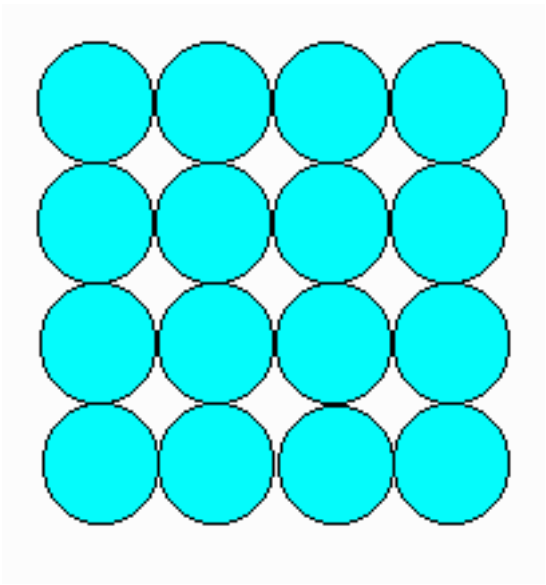
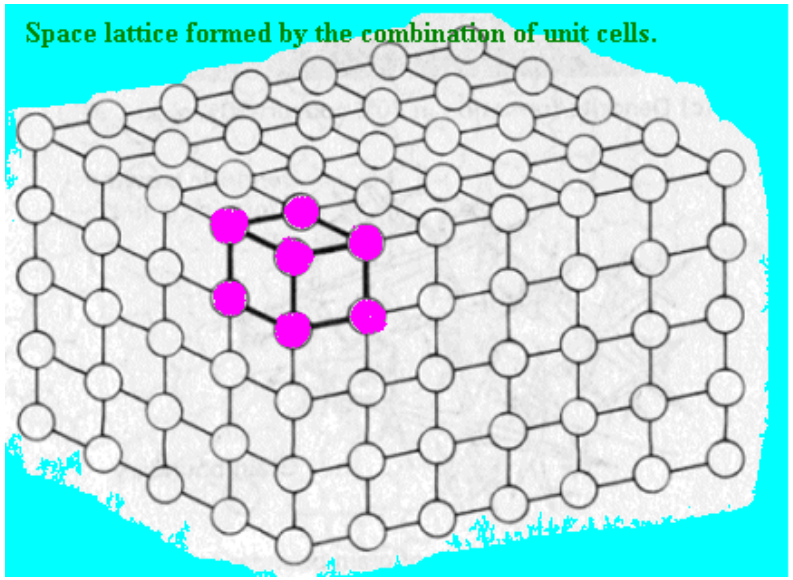
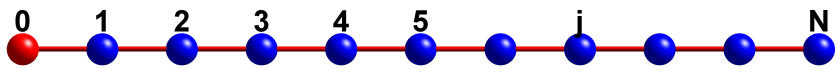
PH 575 Spring 2019

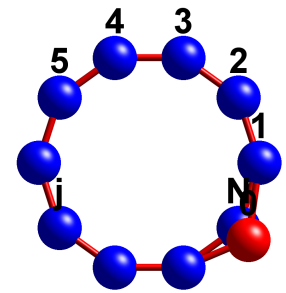
Lecture #7
2 and 3 dimensions: Sutton Ch. 4 pp 74 -> 80





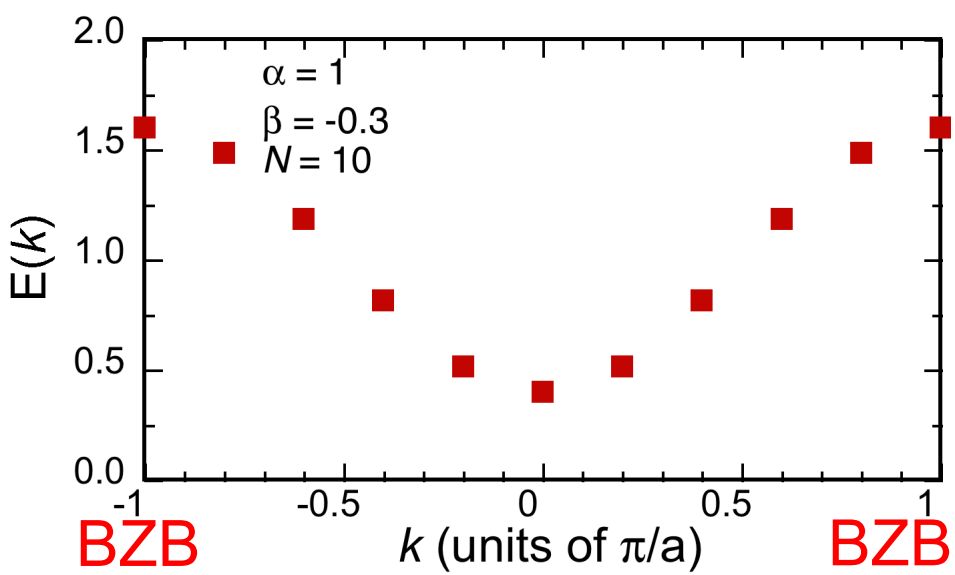
Summary: 1-D Chain, n-n, PBC



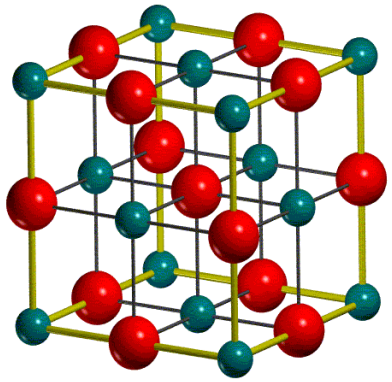


MO $$\left|\Psi_m\right\rangle = \sum_{j=1}^{N} \frac{1}{\sqrt{N}} e^{ij\frac{2\pi m}{N}} \left|j\right\rangle \qquad \left|\Psi_k\right\rangle = \sum_{j=1}^{N} \frac{1}{\sqrt{N}} e^{ijka} \left|j\right\rangle$$

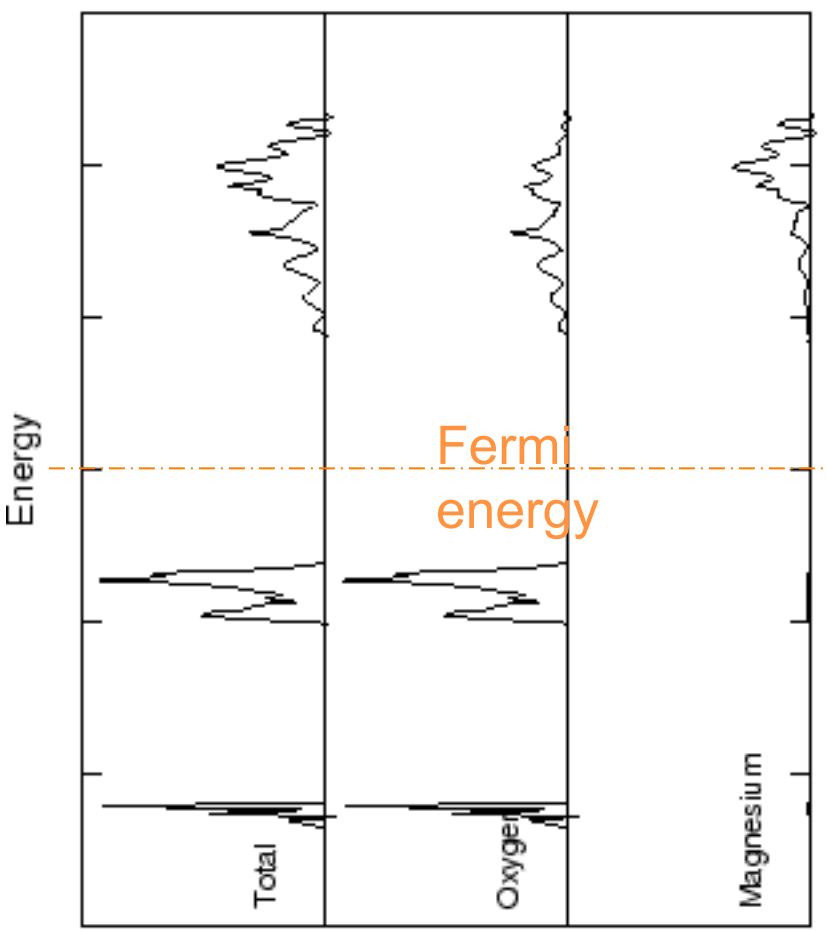
$$E^{(m)} = \alpha + 2\beta\cos\left(\frac{2m\pi}{N}\right) \qquad E(k) = \alpha + 2\beta\cos(ka)$$



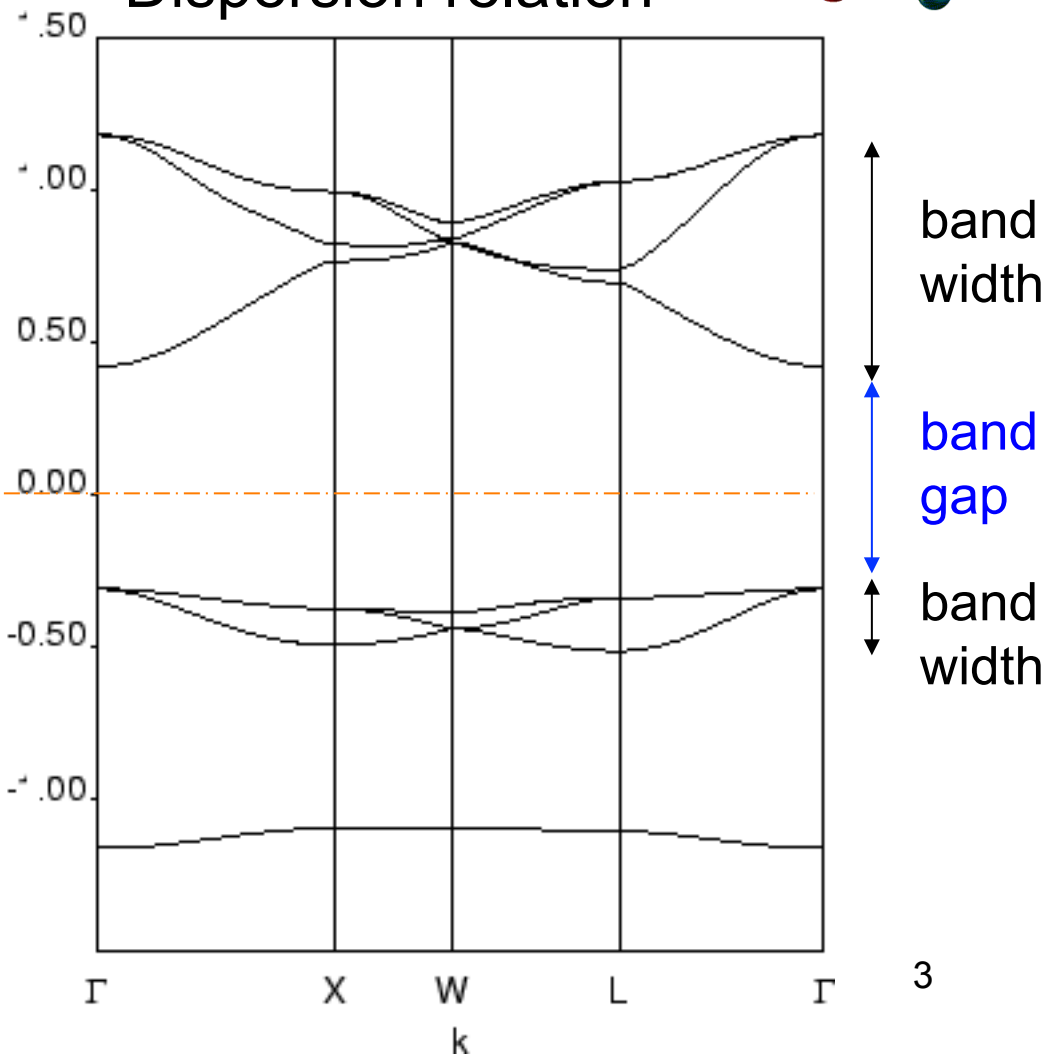
MgO - an ionic crystal



Density of states



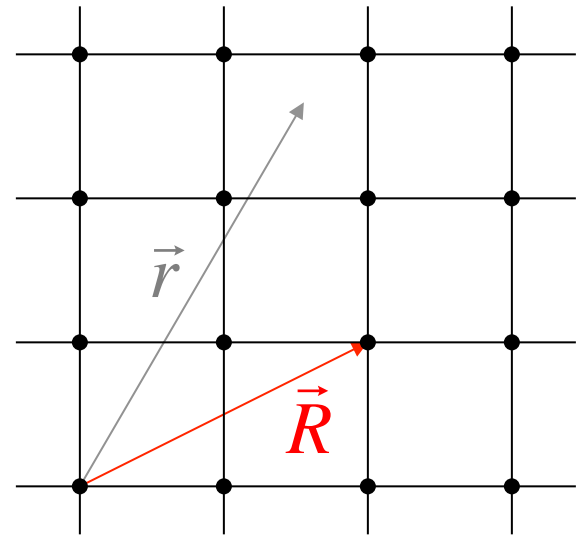
Dispersion relation



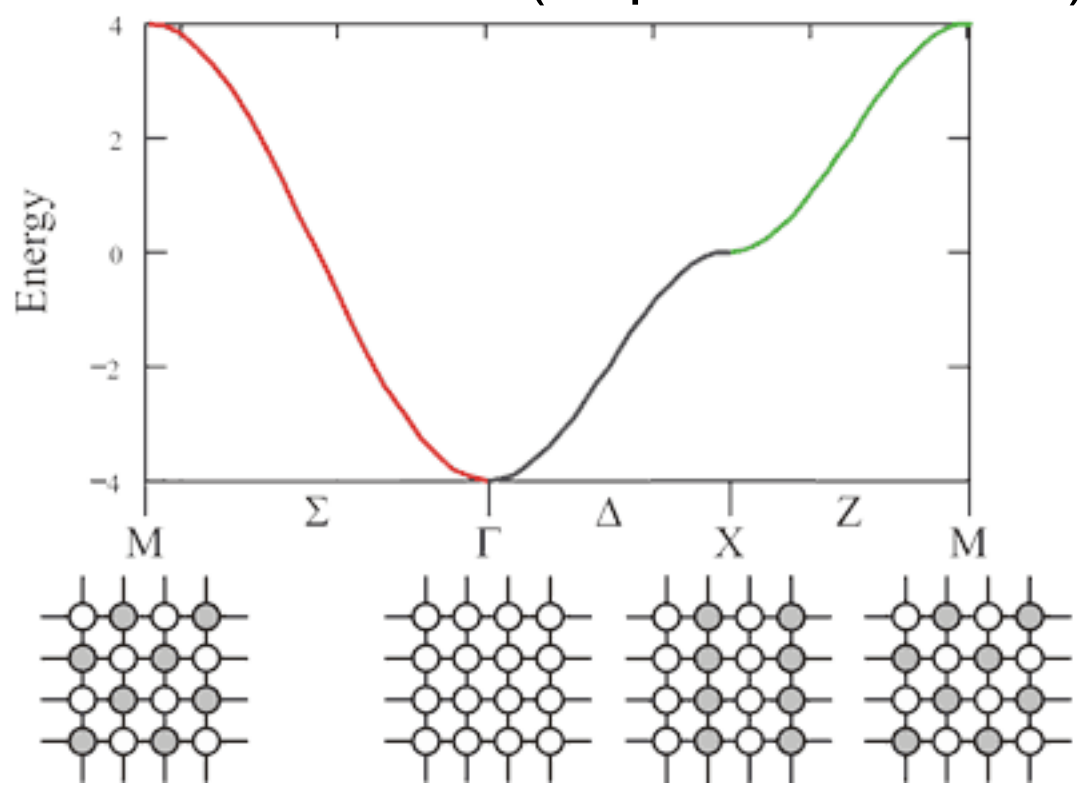
www.crystal.unito.it/tutojan2004/tutorials/G_properties/img47.gif&imgrefurl=http://www.crystal.unito.it/tutojan2004/tutorials/G_properties/properties_tut.html

The 2-dimensional square lattice:

① Band structure (dispersion relation)
② Wave functions (electron density)
③ Brillouin zone
④ Fermi surface



① Band structure (dispersion relation)



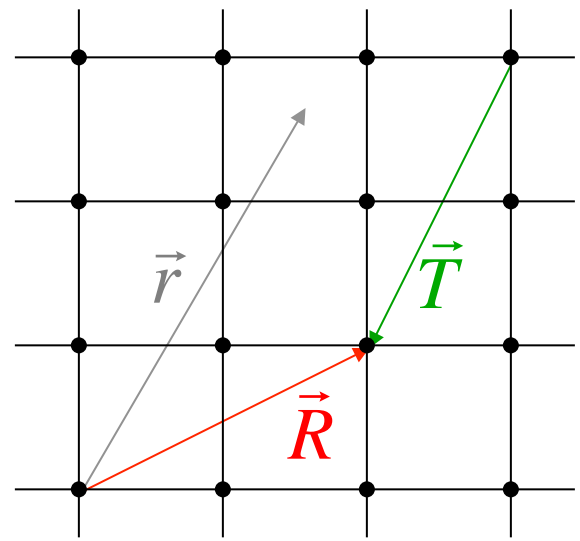
1-D to 2-D

$$x \rightarrow \vec{r}$$
$$k \rightarrow \vec{k}$$
$$|j\rangle \rightarrow |\vec{R}\rangle$$
$$|\Psi_m\rangle \rightarrow |\Psi_{\vec{k}}\rangle$$
$$c_j^{(m)} \rightarrow c_{\vec{k}}(\vec{R})$$

$$\left|\Psi_{\vec{k}}\right\rangle = \sum_{R} c_{\vec{k}}\left(\vec{R}\right)\left|\vec{R}\right\rangle$$ MO made from AOs

By analogy with 1D

$$c_{\vec{k}}\left(\vec{R}\right) = \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{R}}$$



This form ensures

① Normalization

② periodicity in electron density

③ appropriate translational symmetry of the wave function (PH grads, you should study this and ask me about it)

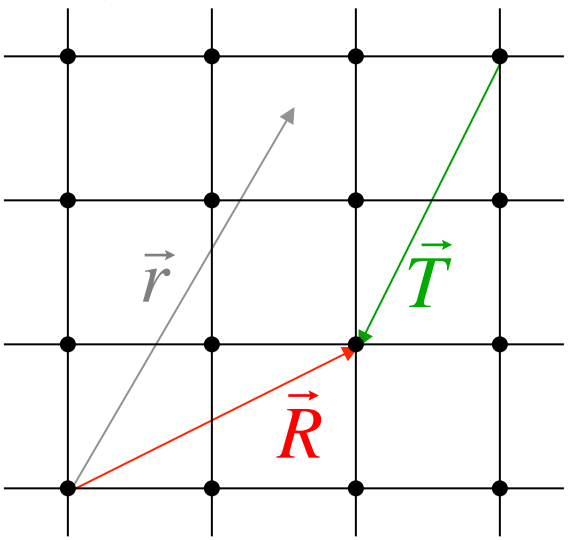
$$\Psi_{\vec{k}}\left(\vec{r}+\vec{T}\right) = e^{i\vec{k}\cdot\vec{T}}\Psi_{\vec{k}}\left(\vec{r}\right)$$

T is any lattice vector. *R* is a special lattice vector that starts from the origin. *N* is the number of atoms (lattice sites).

$$\left|\Psi_{\vec{k}}\right\rangle = \frac{1}{\sqrt{N}}\sum_{R} e^{i\vec{k}\cdot\vec{R}}\left|\vec{R}\right\rangle$$

Apply Schrödinger equation: $\hat{H}\left|\Psi_{\vec{k}}\right\rangle = E\left(\vec{k}\right)\left|\Psi_{\vec{k}}\right\rangle$

$$\sum_{R} e^{i\vec{k}\cdot\vec{R}}\hat{H}\left|\vec{R}\right\rangle = E\left(\vec{k}\right)\sum_{R} e^{i\vec{k}\cdot\vec{R}}\left|\vec{R}\right\rangle$$



Project onto the other atomic orbitals $\left|\vec{R}'\right\rangle$

$$\sum_{R} e^{i\vec{k}\cdot\vec{R}}\left\langle\vec{R}'\right|\hat{H}\left|\vec{R}\right\rangle = E\left(\vec{k}\right)\sum_{R} e^{i\vec{k}\cdot\vec{R}}\left\langle\vec{R}'\middle|\vec{R}\right\rangle$$

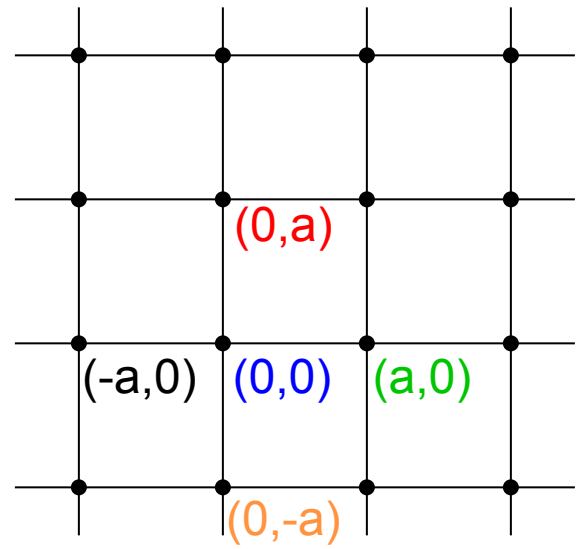
$$\sum_{R} e^{i\vec{k}\cdot\vec{R}}\left\langle\vec{R}'\right|\hat{H}\left|\vec{R}\right\rangle = E\left(\vec{k}\right)e^{i\vec{k}\cdot\vec{R}'}$$

$$E\left(\vec{k}\right) = \sum_{R} e^{i\vec{k}\cdot\left(\vec{R}-\vec{R}'\right)}\left\langle\vec{R}'\right|\hat{H}\left|\vec{R}\right\rangle$$

This is the dispersion relation (3D also) - but we need the Hamiltonian matrix!

$$E\left(\vec{k}\right) = \sum_{R} e^{i\vec{k}\cdot\left(\vec{R}-\vec{R}'\right)} \left\langle \vec{R}' \middle| \hat{H} \middle| \vec{R} \right\rangle$$

$$\left\langle \vec{R}' \middle| \hat{H} \middle| \vec{R} \right\rangle = \begin{cases} \alpha & \text{if } \vec{R} = \vec{R}' \\ \beta & \text{if } \vec{R} \text{ and } \vec{R}' \text{ are n.n} \\ 0 & \text{otherwise} \end{cases}$$



Pick any *R*' to evaluate *E*(*k*) - all give same result. Choose (0, 0).

$$E\left(\vec{k}\right) = \sum_{R} e^{i\vec{k}\cdot\vec{R}} \left\langle \vec{0} \middle| \hat{H} \middle| \vec{R} \right\rangle$$

$$E\left(k_x, k_y\right) = \alpha + \beta e^{ik_x a} + \beta e^{-ik_x a} + \beta e^{ik_y a} + \beta e^{-ik_y a}$$

$$E\left(k_x, k_y\right) = \alpha + 2\beta\cos\left(k_x a\right) + 2\beta\cos\left(k_y a\right)$$

$$E\left(k_x,k_y\right)=\alpha+2\beta\left[\cos\left(k_x a\right)+\cos\left(k_y a\right)\right]$$

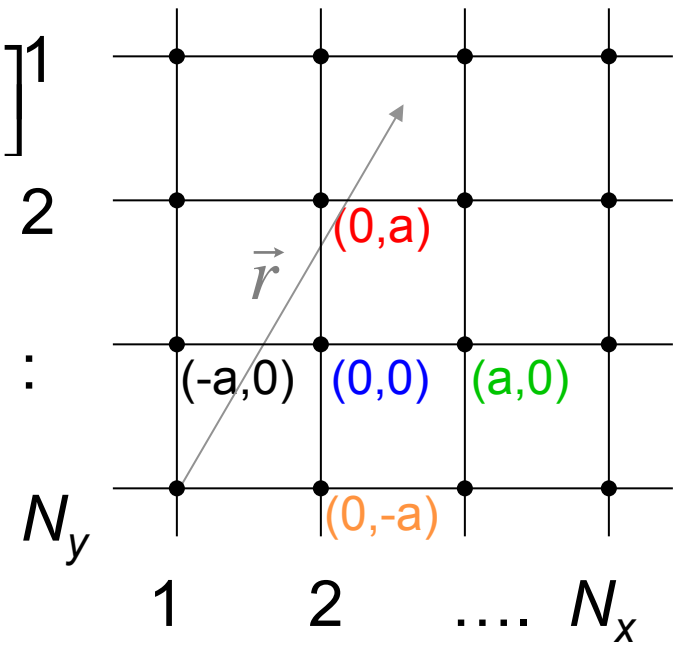
What values can k_x and k_y take?
Unique solutions for (PBC)

$$\frac{-N_x}{2}\le m_x\le\frac{N_x}{2}$$

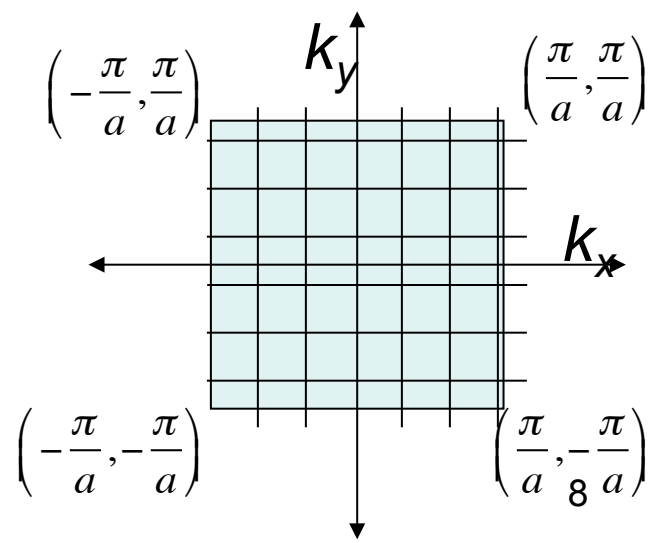
$$\frac{-N_y}{2}\le m_y\le\frac{N_y}{2}$$

$$k_x\equiv\frac{2\pi m_x}{N_x a};k_y\equiv\frac{2\pi m_y}{N_y a}$$

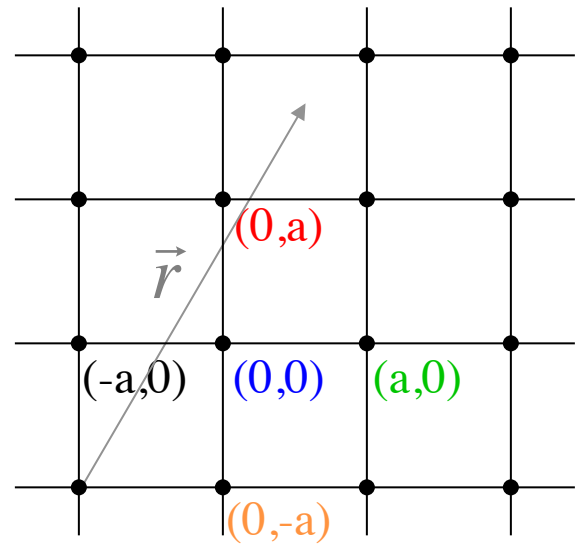
$$-\frac{\pi}{a}\le k_x,k_y\le\frac{\pi}{a}$$



Real space. $N=N_xN_y$ atoms



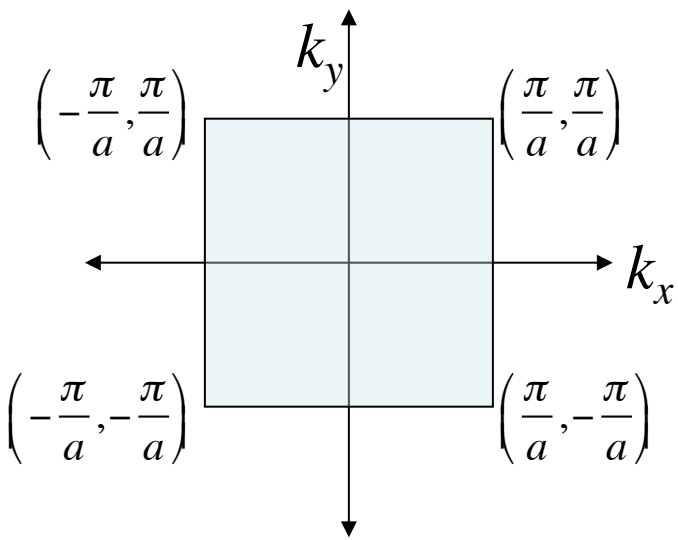
$$E\left(k_x, k_y\right) = \alpha + 2\beta\left[\cos\left(k_x a\right) + \cos\left(k_y a\right)\right]$$

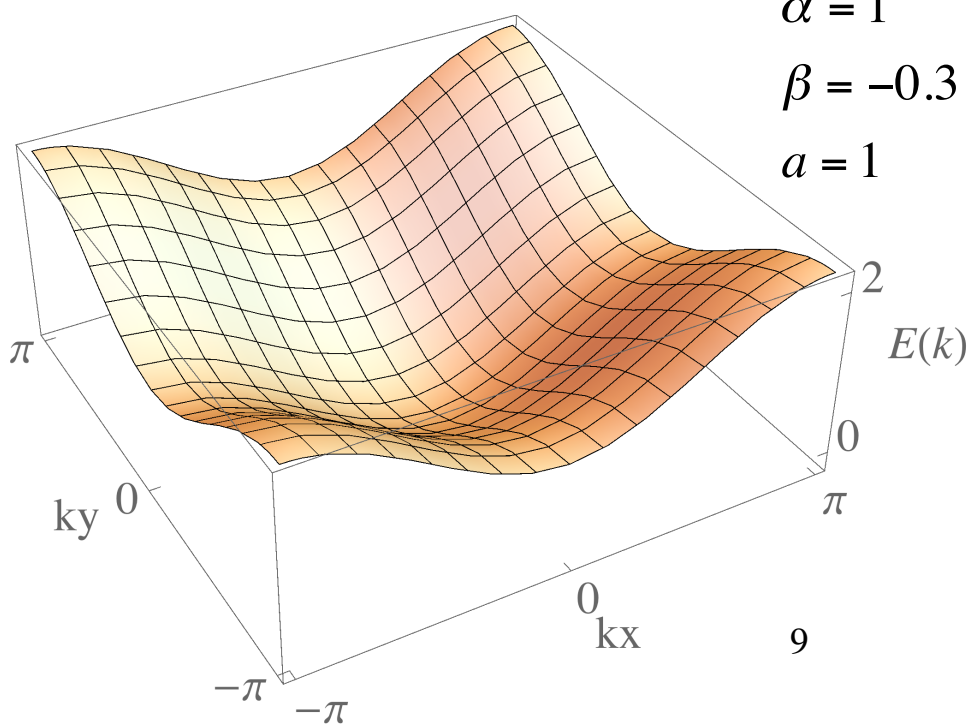


How to represent this in a plot?
What values can k_x and k_y take?

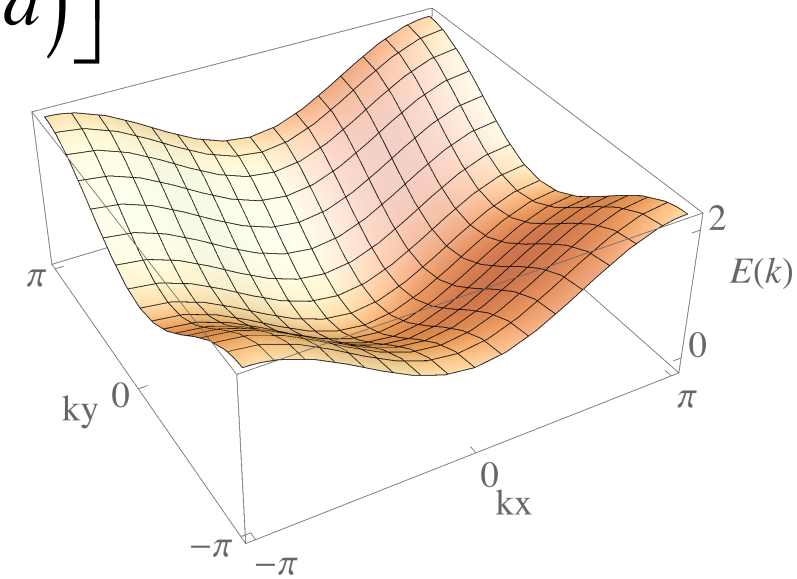
Unique solutions for

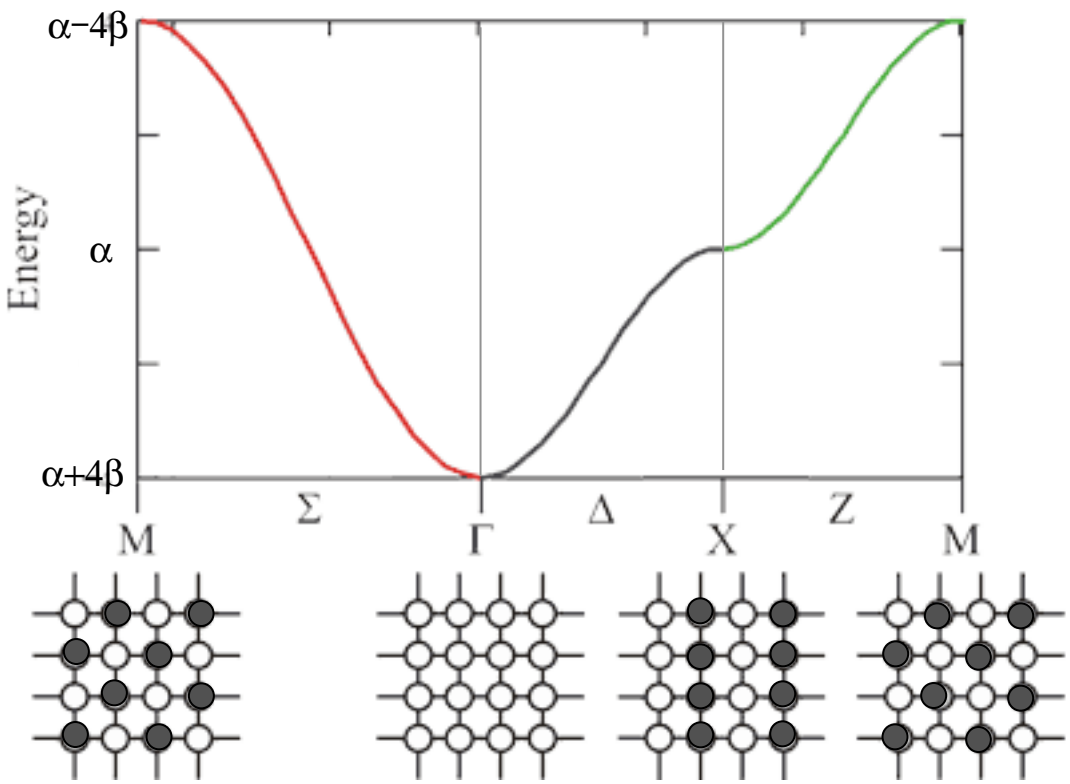
$$-\frac{\pi}{a} \le k_x, k_y \le \frac{\pi}{a}$$

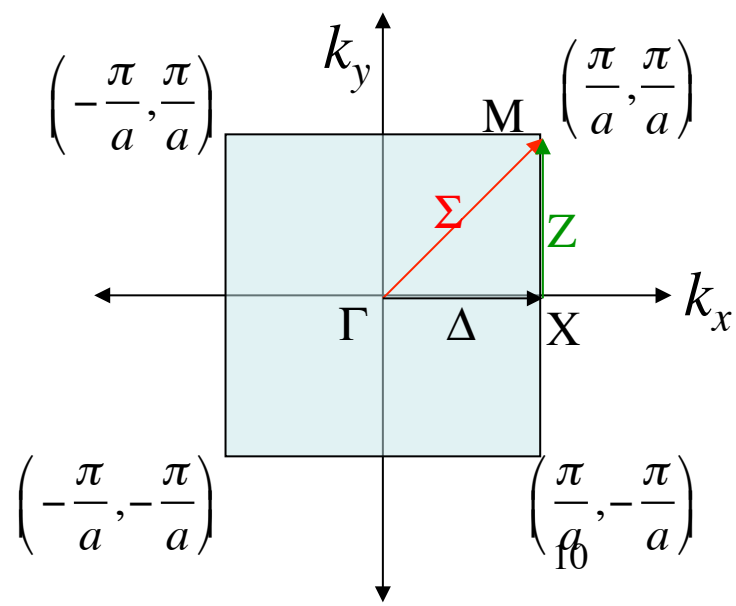


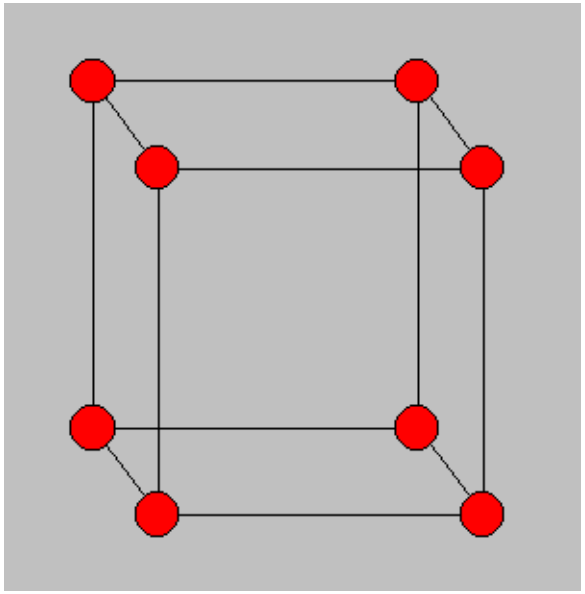


$$E\left(k_x,k_y\right)=\alpha+2\beta\left[\cos\left(k_x a\right)+\cos\left(k_y a\right)\right]$$









Simple cubic lattice

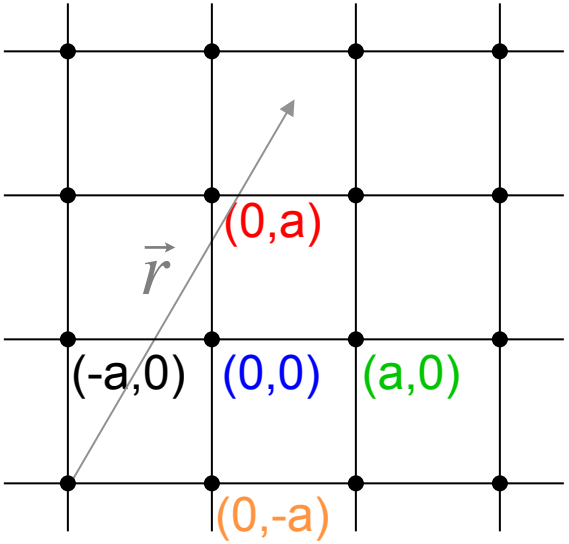
Dispersion relation?

$\mathbf{a}_1 = (a , 0 , 0)$
$\mathbf{a}_2 = (0 , a , 0)$
$\mathbf{a}_3 = (0 , 0 , a)$

$$E(k) = \alpha + 2\beta\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)$$

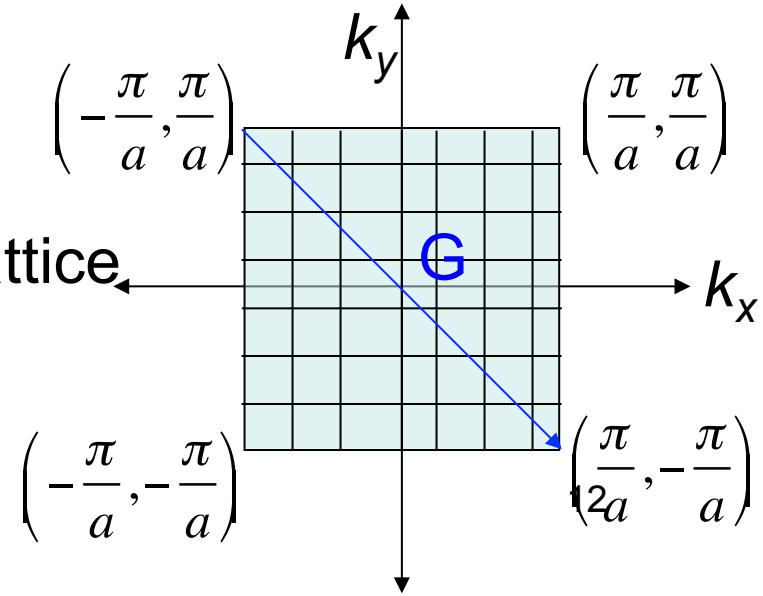
	Band width	#n.n.
1D	4β	2
2D	8β	4
3D	12β	6

Real space lattice



Reciprocal lattice of a square lattice is also square, but this is not true of all lattice types.
First Brillouin zone contains ALL unique *k* points, and they are closer to *k* = 0 than any other.
Just as *T* is a vector that connects 2 lattice points in REAL space, so *G* is a vector that connects 2 points in *k*-space or reciprocal space.

Reciprocal space lattice



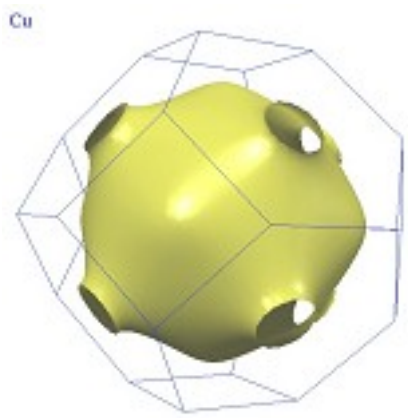
The Fermi surface:

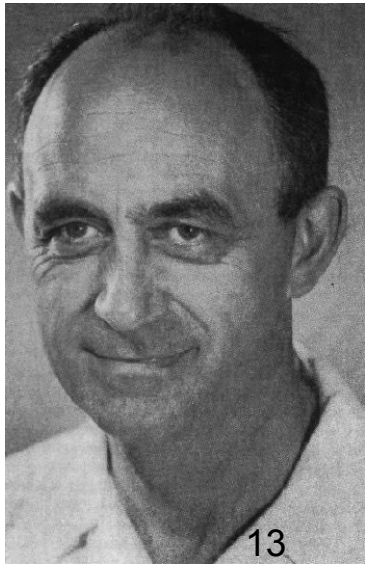
Not all states are occupied with electrons. At T=0, the states fill sequentially form lowest to highest energy, consistent with the Pauli Principle.

Highest occupied state defines the Fermi energy.

Highest occupied states define a surface in k-space called Fermi surface.

Fermi surface is still defined at $T \neq 0$.





Enrico Fermi 1901-1954

$$E(k_x,k_y) = \alpha + 2\beta\left[\cos(k_x a) + \cos(k_y a)\right]$$

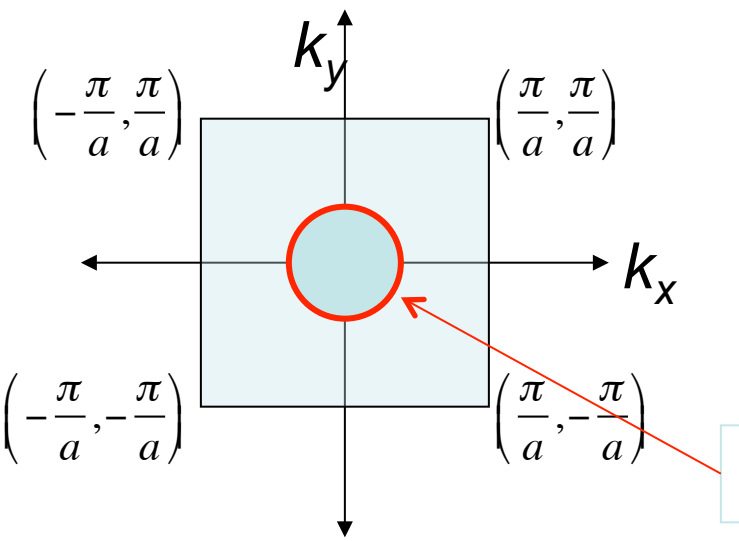
Low filling,
Small E_F,
$k_F \approx 0$

$$E(k_x,k_y) \approx \alpha + 2\beta\left[1 - \tfrac{1}{2}(k_x a)^2 + 1 - \tfrac{1}{2}(k_y a)^2\right]$$

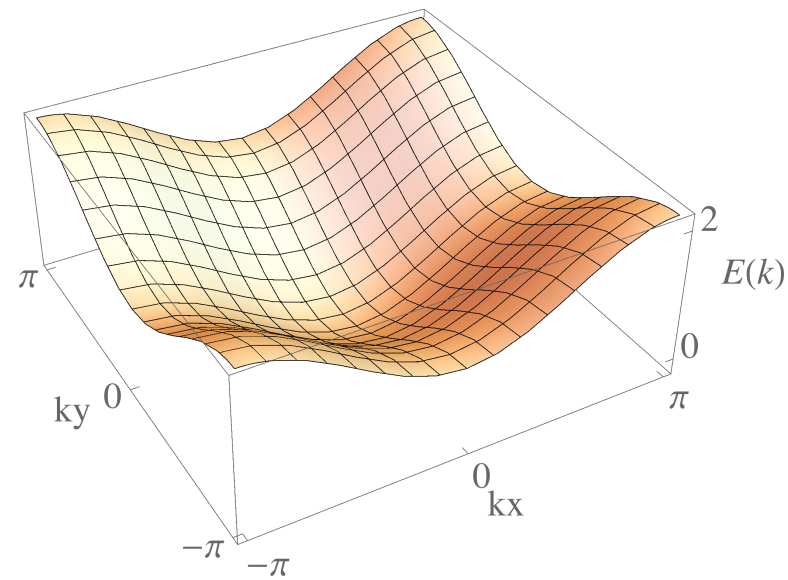
$$E_F = \alpha + 4\beta - \beta a^2\left(k_{F,x}^2 + k_{F,y}^2\right) = \alpha + 4\beta - \beta a^2 k_F^2$$

Circle!

$$k_F = \sqrt{\frac{E_F - \alpha - 4\beta}{-\beta a^2}}$$



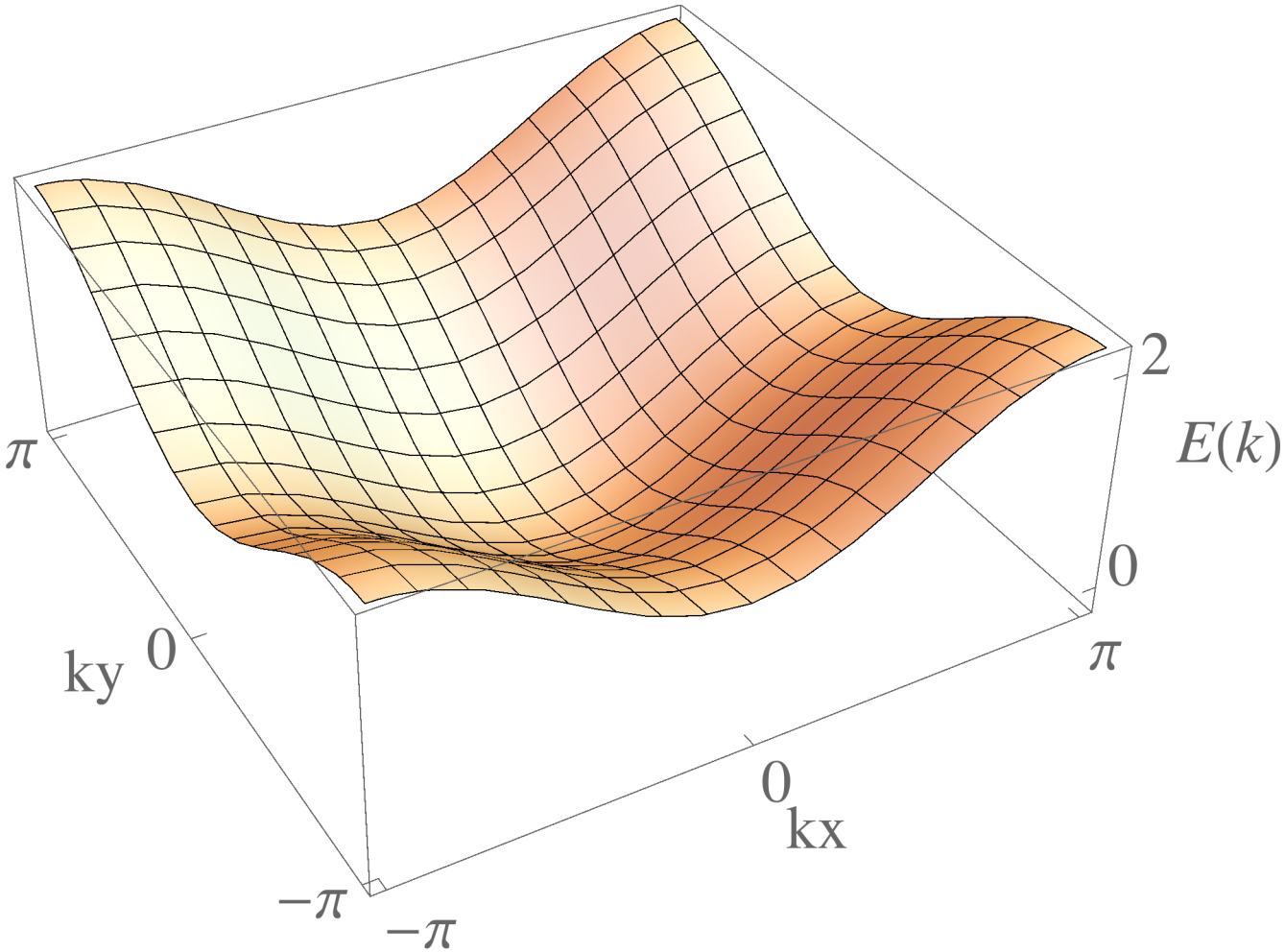
Fermi surface



$\alpha = 1$

$\beta = -0.3$

$a = 1$



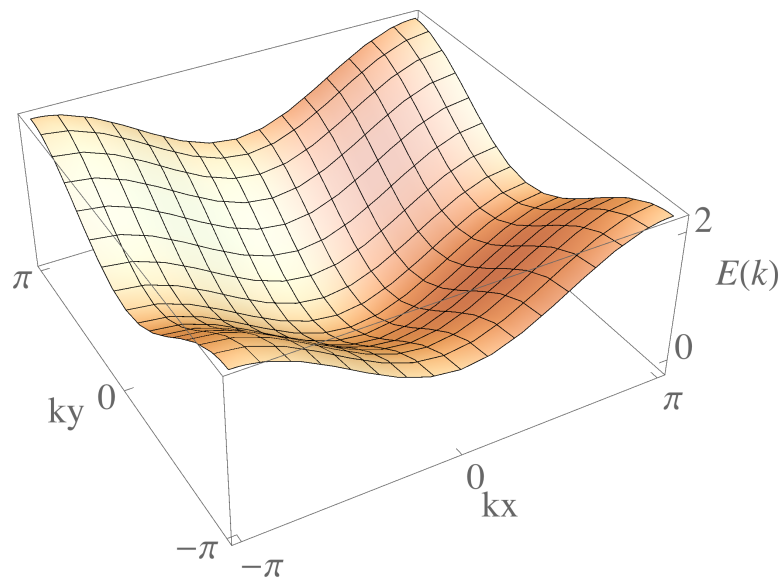
$$E_F = \alpha = \alpha + 2\beta\left[\cos\left(k_{F,x}a\right) + \cos\left(k_{F,y}a\right)\right]$$

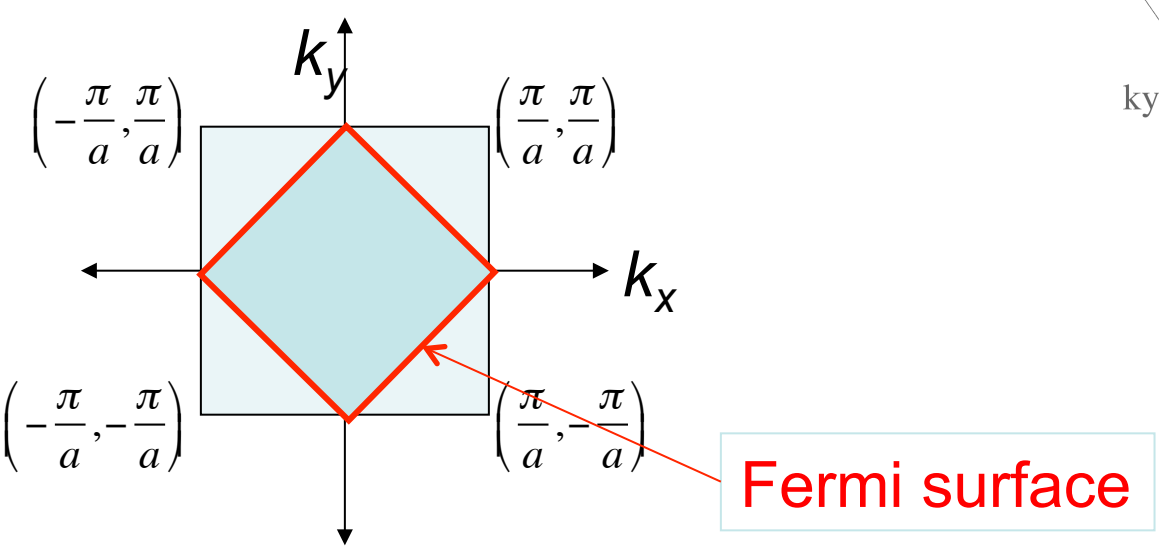
$$\cos\left(k_{F,x}a\right) + \cos\left(k_{F,y}a\right) = 0$$

Half filling
$E_F = \alpha$

$$k_{F,y} = \pm k_{F,x} \pm \pi / a$$

Square!

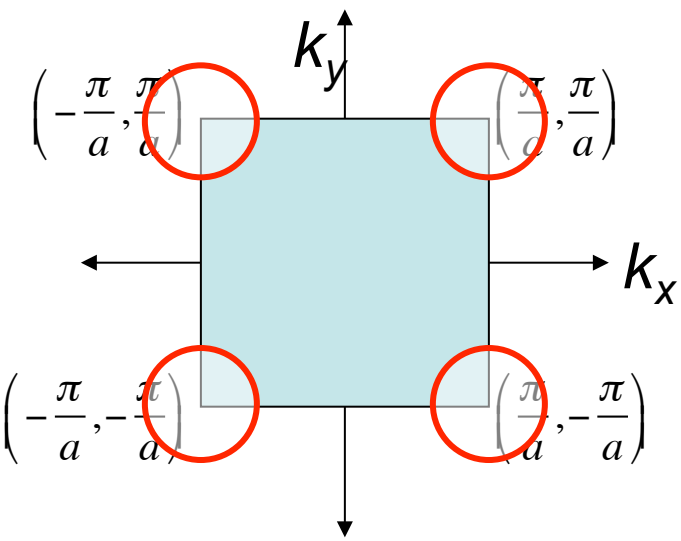


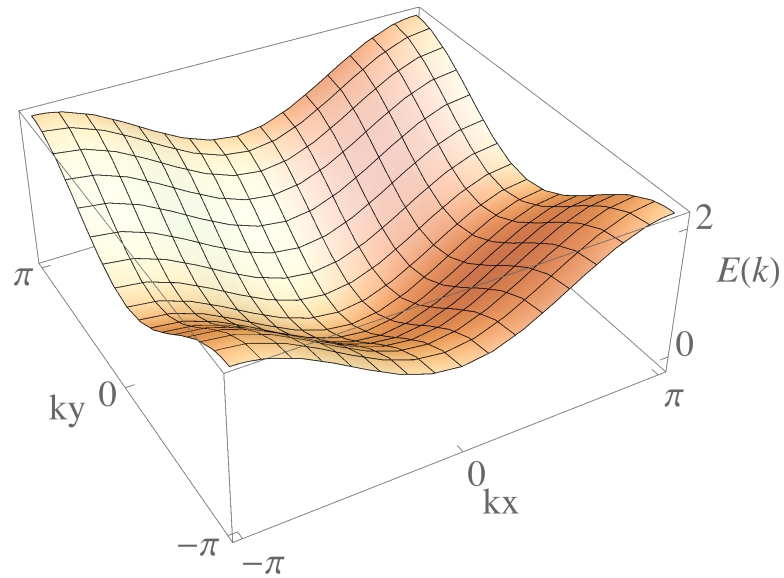


$$E_F = \alpha = \alpha + 2\beta\left[\cos\left(k_{F,x}a\right) + \cos\left(k_{F,y}a\right)\right]$$

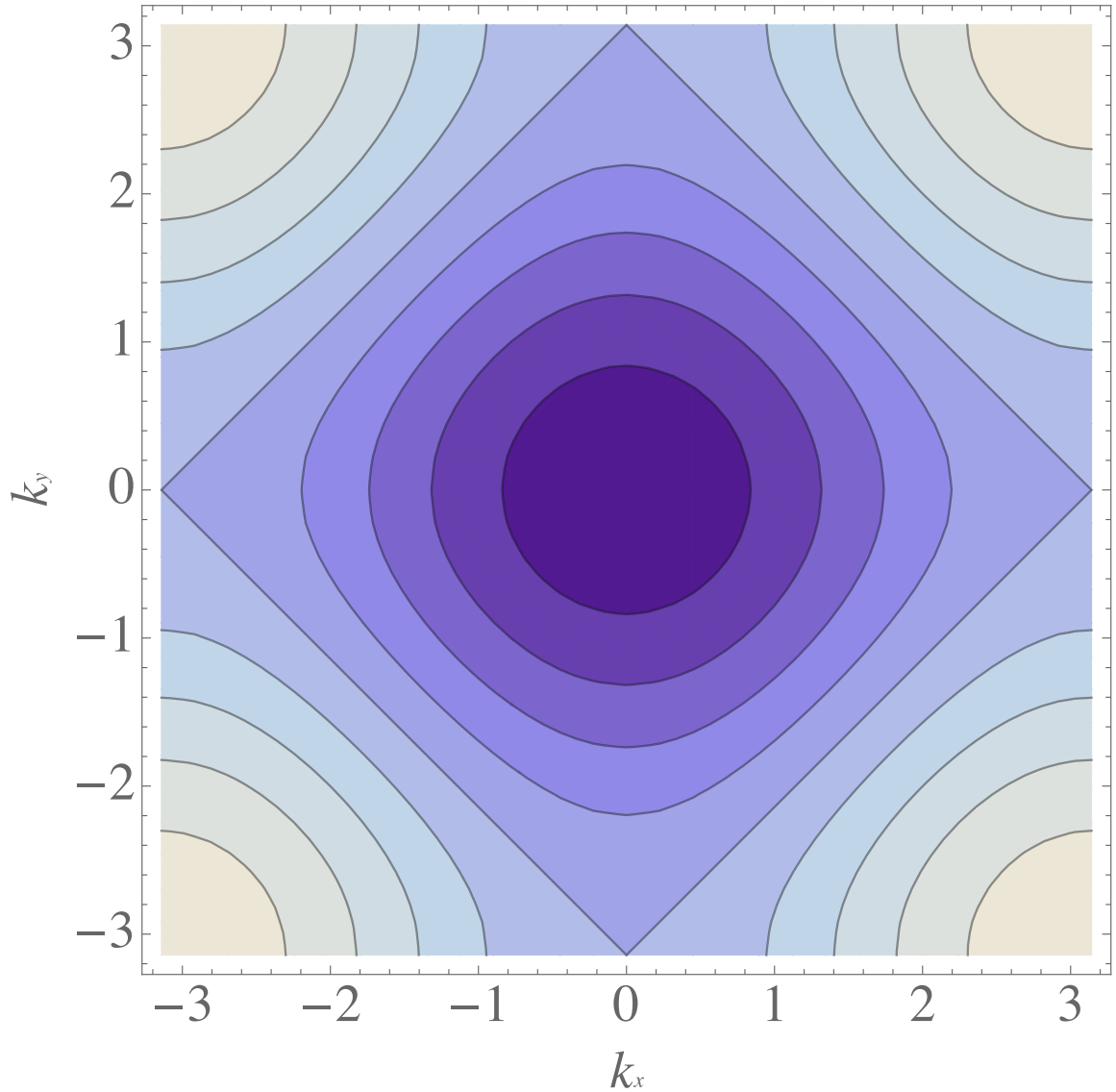
Almost full
$E_F \approx \alpha - 2\beta$,
$k_F \approx \pi/a - \delta$

Expand cosines about π/a - circles again, but "empty" circles, centered on $(\pm\pi/a, \pm\pi/a)$



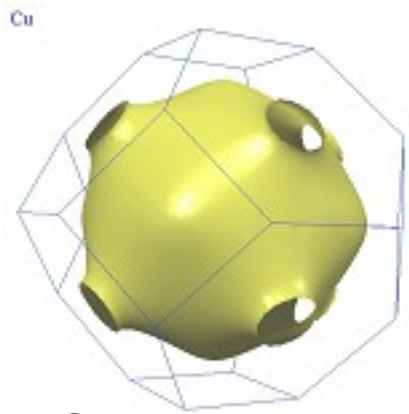


Fermi surface

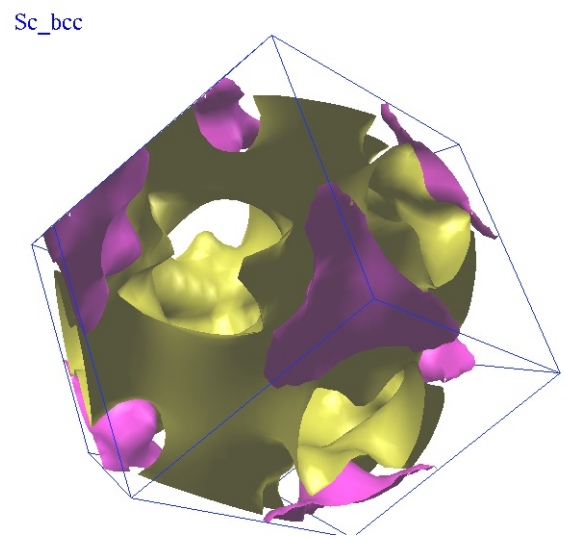


Fermi surfaces for different band fillings

Real Fermi surfaces can be measured by applying magnetic fields and measuring magnetoresistance at low *T* in different directions (Schubnikov-de Haas oscillations). Other methods, too (PES).



Copper



Scandium

http://www.phys.ufl.edu/fermisurface/

Position of the Fermi energy in the bands determines whether the material is a metal or an insulator.

Filled bands imply insulating or semiconducting behavior. (Depends on distance of Fermi energy from band edge compared to thermal energies).

Partially filled bands result in metallic behavior. Thermal energies do not determine number of carriers.