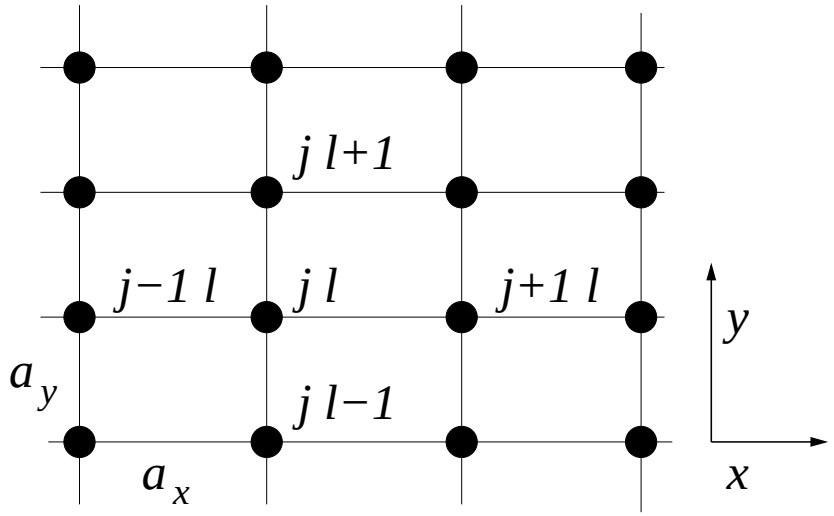
PY4T01 Condensed Matter Theory: Lecture 9

Solids as giant molecules

Consider the following square lattice of atoms



As usual we expand the wave function on a localized atomic orbital basis set $|mn\alpha\rangle$ (supposed orthogonal)

$$|\psi\rangle = \sum_{mn\alpha} \psi_{mn\alpha} |mn\alpha\rangle$$

As usual consider the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$, and project on $\langle jl\beta|$

$$\sum_{mn}^{N_x N_y} \sum_{\alpha}^{N_\alpha} \langle jl\beta|H|mn\alpha\rangle \psi_{mn\alpha} = E \sum_{mn}^{N_x N_y} \sum_{\alpha}^{N_\alpha} \langle jl\beta|mn\alpha\rangle \psi_{mn\alpha}$$

Take only first nearest neighbors coupling (both along x and y). This means $m = j \pm 1$ and $n = l \pm 1$:

$$\sum_{\alpha}^{N_\alpha}[\langle jl\beta|H|jl\alpha\rangle\psi_{jl\alpha}+$$

$$\langle jl\beta|H|(j+1)l\alpha\rangle\psi_{j+1\ l\alpha} + \langle jl\beta|H|(j-1)l\alpha\rangle\psi_{j-1\ l\alpha}+$$

$$\langle jl\beta|H|j\ (l+1)\ \alpha\rangle\psi_{j\ l+1\ \alpha} + \langle jl\beta|H|j\ (l-1)\ \alpha\rangle\psi_{j\ l-1\ \alpha}] =$$

$$= E\sum_{\alpha}^{N_\alpha}\langle jl\beta|jl\alpha\rangle\psi_{jl\alpha}$$

This looks rather complicated, however if we consider a square lattice of H atoms (one s state per atom), then $N_\alpha = 1$ and we obtain

$$(E-\epsilon_0)\psi_{jl} + \gamma_x(\psi_{j+1\ l} + \psi_{j-1\ l}) + \gamma_y(\psi_{j\ l+1} + \psi_{j\ l-1}) = 0$$

This is identical to the previous $1D$ case in both the x and y directions!!! The solution, then must be of the kind:

$$\psi_{jl} = A\mathrm{e}^{ik_x a_x j}\ \mathrm{e}^{ik_y a_y l}$$

By substituting this one obtains:

$$(E - \epsilon_0) + \gamma_x(\mathrm{e}^{ik_x a_x} + \mathrm{e}^{-ik_x a_x}) + \gamma_y(\mathrm{e}^{ik_y a_y} + \mathrm{e}^{-ik_y a_y}) = 0$$

then

$$\boxed{E = \epsilon_0 + 2\gamma_x \cos(k_x a_x) + 2\gamma_y \cos(k_y a_y)}$$

This is an example of band structure in 2D.

Note that:

- Now we have

$$-\pi/a_x < k_x < \pi/a_x$$

$$-\pi/a_y < k_y < \pi/a_y$$

This means that the Brillouin Zone is "different" for k_x and k_y

- The Brillouin Zone for this 2D case is the 2D rectangular area given by

$$-\pi/a_x < k_x < \pi/a_x$$

$$-\pi/a_y < k_y < \pi/a_y$$

- Again the Schrödinger equation is invariant for both (why?)

$$k_x \rightarrow -k_x$$

$$k_y \rightarrow -k_y$$

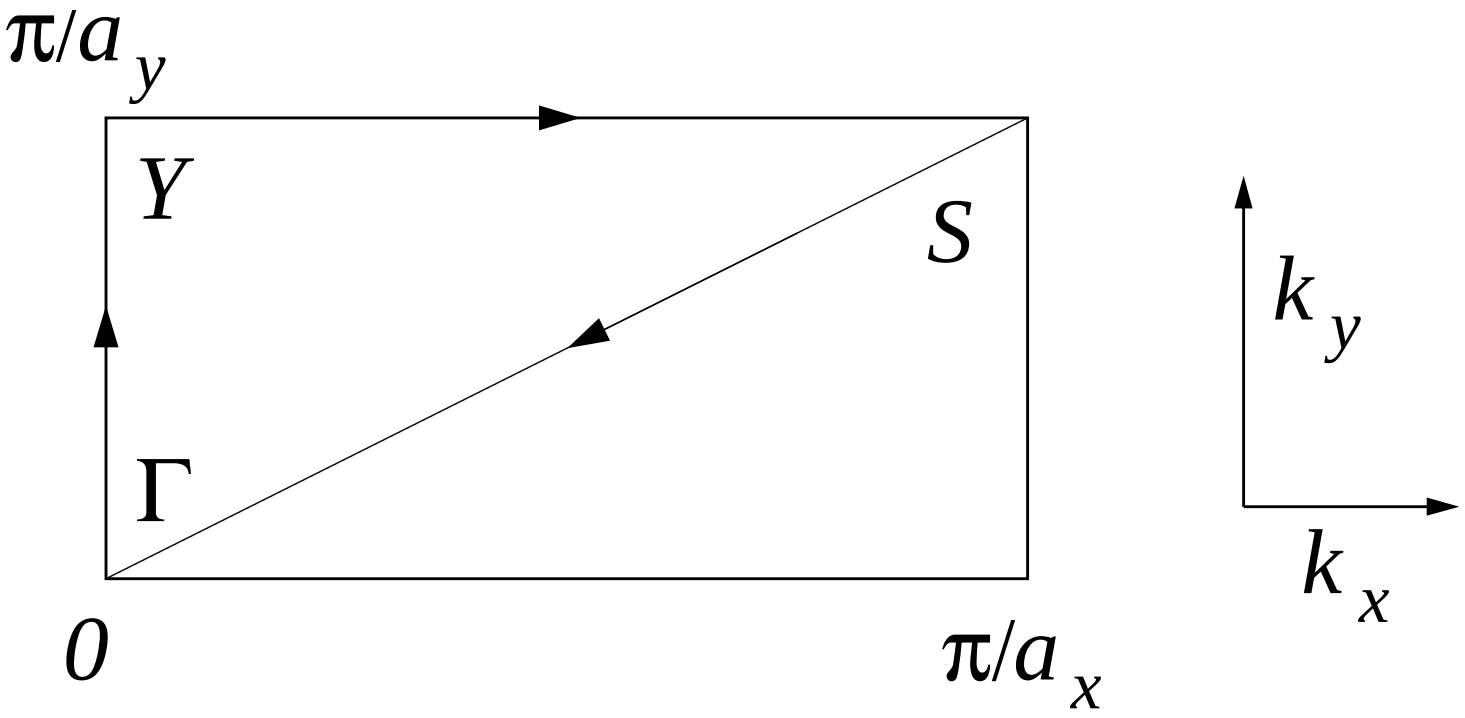
We can reduce the Brillouin zone to (irreducible Brillouin Zone):

$$0 < k_x < \pi/a_x$$

$$0 < k_y < \pi/a_y$$

- Since now the Brillouin Zone is a surface we can plot along different directions. For instance we can do:

$$(k_x, k_y) = (0, 0) \rightarrow (0, \pi/a_y) \rightarrow (\pi/a_x, \pi/a_y) \rightarrow (0, 0)$$



Example: $a_y = 2a_x = 2a_0$

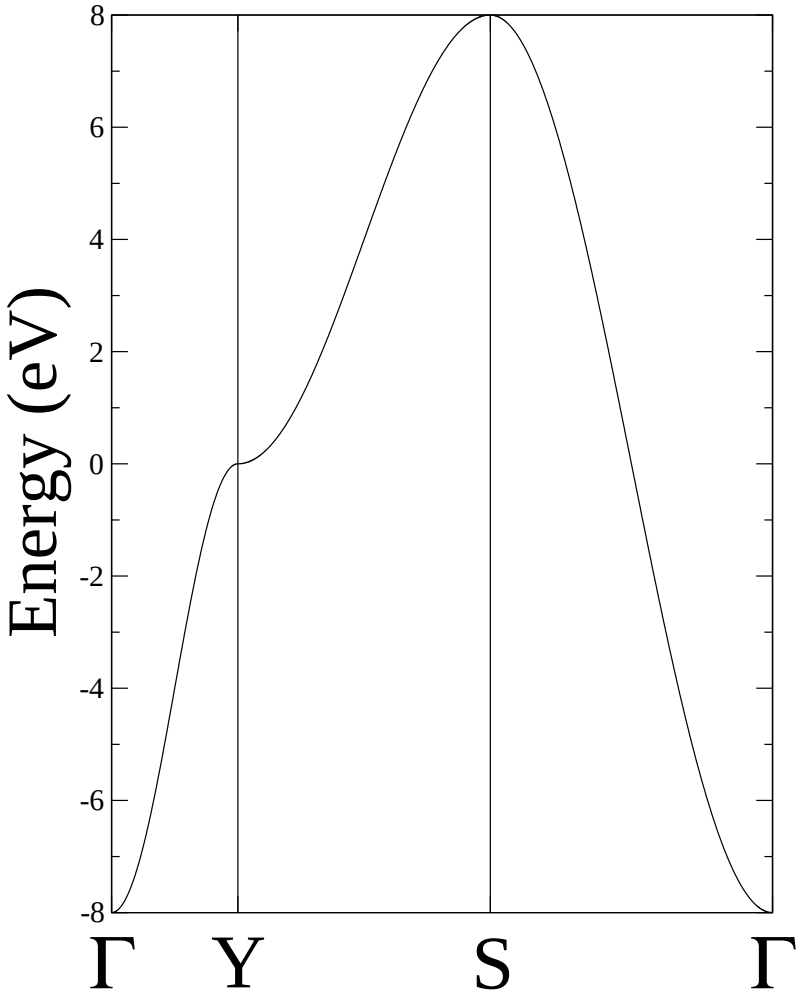
The dispersion relation therefore is:

$$E = \epsilon_0 + 2\gamma_x \cos(k_x a_0) + 2\gamma_y \cos(2k_y a_0)$$

Let's plot the band along the direction:

$$(k_x, k_y) = (0,0) \rightarrow (0, \pi/a_y) \rightarrow (\pi/a_x, \pi/a_y) \rightarrow (0,0)$$

$$(k_x, k_y) = \Gamma \rightarrow Y \rightarrow S \rightarrow \Gamma$$



$\epsilon_0 = 0$
$\gamma_x = -2$
$\gamma_y = -2$

Example: $a_y = a_x = a_0$

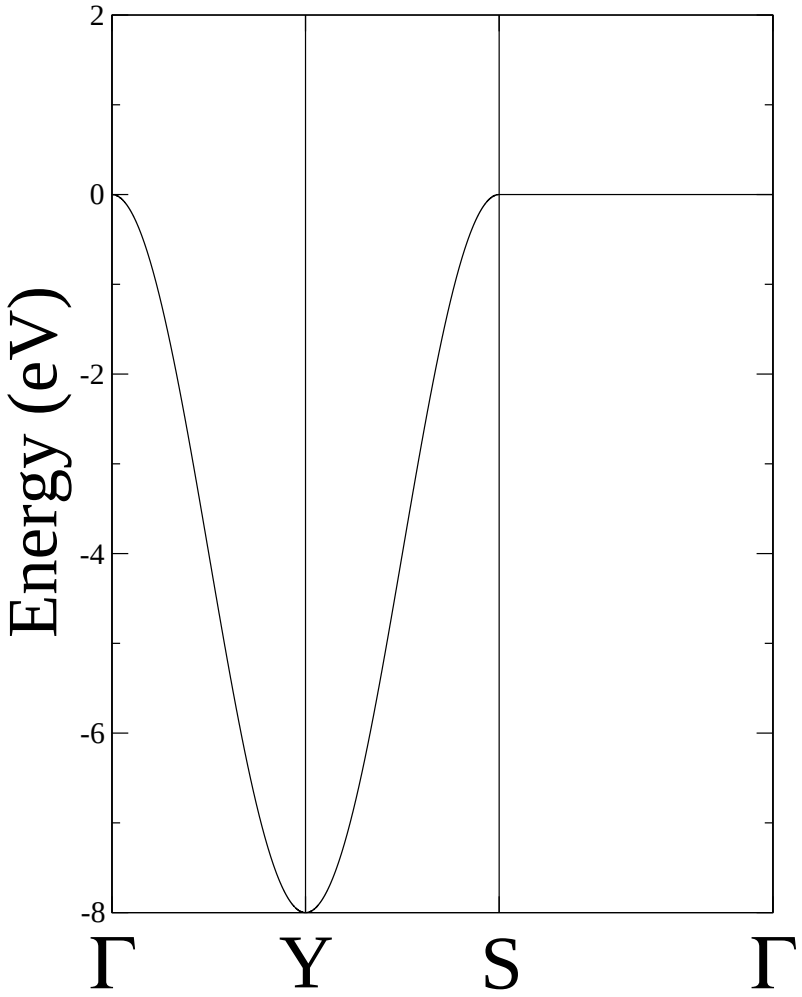
The dispersion relation therefore is:

$$E = \epsilon_0 + 2\gamma_x \cos(k_x a_0) + 2\gamma_y \cos(k_y a_0)$$

Let's plot the band along the same direction:

$$(k_x, k_y) = \Gamma \rightarrow Y \rightarrow S \rightarrow \Gamma$$

But now $\gamma_x = -\gamma_y = -2$, $\epsilon_0 = 0$



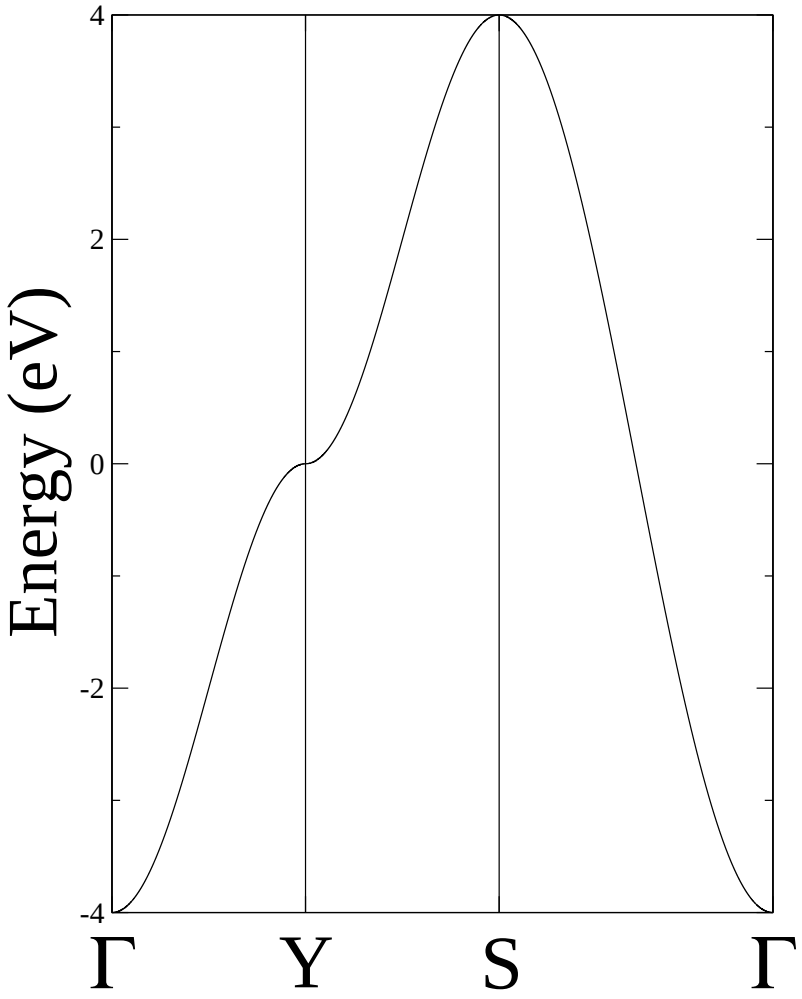
Example: square H lattice

$$a_y = a_x = a_0 \qquad \gamma_x = \gamma_y = \gamma = -1 \qquad \epsilon_0 = 0.$$

$$E_k = \epsilon_0 + 2\gamma[\cos(k_x a_0) + \cos(k_y a_0)]$$

Let's plot the band along the same direction:

$$(k_x, k_y) = \Gamma \rightarrow Y \rightarrow S \rightarrow \Gamma$$



Fermi Surface

In 2D (and 3D) the energy depends on both k_x and k_y.

Can we define a Fermi wave vector?

No!!! but we can define a Fermi Surface. This is the set of k_x and k_y such that

$$E_F = E(k_x, k_y)$$

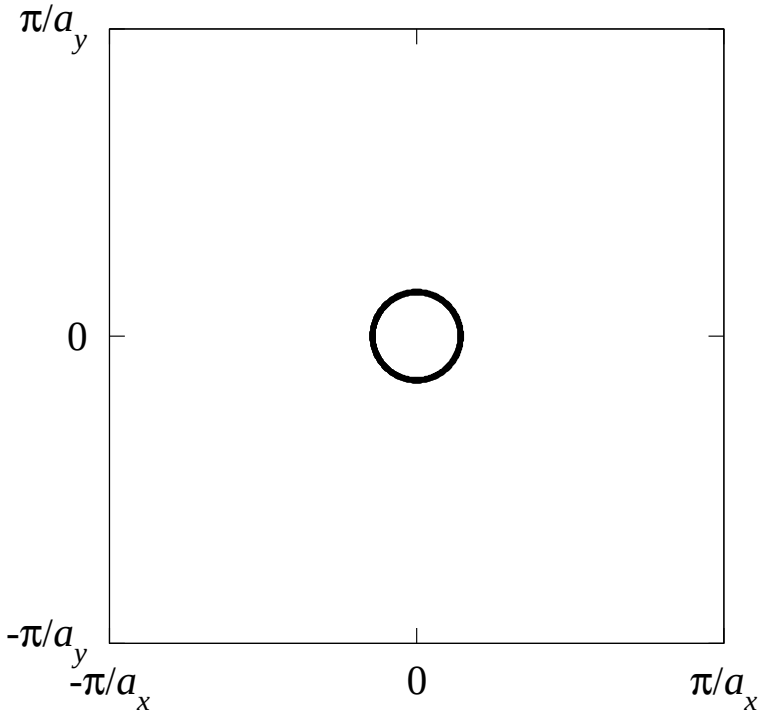
Let us see some examples for the square H lattice. In this case the Fermi surface is defined as:

$$E_F = \epsilon_0 + 2\gamma[\cos(k_x a_0) + \cos(k_y a_0)]$$

- Small band filling ($E_F \simeq \epsilon_0 + 4\gamma$). This means

$$E_F = E(k_x, k_y) \simeq \epsilon_0 + 4\gamma - \gamma a_0^2 (k_x^2 + k_y^2)$$

The Fermi surface then looks like



Note also that in the free electron model in 2D one has

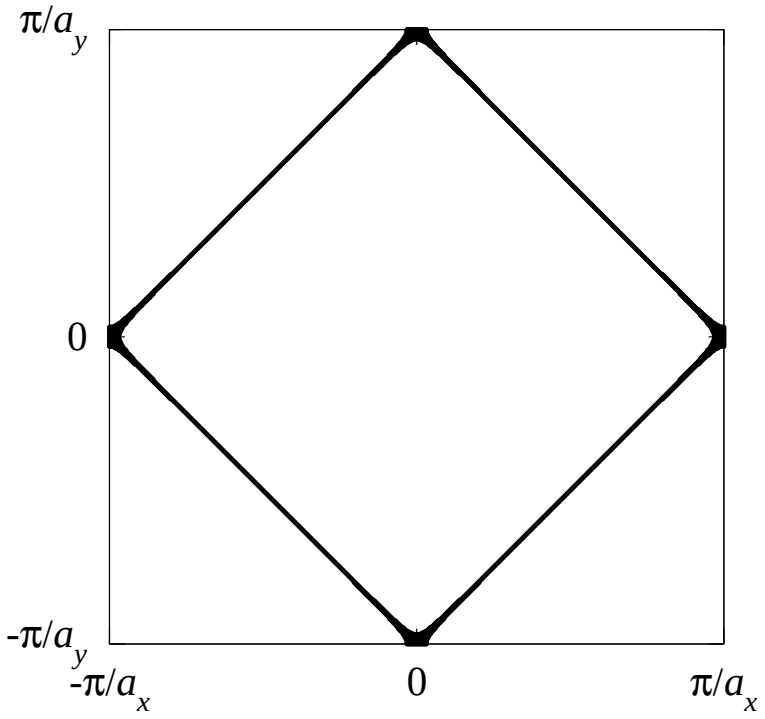
$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$$

Therefore at the bottom of the band electrons behave almost freely with:

$$\frac{\hbar^2}{2m} \rightarrow -a_0^2 \gamma$$

- Band Center ($E_F = \epsilon_0$). This means

$$\cos(k_x a_0) = -\cos(k_y a_0)$$

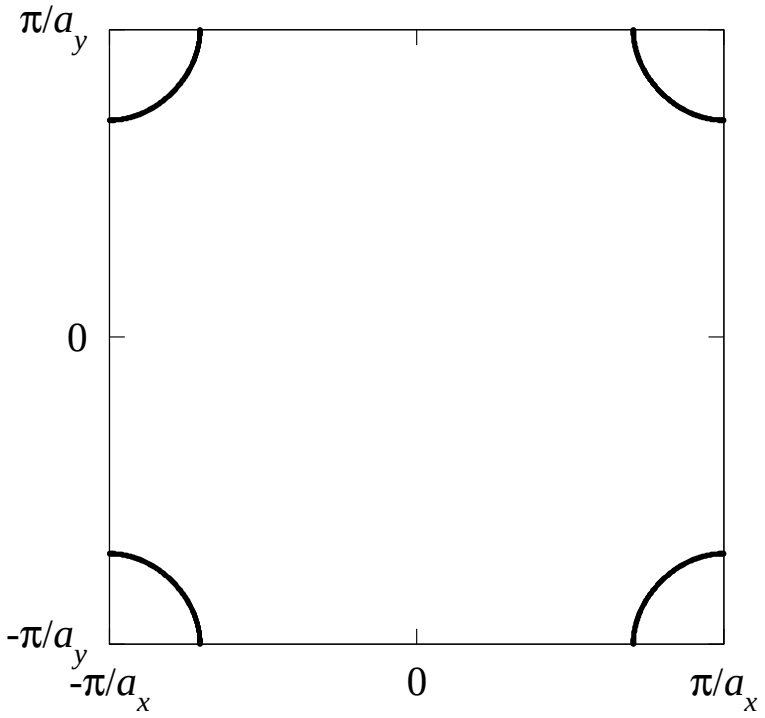


- Band nearly filled ($E_F \simeq \epsilon_0 - 4\gamma$). This means

$$\cos(k_x a_0) + \cos(k_y a_0) \simeq -2 \quad \rightarrow \quad k_x \sim \pi/a_x \;\; k_y \sim \pi/a_y$$

Expanding around π/a we find:

$$E_F = E(k_x, k_y) \simeq \epsilon_0 - 4\gamma + \gamma a_0^2 (k_x^2 + k_y^2)$$



This is similar to the small band filling with

$$-a_0^2\gamma \rightarrow +a_0^2\gamma$$

Density of States

The definition given for one dimensional systems is still valid:

$$d(E) = \sum_{\text{all } E_k} \delta(E - E_k)$$

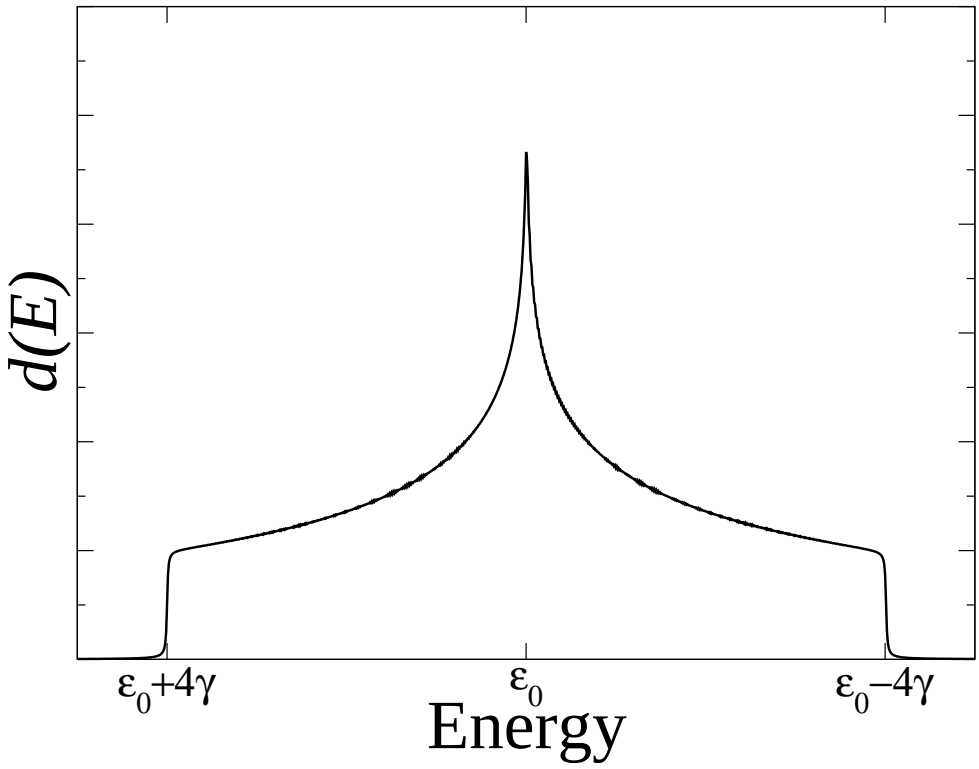
However this time E_k depends on both k_x and k_y:

$$E_k = E(k_x, k_y) = \epsilon_0 + 2\gamma_x \cos(k_x a_x) + 2\gamma_y \cos(k_y a_y)$$

This can be calculated analytically (rather long) $\rightarrow$ numerically

$$d(E) = \sum_{k_x=-\pi/a_x}^{\pi/a_x} \sum_{k_y=-\pi/a_y}^{\pi/a_y} \delta(E - E(k_x, k_y))$$

For the square H lattice one obtains

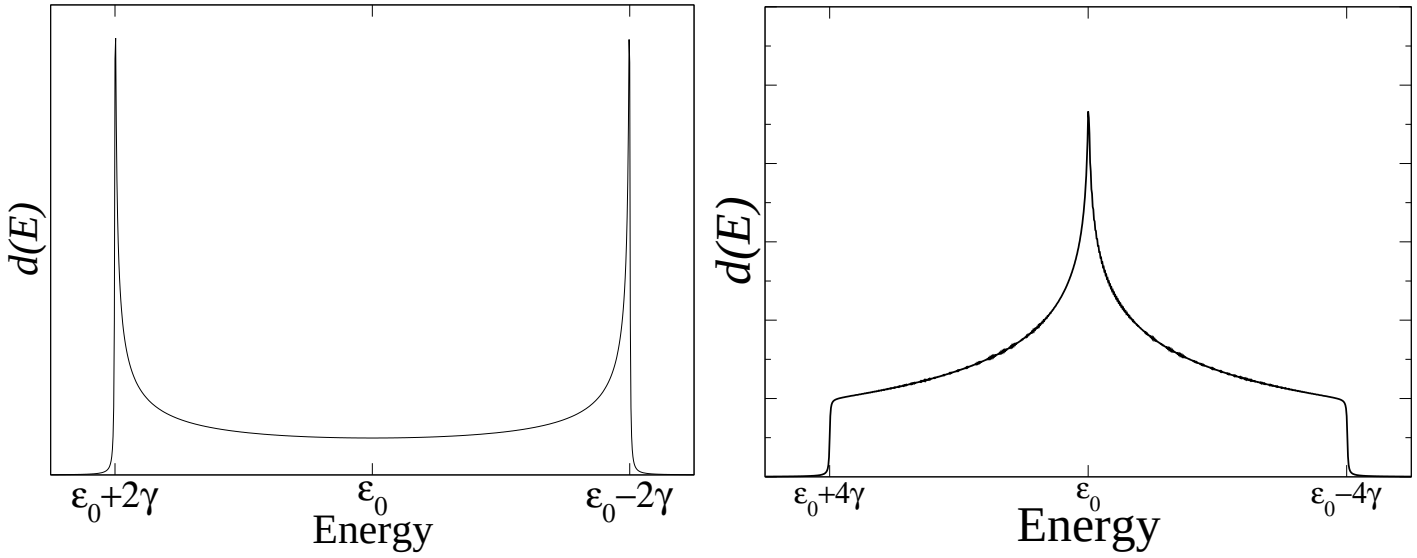


Note that:

- The bandwidth is now 8γ
- The DOS diverges at the band center $E = \epsilon_0$

From 1D to 2D

How does the DOS change?



Consider again the general solution for our square lattice:

$$|\psi_{\vec{k}}\rangle = \sum_{jl}^{N_x N_y} \psi_{jl}|jl\rangle = \sum_{jl}^{N_x N_y} A\mathrm{e}^{ik_x a_x j}\ \mathrm{e}^{ik_y a_y l}|jl\rangle$$

In the limit $N_y = 1$ we have the 1D solution

$$|\psi_k\rangle = \sum_{j}^{N_x} \mathrm{e}^{ik_x a_x j}|j\rangle$$

Consider now $N_y \neq 1$ but also $N_y \neq \infty$. In this case the

boundary conditions for the wave function in the y direction are:

$$\psi_{j0} = \psi_{j\ N_y+1} = 0$$

This gives immediately (it is analogous to the case of the linear chain)

$$|\psi^m_{\vec{k}}\rangle = \sum_{jl}^{N_x N_y} \psi^m_{jl} |jl\rangle$$

with

$$\psi^m_{jl} = \left(\frac{1}{N_x}\right)^{1/2} \left(\frac{2}{N_y+1}\right)^{1/2} \mathrm{e}^{ik_x a_x j} \sin\left(\frac{m\pi}{N_y+1} l\right)$$

for $m = 1, .., N_y$

Therefore the wave function is the product of a standing wave (along y) times a traveling wave (along x). The energy is simply:

$$E_k = \epsilon_0 + 2\gamma \left[\cos(k_x a_0) + \cos\left(\frac{m\pi}{N_y+1}\right)\right]$$

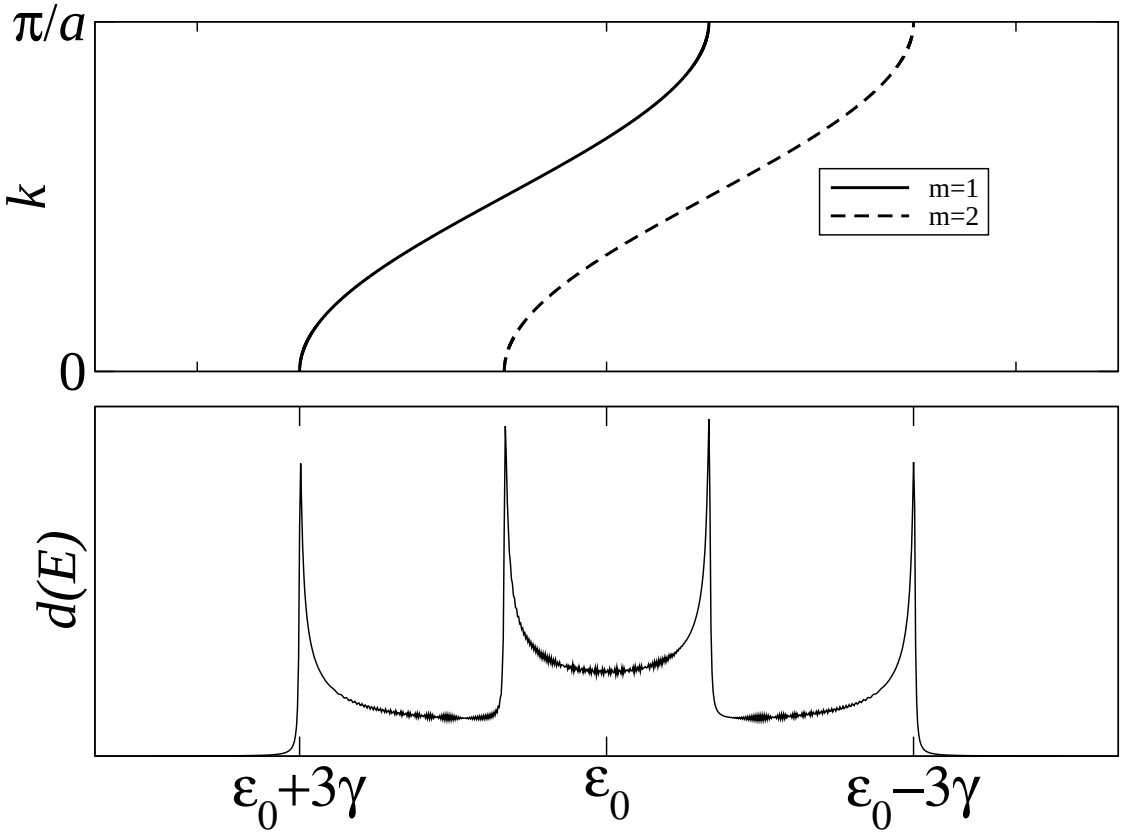
For every standing wave along y (transverse mode) we have a 1D band:

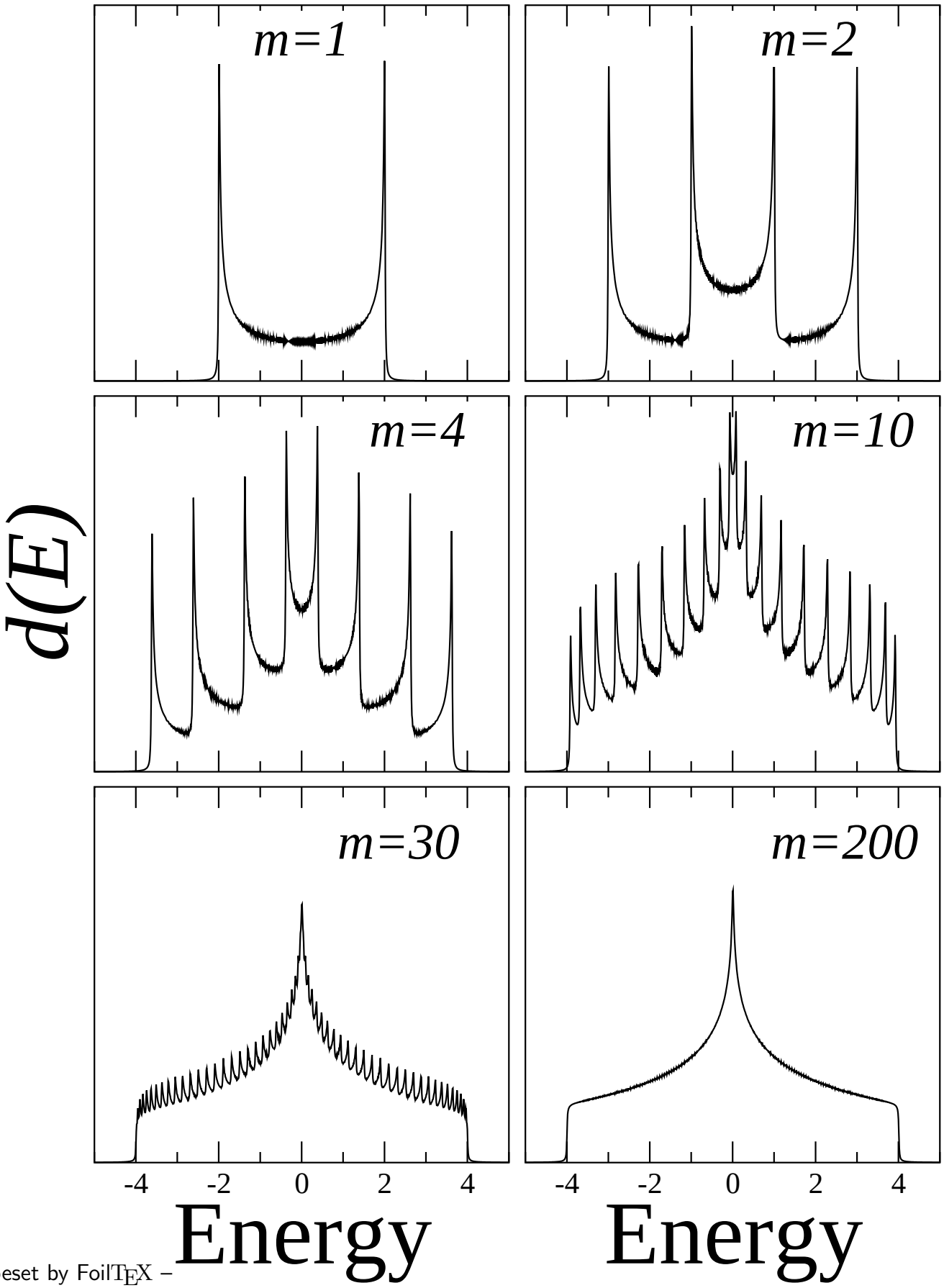
$$E_k = \epsilon_0 + \epsilon_m + 2\gamma \cos(k_x a_x)$$

with

$$\epsilon_m = 2\gamma \cos\left(\frac{m\pi}{N_y + 1}\right)$$

These m-dependent 1D bands are usually called **mini-bands**. This explains how the DOS changes from 1D to 2D.




m=1
m=2
m=4
m=10
m=30
m=200
d(E)
-4
-2
0
2
4
Energy
Energy