Book of Exercises

GDR School on topology

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Contents

1 Preliminary exercises to do before the school

1.1 Tight binding model for 1d chain.

Let?s consider a chain of N identical atoms with only one orbital per atom $\phi_n(\vec{r})$, label $|\phi_n\rangle$, separated by the same distance $a/2$. We will consider the unit cell containing 2 atoms of length a, whose orbitals will be $|\phi_{2m}\rangle$ and $|\phi_{2m+1}\rangle$, with m indexing the considered cell. The reason for this 2 atoms per unit cell is that we will consider 2 different hopping integrals between the atoms of the same cell and between neighboring cells :

$$\begin{aligned}
&\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m+1}\rangle = \langle\phi_{2m+1}|\,\hat{H}\,|\phi_{2m}\rangle = -t\,(1-\delta)\\
&\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m-1}\rangle = \langle\phi_{2m-1}|\,\hat{H}\,|\phi_{2m}\rangle = -t\,(1+\delta)\\
&\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m}\rangle = \epsilon_0\\
&\langle\phi_{2m+1}|\,\hat{H}\,|\phi_{2m+1}\rangle = \epsilon_1
\end{aligned} \tag{1}$$

All the other terms are considered null. The physical origin of this difference in hopping parameter can be an unequal distance between identical atoms (in this case $\epsilon_0 = \epsilon_1$) or just 2 different atoms per cell ($\epsilon_0 \neq \epsilon_1$). We will take the total wave function as a linear combination of the local orbital : $\Psi = \sum_m \alpha_m\,|\phi_{2m}\rangle + \beta_m\,|\phi_{2m+1}\rangle$.

We recall the Bloch theorem : in a spatially periodic system of period $\vec{T}$ the total wavefunction is decomposed in $\Psi(\vec{r}) = u(\vec{r})e^{i\vec{k}.\vec{r}}$ with $u(\vec{r}+\vec{T}) = u(\vec{r})$ a periodic function.

1. What are the limit of the Brillouin zone for a unit cell of length a ?
   Solution.
   The Brillouin zone is $]0 : \frac{2\pi}{a}]$ or $]-\frac{\pi}{a} : \frac{\pi}{a}]$. Be careful that one of the boundary is exluded from the Brillouin zone as it is actually the same point and you don't want to count this point twice.

2. Using the periodicity of the system, calculate $\Psi(x+a)$ as a function of $\phi_{2m}(x)$ and $\phi_{2m+1}(x)$.
   Solution.
   From translational symmetry :

$$\begin{aligned}
&\phi_{2m}(x+a) = \phi_{2m-2}(x)\\
&\phi_{2m+1}(x+a) = \phi_{2m-1}(x)\\
\Psi(x+a) \quad &= \sum_m \alpha_m\phi_{2m}(x+a) + \beta_m\phi_{2m+1}(x+a)\\
&= \sum_m \alpha_m\phi_{2m-2}(x) + \beta_m\phi_{2m-1}(x)\\
&\underset{m'=m-1}{=} \sum_{m'} \alpha_{m'+1}\phi_{2m"}(x) + \beta_{m'+1}\phi_{2m'+1}(x)
\end{aligned} \tag{2}$$

3. Using the block theorem, find the expression of $\Psi(x+a)$ as function of $\Psi(x)$
   Solution.
   From Bloch theorem :
   $\Psi(x) = u(x)e^{ikx}$ with $u(x+a) = u(x)$
   Then $\Psi(x+a) = \Psi(x)e^{ika}$

4. Comparing the two expressions of $\Psi(x+a)$, deduce the relation between α_{m+1} and α_m or β_{m+1} and β_m
   Solution.
   $\alpha_{m+1} = e^{ika}\alpha_m$ and $\alpha_{m+1} = e^{ika}\beta_m$

5. Calculate the term $<\phi_{2n}|\mathcal{H}|\Psi_k>$ (ϕ_{2n} being one orbital of the first atom of the unit cell, labelled with an even index $2n$), first using the Schrödinger equation to make appear E_k, the energy of the wavefunction Ψ_k, and secondly expanding $|\Psi_k>$ to make appear the hopping integrals of the kind $\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m+1}\rangle$ that we will replace by the corresponding value (see Eq. 1). By comparing the two methods, derive the first equation relating E_k, α_n, β_n, t and δ.

Solution.

$$\begin{aligned}
< \phi_{2n}|\mathcal{H}|\Psi_k > &= E_k < \phi_{2n}|\Psi_k >= E_k e^{ika}\alpha_n \\
&= \sum_m \alpha_m < \phi_{2n}|\mathcal{H}|\phi_{2m} > + \beta_m < \phi_{2n}|\mathcal{H}|\phi_{2m+1} > \\
&\text{Non zero term when m=n or m=n-1} \\
&= \alpha_n < \phi_{2n}|\mathcal{H}|\phi_{2n} > + \beta_n < \phi_{2n}|\mathcal{H}|\phi_{2n+1} > + \beta_{n-1} < \phi_{2n}|\mathcal{H}|\phi_{2n-1} > \\
&= \alpha_n\epsilon_0 + \beta_n(-t(1-\delta)) + \beta_n e^{-i1ka}(-t(1+\delta)) \\
\Rightarrow \quad & (E_k - \epsilon_0)\alpha_n + \beta_n\left[t(1-\delta) + t(1+\delta)e^{-ika}\right] = 0
\end{aligned} \tag{3}$$

6. Apply the same method for the term $< \phi_{2n+1}|\mathcal{H}|\Psi_k >$ (ϕ_{2n+1} being one orbital of the second atom of the unit cell, labelled with an odd index $2n+1$) to find a second equation.

Solution.

$$\begin{aligned}
< \phi_{2n+1}|\mathcal{H}|\Psi_k > &= E_k < \phi_{2n+1}|\Psi_k >= E_k e^{ika}\beta_n \\
&= \sum_m \alpha_m < \phi_{2n+1}|\mathcal{H}|\phi_{2m} > + \beta_m < \phi_{2n+1}|\mathcal{H}|\phi_{2m+1} > \\
&\text{Non zero term when m=n or m=n+1} \\
&= \alpha_n < \phi_{2n+1}|\mathcal{H}|\phi_{2n} > + \alpha_{n+1} < \phi_{2n+1}|\mathcal{H}|\phi_{2n+2} > + \beta_n < \phi_{2n+1}|\mathcal{H}|\phi_{2n+1} > \\
&= \alpha_n(-t(1-\delta)) + \alpha_n e^{i1ka}(-t(1+\delta)) + \beta_n\epsilon_1 \\
\Rightarrow \quad & (E_k - \epsilon_1)\beta_n + \alpha_n\left[t(1-\delta) + t(1+\delta)e^{ika}\right] = 0
\end{aligned} \tag{4}$$

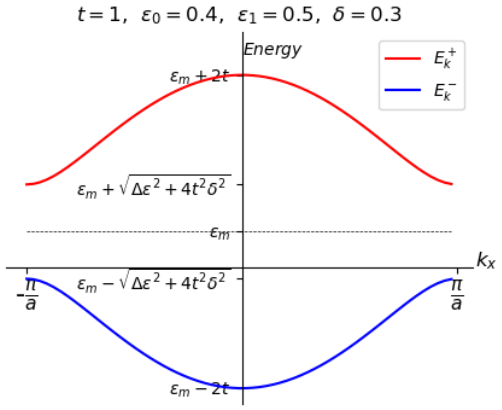
7. Using the two equations, find the two eigenvalues E_k.

Solution.

$$\begin{aligned}
&\begin{bmatrix} (E_k - \epsilon_0) & \left[t(1-\delta) + t(1+\delta)e^{-ika}\right] \\ \left[t(1-\delta) + t(1+\delta)e^{ika}\right] & (E_k - \epsilon_1) \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\
&\Rightarrow (E_k - \epsilon_0)(E_k - \epsilon_1) - t^2\left[(1-\delta) + (1+\delta)e^{-ika}\right]\left[(1-\delta) + (1+\delta)e^{ika}\right] = 0 \\
&\Rightarrow (E_k - \epsilon_0)(E_k - \epsilon_1) - t^2\left|(1-\delta) + (1+\delta)e^{-ika}\right|^2 = 0 \\
&\Rightarrow (E_k - \epsilon_0)(E_k - \epsilon_1) - t^2\left|(1-\delta)e^{i\frac{ka}{2}} + (1+\delta)e^{-i\frac{ka}{2}}\right|^2 = 0 \\
&\Rightarrow (E_k - \epsilon_0)(E_k - \epsilon_1) - 4t^2\left[cos^2(\frac{ka}{2}) + \delta^2 sin^2(\frac{ka}{2})\right] = 0 \\
&\text{Rewriting :} (E_k - \epsilon_0)(E_k - \epsilon_1) = (E_k - \epsilon_m)^2 - \Delta\epsilon^2 \\
&\text{with : } \epsilon_m = \tfrac{\epsilon_1 + \epsilon_0}{2} \text{ the mean value, and } \Delta\epsilon = \tfrac{\epsilon_1 - \epsilon_0}{2} \text{ the deviation from the mean value} \\
&\Rightarrow (E_k - \epsilon_m)^2 = \Delta\epsilon^2 + 4t^2\left[cos^2(\frac{ka}{2}) + \delta^2 sin^2(\frac{ka}{2})\right] \\
&\Rightarrow E_k^{\pm} = \epsilon_m \pm \sqrt{\Delta\epsilon^2 + 4t^2\left(cos^2(\frac{ka}{2}) + \delta^2 sin^2(\frac{ka}{2})\right)}
\end{aligned} \tag{5}$$

8. Plot the two bands, and calculate the gap to show that it depends only on $\Delta\epsilon$ and δ, and that it vanishes when $\Delta\epsilon = \delta = 0$.

Solution.



The gap at the zone boundary is $\Delta = 2\sqrt{\Delta\epsilon^2 + 4t^2\delta^2}$

1.2 Tight binding model for 1d chain : second quantization formalism.

We will see now how to write the same system using second quantization. In second quantization, we think in term of the occupation of the sites with creation and annihilation operators that add or remove electrons on specific site. For example, the operator $c_i^\dagger$ will add an electron on the site i and $c_i^\dagger c_i$ counts the number of electron on the site i. For our 1d chain model, we can consider two sublattices : the atoms on A (corresponding to the $2m$) and the atoms on B (corresponding to $2m+1$). The previous Hamitonian can be rewritten :

$$\hat{H} = \sum_m^N \left[\epsilon_0 c_{A,m}^\dagger c_{A,m} + \epsilon_1 c_{B,m}^\dagger c_{B,m} + t(1-\delta)c_{A,m}^\dagger c_{B,m} + t(1+\delta)c_{B,m}^\dagger c_{A,m+1} + h.c.\right] \tag{6}$$

where the sum is made over N unit cells, the third term being the hopping parameter between atoms of the same unit cell and the fourth term is the hopping parameter between first neighbours of different unit cells. The $h.c.$ stands for the hermitian conjugate of these two terms so that the total Hamiltonian si hermitian. Here $h.c.$ stands for $t(1-\delta)c_{B,m}^\dagger c_{A,m} + t(1+\delta)c_{A,m+1}^\dagger c_{B,m}$ and means that hopping from A, m to B, m is the same as hopping from $B, m1$ to A, m.

9. Transform the Hamitlonian from real space to momentum space using the relations :

$$\begin{aligned} c_{A,m} &= \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{k}.\vec{r}_m} c_{A,k}, \quad c_{A,m}^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}.\vec{r}_m} c_{A,k}^\dagger \\ c_{B,m} &= \frac{1}{\sqrt{N}}\sum_k e^{-i\vec{k}.\vec{r}_m} c_{B,k}, \quad c_{B,m}^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}.\vec{r}_m} c_{B,k}^\dagger \end{aligned} \tag{7}$$

and show that it can take the following form :

$$\hat{H} = \sum_k \begin{pmatrix} c_{k,A}^\dagger & c_{k,B}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_0 & t(1-\delta) + t(1+\delta)e^{ika} \\ t(1-\delta) + t(1+\delta)e^{-ika} & \epsilon_1 \end{pmatrix} \begin{pmatrix} c_{k,A} \\ c_{k,B} \end{pmatrix} \tag{8}$$

Solution.
Let's start with the first two term :

$$\begin{aligned}\sum_m^N \epsilon_0 c_{A,m}^\dagger c_{A,m} &= \frac{1}{N}\sum_k \sum_m^N \epsilon_0 e^{i\vec{k}.\vec{r}_m} c_{A,k}^\dagger e^{-i\vec{k}.\vec{r}_m} c_{A,k} = \sum_k \epsilon_0 c_{A,k}^\dagger c_{A,k} \\ \sum_m^N \epsilon_1 c_{B,m}^\dagger c_{B,m} &= \frac{1}{N}\sum_k \sum_m^N \epsilon_1 e^{i\vec{k}.\vec{r}_m} c_{B,k}^\dagger e^{-i\vec{k}.\vec{r}_m} c_{B,k} = \sum_k \epsilon_1 c_{B,k}^\dagger c_{B,k}\end{aligned} \tag{9}$$

For the third term we have :

$$\begin{aligned}\sum_m^N t(1-\delta) c_{A,m}^\dagger c_{B,m} &= \frac{1}{N}\sum_k \sum_m^N t(1-\delta) e^{i\vec{k}.\vec{r}_m} c_{A,k}^\dagger e^{-i\vec{k}.\vec{r}_m} c_{B,k} \\ &= \sum_k t(1-\delta) c_{A,k}^\dagger c_{B,k} \frac{1}{N}\sum_m^N e^{i\vec{k}.\vec{r}_m} e^{-i\vec{k}.\vec{r}_m} \\ &= \sum_k t(1-\delta) c_{A,k}^\dagger c_{B,k}\end{aligned} \tag{10}$$

and the hermitian conjugate :

$$\begin{aligned}\sum_m^N t(1-\delta) c_{B,m}^\dagger c_{A,m} &= \frac{1}{N}\sum_k \sum_m^N t(1-\delta) e^{i\vec{k}.\vec{r}_m} c_{B,k}^\dagger e^{-i\vec{k}.\vec{r}_m} c_{A,k} \\ &= \sum_k t(1-\delta) c_{B,k}^\dagger c_{A,k} \frac{1}{N}\sum_m^N e^{i\vec{k}.\vec{r}_m} e^{-i\vec{k}.\vec{r}_m} \\ &= \sum_k t(1-\delta) c_{B,k}^\dagger c_{A,k}\end{aligned} \tag{11}$$

For the fourth term we have :

$$\begin{aligned}\sum_m^N t(1+\delta) c_{B,m}^\dagger c_{A,m+1} &= \frac{1}{N}\sum_k \sum_m^N t(1+\delta) e^{i\vec{k}.\vec{r}_m} c_{B,k}^\dagger e^{-i\vec{k}.\vec{r}_{m+1}} c_{A,k} \\ &= \sum_k t(1+\delta) c_{B,k}^\dagger c_{A,k} \frac{1}{N}\sum_m^N e^{i\vec{k}.\vec{r}_m} e^{-i\vec{k}.\vec{r}_m} e^{-ika} \\ &= \sum_k t(1+\delta) c_{B,k}^\dagger c_{A,k} e^{-ika}\end{aligned} \tag{12}$$

and the hermitian conjugate :

$$\begin{aligned}\sum_m^N t(1+\delta) c_{A,m+1}^\dagger c_{B,m} &= \frac{1}{N}\sum_k \sum_m^N t(1+\delta) e^{i\vec{k}.\vec{r}_{m+1}} c_{A,k}^\dagger e^{-i\vec{k}.\vec{r}_m} c_{A,k} \\ &= \sum_k t(1+\delta) c_{A,k}^\dagger c_{B,k} \frac{1}{N}\sum_m^N e^{i\vec{k}.\vec{r}_m} e^{-i\vec{k}.\vec{r}_m} e^{ika} \\ &= \sum_k t(1+\delta) c_{A,k}^\dagger c_{B,k} e^{ika}\end{aligned} \tag{13}$$

So the Hamiltonian writes :

$$\begin{aligned}\hat{H} &= \sum_k \epsilon_0 c_{A,k}^\dagger c_{A,k} + \epsilon_1 c_{B,k}^\dagger c_{B,k} \\ &= +t(1-\delta) c_{A,k}^\dagger c_{B,k} + t(1-\delta) c_{B,k}^\dagger c_{A,k} + t(1+\delta) c_{B,k}^\dagger c_{A,k} e^{-ika} + t(1+\delta) c_{A,k}^\dagger c_{B,k} e^{ika}\end{aligned} \tag{14}$$

So we have :

$$\hat{H} = \sum_k \begin{pmatrix} c_{k,A}^\dagger & c_{k,B}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_0 & t(1-\delta) + t(1+\delta) e^{ika} \\ t(1-\delta) + t(1+\delta) e^{-ika} & \epsilon_1 \end{pmatrix} \begin{pmatrix} c_{k,A} \\ c_{k,B} \end{pmatrix} \tag{15}$$

10. Rewrite the Hamiltonian matrix :

$$h = \begin{pmatrix} \epsilon_0 & t(1-\delta) + t(1+\delta)e^{ika} \\ t(1-\delta) + t(1+\delta)e^{-ika} & \epsilon_1 \end{pmatrix} \tag{16}$$

in the Pauli matrix basis and the identity, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$

Solution.

$$h = \epsilon_m \sigma_0 + \Delta\epsilon\sigma_z + (t(1-\delta) + t(1+\delta)cos(ka))\,\sigma_x + (t(1+\delta)sin(ka))\,\sigma_y \tag{17}$$

11. Once the Hamiltonian is in the form $h = \vec{D}_k.\vec{\sigma} + \epsilon_k\sigma_0$, the eigenvalues are given by $E_k^{\pm} = \epsilon_k \pm |\vec{D}_k|$. Calculate the eigenvalues.

Solution.

$$\begin{aligned} E_k^{\pm} &= \epsilon_m \pm \sqrt{\Delta\epsilon^2 + (t(1-\delta) + t(1+\delta)cos(ka))^2 + (t(1+\delta)sin(ka))^2} \\ &= \epsilon_m \pm \sqrt{\Delta\epsilon^2 + 4t^2cos^2(\frac{ka}{2}) + 4t^2\delta^2sin^2(\frac{ka}{2})} \end{aligned} \tag{18}$$

1.3 Tight binding model for 2d square lattice in second quantization

We consider now a square lattice in 2 dimension (x and y) of parameter a, with one atom per unit cell and one orbital per atom. In second-quatization, we can write the Hamiltonian :

$$\hat{H} = \sum_{m,n}^{N} \left[\epsilon_0 c_{m,n}^{\dagger} c_{m,n} - t c_{m,n}^{\dagger} c_{m+1,n} + t c_{m,n}^{\dagger} c_{m,n+1} + h.c.\right] \tag{19}$$

where (m,n) refers to the coordinate of the unit cell (and thus the atom) and $-t$ (t>0) the hopping parameter between first neighbour atoms.

12. Transform the Hamitlonian from real space to momentum space using the relations :

$$c_{m,n} = \frac{1}{\sqrt{N^2}} \sum_k e^{-i\vec{k}.\vec{r}_{m,n}} c_k, \quad c_{m,n}^{\dagger} = \frac{1}{\sqrt{N^2}} \sum_k e^{i\vec{k}.\vec{r}_{m,n}} c_k^{\dagger} \tag{20}$$

Solution.
Let's start with the first term :

$$\sum_{m,n}^{N} \epsilon_0 c_{m,n}^{\dagger} c_{m,n} = -\frac{1}{N^2} \sum_{k} \sum_{m}^{N} \sum_{n}^{N} \epsilon_0 e^{i\vec{k}.\vec{r}_{m,n}} c_k^{\dagger} e^{-i\vec{k}.\vec{r}_{m,n}} c_k = \sum_{k} \epsilon_0 c_k^{\dagger} c_k \tag{21}$$

For the second term we have :

$$\begin{aligned} \sum_{m,n}^{N} -t c_{m,n}^{\dagger} c_{m+1,n} &= -\frac{1}{N^2} \sum_{k} \sum_{m}^{N} \sum_{m}^{N} t e^{i\vec{k}.\vec{r}_{m,n}} c_k^{\dagger} e^{-i\vec{k}.\vec{r}_{m+1,n}} c_k \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{i\vec{k}.\vec{r}_{m,n}} e^{-i\vec{k}.\vec{r}_{m,n}} e^{-ik_x a} \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{-ik_x a} \end{aligned} \tag{22}$$

and the hermitian conjugate :

$$\begin{aligned} \sum_{m,n}^{N} -t c_{m+1,n} c_{m,n}^{\dagger} &= -\frac{1}{N^2} \sum_{k} \sum_{m}^{N} \sum_{m}^{N} t e^{i\vec{k}.\vec{r}_{m+1,n}} c_k^{\dagger} e^{-i\vec{k}.\vec{r}_{m,n}} c_k \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{i\vec{k}.\vec{r}_{m,n}} e^{-i\vec{k}.\vec{r}_{m,n}} e^{ik_x a} \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{ik_x a} \end{aligned} \tag{23}$$

For the third term we have :

$$\begin{aligned} \sum_{m,n}^{N} -t c_{m,n}^{\dagger} c_{m,n+1} &= -\frac{1}{N^2} \sum_{k} \sum_{m}^{N} \sum_{m}^{N} t e^{i\vec{k}.\vec{r}_{m,n}} c_k^{\dagger} e^{-i\vec{k}.\vec{r}_{m,n+1}} c_k \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{i\vec{k}.\vec{r}_{m,n}} e^{-i\vec{k}.\vec{r}_{m,n}} e^{-ik_y a} \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{-ik_y a} \end{aligned} \tag{24}$$

and the hermitian conjugate :

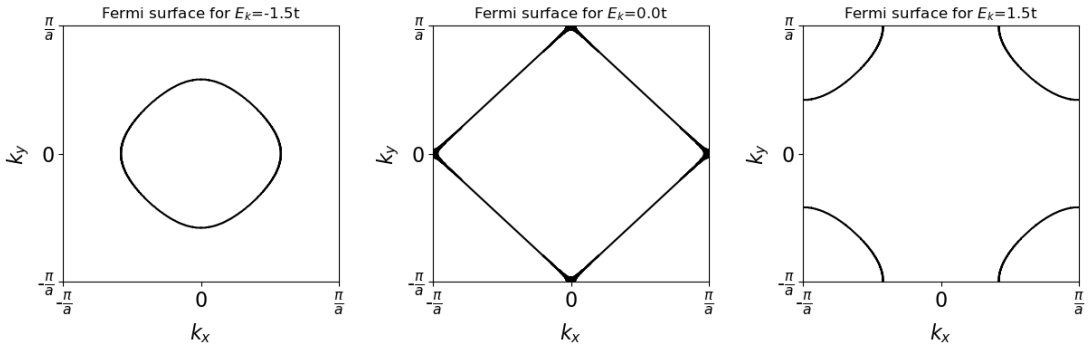
$$\begin{aligned} \sum_{m,n}^{N} -t c_{m,n+1} c_{m,n}^{\dagger} &= \frac{1}{N^2} \sum_{k} \sum_{m}^{N} \sum_{m}^{N} t e^{i\vec{k}.\vec{r}_{m,n+1}} c_k^{\dagger} e^{-i\vec{k}.\vec{r}_{m,n}} c_k \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{i\vec{k}.\vec{r}_{m,n}} e^{-i\vec{k}.\vec{r}_{m,n}} e^{ik_y a} \\ &= \sum_{k} -t c_k^{\dagger} c_k e^{ik_y a} \end{aligned} \tag{25}$$

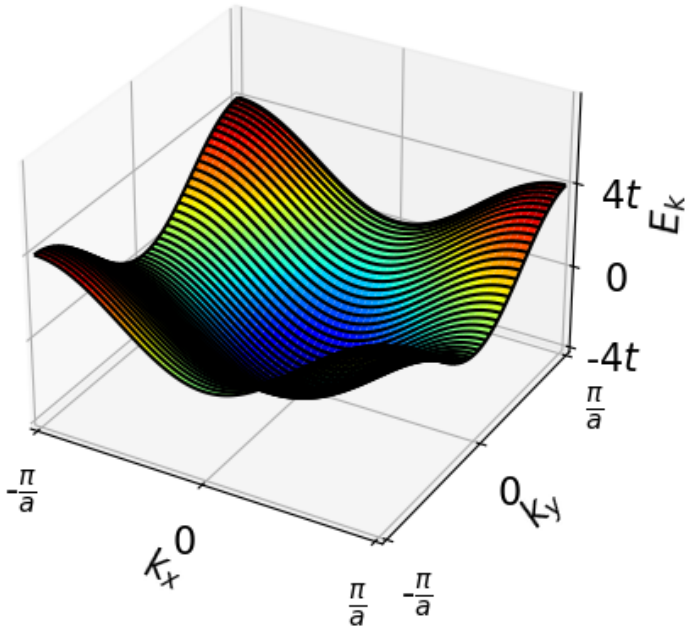
So we have ultimately :

$$\hat{H} = \sum_{k} -2t \left[cos(k_x a) + cos(k_y a) \right] c_k^{\dagger} c_k \tag{26}$$

13. Draw the Fermi surface for $E_k < 0$, $E_k = 0$ and $E_k > 0$.

Solution.


Fermi surface for E_k=-1.5t
Fermi surface for E_k=0.0t
Fermi surface for E_k=1.5t
k_y
k_x
$\frac{\pi}{a}$
0
$-\frac{\pi}{a}$


4t
E_k
0
-4t
$\frac{\pi}{a}$
$-\frac{\pi}{a}$
k_x
k_y