - H_{22})^2 + |H_{12}|^2}}{2}.$$

Merging of the bands demands three conditions: $H_{11} = H_{22}$ and $H_{12} = 0$. We have only two parameters: (k_1, k_2) , hence generally the bands don't merge.

Tight binding hamiltonian for σ bands

$$\hat{H}(\mathbf{k}) = E_0(\mathbf{k})\hat{I} + \mathbf{R}(\mathbf{k}) \cdot \hat{\sigma},$$

where $E_0(\mathbf{k})$ and $\mathbf{R}(\mathbf{k}) = (R_1(\mathbf{k}), R_2(\mathbf{k}), R_3(\mathbf{k}))$ are real functions of \mathbf{k} , and $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices.

The dispersion law

$$\varepsilon_{\pm}(\mathbf{k}) = E_0(\mathbf{k}) \pm |\mathbf{R}(\mathbf{k})|$$

shows that a contact takes place where $\mathbf{R}(\mathbf{k}) = 0$, that is three conditions ($R_1 = R_2 = R_3 = 0$) should be satisfied.

Symmetry

Let the Hamiltonian $\hat{H}(\mathbf{k})$ be invariant under a symmetry operation \mathcal{A} . The operation can be unitary

$$\hat{U}\hat{H}(\mathbf{k})\hat{U}^{-1} = \hat{H}(\mathbf{k})$$

or antiunitary

$$\hat{U}\hat{H}^*(\mathbf{k})\hat{U}^{-1} = \hat{H}(\mathbf{k})$$

Symmetry and constraints

$$\hat{H} = E_0 \hat{I} + \mathbf{R} \cdot \hat{\sigma} \iff \hat{H}^* = E_0 \hat{I} - \sigma_2 (\mathbf{R} \cdot \hat{\sigma}) \sigma_2,$$

$$\hat{U} \hat{H}^*(\mathbf{k}) \hat{U}^{-1} = \hat{H}(\mathbf{k}) \iff \left\{ \hat{U} \sigma_2, \mathbf{R} \cdot \hat{\sigma} \right\} = 0$$

Any 2×2 unitary matrix can be expressed as

$$\hat{U} = e^{i\phi} \left(\omega_0 \hat{I} + i\boldsymbol{\omega} \cdot \hat{\sigma} \right)$$

$$\left\{ \hat{U} \sigma_2, \mathbf{R} \cdot \hat{\sigma} \right\} = 0 \iff \omega_2 \mathbf{R} = 0, \quad \mathbf{s} \cdot \mathbf{R} = 0,$$

where $\mathbf{s} = (\omega_3, \omega_0, -\omega_1)$.

Let \mathcal{A} is a product of spacial inversion \mathcal{I} and time inversion \mathcal{T} . Both \mathcal{I} and \mathcal{T} give rise to the inversion of \mathbf{k} -points $\mathbf{k} \leftrightarrow -\mathbf{k}$, and thus the general \mathbf{k} -points are kept unchanged after the space-time inversion.

Since $(\mathcal{IT})^2 = I$, we get

$$\hat{U}\hat{U}^* = I \iff \hat{U} = \hat{U}^T \Rightarrow \omega_2 = 0.$$

Hence we get a single constraint on \mathbf{R}

$$\mathbf{s} \cdot \mathbf{R} = 0.$$

Because

$$\hat{H}(\mathbf{k}) = E_0(\mathbf{k})\hat{I} + \mathbf{R}(\mathbf{k}) \cdot \hat{\sigma},$$

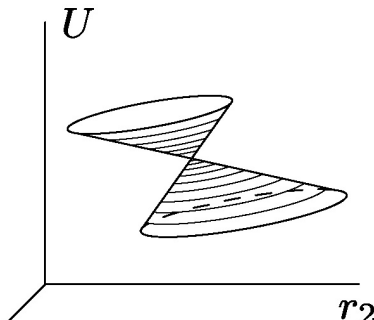
where $\mathbf{R}(\mathbf{k}) = (R_1(\mathbf{k}), R_2(\mathbf{k}), R_3(\mathbf{k}))$, it is plausible to expect that the bands merge at some point (points).

In the vicinity of a merging point

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}, \quad (4)$$

where each element is a linear function of k_x, k_y

$$E = c_i k_i \pm \sqrt{d_{ij} k_i k_j}. \quad (5)$$



Because any vector in the k_x, k_y plane compatible with the symmetry C_{3v} is identically equal to zero, and any tensor of rank two compatible with the symmetry is proportional to the unity tensor, the dispersion law is just

$$E \approx \pm |\mathbf{k}|, \quad (6)$$

and can be presented by two circular cones, with the axis perpendicular to the k_x, k_y plane.

Degenerate $\mathbf{k} \cdot \mathbf{p}$ perturbation theory

$$H = \frac{\hat{\mathbf{p}}^2}{2m} + U(r)$$

The dispersion law in the vicinity of the point k_0 is given by the effective Hamiltonian

$$H_{eff}(\mathbf{k}) = \frac{\mathbf{k} \cdot \mathbf{p}}{m},$$

more explicitly

$$H_{eff}(\mathbf{k}) = \hat{\mathbf{A}} \cdot \mathbf{k},$$

where

$$\mathbf{A}_{\mu\mu'} = \frac{1}{m} \langle k_0\mu | \mathbf{p} | k_0\mu' \rangle .$$

Dirac Hamiltonian

From the symmetry considerations follows that

$$\{\hat{A}^x, \hat{A}^x\} = \{\hat{A}^y, \hat{A}^y\} \sim I, \quad \{\hat{A}^x, \hat{A}^y\} = 0.$$

Hence effective Hamiltonian can be written as

$$H_{eff}(\mathbf{k}) = v\sigma \cdot \mathbf{k},$$

or as

$$H_{eff}(\mathbf{k}) = v\sigma^* \cdot \mathbf{k}.$$

In the absence of spin-orbit coupling electron spin can be taken into account in a trivial way: any degeneracy which we spoke about previously should be multiplied by factor of two. Thus at a general point of the zone the representation which was singly degenerate in the absence of spin, becomes doubly degenerate. This degeneracy remains even when spin-orbit coupling is taken into account. However, at points of high symmetry in the zone spin-orbit coupling may cause partial splitting. We'll restrict ourselves by the analysis of the splitting of the states realizing representations E' and E'' at the point K in the framework of group theory.

Let the coordinate parts of the wave-functions realize a representation R_i of the group of wave vector. The spin functions transform like $D_{1/2}$ representation of the rotation group, thus spin-dependent wave-functions realize representation, which is just the direct product of the above mentioned ones: $R_i \times D_{1/2}$. Because $D_{1/2}$ is a two-valued irreducible representation, we get a two valued representation of the group of wave vector. This two-valued representation of the space group is an irreducible representation at a general point of the zone, but is typically a reducible representation in the points of high symmetry. To find (the characters of) two-valued irreducible representations, 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 decomposition of the representation $R_i \times D_{1/2}$ with respect to two-valued irreducible representations of the group of the wave vector. can be readily obtained by using the tables of the characters. The characters of the group $D_{1/2}$ follow from the general results for the representations D_J :

$$\chi_j(\phi) = \frac{\sin\left(J + \frac{1}{2}\right)\phi}{\sin\frac{1}{2}\phi} \quad (7)$$

$$S(\phi) = IC(\phi + \pi), \quad (8)$$

where π is the angle of rotation about the axis, and the inversion I multiplies all ψ_{JM} by ± 1 .

D_{3h}	E	$2C_3$	$2S_3$
E'	2	-1	-1
E''	2	-1	1

$O(3)$	E	Q	C_3	C_3^2	S_3	S_3^2
			C_3^2Q	C_3Q	S_3^2Q	S_3Q
$D_{1/2}$	2	-2	1	-1	$-\sqrt{3}$	$\sqrt{3}$

D'_{3h}	E	Q	σ_h	C_3	C_3^2	S_3	S_3^2	$3U_2$	$3\sigma_v$
			$\sigma_h Q$	$C_3^2 Q$	$C_3 Q$	$S_3^2 Q$	$S_3 Q$	$3U_2 Q$	$3\sigma_v Q$
E'_1	2	-2	0	1	-1	$-\sqrt{3}$	$\sqrt{3}$	0	0
E'_2	2	-2	0	1	-1	$\sqrt{3}$	$-\sqrt{3}$	0	0
E'_3	2	-2	0	-2	2	0	0	0	0

Splitting of the levels at the point K due to spin-orbit coupling

$$E' = E'_2 + E'_3$$
$$E'' = E'_1 + E'_3.$$

Thus the four-fold degeneracy (including spin) of the bands which were merging at the point K is partially removed, and only two-fold (Kramers) degeneracy is left. In other words, spin-orbit coupling in graphene opens a gap and gives fermionic excitations a small mass.

WE (HOPEFULLY) GOT AN ADDITIONAL MOTIVATION TO STUDY IN DEPTH GROUP THEORY AND TO APPLY IT TO SOLID STATE PHYSICS.

I ENJOYED YOUR PATIENCE AND YOUR QUESTIONS AND HOPE TO SEE YOU AGAIN AT THE NEXT TAINAN WORKSHOP.