

Electronic structure of solids

Homework

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Exercise 1

As an introduction for this and the next exercise, the eigenstates and eigenenergies of the free electron approximation are:

$$\phi_{\mathbf{K}}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{V}} e^{i(\mathbf{k}+\mathbf{K})\mathbf{r}} \quad (1)$$

$$\varepsilon_{\mathbf{K}}(\mathbf{k}) = \frac{\hbar^2}{2m} (\mathbf{k} + \mathbf{K})^2 \quad (2)$$

where \mathbf{K} notes the band.

Degenerate perturbation theory

In this exercise we investigate a cubic system on the ΓX line which can be parametrized as $\frac{\pi}{a}(0, 0, \kappa)$ where a is the lattice constant and $\kappa \in [0, 1]$. In this case the bands corresponding to

$$\mathbf{K}_D = \frac{2\pi}{a}(1, 0, 0) \quad \mathbf{K}_E = \frac{2\pi}{a}(0, 1, 0) \quad (3)$$

$$\mathbf{K}_F = \frac{2\pi}{a}(-1, 0, 0) \quad \mathbf{K}_G = \frac{2\pi}{a}(0, -1, 0) \quad (4)$$

are degenerate with the energy

$$\varepsilon_{\mathbf{K}}(\mathbf{k}) = \frac{\hbar^2 \pi^2}{2ma^2} (\kappa^2 + 4)^2 \quad (5)$$

what we get from Eq.(2) after substituting the \mathbf{K} values above. The wavefunctions corresponding to these states are:

$$\phi_{\mathbf{K}_{D/F}}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\frac{\pi}{a}(\kappa z \pm 2x)} \quad (6)$$

$$\phi_{\mathbf{K}_{E/G}}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\frac{\pi}{a}(\kappa z \pm 2y)} \quad (7)$$

In order to find how the degenerations are split I going to use degenerate perturbation theory and I going to diagonalize the 4×4 Hamiltonian matrix spanned by the four degenerate wavefunction. The matrix element of the perturbation potential what we turn on to lift the degeneracies is:

$$V_{\mathbf{K}, \mathbf{K}'} = \int d^3r \phi_{\mathbf{K}}^*(\mathbf{k}, \mathbf{r}) V(\mathbf{r}) \phi_{\mathbf{K}'}(\mathbf{k}, \mathbf{r}) \quad (8)$$

$$= \frac{1}{V} \int d^3r V(\mathbf{r}) e^{i(\mathbf{K}-\mathbf{K}')\mathbf{r}} = V_{\mathbf{K}-\mathbf{K}'} \quad (9)$$

which has the property $V_{\mathbf{K}-\mathbf{K}'}^* = V_{\mathbf{K}'-\mathbf{K}}$ for a real potential.

The matrix what we have to diagonalize is:

$$H = \begin{pmatrix} \varepsilon & V_{DE} & V_{DF} & V_{DG} \\ V_{ED} & \varepsilon & V_{EF} & V_{EG} \\ V_{FD} & V_{FE} & \varepsilon & V_{FG} \\ V_{GD} & V_{GE} & V_{GF} & \varepsilon \end{pmatrix} \quad (10)$$

It contains matrix elements for the following wavenumber differences:

$$\mathbf{K}_D - \mathbf{K}_E = \frac{2\pi}{a}(1, -1, 0) \quad \mathbf{K}_D - \mathbf{K}_F = \frac{2\pi}{a}(2, 0, 0) \quad \mathbf{K}_D - \mathbf{K}_G = \frac{2\pi}{a}(1, 1, 0) \quad (11)$$

$$\mathbf{K}_E - \mathbf{K}_F = \frac{2\pi}{a}(1, 1, 0) \quad \mathbf{K}_E - \mathbf{K}_G = \frac{2\pi}{a}(0, 2, 0) \quad \mathbf{K}_F - \mathbf{K}_G = \frac{2\pi}{a}(-1, 1, 0) \quad (12)$$

and the opposite of them in the lower triangle. If we use the fact that we have cubic symmetry it turns out that we have only two different matrix element, V_1 corresponds to $\Delta K = \frac{2\pi}{a}(1, 1, 0)$ and V_2 corresponds to $\Delta K = \frac{2\pi}{a}(2, 0, 0)$. The matrix which we have to deal with is simplified a lot after this considerations:

$$H = \begin{pmatrix} \varepsilon & V_1 & V_2 & V_1 \\ V_1 & \varepsilon & V_1 & V_2 \\ V_2 & V_1 & \varepsilon & V_1 \\ V_1 & V_2 & V_1 & \varepsilon \end{pmatrix} \quad (13)$$

This is a very simple matrix so we can try to solve the eigenvalue equation intuitively to save time. There is a trivial eigenvector $\mathbf{v}_1 = (1, 1, 1, 1)$ with eigenvalue $\varepsilon + 2V_1 + V_2$. The previous state has a pair, where V_1 appears with minus sign, this is $\mathbf{v}_2 = (1, -1, 1, -1)$ with self energy $\varepsilon - 2V_1 + V_2$. The remaining two is then when we take zero from V_1 , a guess is $\mathbf{v}_3 = (1, 0, -1, 0)$, it turns out this is a good eigenvector too with energy $\varepsilon - V_2$, and the last one can be found by find the last member of the orthogonal set, $\mathbf{v}_4 = (0, 1, 0, -1)$ with energy $\varepsilon - V_2$.

So I found the four eigenvector of the Hamiltonian on the degenerate subspace, and they tell that in a cubic crystal on the ΓX line there are two non-degenerate and a double degenerate band.

Group theory

An other way to investigate the problem is group theory. The small group of the \mathbf{K} vector is C_{4v} . I have to construct a representation of this group on the four degenerate state noted by the \mathbf{K} vectors, it going to be a 4 dimension representation with permutation matrices. The generators of the representation is:

$$\Gamma_{C_4} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (14)$$

$$\Gamma_{\sigma_v^x} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad (15)$$

the further transformations can be generated by the multiplication table, namely:

$$\Gamma_{C_2} = \Gamma_{C_4}^2 \quad (16)$$

$$\Gamma_{C_4^3} = \Gamma_{C_4}^3 \quad (17)$$

$$\Gamma_{\sigma_v^y} = \Gamma_{\sigma_v^x} \Gamma_{C_2} \quad (18)$$

$$\Gamma_{\sigma_d^1} = \Gamma_{\sigma_v^x} \Gamma_{C_4} \quad (19)$$

$$\Gamma_{\sigma_d^2} = \Gamma_{\sigma_v^x} \Gamma_{C_4^3} \quad (20)$$

After we have all the representing matrices we can calculate the irreducible decomposition of our representation, the irreducible characters and the characters of our representation show in Tab..

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	-1	1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	2	0	0
Γ	4	0	0	2	0

Table 1: The irreducible characters

We can calculate the coefficients of an irreducible representation as:

$$m_\mu = \frac{1}{\dim G} \sum_{g \in G} \chi_\mu(g)^* \chi(g) \quad (21)$$

with the usage of the previous equation on our representation we get:

$$\Gamma = A_1 \oplus B_1 \oplus E \quad (22)$$

this is the first result of this calculation, we arrived to the same level structure as before, namely we have two one dimension and a two dimension representation. We can find the eigenvectors for these representations if we construct the projectors which project to the irreducible subspaces,

$$P^\mu = \frac{n_\mu}{\dim(G)} \sum_{g \in G} \chi^\mu(g)^* \Gamma(g) \quad (23)$$

after checking the action of the projectors to the standard basis vectors of the euclidean space we end up with the same subspace structure:

$$v_{A_1} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad v_{B_1} = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \quad v_E = \alpha \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} \quad (24)$$

and of course by checking the eigenvalue equation we get the same energies:

$$\varepsilon_{A_1} = \varepsilon + 2V_1 + V_2 \quad \varepsilon_{B_1} = \varepsilon - 2V_1 + V_2 \quad \varepsilon_E = \varepsilon - V_2 \quad (25)$$

Exercise 2

Degenerate perturbation theory

Now we are going to investigate the ΓR line of a cubic crystal which can be parametrized as $\frac{\pi\kappa}{a}(1, 1, 1)$ where $\kappa \in [0, 1]$. In this case we have a threefold degeneracy for the bands with the following \mathbf{K} vectors:

$$\mathbf{K}_B \frac{2\pi}{a}(0, 0, -1) \quad \mathbf{K}_F \frac{2\pi}{a}(-1, 0, 0) \quad \mathbf{K}_C \frac{2\pi}{a}(0, -1, 0) \quad (26)$$

with degenerate energy:

$$\varepsilon(\mathbf{k}) = \varepsilon_0(2\kappa^2 + (\kappa - 2)^2) \quad (27)$$

and wavefunctions:

$$\phi_B = \frac{1}{\sqrt{V}} e^{i\frac{\pi}{a}(\kappa x + \kappa y + (\kappa - 2)z)} \quad (28)$$

$$\phi_F = \frac{1}{\sqrt{V}} e^{i\frac{\pi}{a}(\kappa y + \kappa z + (\kappa - 2)x)} \quad (29)$$

$$\phi_G = \frac{1}{\sqrt{V}} e^{i\frac{\pi}{a}(\kappa x + \kappa z + (\kappa - 2)y)} \quad (30)$$

By following the steps what we made above first we construct the Hamiltonian matrix of the degenerate subspace for a small perturbation:

$$H = \begin{pmatrix} \varepsilon & V_{BF} & V_{BG} \\ V_{FB} & \varepsilon & V_{FG} \\ V_{GB} & V_{GF} & \varepsilon \end{pmatrix} \quad (31)$$

in this case the wavenumber differences for the matrix elements are:

$$\mathbf{K}_B - \mathbf{K}_F = \frac{2\pi}{a}(1, 0, -1) \quad \mathbf{K}_B - \mathbf{K}_G = \frac{2\pi}{a}(0, 1, -1) \quad \mathbf{K}_F - \mathbf{K}_G = \frac{2\pi}{a}(-1, 1, 0) \quad (32)$$

since we have cubic symmetry these \mathbf{K} vectors can be transformed to each other and minus sign also can be transformed out so the simplified matrix is:

$$H = \begin{pmatrix} \varepsilon & V_1 & V_1 \\ V_1 & \varepsilon & V_1 \\ V_1 & V_1 & \varepsilon \end{pmatrix} \quad (33)$$

The next step is to solve the eigenvalue problem. We follow same arguments as before, this matrix also has the trivial $\mathbf{v}_1 = (1, 1, 1)$ eigenstate with $\varepsilon + 2V_1$. An other good eigenvector is $\mathbf{v}_2 = (2, -1, -1)$ which has $\varepsilon - V_1$ energy. Then we have to find the third orthogonal vector, which we can do by finding a third orthogonal vector, this is $\mathbf{v}_3 = (0, 1, -1)$ and this state has the same energy as the second one. So there is a non-degenerate and a two times degenerate band.

Group theory

For group theory investigation first of all we need to transform our \mathbf{K} vectors to the system K' where the 111 direction is parallel with the z axis. In the natural basis the \mathbf{K} vectors are the negative basis vectors, if we can construct the form of them in the new basis we have found the transformation. If we look the cube parallel with the main diagonal we see that the x, y and z vectors form a triangle where the vectors are separated by 120° , this is going to be the structure in the (x', y') plane in the new coordinate system. The only thing remained is to calculate the z' component of the vectors which going to be equal for each of them. After simple geometrical considerations the z' component of our \mathbf{K} vectors is $\frac{1}{\sqrt{3}}$, so the transformation is:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \Rightarrow \begin{pmatrix} -\frac{\sqrt{6}}{2\sqrt{3}} \\ -\frac{\sqrt{2}}{2\sqrt{3}} \\ \frac{2}{2\sqrt{3}} \end{pmatrix} \begin{pmatrix} \frac{\sqrt{6}}{2\sqrt{3}} \\ -\frac{\sqrt{2}}{2\sqrt{3}} \\ \frac{2}{2\sqrt{3}} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{\sqrt{2}}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \quad (34)$$

I note that our \mathbf{K} are minus these vectors but it only means a minus sign in the z component which doesn't affect the symmetry calculations because it doesn't change for any symmetry transformation.

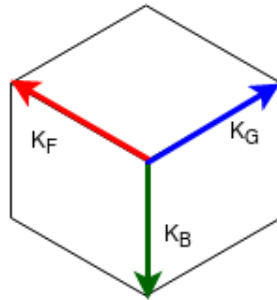


Figure 1: The \mathbf{K} vectors

The small group of the \mathbf{K} vectors in this case is \mathbf{C}_{3v} . We can build up a 3 dimensional representation of the group by permutation matrices. The two generator matrix is:

$$\Gamma_{C_3} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad \Gamma_{\sigma_v} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (35)$$

The other matrices can be generated as:

$$\Gamma_{C_3^2} = \Gamma_{C_3} \Gamma_{C_3} \quad (36)$$

$$\Gamma_{\sigma_v^2} = \Gamma_{\sigma_v} \Gamma_{C_3} \quad (37)$$

$$\Gamma_{\sigma_v} = \Gamma_{\sigma_v} \Gamma_{C_3^2} \quad (38)$$

The character table of the group and characters of our representation is:

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

Table 2: The irreducible characters

If we reduce the representation as in the previous example we get:

$$\Gamma = A_1 \oplus E \quad (39)$$

which means we have a non-degenerate and a two times degenerate subspace, now we can project the subspaces corresponds to these representation with the projectors used in the exercise above. After we acted on the standard basis vectors with the projectors we get the same structure as for the degenerate perturbation theory, namely:

$$\mathbf{v}_{A_1} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \mathbf{v}_E = \alpha \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \quad (40)$$

with energies $\varepsilon_{A_1} = \varepsilon + 2V_1$ and $\varepsilon_E = \varepsilon - V_1$.

Exercise 3

In this and the following exercise we going to investigate the the model of a 1 dimensional chain with two atoms per unit cell with γ_1 intracell and γ_2 intercell hopping. The real space Hamiltonian of the system is:

$$H_{ij}^{\alpha\beta} = \varepsilon_\alpha \delta_{\alpha\beta} \delta_{ij} + \gamma_1 (1 - \delta_{\alpha\beta}) \delta_{ij} + \gamma_2 (\delta_{\alpha A} \delta_{\beta B} \delta_{i,j+1} + \delta_{\alpha B} \delta_{\beta A} \delta_{i+1,j}) \quad (41)$$

where i, j are indexing the cells and α, β are indexing the atoms in the unit cell. This a chain with two atoms per unit cell, show on Fig.3

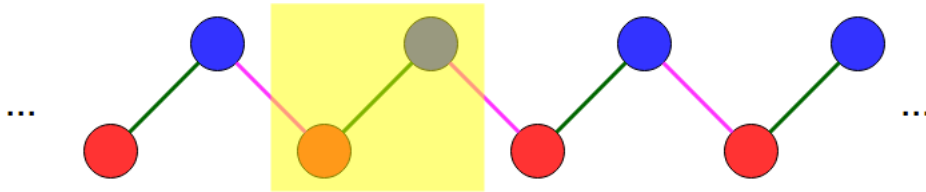


Figure 2: The chain contains two atoms per unit cell, which shaded with yellow and two different hopping(γ_1, γ_2) with different colours

For simplicity we take the on-site energies to zero, in this case the matrix form of the Hamiltonian is:

$$H = \begin{pmatrix} 0 & \gamma_1 & 0 & 0 & \dots \\ \gamma_1 & 0 & \gamma_2 & 0 & \\ 0 & \gamma_2 & 0 & \gamma_1 & \\ 0 & 0 & \gamma_1 & \ddots & \ddots \\ \vdots & & & \ddots & \ddots \end{pmatrix} \quad (42)$$

We want to calculate the spectrum of this Hamiltonian, we can simply do that if we perform a Bloch Wannier tranform and we go to momentum space. We have two internal degrees of freedom, so the bulk momentum space Hamiltonian going to be a 2×2 matrix:

$$H(k) = \begin{pmatrix} 0 & \gamma_1 + \gamma_2 e^{-ika} \\ \gamma_1 + \gamma_2 e^{ika} & 0 \end{pmatrix} \quad (43)$$

A 2 hermitian matrix can be decomposed on the Pauli matrices and can be written in the form $H = d(k)_0 \sigma_0 + \mathbf{d}(k) \cdot \boldsymbol{\sigma}$. In this case the decomposition looks like:

$$H(k) = (\gamma_1 + \gamma_2 \cos(ka)) \sigma_x + \gamma_2 \sin(ka) \sigma_y \quad (44)$$

and this is a perfect form to determine the dispersion relation because $H(k)^2 = E(k)^2 \mathbb{I}_2$ and $H(k)^2 = d_0^2 + \mathbf{d}(k)^2$ due to the properties of the Pauli matrices. So the dispersion relation is:

$$E_{\pm}(k) = \pm \sqrt{(\gamma_1 + \gamma_2 \cos(ka))^2 + \gamma_2^2 \sin^2(ka)} \quad (45)$$

$$= \pm \sqrt{\gamma_1^2 + 2\gamma_1\gamma_2 \cos(ka) + \gamma_2^2} \quad (46)$$

from this dispersion relation we want to derive the condition for the existence of a gap. The point where the gap is the smallest is at the sides of the Brilloune zone at $\pm \frac{\pi}{a}$, in this point the cosine function is -1 , if substitute this to the dispersion relation we get

$$E_{\pm}(k) = \pm |\gamma_1 - \gamma_2| \quad (47)$$

so the gap is

$$E_{\text{gap}} = |E_+ - E_-| = 2|\gamma_1 - \gamma_2|, \quad (48)$$

which means there is always going to be a gap expect when $\gamma_1 = \gamma_2$.

Exercise 4

Now we consider a semi infinity chain and we are looking for a localized edge state on the one remained edge. The energy of the edge state is deeply in the gap, in that case we assume that it is zero and try to find the eigenvector for this state. The real space Hamiltonian of the system is the same as before:

$$H = \begin{pmatrix} 0 & \gamma_1 & 0 & 0 & \dots \\ \gamma_1 & 0 & \gamma_2 & 0 & \\ 0 & \gamma_2 & 0 & \gamma_1 & \\ 0 & 0 & \gamma_1 & \ddots & \ddots \\ \vdots & & & \ddots & \ddots \end{pmatrix} \quad (49)$$

we are going to solve the eigenvalue equation where the eigenstate is:

$$\mathbf{x} = \begin{pmatrix} a_0 \\ b_0 \\ a_1 \\ b_1 \\ \vdots \end{pmatrix} \quad (50)$$

where the a_i and b_i numbers are the coefficient of the wavefunction on a given sites. The eigenvalue equation is separated to a set of simple linear equations:

$$\gamma_1 b_0 = 0 \quad (51)$$

$$\gamma_2 b_{i-1} + \gamma_1 b_i = 0 \quad (52)$$

$$\gamma_1 a_i + \gamma_2 a_{i+1} = 0 \quad (53)$$

The first thing what we can see is that the equations for a_i and b_i are decoupled, so they give us two independent eigenvectors. From the last two equation we get two recursive formula, one for the coefficients on the A sublattice and and for the B . The recursive formula on the A sublattice is:

$$a_{i+1} = -\frac{\gamma_1}{\gamma_2} a_i \quad (54)$$

the solution of this for the m th cell is:

$$a_m = \left(-\frac{\gamma_1}{\gamma_2}\right)^m a_0 \quad (55)$$

the probability of the electron is on the a_i site is a_i^2 so we need to consider only the absolute value of the coefficients:

$$|a_m| = \left(\frac{\gamma_1}{\gamma_2}\right)^m a_0 \quad (56)$$

We can use a simple trick to transform this equation to an exponential one:

$$|a_m| = \left(e^{\log \frac{\gamma_1}{\gamma_2}}\right)^m a_0 \quad (57)$$

$$= e^{-m \log \frac{\gamma_2}{\gamma_1}} a_0 = e^{-m/\xi} \quad (58)$$

where ξ is the localization length, which can be written as:

$$\xi = \frac{1}{\log \gamma_2 - \log \gamma_1} \quad (59)$$

So we get an exponentially decaying wavefunction living on the A sublattice and localized to the left edge with localization length ξ if $\gamma_2 > \gamma_1$, so if the intercell hopping is the stronger.

We didn't said anything about the b_i numbers yet. We saw $b_0 = 0$ so on the left edge there is no electron on the B sublattice. It turns out if we take a finite chain b_N going to be finite and we can start the recursion from the right edge. This going to be the edge state of the right edge.

Exercise 9

In this exercise I going to solve the CPA condition iteratively for the one dimensional chain of a two component compound. This is the simplest case of CPA, because in that case all of the quantities are scalar. The two components has energies $\pm\varepsilon_0$ and we apply a positive V potential to couple them. We are going to work with dimensionless quantities:

$$x_0 = \frac{\varepsilon_0}{2V} \quad x_c = \frac{\varepsilon_c}{2V} \quad \omega = \frac{z}{2V} \quad (60)$$

here the ω plays the role of the dimensionless complex energy and all of our quantities are depend on ω , the c in subscript notes the quantities corresponding to the coherent medium of the CPA.

The CPA condition in this formalism is:

$$x_c = (2c - 1)x_0 + \frac{x_0^2 - x_c^2}{\sqrt{\omega - x_c^2} - 1} \quad (61)$$

where $c \in [0, 1]$ the concentration. This in an implicit equation of x_c and it is impossible to express x_c as a function of the other variables, so we need other ways to solve this equation.

- (a) The first simplest thin what we can try is successive approximation. We start from $x_c^{(1)} = (2c - 1)x_0$, the virtual crystal approximation and we calculate x_c from the right hand side of Eq.(60) and this going to be the next guess. We can stabilize this process with a mixing procedure when we use only an α portion of the calculated guess. Later it going to turn out that this method has very bad convergence properties.
- (b) There is an other way to solve Eq.(60) named after Ginatempo and Staunton. In this method we have an iteration shame to the change in the x_c coherent energy. The method can be illustrated as:

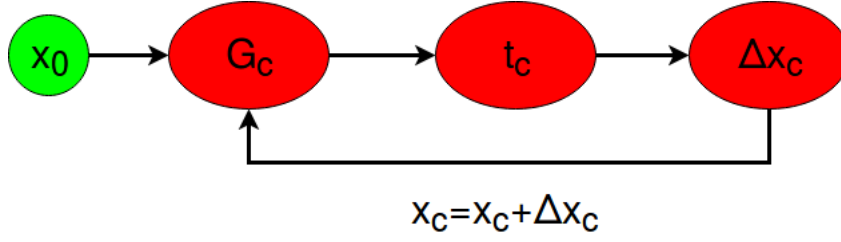


Figure 3: The flow chart of the Ginatempo–Staunton method

The quantities what are appear is:

$$G_c^{(n)}(\omega) = \frac{1}{\sqrt{\omega - x_c^{(n)2} - 1}} \quad (62)$$

$$t_c^{(n)}(\omega) = \frac{c(x_0 - x_c^{(n)})}{1 - (x_0 - x_c^{(n)})G_c^{(n)}} - \frac{(1-c)(x_0 + x_c^{(n)})}{1 + (x_0 + x_c^{(n)})G_c^{(n)}(\omega)} \quad (63)$$

$$\Delta x_c(\omega) = \frac{t_c^{(n)}(\omega)}{1 + t_c^{(n)}(\omega)G_c^{(n)}(\omega)} \quad (64)$$

At this point I note that when I calculate the Green's function in the denominator I have to take the square root with *positive* imaginary part in order to have a well behaving DOS. It can be seen if a make the following consideration: in this case the Green's function has negative imaginary part and then if a take the DOS as in Eq.(67) it going to be positive, but in the other case I going to have negative DOS what is not physical.

I did the calculation for both methods. The energy of each band, if they are not in the compound, change between $x_0 \pm 1$, so I calculate for $\omega \in [-x_0 - 2, x_0 + 2]$ in order to see the cutoff in the DOS. Furthermore we know that the Green's function is singular on the spectrum so we need to take a small imaginary part to perform the calculations, I used $0.02i$ as imaginary part. For the (a) method I used $\alpha = 0.2$ and I calculated the next iteration as:

$$x_c^{(n+1)} = \alpha x_c^{(n)\text{out}} + (1 - \alpha)x_c^{(n)\text{in}} \quad (65)$$

where in/out notes the input and the output of the self-consistent equation in the n th iteration. I plotted the DOS from this calculation in the same iteration when the other method converged. So I can compare them graphically.

For the Ginatempo–Staunton method I used the same initial value and the same energy points. The only additional detail is the convergence condition. In order to check the convergence I introduced an error array from the CPA condition:

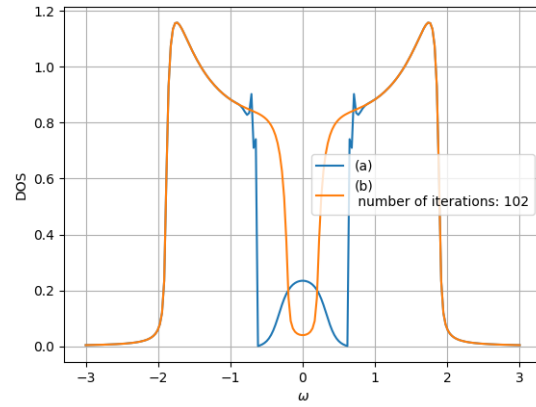
$$e^{(n)}(\omega) = x_c^{(n)} - (2c - 1)x_0 + \frac{x_0^2 - (x_c^{(n)})^2}{\sqrt{\omega - x_c^{(n)2} - 1}} \quad (66)$$

and I my condition is $|e^{(n)}(\omega)| < \epsilon$ where $|\cdot|$ is the euclidean norm of the error as a vector of the discrete ω and I set the tolerance value to $\epsilon = 1e - 10$. The results of my calculations are shown on Fig.4, where I plotted the DOS:

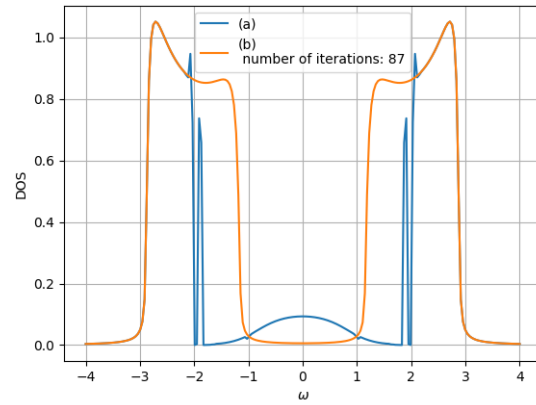
$$D(\omega) = -\text{Im} G_c(\omega) \quad (67)$$

The first case on Fig. 4 is specific because for $x_0 = 1$ the two bands touch each other at $\omega = 0$, but because they are in an alloy there going to be a gap, or more precisely the DOS going to decrease dramatically. The second case is when we open the gap, in this case the band are repel each other. Finally in the third case we investigated an asymmetric compound are we can say that this is a doped material, in that case the doping create a tight conduction band above the wide band of the initial material.

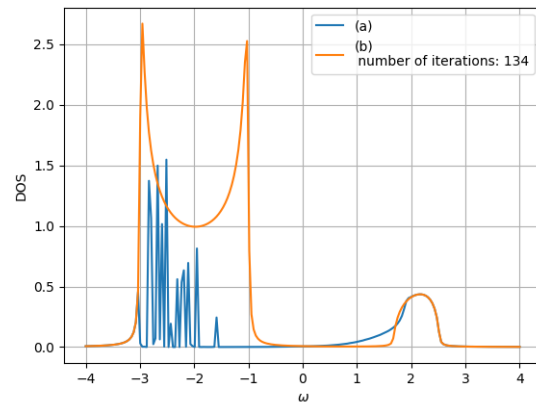
We can also see that the (a) method behaves worse and worse as the system becomes more specific. In the first case it seems like it going to converge on the second graph appears strange peaks and at the third it become awful.



(a) $c = 0.5, x_0 = 1$



(b) $c = 0.5, x_0 = 2$



(c) $c = 0.1, x_0 = 1$

Figure 4: The plot of the DOS of two component 1D compounds with specific c and x_0 parameters. (a) notes the successive approximation and (b) notes the Ginatempo–Staunton method, the (a) is plotted for as many iteration as what needed for (b) to converge