Computational Material Science

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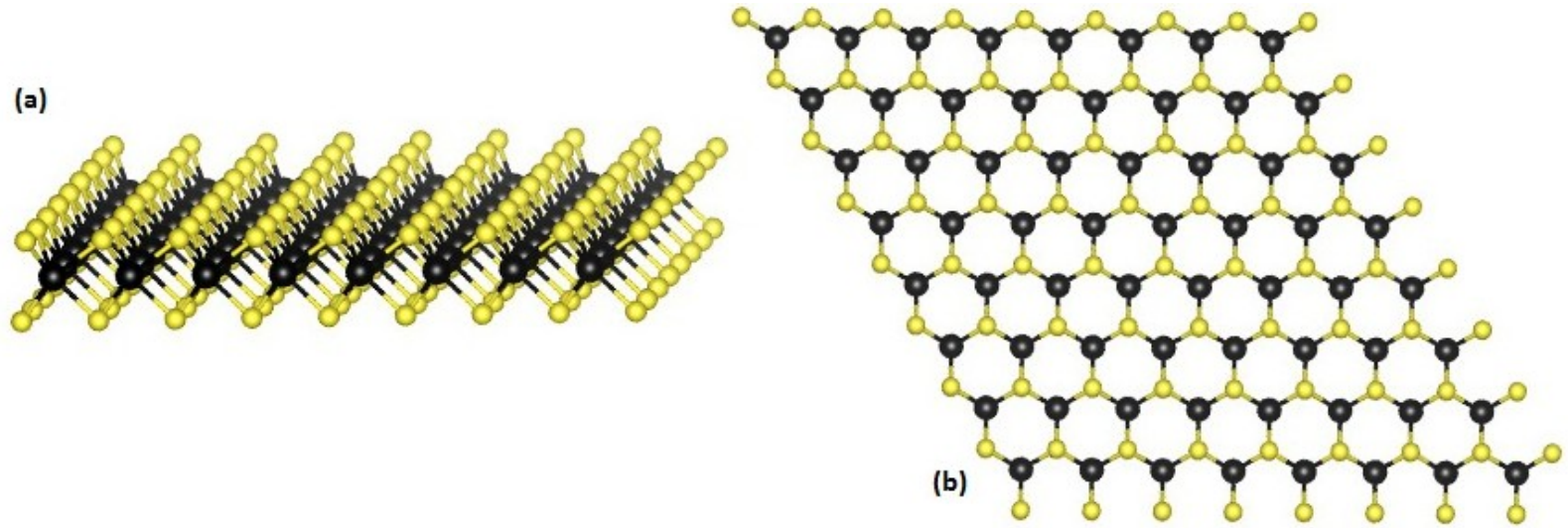
TU Wien

Bloch wave function - what is it?

In most 'real life' cases, the wave functions are hidden somewhere in the memory of our computer. However, looking at their shape sometimes can provide a better intuition about 'how the theory actually works'.

This is such an example.

Transition metal dichalcogenides (e.g. MoS_2):



source Wikipedia

Bloch theorem for lattice models

$$H = \sum_{\mathbf{R}} \sum_{\mathbf{S}} t(\mathbf{S}) c^{\dagger}_{\mathbf{R}+\mathbf{S}} c_{\mathbf{R}}$$

periodicity

lattice site coincides with the unit cell
(not the most general case)

Unitary transformation (very common trick for periodic systems):

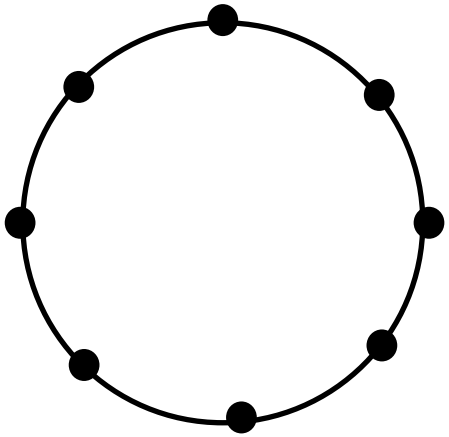
$$c_{\mathbf{R}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{k}}$$

$$H = \frac{1}{N} \sum_{\mathbf{R}} \sum_{\mathbf{S}} \sum_{\mathbf{k},\mathbf{k}'} t(\mathbf{S}) e^{-i\mathbf{k}\cdot(\mathbf{R}+\mathbf{S})} c^{\dagger}_{\mathbf{k}} e^{i\mathbf{k}'\cdot\mathbf{R}} c_{\mathbf{k}'}$$

$$= \sum_{\mathbf{k},\mathbf{k}'} \underbrace{\left(\frac{1}{N} \sum_{\mathbf{R}} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} \right)}_{\delta_{\mathbf{k}\mathbf{k}'}} \underbrace{\left(\sum_{\mathbf{S}} e^{-i\mathbf{k}\cdot\mathbf{S}} t(\mathbf{S}) \right)}_{t(\mathbf{k})} c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}'} = \sum_{\mathbf{k}} t(\mathbf{k}) c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}}$$

Example: 1D chain with nn hopping

$$H = t\sum_{i=1}^{N-1}\left(c_{i+1}^{\dagger}c_i + c_i^{\dagger}c_{i+1}\right) + t\left(c_1^{\dagger}c_N + c_N^{\dagger}c_1\right)$$



Hopping matrix (Hamiltonian):

$$h = \begin{pmatrix} 0 & t & 0 & 0 & \dots & 0 & t \\ t & 0 & t & 0 & \dots & 0 & 0 \\ 0 & t & 0 & t & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & t \\ t & 0 & 0 & 0 & \dots & t & 0 \end{pmatrix}$$

Basis transformation:

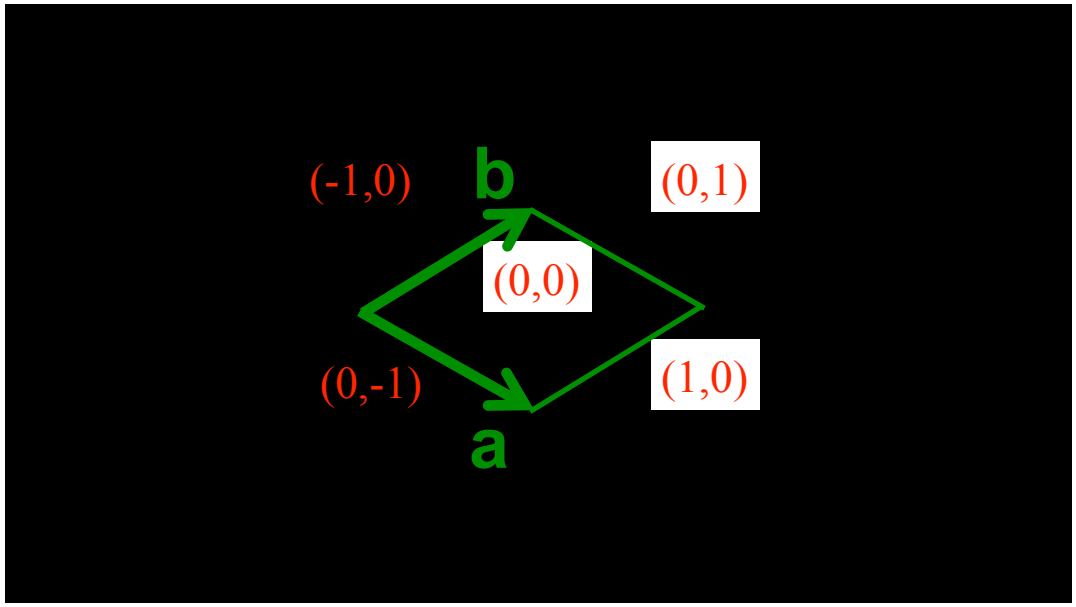
$$\begin{pmatrix} \vdots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \rightarrow \frac{1}{\sqrt{N}} \begin{pmatrix} \vdots \\ e^{ikl} \\ e^{ik(l+1)} \\ e^{ik(l+2)} \\ e^{ik(l+3)} \\ e^{ik(l+4)} \\ \vdots \end{pmatrix}$$

Dispersion:

$$t(k) = 2t\cos\left(\frac{2\pi}{N}k\right), \quad k = 0, 1, \dots, N-1$$

Diagonalize h directly for N=3. What eigenstates do you get?
Generalize the problem for square and cubic lattices.

Example: Honeycomb lattice



$$H = t \sum_{\mathbf{R}} \left(c^{\dagger}_{\mathbf{R}} d_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}} c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(1,0)} d_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}+(-1,0)} c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(0,1)} d_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}+(0,-1)} c_{\mathbf{R}} \right)$$

After FT:

$$H = t \sum_{k_a, k_b} (1 + e^{ik_a} + e^{ik_b}) c^{\dagger}_{\mathbf{k}} d_{\mathbf{k}} + h.c.$$

Example: Honeycomb lattice

$$H = t\sum_{\mathbf{R}}\left(c^{\dagger}_{\mathbf{R}}d_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}}c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(1,0)}d_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}+(-1,0)}c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+(0,1)}d_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}+(0,-1)}c_{\mathbf{R}}\right)$$

After FT:

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At each k-point $\mathbf{k}=(k_a,k_b)$ we have a 2x2 matrix to diagonalize:

$$h(k_a,k_b) = \begin{pmatrix} 0 & 1 + e^{ik_a} + e^{ik_b} \\ 1 + e^{-ik_a} + e^{-ik_b} & 0 \end{pmatrix}$$

Finally we get the dispersion relation:

$$\epsilon(\mathbf{k}) = \pm\sqrt{3 + 2\left(\cos(k_a) + \cos(k_b) + \cos(k_a - k_b)\right)}$$

Example: Honeycomb lattice

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At each k-p

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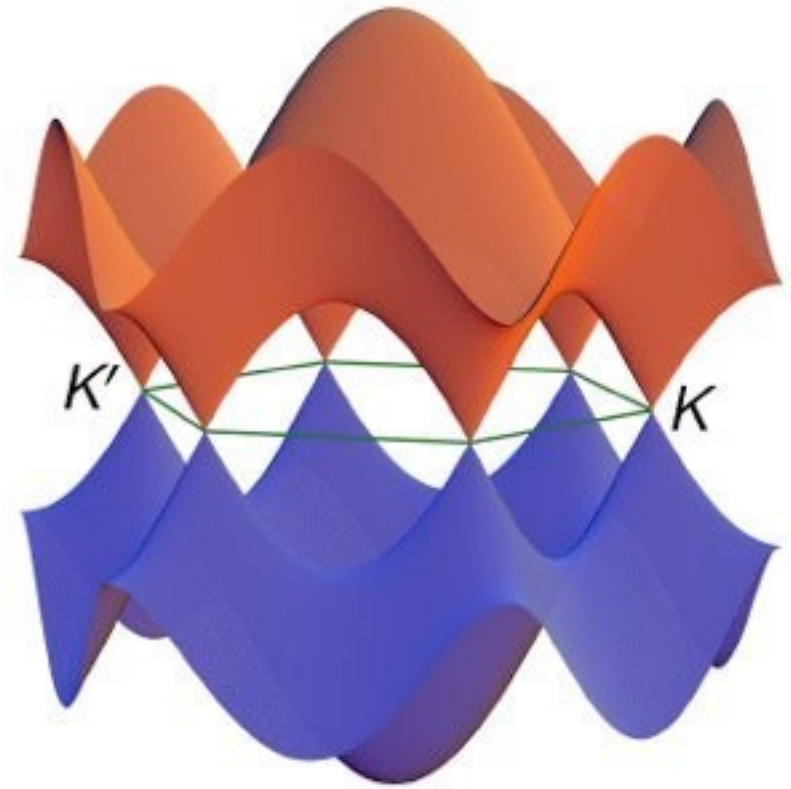
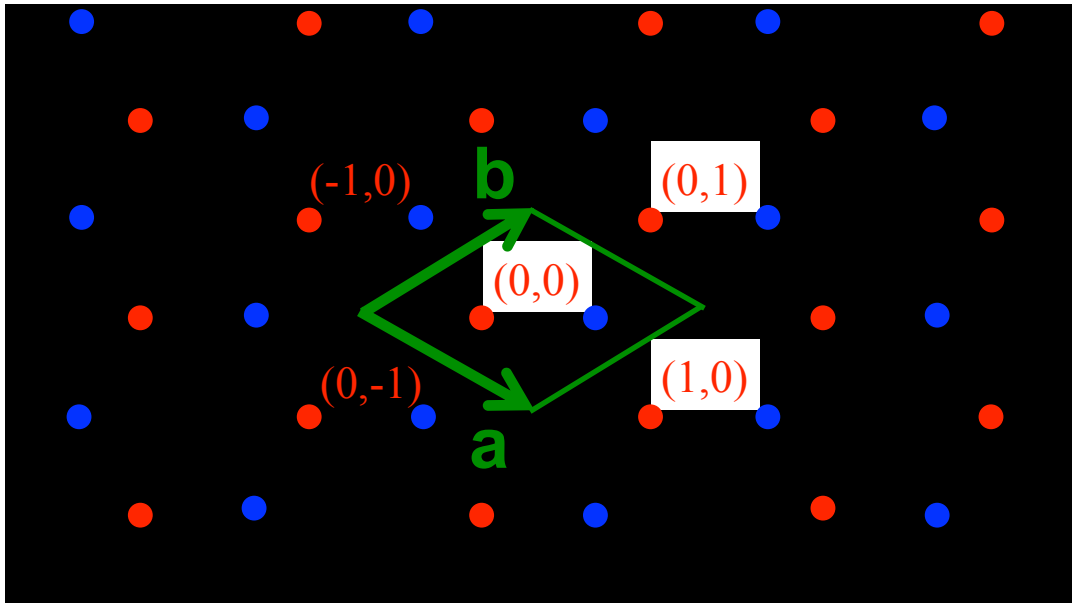
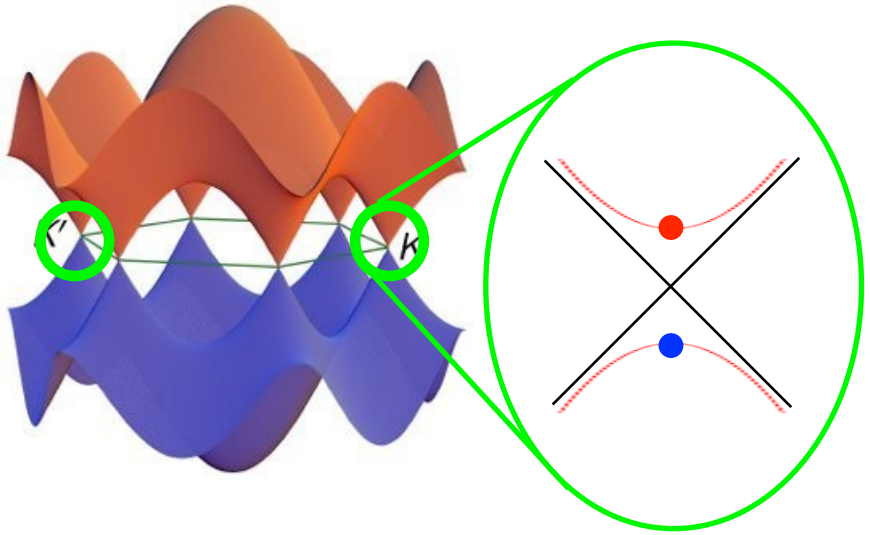


Transition metal dichalcogenides (TMDs)





$$H = t \sum_{k_a, k_b} (1 + e^{ik_a} + e^{ik_b}) c_k^\dagger d_k + h.c. + \Delta \sum_k \left(c_k^\dagger c_k - d_k^\dagger d_k \right)$$

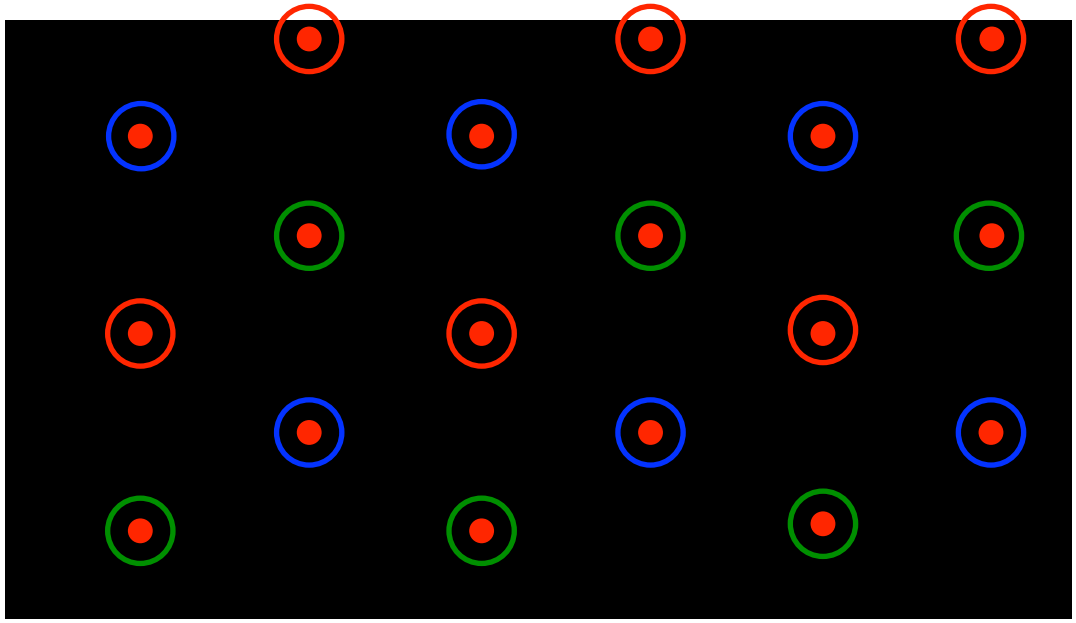
At K and K' the off-diagonal element vanishes:

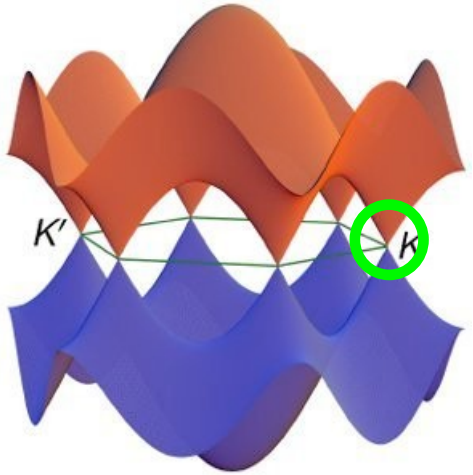
$$\mathbf{K} = (\pm \frac{2\pi}{3}, \mp \frac{2\pi}{3})$$

How does the wave function at K look?

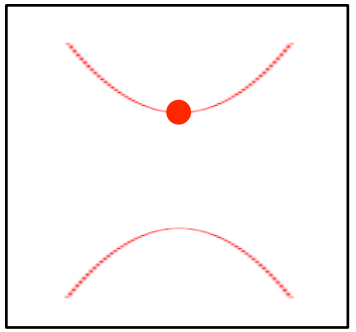
$$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$$

Wave function at K





$$H = t \sum_{k_a, k_b} (1 + e^{ik_a} + e^{ik_b}) c_{\mathbf{k}}^{\dagger} d_{\mathbf{k}} + h.c. + \Delta \sum_{\mathbf{k}} \left(c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} - d_{\mathbf{k}}^{\dagger} d_{\mathbf{k}} \right)$$

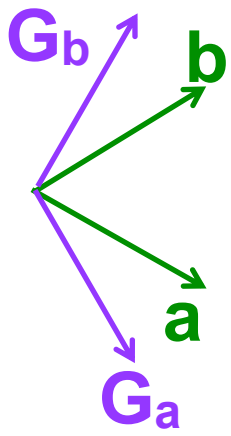


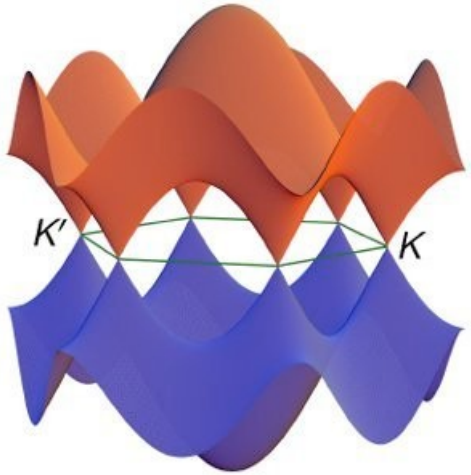
$$h(\mathbf{K}) = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix}$$

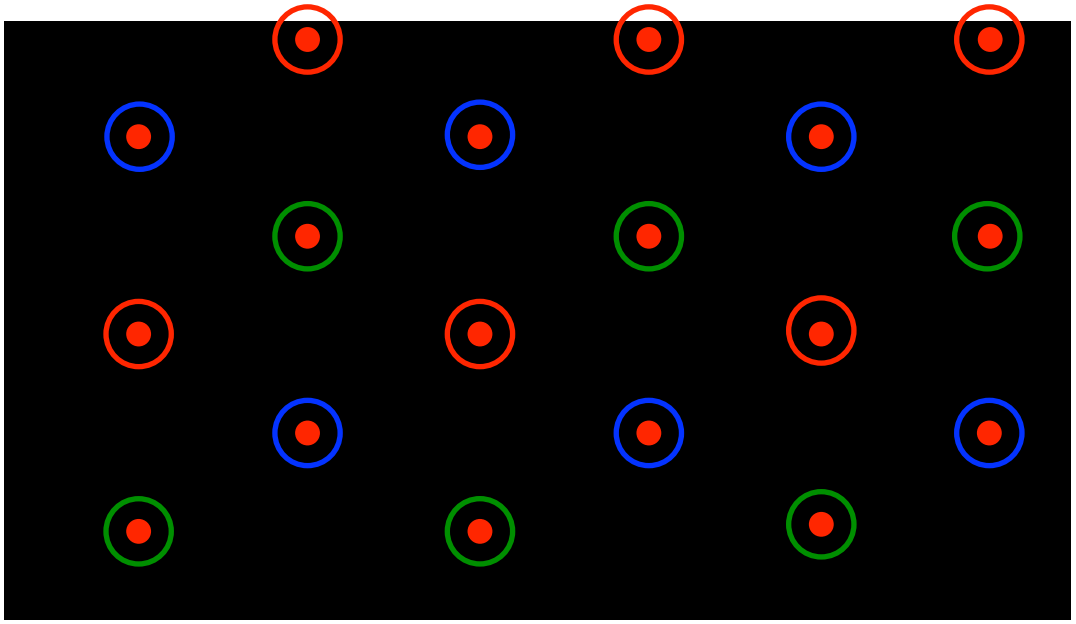
How does the wave function at K look?

$$\psi(\mathbf{R} = m, n) \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(i\frac{2\pi}{3}(m - n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$

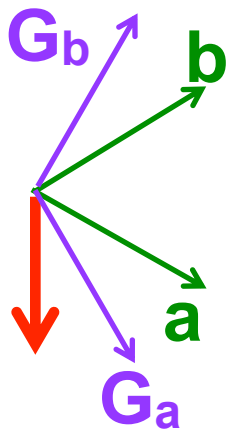
Are different K points equivalent?

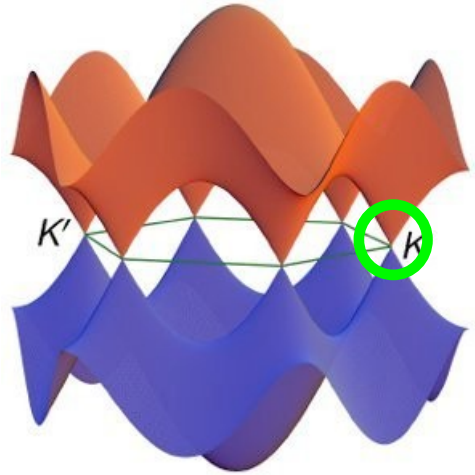


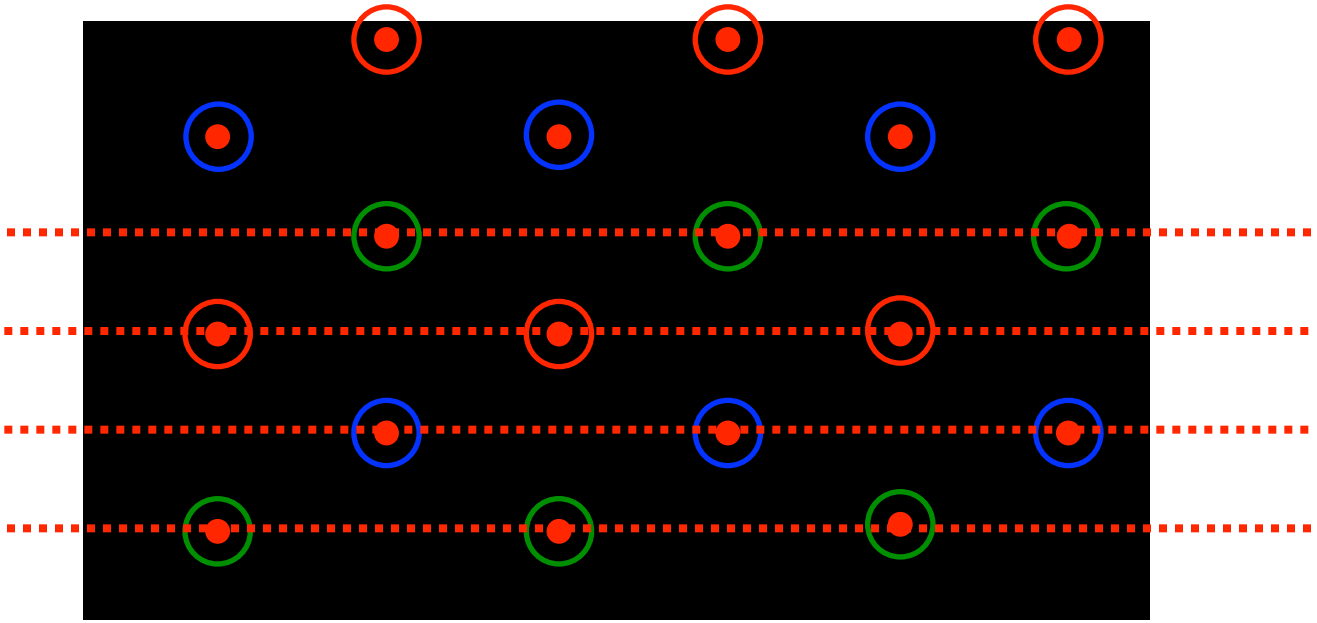




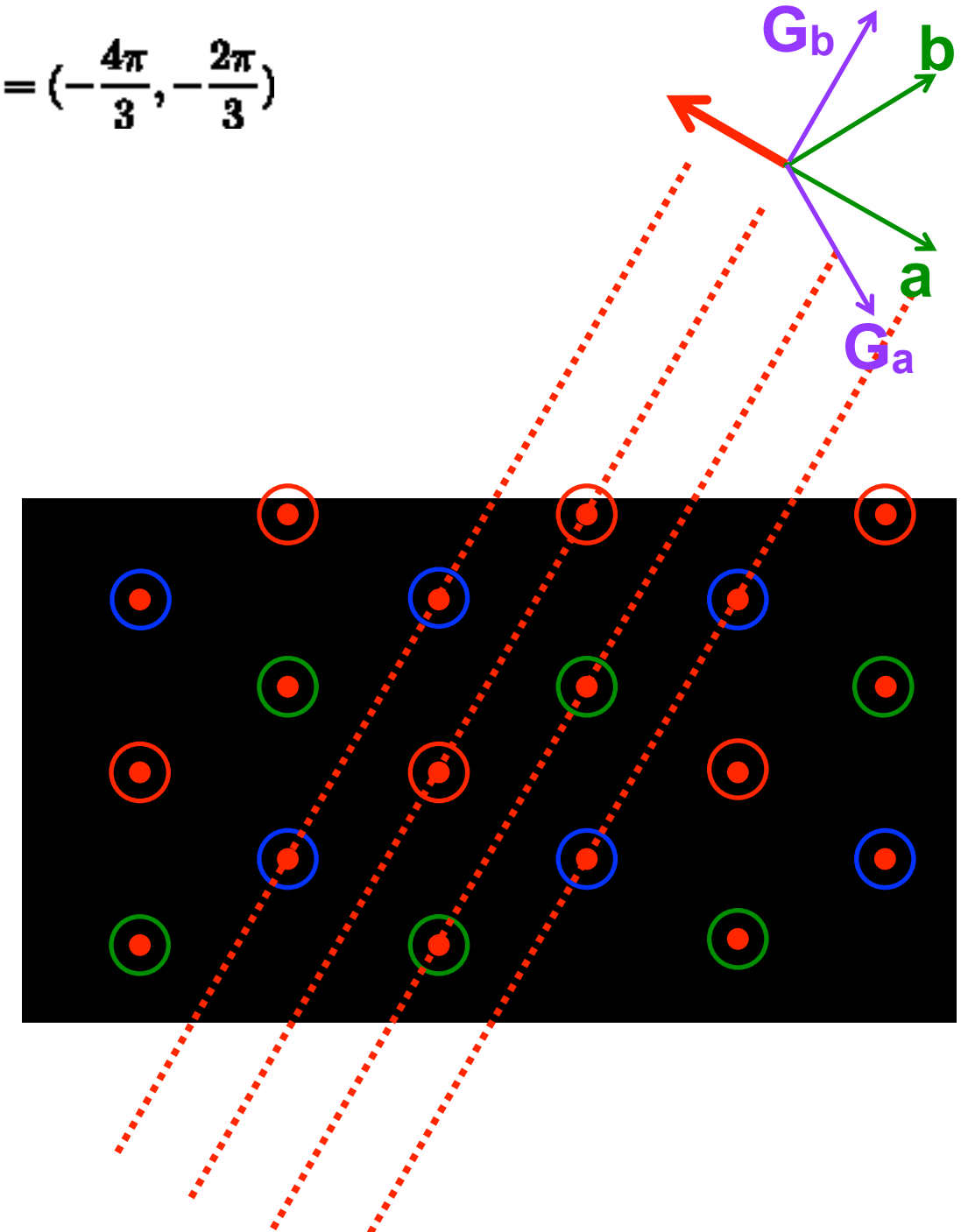
$$\mathbf{K} = \left(\frac{2\pi}{3}, -\frac{2\pi}{3}\right)$$

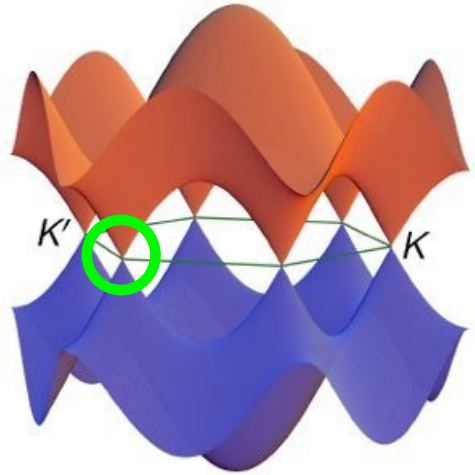




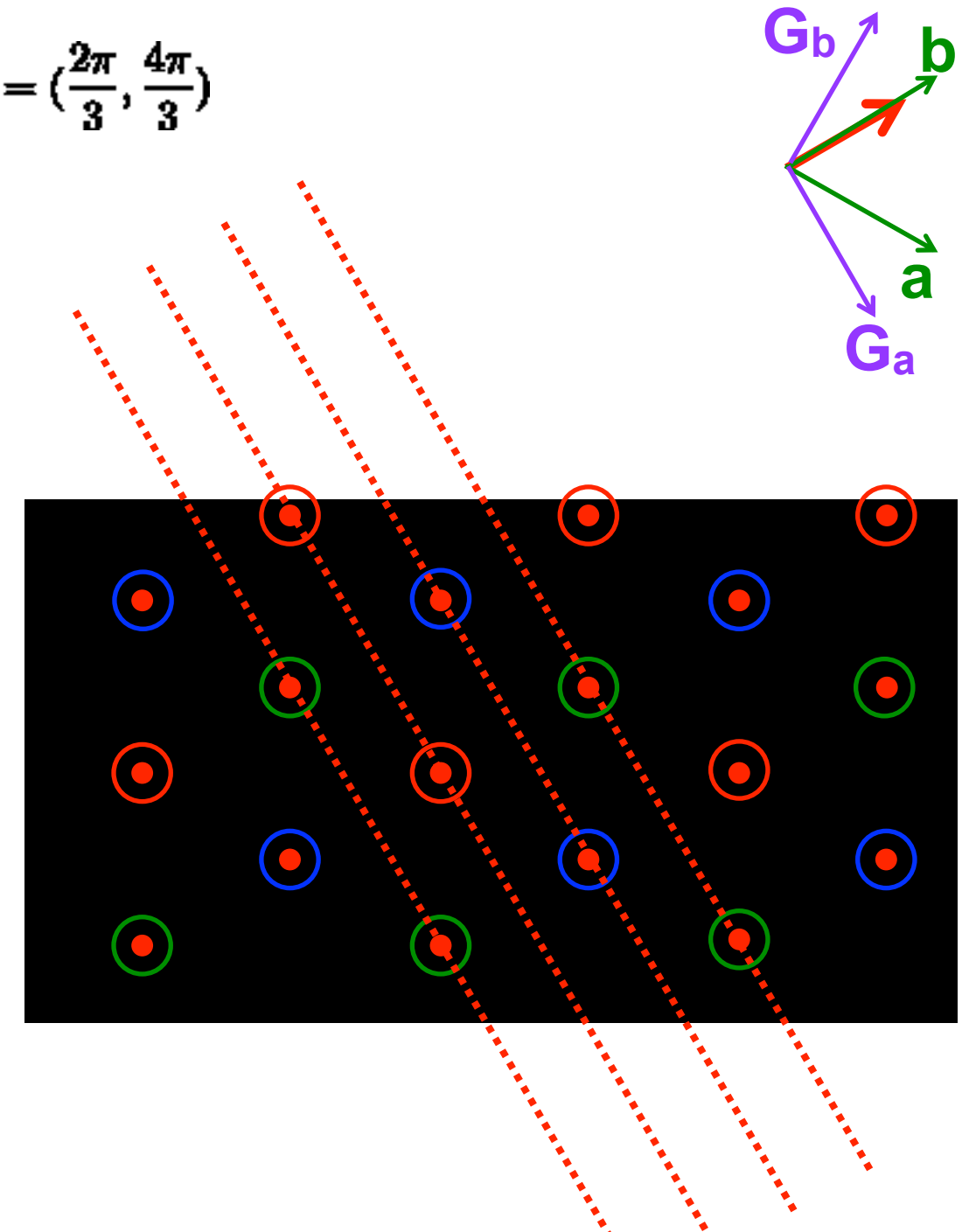


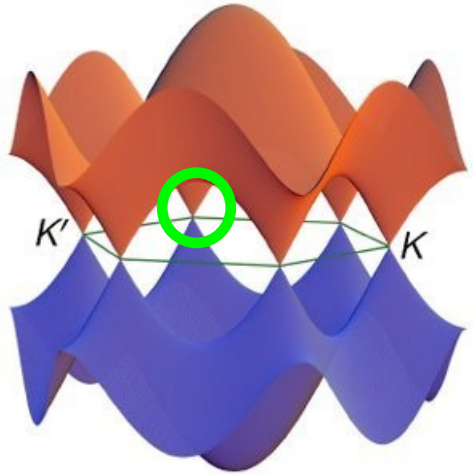
$$\mathbf{K} = (-\frac{4\pi}{3}, -\frac{2\pi}{3})$$





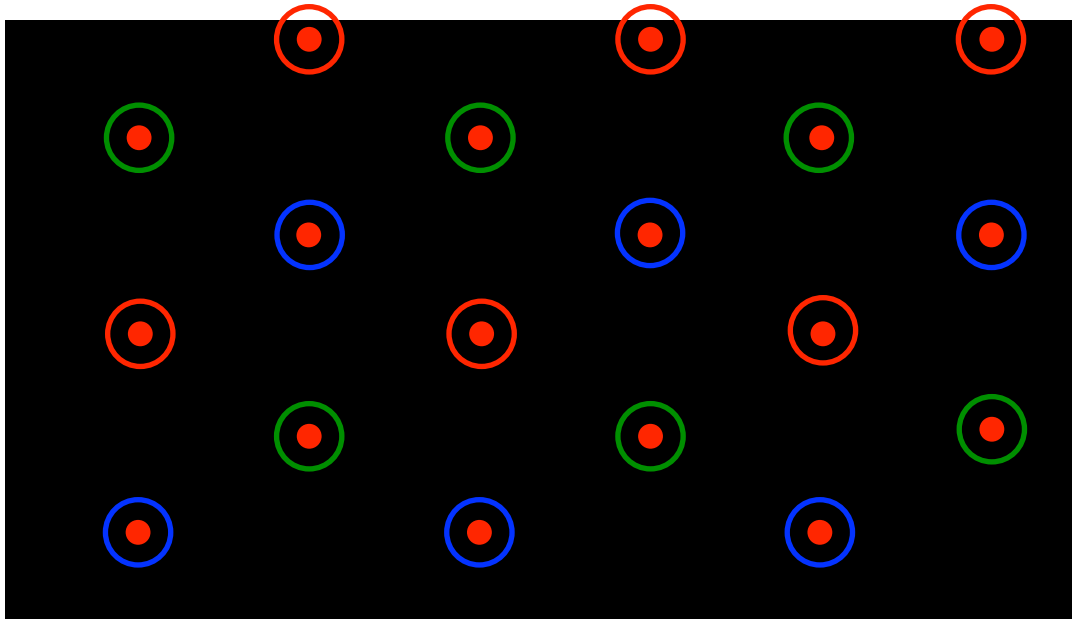
$$\mathbf{K} = \left(\frac{2\pi}{3}, \frac{4\pi}{3}\right)$$

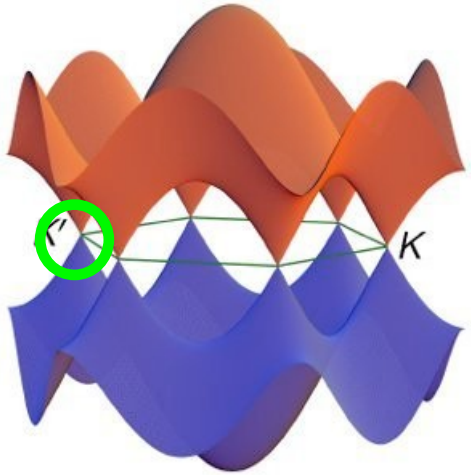




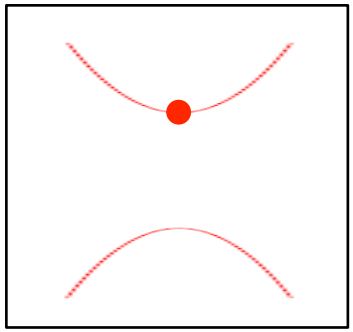
$$\mathbf{K}' = (-\frac{2\pi}{3}, \frac{2\pi}{3})$$

Wave function at K'



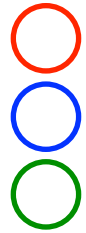


$$H = t \sum_{k_a, k_b} (1 + e^{ik_a} + e^{ik_b}) c_{\mathbf{k}}^{\dagger} d_{\mathbf{k}} + h.c. + \Delta \sum_{\mathbf{k}} \left(c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} - d_{\mathbf{k}}^{\dagger} d_{\mathbf{k}} \right)$$



How does the wave function at K look?

$$\psi(\mathbf{R} = m, n) \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(i\frac{2\pi}{3}(m-n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$



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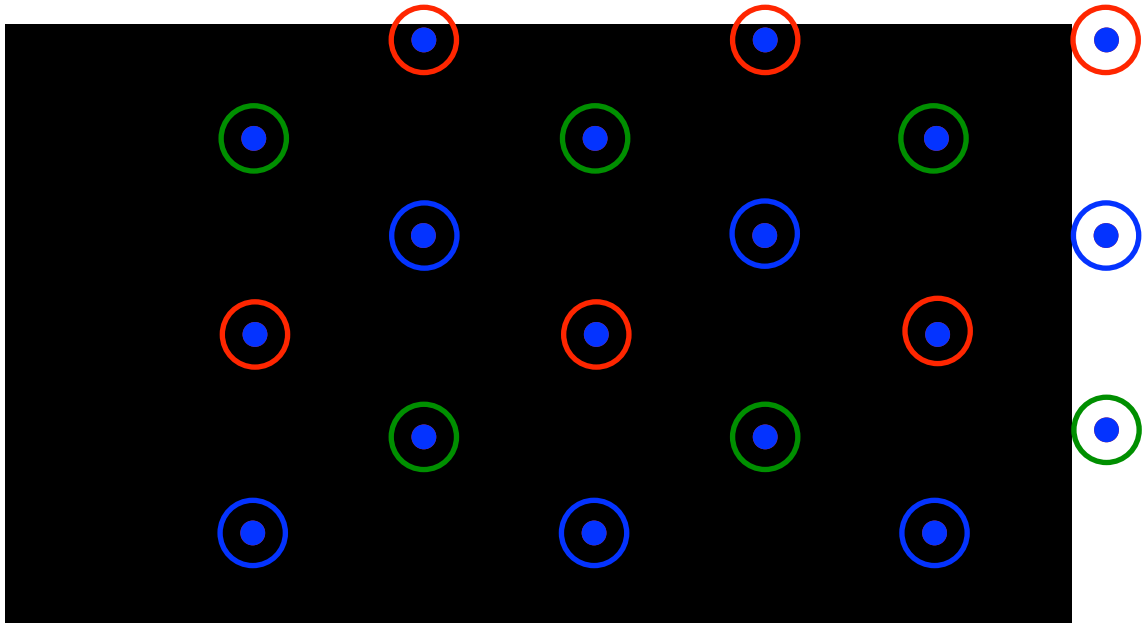
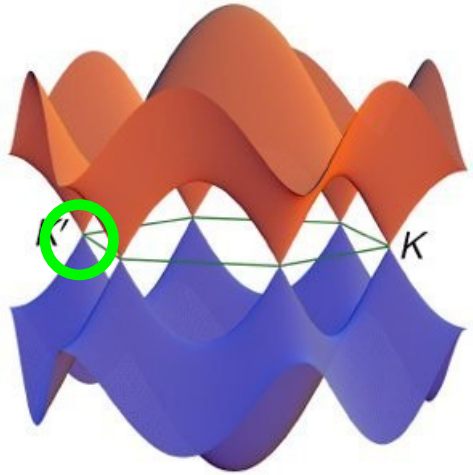
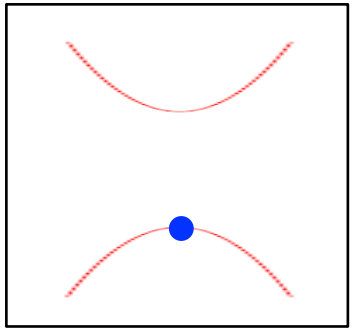
Wave function at K'





$$H = t \sum_{k_a, k_b} (1 + e^{ik_a} + e^{ik_b}) c_k^\dagger d_k + h.c. + \Delta \sum_k \left(c_k^\dagger c_k - d_k^\dagger d_k \right)$$



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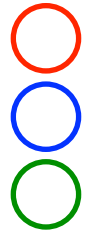

Is this an eigenstate?

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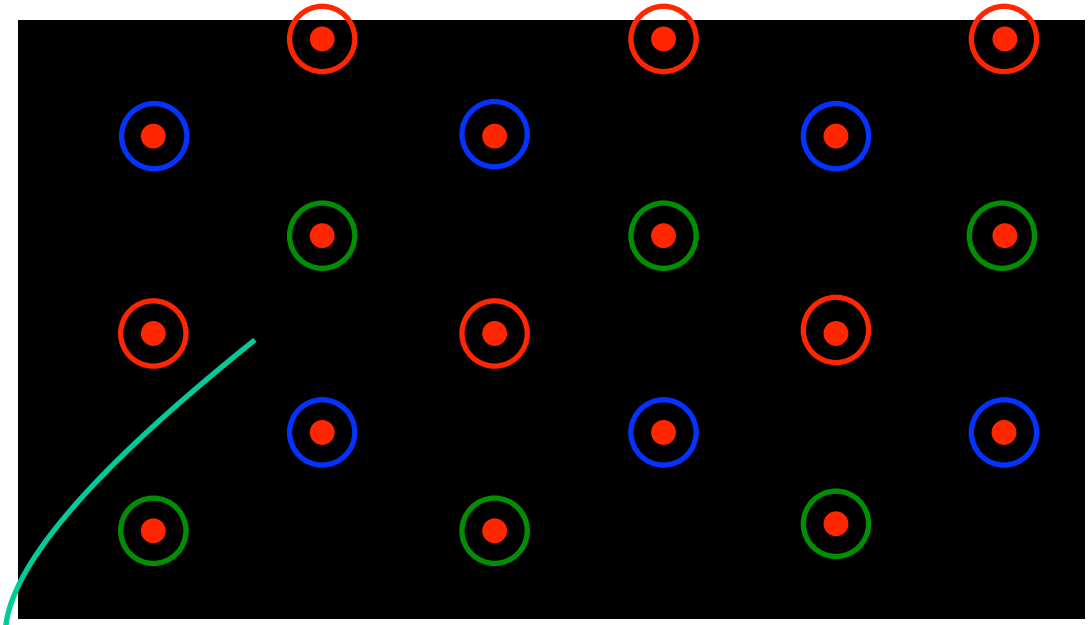
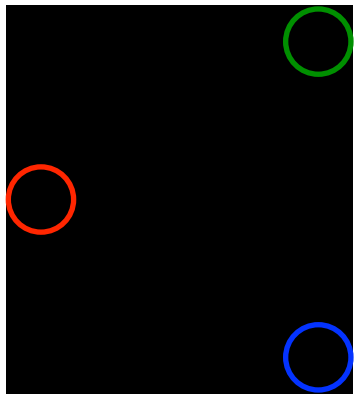
H  = 0

Σ 

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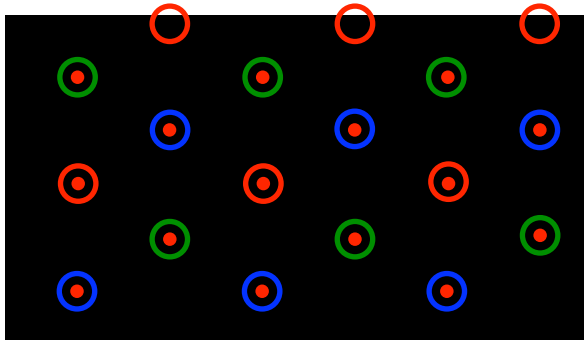
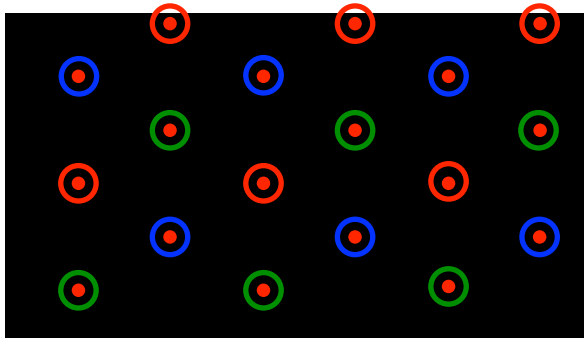
Are function at K and K' mutually orthogonal?

$\sum_{\text{sites}}$  $*$ $\cdot$ 

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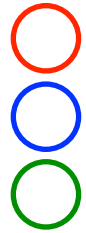

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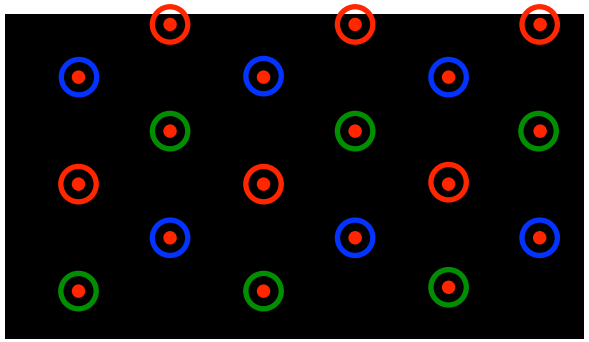
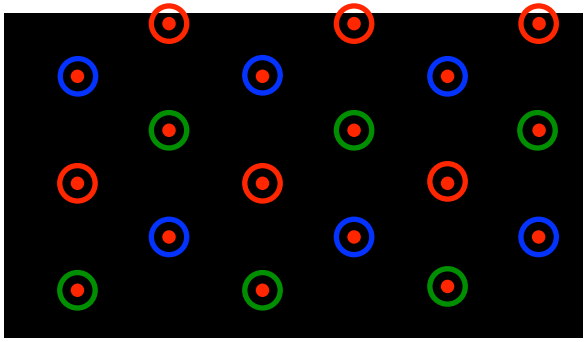
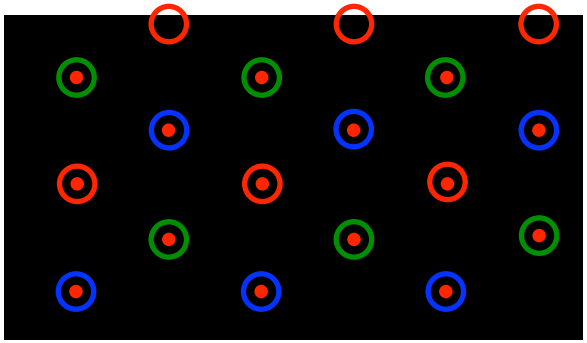
$\sum_{\text{sites}}$  . 

$=$ $\sum_{\text{sites}}$  $= 0$

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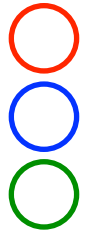
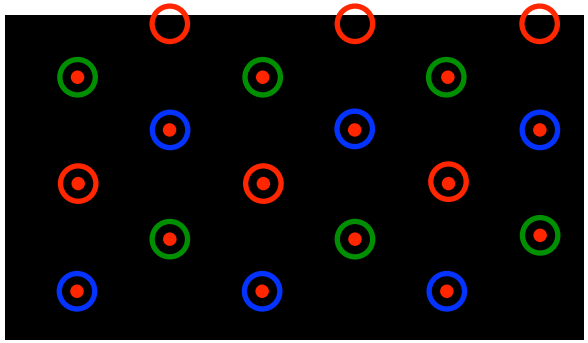


Linear superposition of |K > and |K'>?



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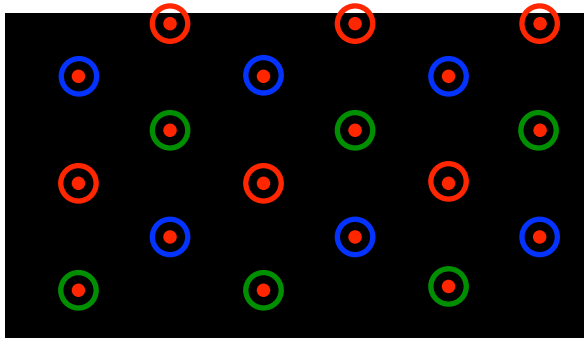

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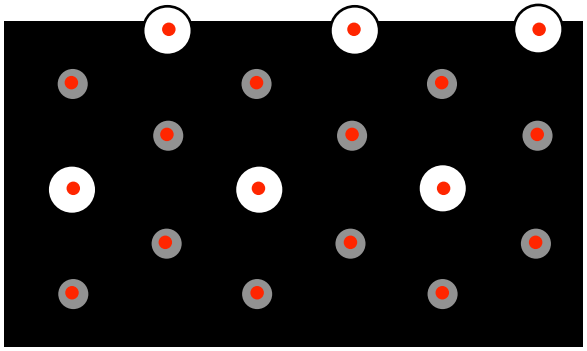

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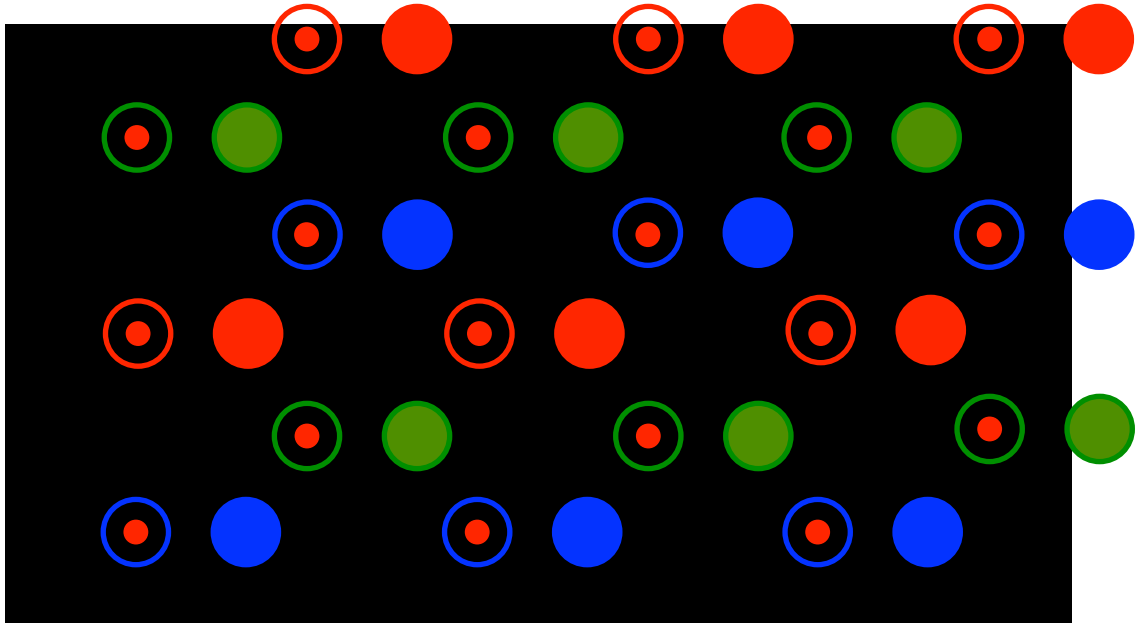
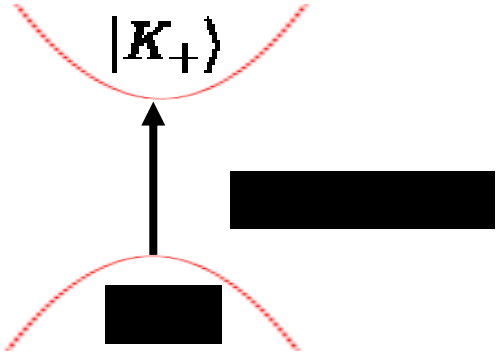
$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$

Optical transitions (at K)

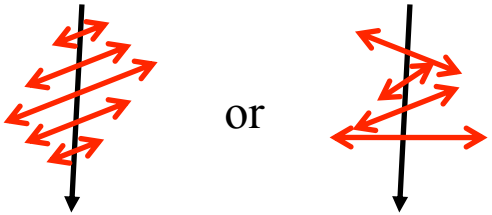




Peierls substitution:

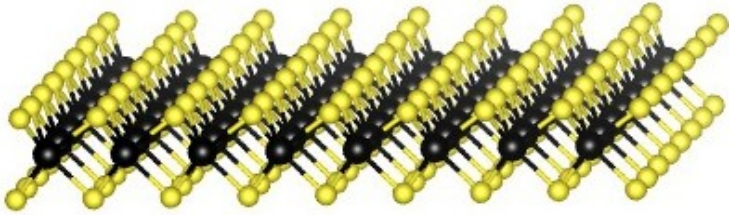
$$t \rightarrow te^{\pm iA} \approx t \pm itA$$

A is related to the vector potential of the elmag. field



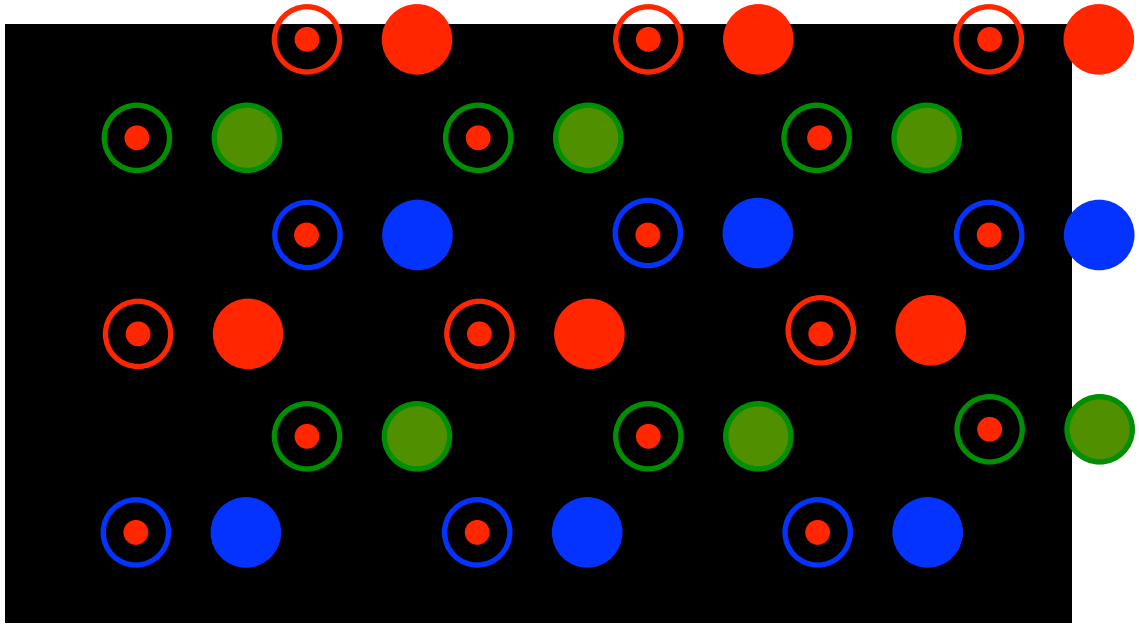
or

light

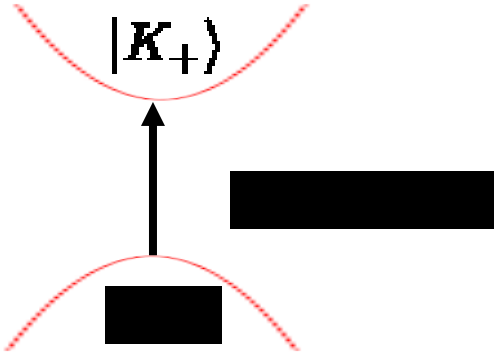


$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$

Optical transitions (at K)



$$\psi(\mathbf{R} = m, n) \propto \exp(i\frac{2\pi}{3}(m-n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$

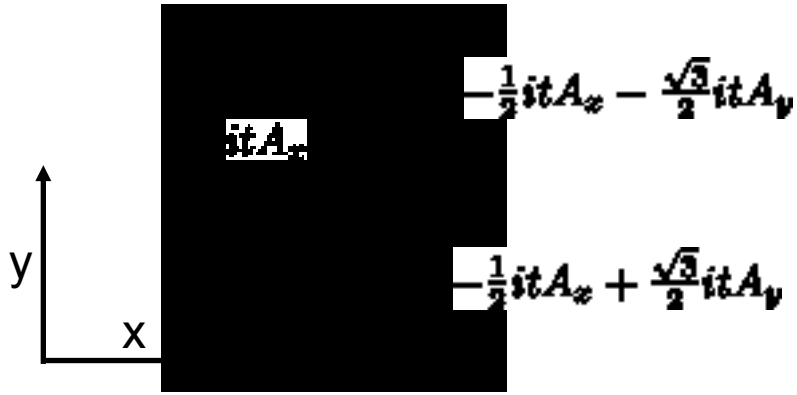


Peierls substitution:

$$t \rightarrow te^{\pm iA} \approx t \pm itA$$

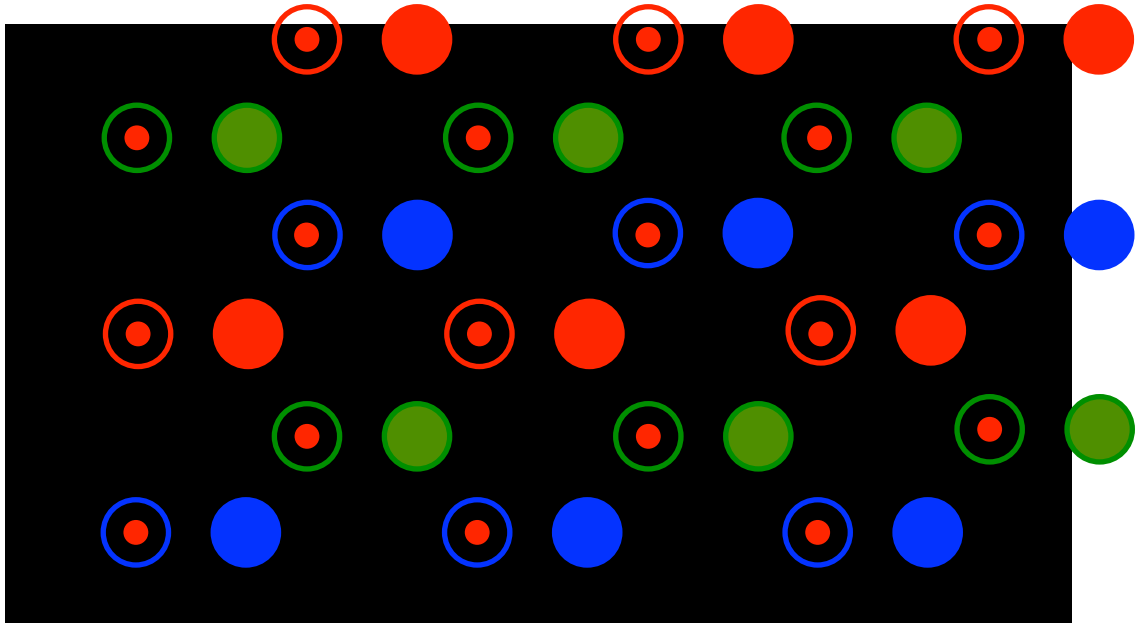
A is related to the vector potential of the elmag. field

When driven by external field electron picks a direction dependent phase on any given bond:



$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$

Optical transitions (at K)



$$\psi(\mathbf{R} = m, n) \propto \exp(i\frac{2\pi}{3}(m-n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$

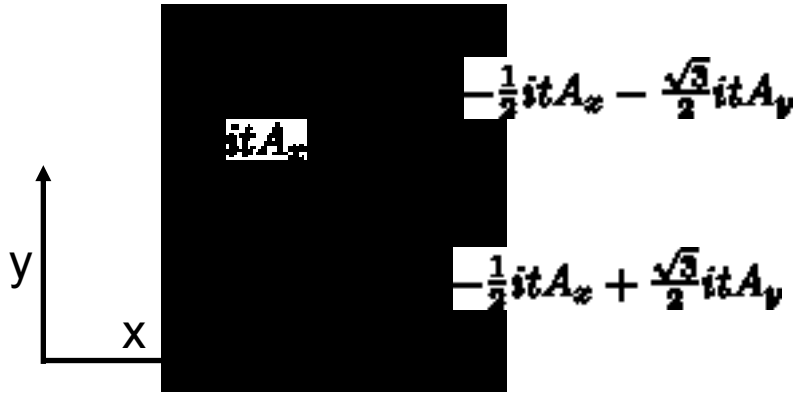
$$iA_x - iA_x\tfrac{1}{2}(e^{i\frac{2\pi}{3}} + e^{-i\frac{2\pi}{3}}) - \tfrac{\sqrt{3}}{2}iA_y(e^{i\frac{2\pi}{3}} - e^{-i\frac{2\pi}{3}}) = \tfrac{3}{2}(iA_x + A_y)$$

Peierls substitution:

$$t \to te^{\pm iA} \approx t \pm itA$$

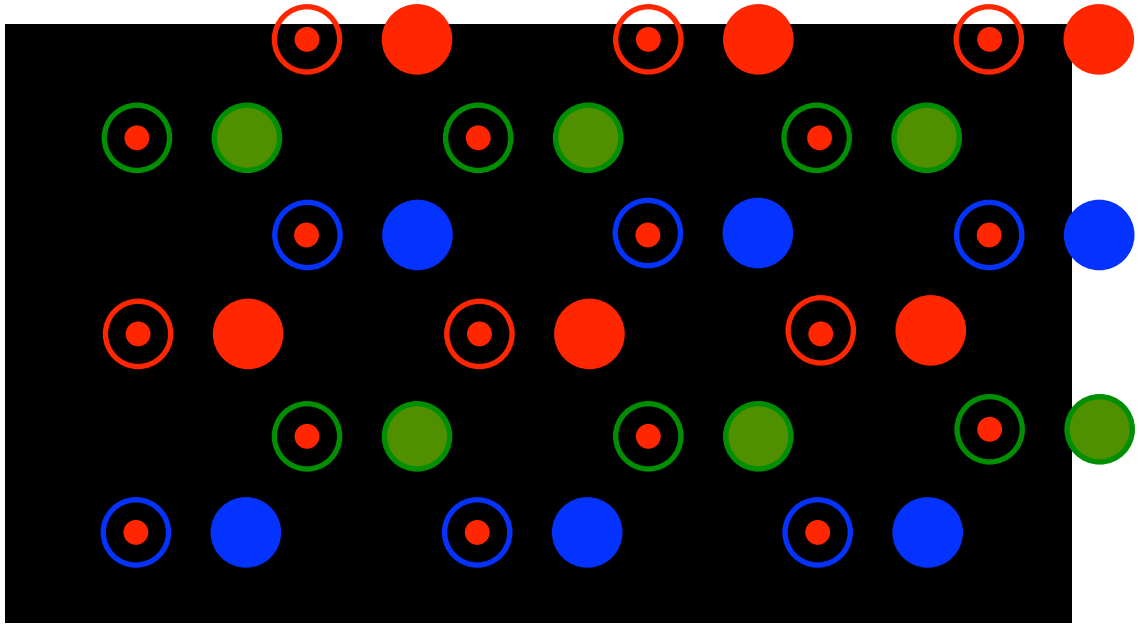
A is related to the vector potential of the elmag. field

When driven by external field electron picks a direction dependent phase on any given bond:



$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$

Optical transitions (at K)



$$\psi(\mathbf{R} = m, n) \propto \exp(i\frac{2\pi}{3}(m-n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$

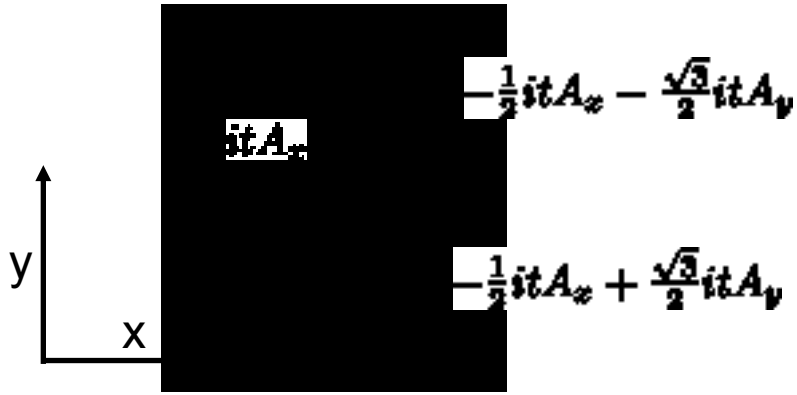
$$iA_x e^{i\frac{2\pi}{3}} - iA_x \tfrac{1}{2}(1 + e^{-i\frac{2\pi}{3}}) - \tfrac{\sqrt{3}}{2} iA_y (e^{-i\frac{2\pi}{3}} - 1) = \tfrac{3}{2}(iA_x + A_y) e^{i\frac{2\pi}{3}}$$

Peierls substitution:

$$t \rightarrow te^{\pm iA} \approx t \pm itA$$

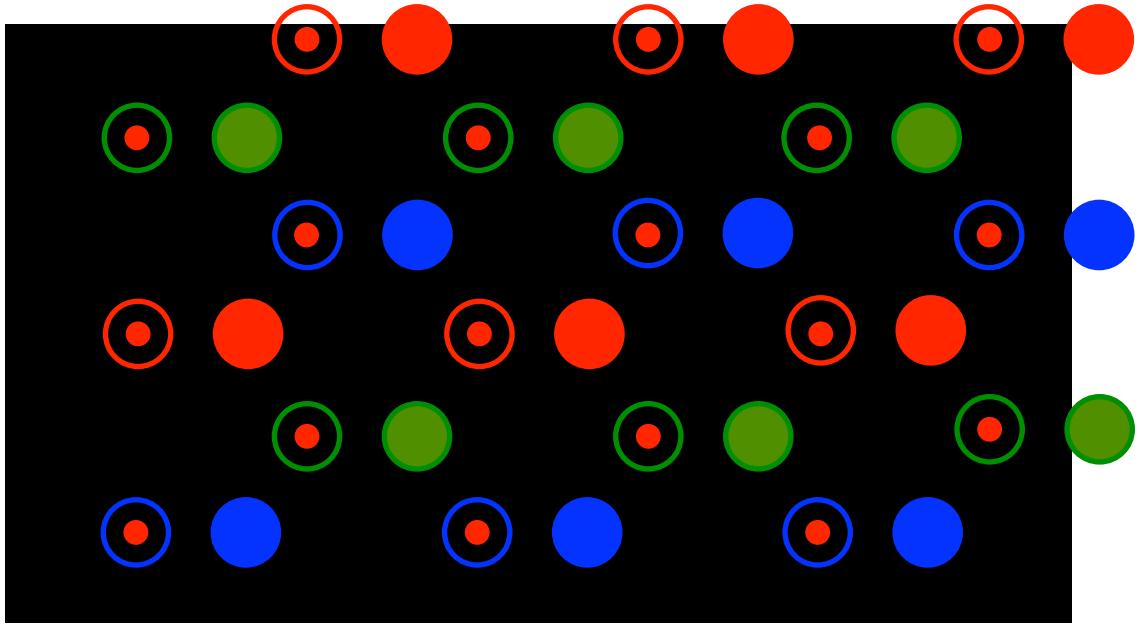
A is related to the vector potential of the elmag. field

When driven by external field electron picks a direction dependent phase on any given bond:



$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$

Optical transitions (at K)



$$\psi(\mathbf{R} = m, n) \propto \exp(i\frac{2\pi}{3}(m-n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$

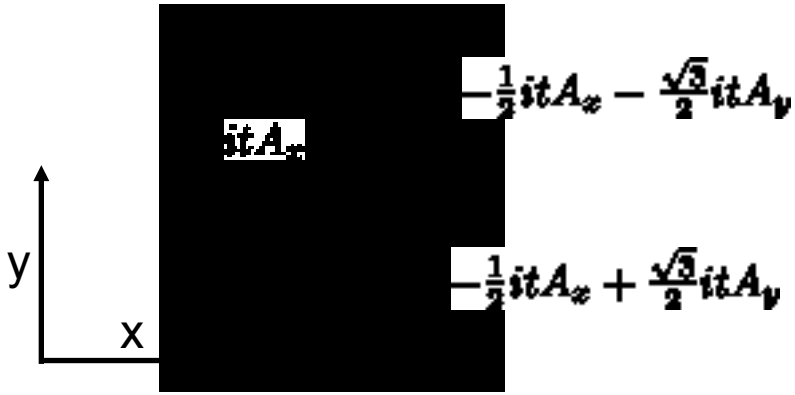
$$iA_x e^{-i\frac{2\pi}{3}} - iA_x \tfrac{1}{2}(1 + e^{i\frac{2\pi}{3}}) - \tfrac{\sqrt{3}}{2} iA_y (1 - e^{i\frac{2\pi}{3}}) = \tfrac{3}{2}(iA_x + A_y)e^{-i\frac{2\pi}{3}}$$

Peierls substitution:

$$t \to te^{\pm iA} \approx t \pm itA$$

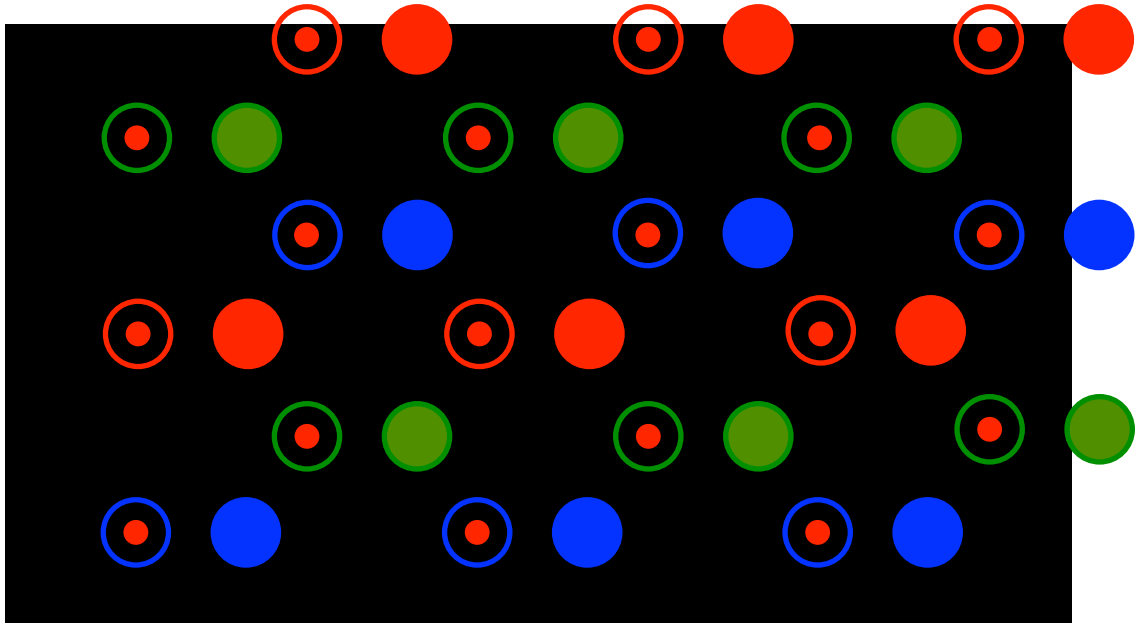
A is related to the vector potential of the elmag. field

When driven by external field electron picks a direction dependent phase on any given bond:

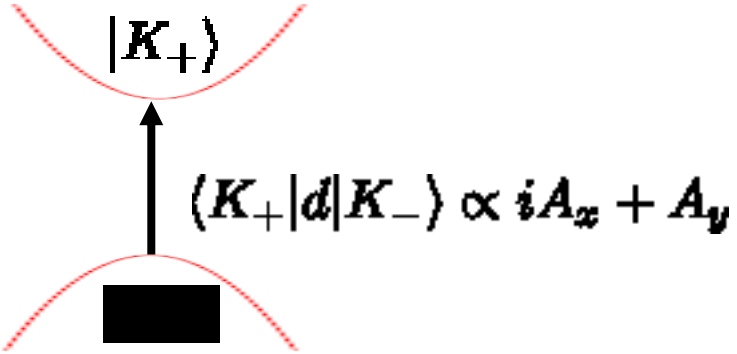


Optical transitions (at K and K')

$$\mathbf{K} = (\frac{2\pi}{3}, -\frac{2\pi}{3})$$



$$\psi(\mathbf{R} = m, n) \propto \exp(i\frac{2\pi}{3}(m-n)) = \begin{cases} 1 \\ \epsilon = e^{i\frac{2\pi}{3}} \\ \epsilon^* \end{cases}$$



circular polarization:

$\mathbf{A} \propto (1, i)$ excites optical transition at K

$\mathbf{A} \propto (1, -i)$ does not excite optical transition at K

You can show that at K' the role of circular polarizations is exchanged.

=> **You can choose the valley K or K' by using a circularly polarized light.**

Summary

- Continuous and lattice models of solids
- Translational symmetry (unit cell, basis vectors)
- Bloch theorem
- Simple lattice models and their diagonalization
- Density of states its calculation

Next time

- Basics of the density functional theory

Project no. 1

Calculate the band structure and density of states for 2D Kagome and 3D pyrochlore lattices.

Are there any bands with special properties?

How does the the band structure change when we add a sublattice site potentials?