Chair of Experimental Solid State Physics, LMU Munich

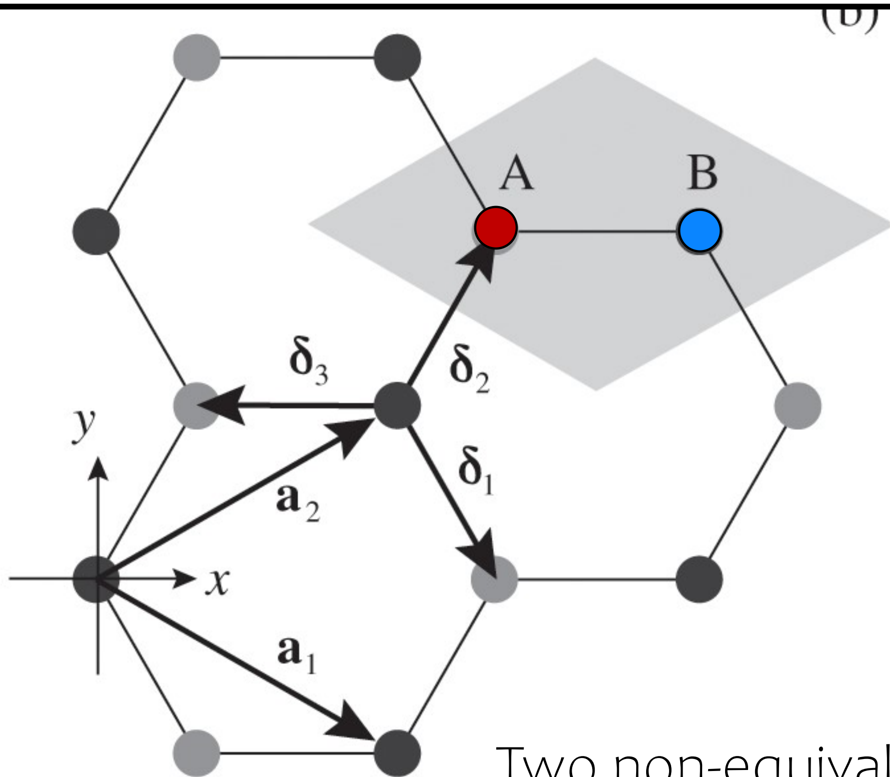
“Introduction to Graphene and 2D Materials”

SS24 Lecture 3, 29/4/2024

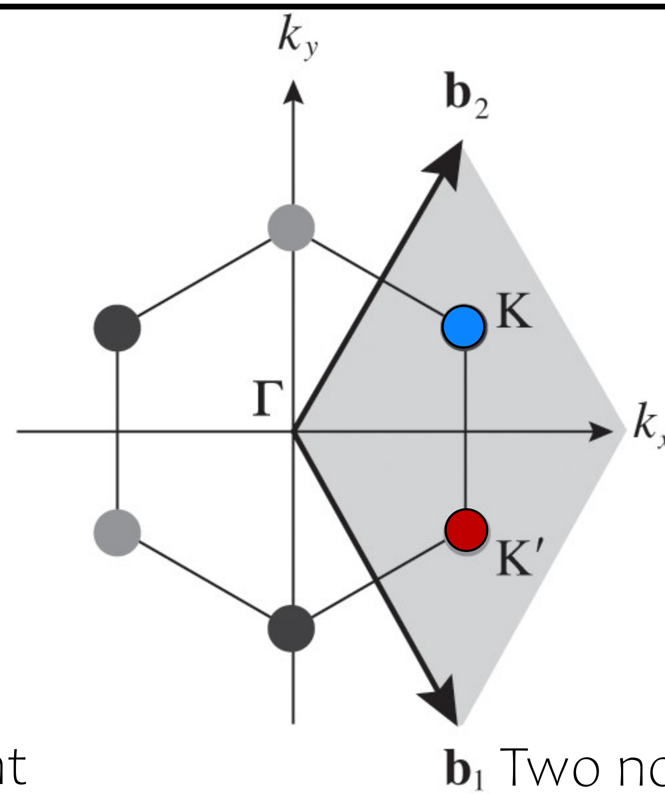
Outline - Lecture 3

- Short reminders on graphene's, Bravais lattice, reciprocal lattice, tight binding model, and band-structure.
- Quick calculation of the density of states (DOS).
- Expansion of the dispersion around the K and K' points, results in the Dirac equation.
- Derivation and visualization of the pseudo-spin, and its helical locking to the momentum.
- Demonstration of the absence of back-scattering.
- Visualizing the phase of the orbital wave-functions with Fermi energy.

Graphene lattice and reciprocal lattice



Two non-equivalent
A and B sub-lattices



Two non-equivalent
K and K' points

- A and B sub-lattices translate into the K and K' points in the BZ.
- Symmetries of the real and reciprocal space protect the Dirac points:

  - inversion symmetry (C_2 or A → B)
  - time reversal symmetry (T or k → -k)
  - 120° rotation symmetry (C_3 or 0° → 120°)

A and B basis representation

- One can also rewrite this in a matrix form in the basis of the A and B wave-functions:

$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix} \psi_{\vec{k}A}(\vec{r}) \\ \psi_{\vec{k}B}(\vec{r}) \end{pmatrix} \rightarrow \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix}$$

spinor representation

- Here the A and B sublattice sites act as two orthogonal wave-functions, and one can make the same analogy as for the spinor of the 2 states of the spin. We will show that this description can be explained as the isospin.

$$H(\vec{k}) = \begin{bmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{bmatrix}$$

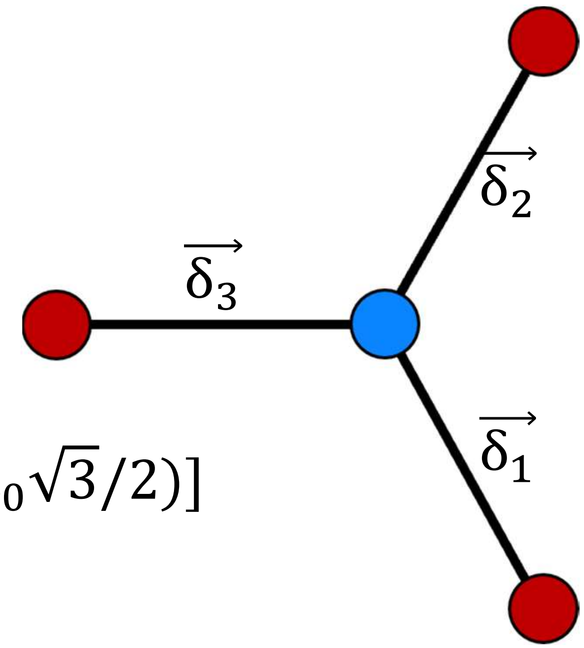
- Solving the Hamiltonian for the AA and BB combination leads only to the self energies, which by symmetry are just zero:

$$H_{AA} = H_{BB} = 0$$

Graphene band structure via tight binding derivation

- For the H_{AB} and H_{BA} only translation vectors to the nearest neighbor sites give finite values. For the A lattice sites (3 adjacent B sites) these vectors are just the nearest neighbor vectors. And for B analogously:

$$\overrightarrow{\delta_1} = \frac{a_0}{2}(1, -\sqrt{3}),\ \overrightarrow{\delta_2} = \frac{a_0}{2}(1, \sqrt{3}),\ \overrightarrow{\delta_3} = a_0(-1{,}0)$$



- Leading to:

$$H_{AB} = \gamma_0 \sum_n e^{-i\vec{k}\overrightarrow{\delta_n}} = \gamma_0[e^{-ik_x a_0} + 2e^{ik_x a_0/2}\cos(k_y a_0\sqrt{3}/2)]$$

$$H_{BA} = \gamma_0 \sum_n e^{i\vec{k}\overrightarrow{\delta_n}} = \gamma_0[e^{ik_x a_0} + 2e^{-ik_x a_0/2}\cos(k_y a_0\sqrt{3}/2)]$$

- With γ_0:

$$\gamma_0 = \int u_A^*(\vec{r})H(\vec{r})u_B\left(\vec{r} + \overrightarrow{\delta_3}\right) \sim 2.8eV$$

A and B basis representation

- One can also rewrite this in a matrix form in the basis of the A and B wave-functions:

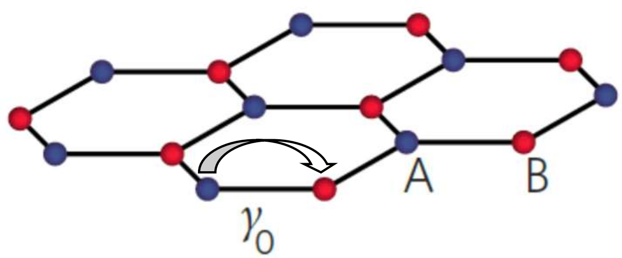
$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix} \psi_{\vec{k}A}(\vec{r}) \\ \psi_{\vec{k}B}(\vec{r}) \end{pmatrix} \rightarrow \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix}$$

spinor representation

$$H(\vec{k}) = \gamma_0 \begin{bmatrix} 0 & [e^{-ik_x a_0} + 2e^{ik_x a_0/2}\cos(k_y a_0\sqrt{3}/2)] \\ [e^{ik_x a_0} + 2e^{-ik_x a_0/2}\cos(k_y a_0\sqrt{3}/2)] & 0 \end{bmatrix}$$

$$\gamma_0 = \int u_A^*(\vec{r})H(\vec{r})u_B\left(\vec{r} + \overrightarrow{\delta_3}\right) \sim 2.8eV$$

$\gamma = \gamma_0$ can be interpreted as the hopping parameter of an electron tunneling from A to B lattice sites.



Graphene band-structure – Dirac cones

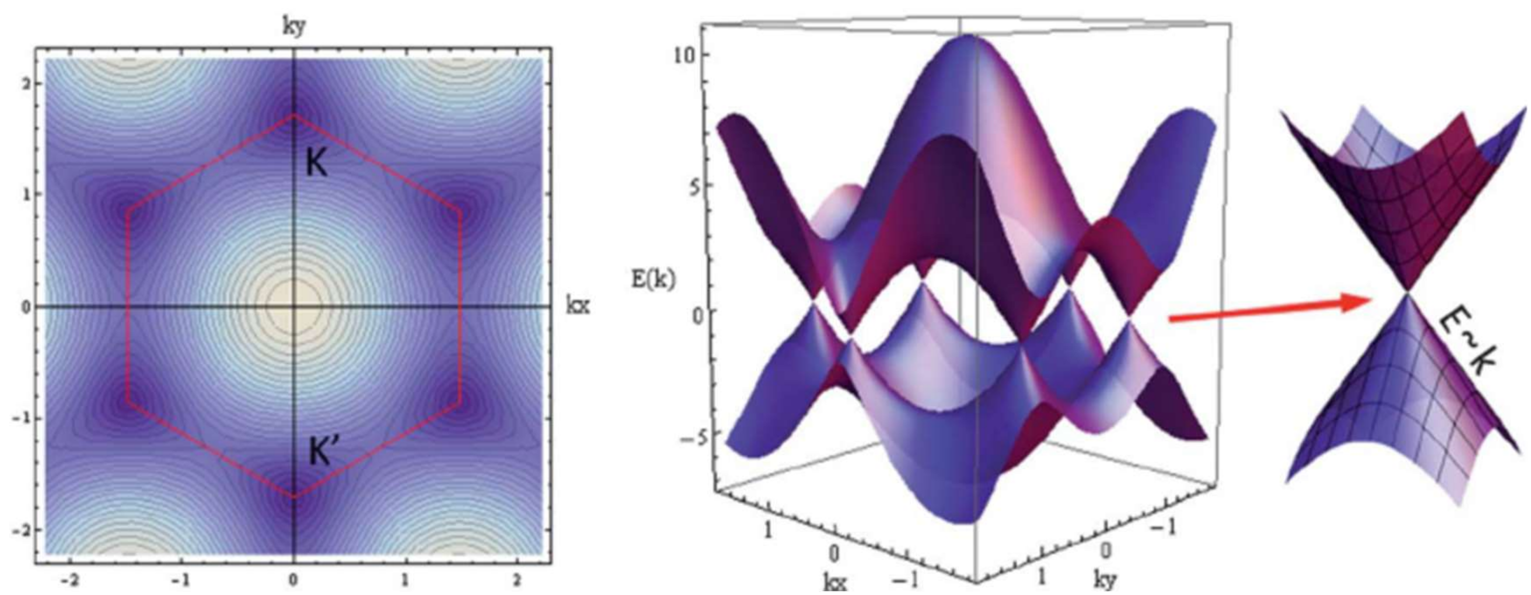
- Solve Schroedinger's equation to get Energy Eigenstates:

$$\varepsilon_m = \int d^3r\, \psi_m^*(\mathbf{r}) H(\mathbf{r}) \psi_m(\mathbf{r})$$

- The final solution of the Eigenenergies of the Hamiltonian have the form:

$$E(\vec{k}) = \pm\gamma_0\sqrt{3 + 2\cos(\sqrt{3}k_y a_0) + 4\cos(3k_x a_0/2)\cos(\sqrt{3}k_y a_0/2)}$$

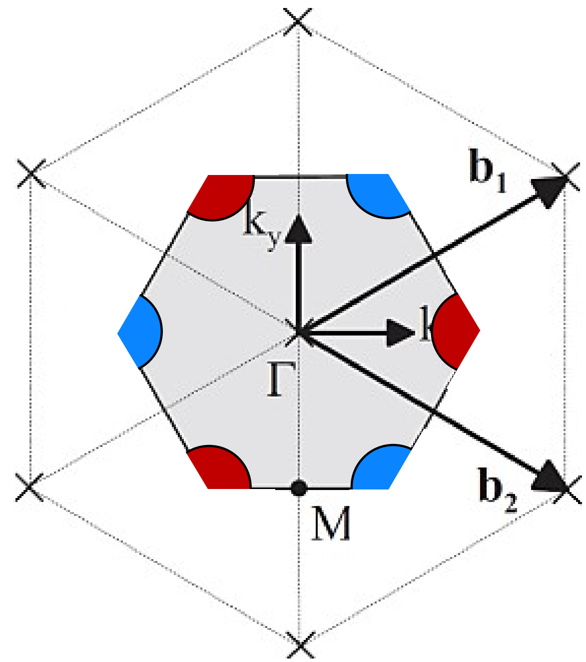
- Dirac cones are formed in the K and K' points. Here the electrons can be shown to be massless and the dispersion relation described by the Dirac equation.



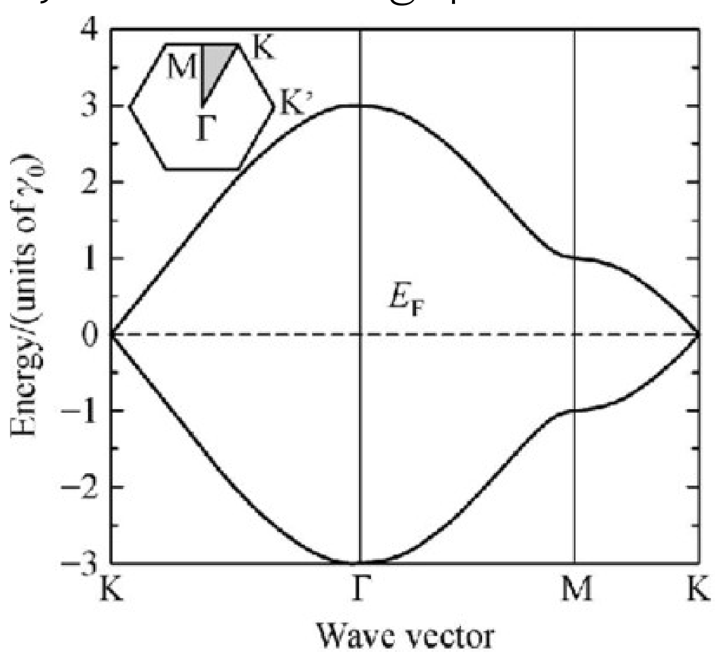
Dirac cones in the K and K’ points

- Linear dispersion relation → Effective mass of the electrons is zero $m^* = 0$.

$$m^* = \pm\hbar\left(\frac{d^2E_k}{dk^2}\right)^{-1} \sim 0 \qquad v_F = \frac{\sqrt{3}a_0\gamma}{2\hbar} \sim \frac{c}{300} \sim 10^6\, m/s$$

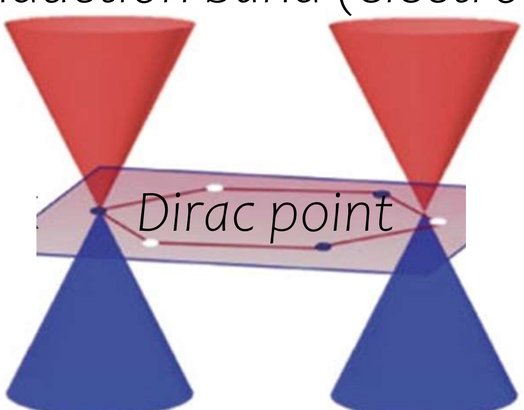


- Dirac cones are formed in the K and K’ points → 2 valleys → no band-gaps.



Valley K’ *Valley K*

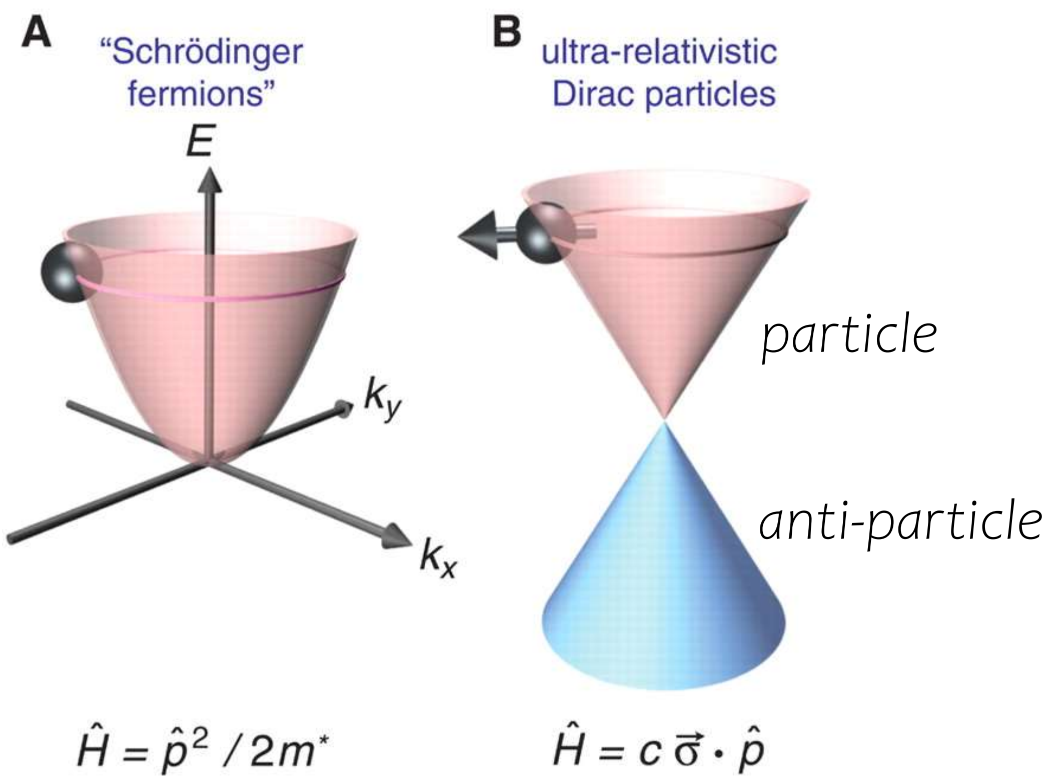
conduction band (electrons)



valence band (holes)

Analogy to Dirac equation

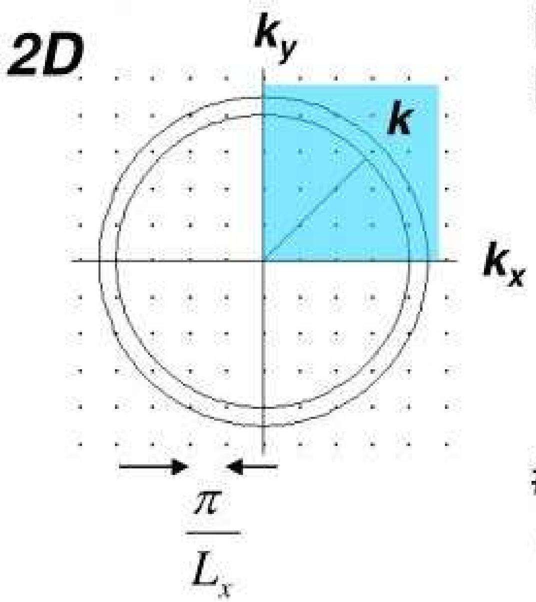
- Non-relativistic particles – Schroedinger equation – no spin vs. momentum locking.
- Relativistic particles – Dirac equation – spin and momentum are locked.



- $(i\hbar\gamma^{\mu}\partial^{\mu} - mc)\psi = 0$
- $H(\vec{p}) = c\vec{\sigma}\vec{p}$
  ($\vec{\sigma}$ *Pauli matrizes*)
- *v = c , m = 0*
- *spin // momentum*

→ *"Helicity" (or "chirality" for particles with mass)*

Density of states (DOS) calculations in 2D



For quantum particles confined in a 2D “box” (e.g., electrons in FET):

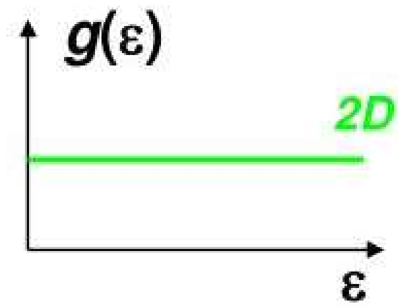
$$k_x = \frac{\pi n_x}{L_x} \qquad k_y = \frac{\pi n_y}{L_y} \qquad k = \sqrt{{k_x}^2 + {k_y}^2}$$

$$N(k) = \frac{1}{4}\,\frac{\pi k^2}{\frac{\pi}{L_x} \times \frac{\pi}{L_y}} = \frac{k^2 (area)}{4\pi} \qquad G(k) = \frac{k^2}{4\pi} A \qquad G(\varepsilon) = \frac{A}{4\pi}\,\frac{2m\varepsilon}{\hbar^2}$$

states within ¼ of a circle of radius ***k***

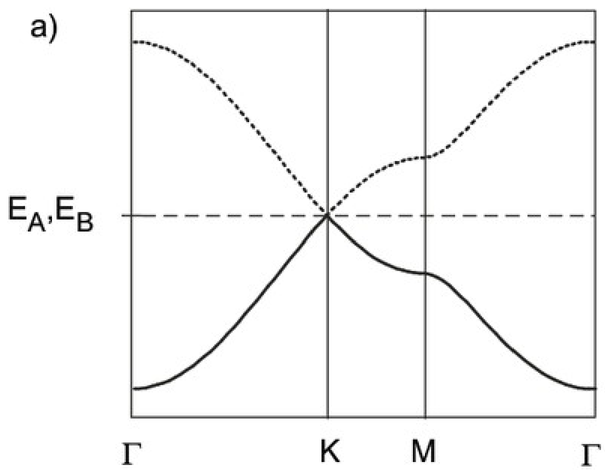
$$g^{2D}(\varepsilon) = \frac{A(2s+1)m}{2\pi\hbar^2}$$

- does not depend on **ε**

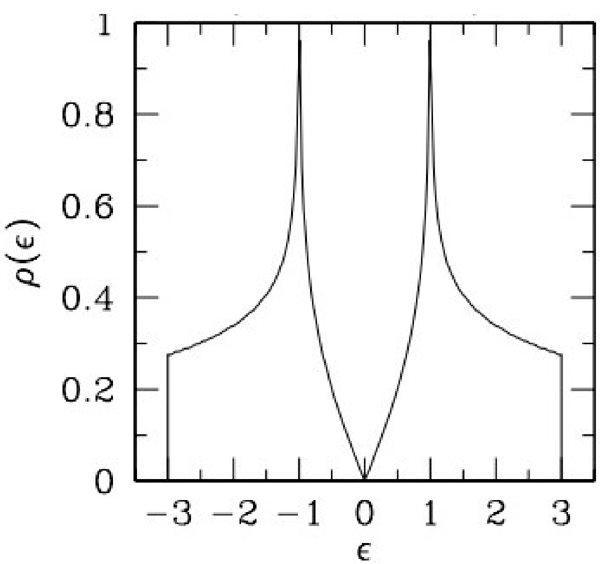


DOS and E_F in graphene

Band structure:



DOS vs. E:



Energy dispersion:

$$E(\vec{\kappa}) \sim \hbar v_F \vec{\kappa}$$

Number of states in $d\kappa$:

$$N(\kappa)d\kappa = \frac{2\pi K dK}{(\frac{2\pi}{L_x})(\frac{2\pi}{L_y})} \times 2\text{ (spin)} \times 2\text{ (valley)} = 2A\,\frac{EdE}{\pi(\hbar v_F)^2}$$

Number of states (per area) vs. E:

$$g(E) = \frac{2E}{\pi(\hbar v_F)^2}$$

Carrier density vs. E_F:

$$n(E_F) = \int_0^{E_F} g(E)\,dE = \frac{E^2}{\pi(\hbar v_F)^2}$$

E_F vs. n:

$$E_F(n) = \hbar v_F\sqrt{\pi n}$$

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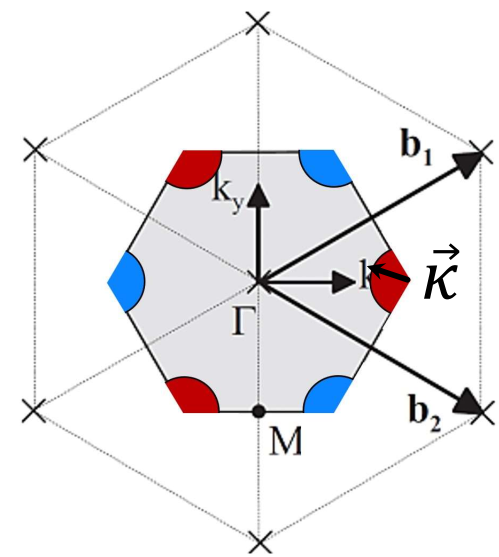
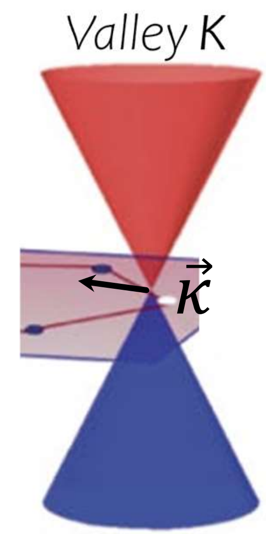
Low energy expansion around K

- We take low energy expansion for small momentum $\vec{k}$ around the $\vec{K}$ and $\vec{K}'$ for low energy:

$$\vec{k} = \vec{K} + \vec{\kappa} \qquad \vec{K} = \left(\frac{4\pi}{3a_0}, 0\right) = -\overrightarrow{K'}$$





- Then Hamiltonian elements become:

$$\sum_n e^{i\vec{k}\overrightarrow{\delta_n}} = e^{ik_y a_0/\sqrt{3}} + e^{-ik_y a_0/2\sqrt{3}} \cos\left(\frac{k_x a_0}{2}\right) \sim \frac{\sqrt{3}a_0}{2}(\kappa_x - i\kappa_y)$$

- And the Hamiltonian around the K point takes the form:

$$H(\vec{k}) = \begin{bmatrix} 0 & -\gamma \sum_n e^{i\vec{k}\overrightarrow{\delta_n}} \\ -\gamma \sum_n e^{-i\vec{k}\overrightarrow{\delta_n}} & 0 \end{bmatrix} \sim \hbar v_F \begin{bmatrix} 0 & \kappa_x - i\kappa_y \\ \kappa_x + i\kappa_y & 0 \end{bmatrix}$$

Dirac-like equation with pseudospin

- For one K point we have a two-component wave function:

$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix} \psi_{\vec{k}A}(\vec{r}) \\ \psi_{\vec{k}B}(\vec{r}) \end{pmatrix} \sim \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \begin{pmatrix} 1 \\ e^{i\theta_\kappa} \end{pmatrix} \rightarrow \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \qquad \theta_\kappa = arctan(\kappa_y/\kappa_x)$$

- The Hamiltonian then takes an effective form of the Dirac Weyl Hamiltonian:

B to A hopping

$$H(\vec{K}) \sim \hbar v_F \begin{bmatrix} 0 & \kappa_x - i\kappa_y \\ \kappa_x + i\kappa_y & 0 \end{bmatrix} = \hbar v_F(\sigma_x \kappa_x + \sigma_y \kappa_y) = \hbar v_F \vec{\sigma}\vec{\kappa}$$

A to B hopping

- Where $\boldsymbol{\sigma_x}$ and $\boldsymbol{\sigma_y}$ are Pauli spin matrizes:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};$$

- Bloch function amplitudes on the A and B lattice sites (“pseudospin”) mimic the spin components of the relativistic Dirac fermions.

Dirac equation for both valleys K and K'

- Including now expansions around both K and K' points we obtain a four-component wave-function from the A and B lattice sites and at K and K' points:

$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix} \psi_{\vec{k}A,K}(\vec{r}) \\ \psi_{\vec{k}B,K}(\vec{r}) \\ \psi_{\vec{k}A,K'}(\vec{r}) \\ \psi_{\vec{k}B,K'}(\vec{r}) \end{pmatrix}$$

Sub-lattice index A and B

Valley index K and K'

- The Hamiltonian then takes an effective form of the Dirac Weyl Hamiltonian:

$$H(\vec{\kappa}) \sim \hbar v_F \begin{bmatrix} 0 & \kappa_x - i\kappa_y & 0 & 0 \\ \kappa_x + i\kappa_y & 0 & 0 & 0 \\ 0 & 0 & 0 & -\kappa_x - i\kappa_y \\ 0 & 0 & -\kappa_x + i\kappa_y & 0 \end{bmatrix} = \begin{bmatrix} 0 & \hbar v_F \vec{\sigma}\vec{\kappa} \\ -\hbar v_F \vec{\sigma}^* \vec{\kappa} & 0 \end{bmatrix}$$

$H(\vec{K})$

$H(\overrightarrow{K'})$

- Hamiltonians around $H(\vec{K})$ and $H(\overrightarrow{K'})$ are connected by time reversal symmetry.

Helicity (Chirality)

- For one K point we have a two-component wave function:

$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix} \psi_{\vec{k}A}(\vec{r}) \\ \psi_{\vec{k}B}(\vec{r}) \end{pmatrix} = \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \begin{pmatrix} 1 \\ e^{i\theta_\kappa} \end{pmatrix} \rightarrow \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \qquad \theta_\kappa = arctan(\kappa_y/\kappa_x)$$

- Hamiltonian around the K point contains the helicity operator $\hat{h} = \vec{\sigma}\vec{n}$:

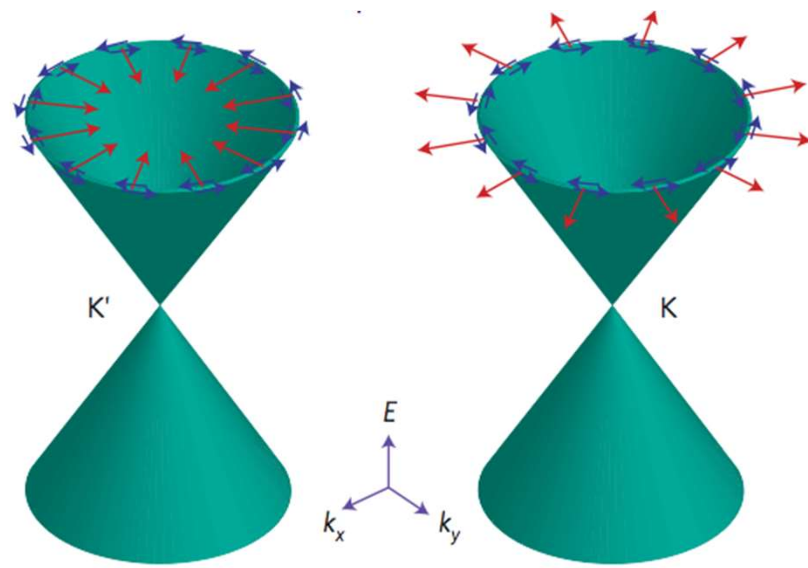
$$H(\vec{K}) \sim \hbar v_F \vec{\sigma}\vec{\kappa} = \hbar v_F \kappa \vec{\sigma}\vec{n} = \hbar v_F \kappa \hat{h}$$

"Helicity" – projection of the spin onto the momentum – is conserved (since energy is conserved).

- *Pseudospin direction is linked to momentum*

→ *in K* $\vec{\sigma}\vec{n}$ *= 1 (electrons),* $\vec{\sigma}\vec{n}$ *= -1 (holes)*

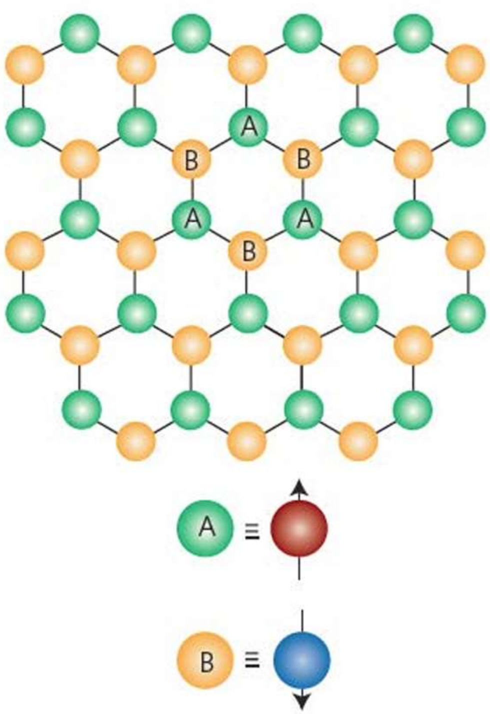
→ *in K'* $\vec{\sigma}\vec{n}$ *= -1 (electrons),* $\vec{\sigma}\vec{n}$ *= 1 (holes)*



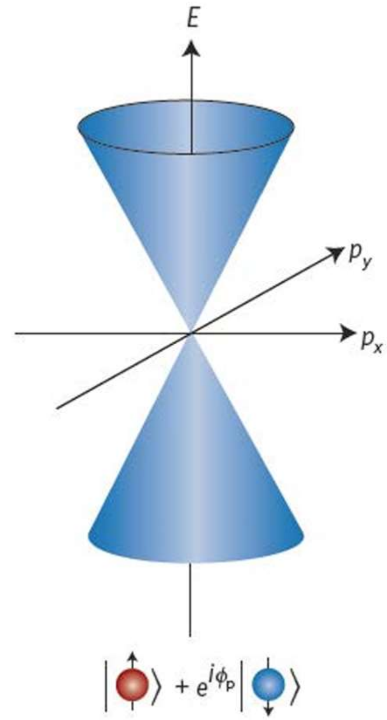
Pseudo-spin

$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix} \psi_{\vec{k}A}(\vec{r}) \\ \psi_{\vec{k}B}(\vec{r}) \end{pmatrix} \sim \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \begin{pmatrix} 1 \\ e^{i\theta_\kappa} \end{pmatrix} \rightarrow \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \qquad \theta_\kappa = arctan(\kappa_y/\kappa_x)$$

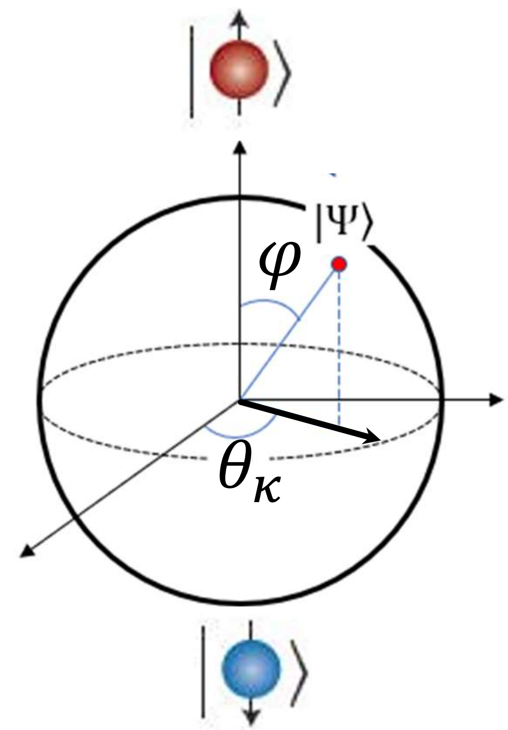
Real space:



Wave functions:



Bloch sphere representation:



- Pseudo-spin is oriented at the equator → A and B have same amplitudes.

Backscattering is forbidden – conservation of helicity

$$\psi_{\vec{k}}(\vec{r}) \sim \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \binom{1}{e^{i\theta_\kappa}}$$

$$H(\vec{k}) \sim \begin{bmatrix} 0 & \hbar v_F \vec{\sigma}\vec{\kappa} \\ -\hbar v_F \vec{\sigma}^* \vec{\kappa} & 0 \end{bmatrix}$$

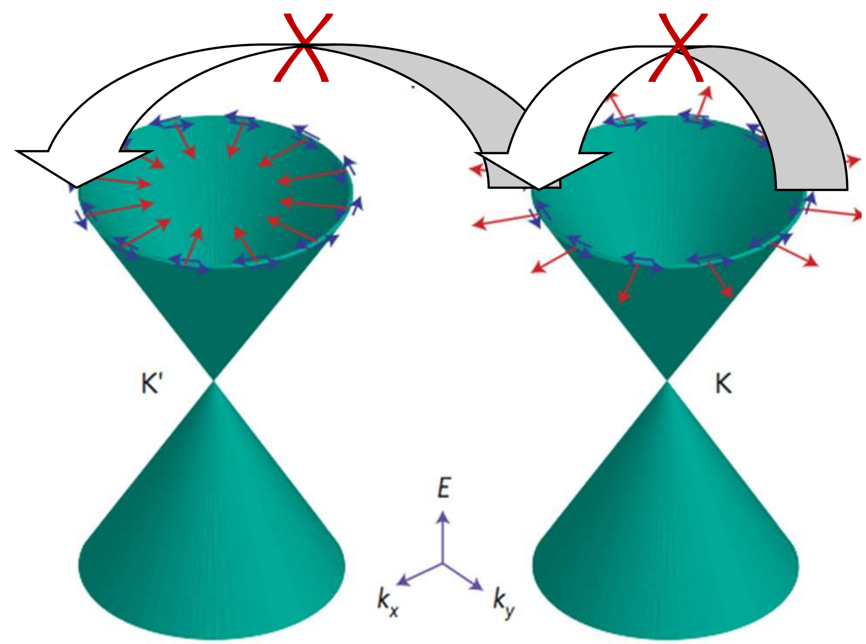
Conservation of helicity $\hat{h} = \vec{\sigma}\vec{n}$ dictates:

- No back-scattering within the Dirac cones (pseudo-spin has to flip). This can be calculated by calculating the scattering probability between:

$$\psi_{\vec{k}}(\vec{r}) \sim \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \binom{1}{0}$$

$$\rightarrow$$

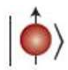
$$\psi_{\vec{k}}(\vec{r}) \sim \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \binom{1}{e^{i2\pi}}$$



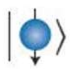
- Analogously there is no back-scattering between cones.

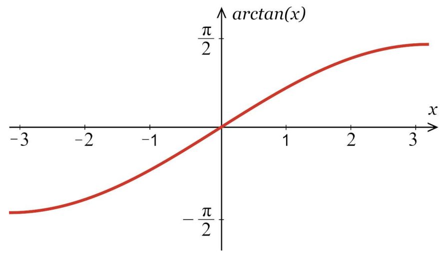
Helicity (Chirality) and Pseudo-spin texture

Wave-functions resemble spin:



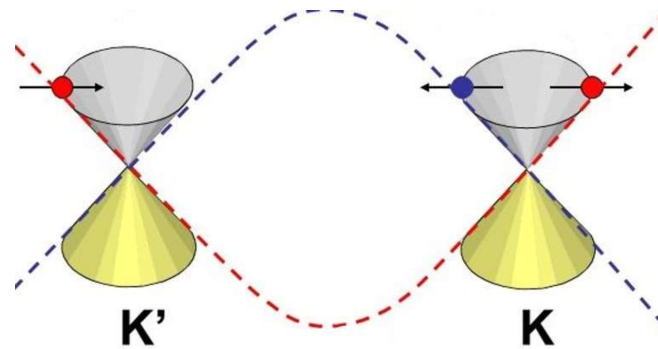
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\vec{\kappa}\vec{r}} \\ e^{i(\vec{\kappa}\vec{r}+\theta_\kappa)} \end{pmatrix}$$





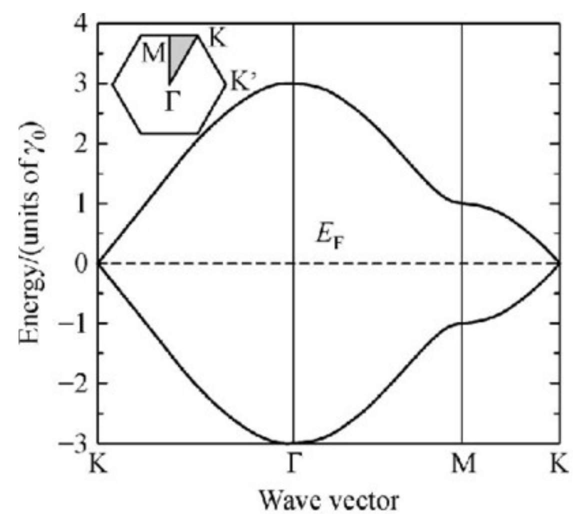
$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

- Hamiltonian around the K point contains the helicity operator $\hat{h} = \vec{\sigma}\vec{n}$:



$$H(\vec{K}) \sim \hbar v_F \vec{\sigma}\vec{\kappa} = \hbar v_F \kappa \vec{\sigma}\vec{n} = \hbar v_F \kappa \hat{h}$$

- *"Helicity" – projection of the spin onto the momentum – is conserved (since energy is conserved).*



- *Pseudospin direction aligned to $\vec{\kappa}$:*

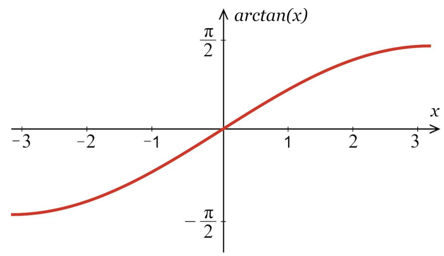
→ *in K $\vec{\sigma}\vec{n}$ = 1 (electrons), $\vec{\sigma}\vec{n}$ = -1 (holes)*

→ *in K' $\vec{\sigma}\vec{n}$ = -1 (electrons), $\vec{\sigma}\vec{n}$ = 1 (holes)*

Spin (SU(2)) X Pseudo-spin (SU(2)) = SU(4)

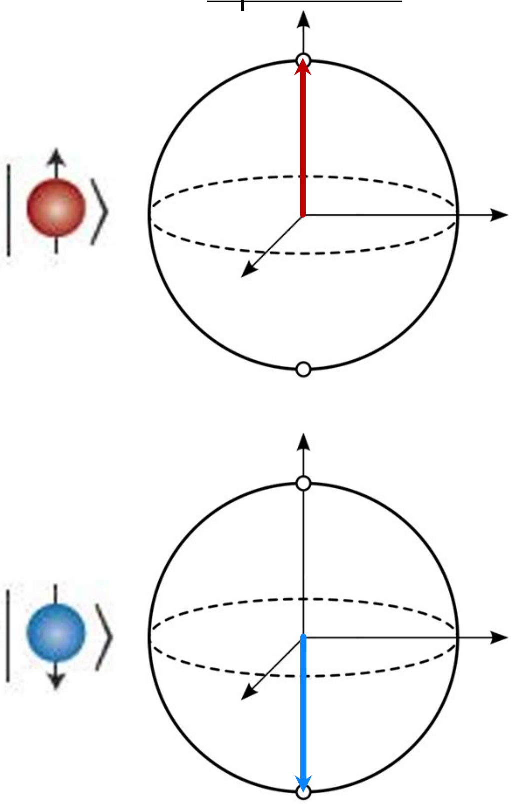
Wave-functions resemble spin:

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\vec{\kappa}\vec{r}} \\ e^{i(\vec{\kappa}\vec{r}+\theta_\kappa)} \end{pmatrix}$$

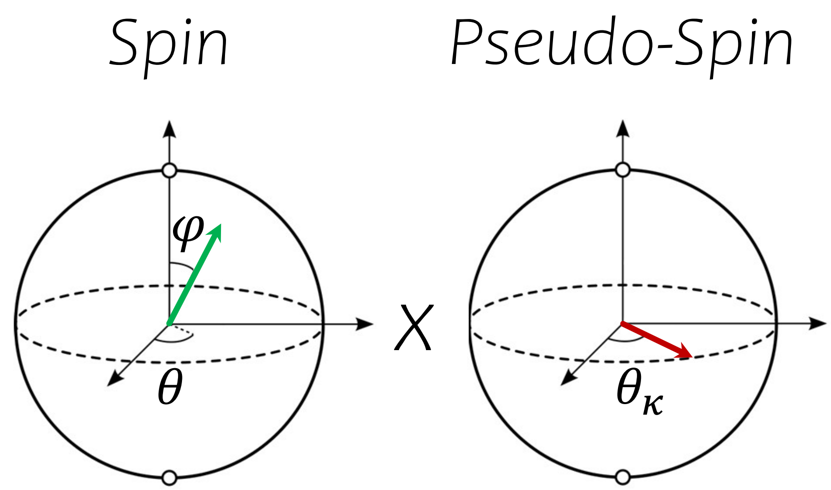


$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

Spinors:



Two quantum numbers spin and pseudo-spin:



SU(2) x SU(2) = SU(4)

→ Also convenient to translate to SU(4) basis of spin x valley.

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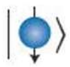
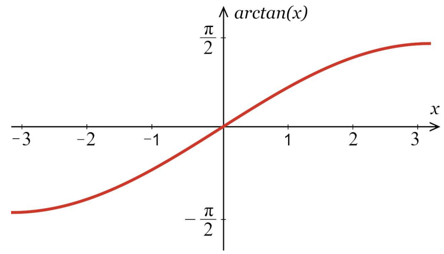
Relating the phase of wave-functions to carbon atoms

Wave-functions resemble spin:

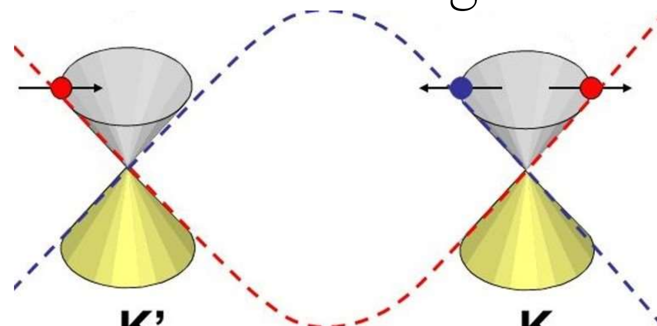
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\vec{\kappa}\vec{r}} \\ e^{i(\vec{\kappa}\vec{r}+\theta_\kappa)} \end{pmatrix}$$





$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

anti-bonding

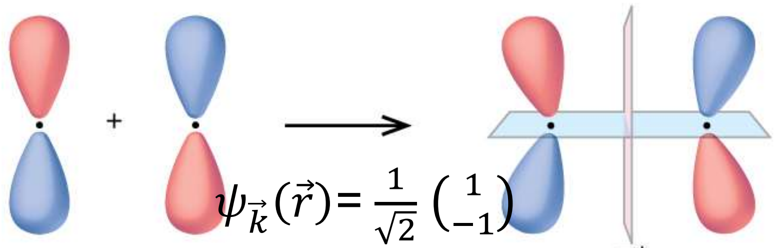


K'

bonding

K

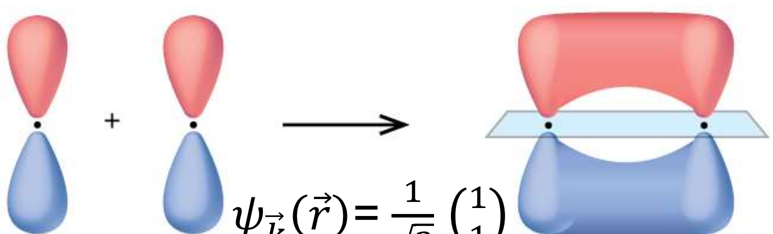
Anti-bonding (anti-symmetric) wave-functions – high energy:



$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

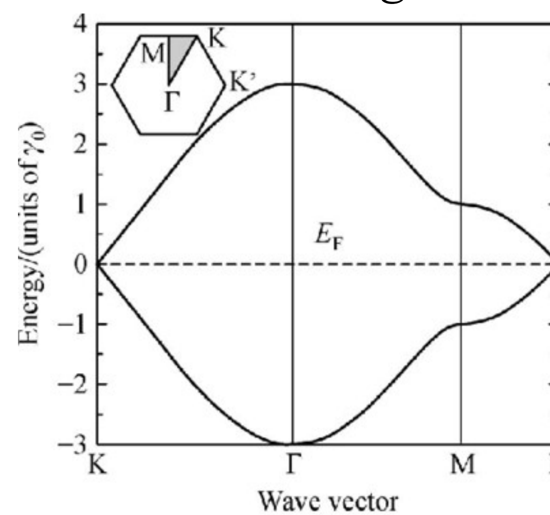
π_p^*

Bonding (symmetric) wave-functions – high energy:

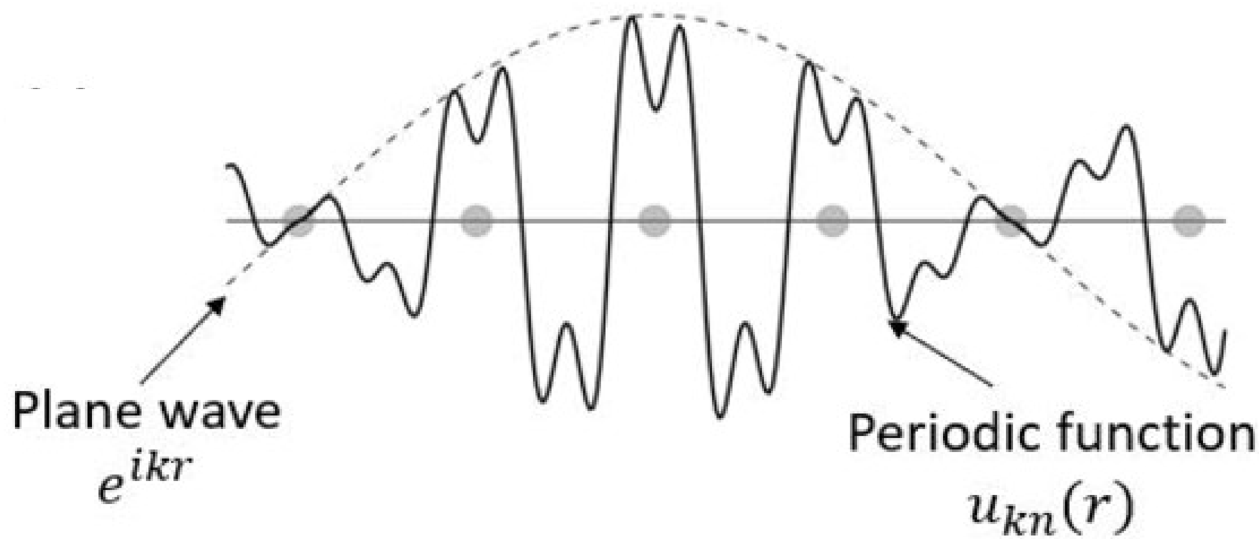


$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

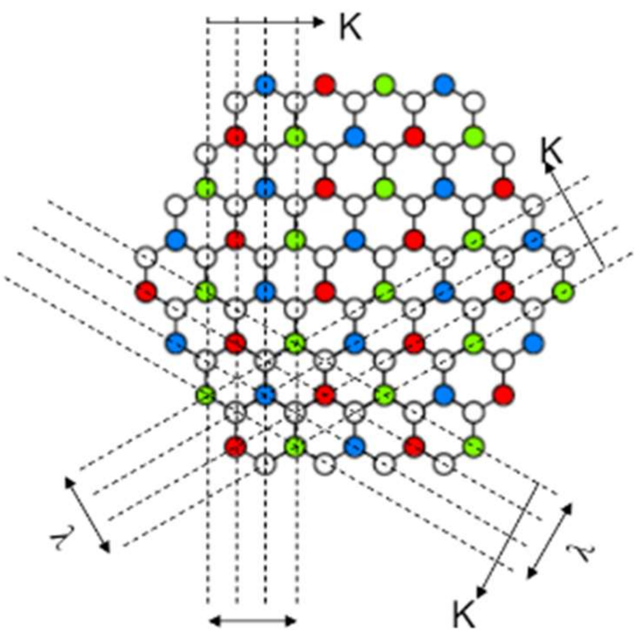
π_p



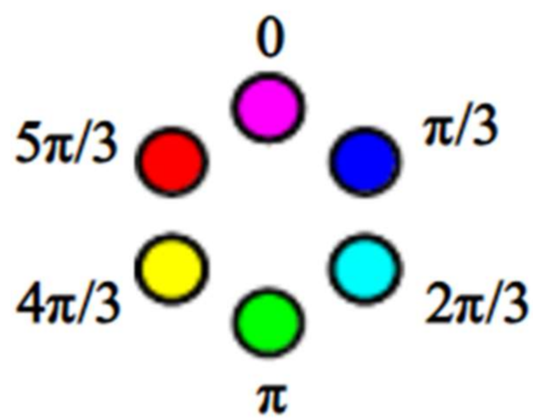
Phase changes under hopping from A to B



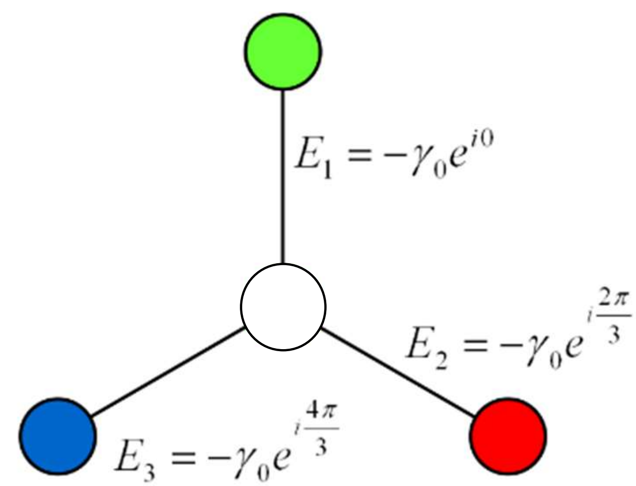
Propagation directions:



Phase:

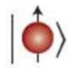


Phase changes under hopping:

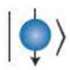


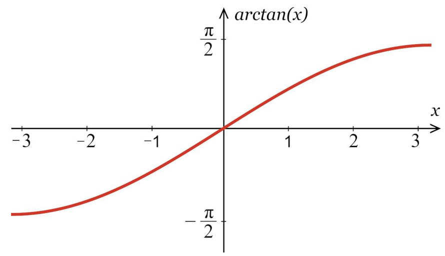
Visualizing wave-functions in real-space

Wave-functions resemble spin:



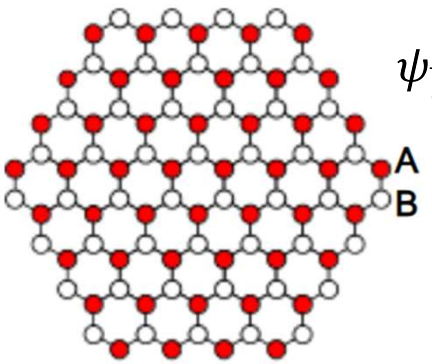
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\vec{\kappa}\vec{r}} \\ e^{i(\vec{\kappa}\vec{r}+\theta_\kappa)} \end{pmatrix}$$



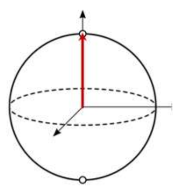


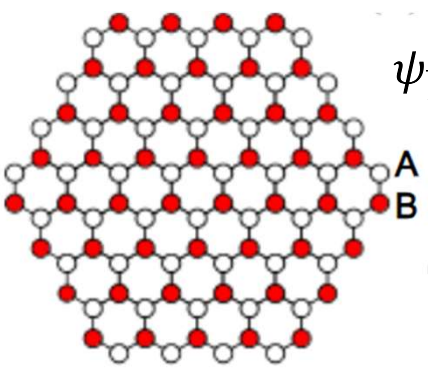
$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

Γ – point, $\vec{k} = 0$:

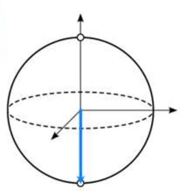


$\psi_{\vec{k}}(\vec{r}) = \binom{1}{0}$

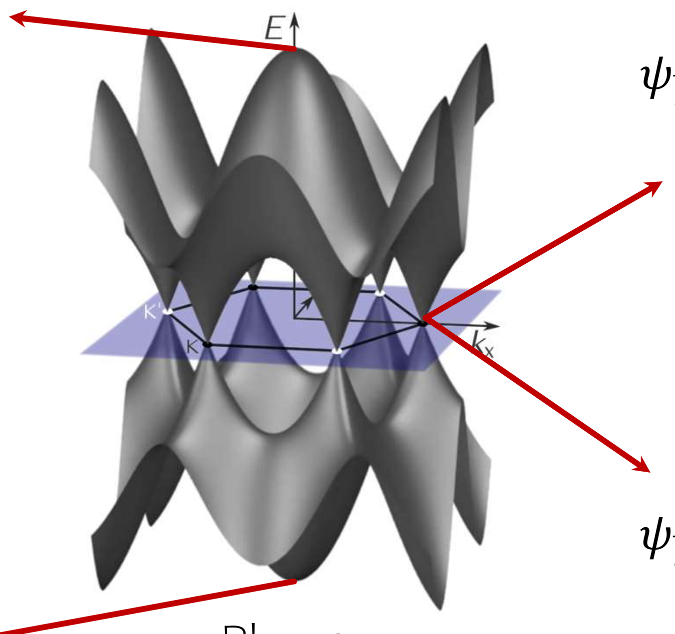




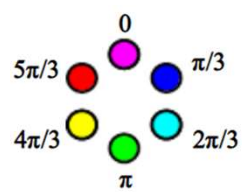
$\psi_{\vec{k}}(\vec{r}) = \binom{0}{1}$



Band-structure:

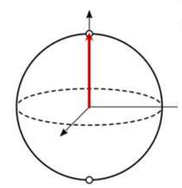


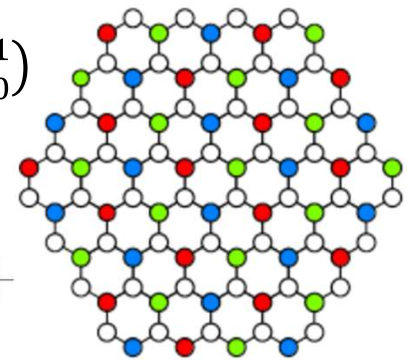
Phase:



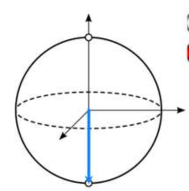
K – point, $\vec{k} = \vec{K}$:

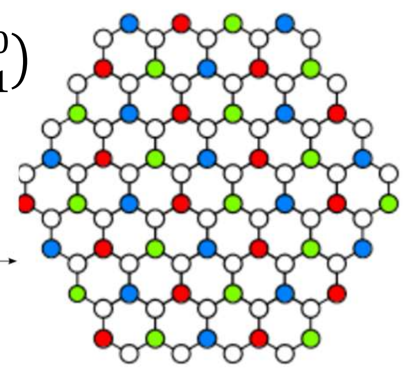
$\psi_{\vec{k}}(\vec{r}) = \binom{1}{0}$





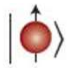
$\psi_{\vec{k}}(\vec{r}) = \binom{0}{1}$



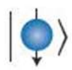


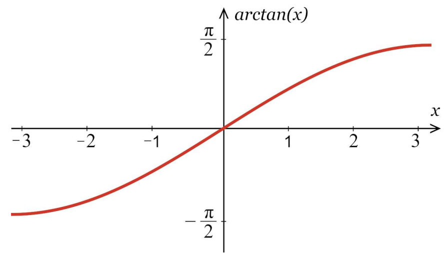
Visualizing wave-functions in real-space

Wave-functions resemble spin:



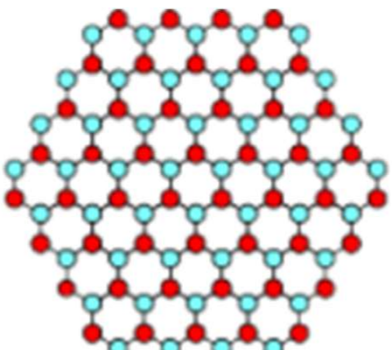
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\vec{\kappa}\vec{r}} \\ e^{i(\vec{\kappa}\vec{r}+\theta_\kappa)} \end{pmatrix}$$





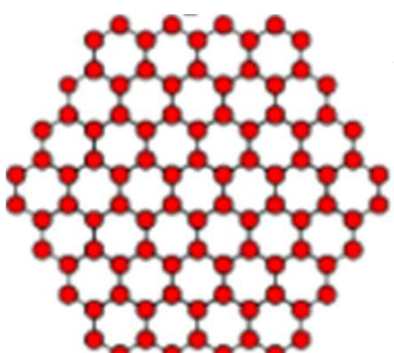
$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

Γ – point, $\vec{k} = 0$:



anti-bonding

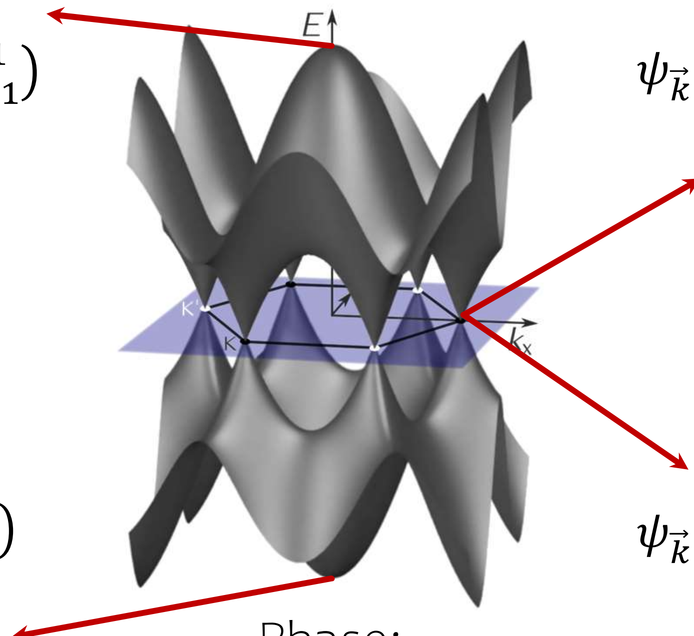
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \binom{1}{-1}$$



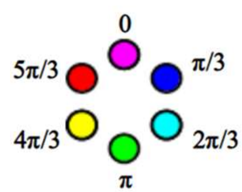
bonding

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \binom{1}{1}$$

Band-structure:

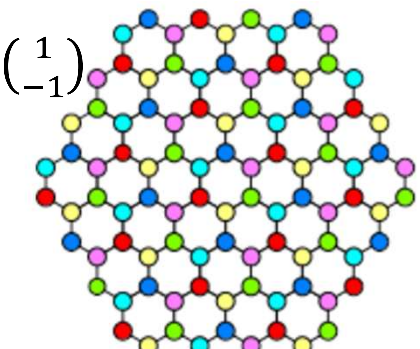


Phase:



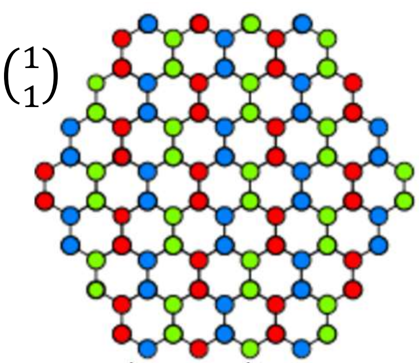
K – point, $\vec{k} = \vec{K}$:

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \binom{1}{-1}$$



anti-bonding

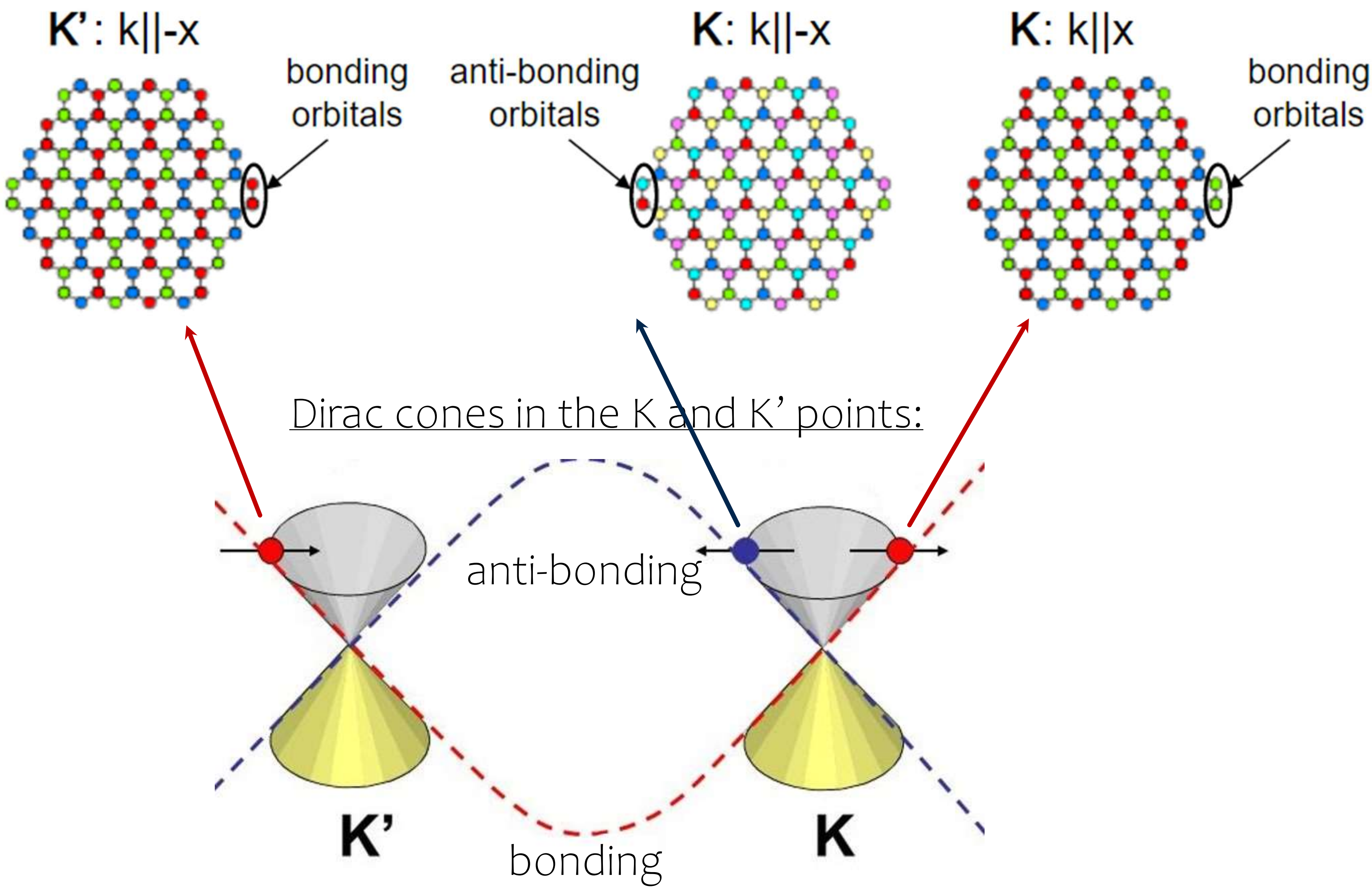
$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{2}} \binom{1}{1}$$



bonding

Real-space wave-functions and pseudo-spin texture

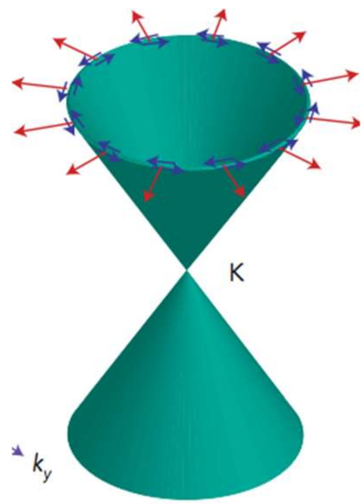
Real space wave-functions:

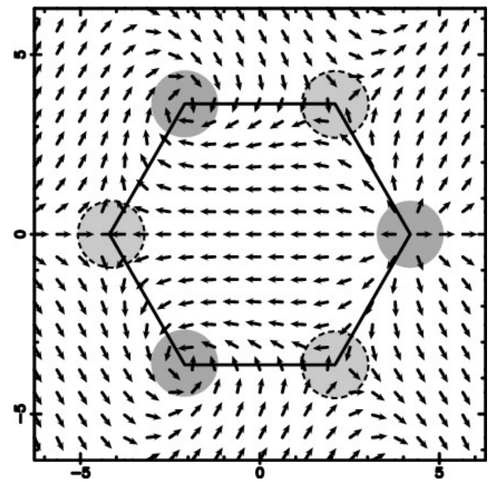


LMU Ludwig-Maximilians-Universität München
Chair of Experimental Solid State Physics

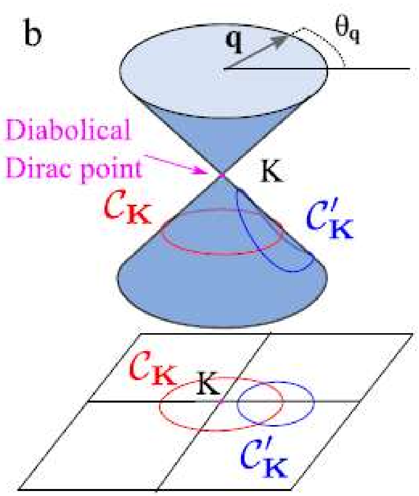
Berry curvature in graphene

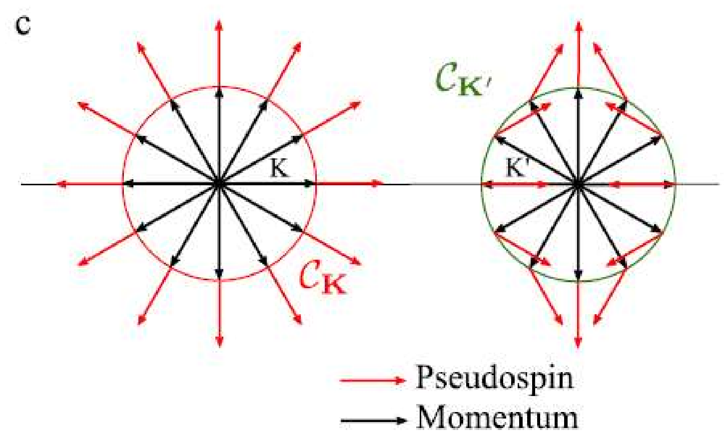
Pseudo-spin textures in k-space:





Trajectories around Dirac point in k-space:





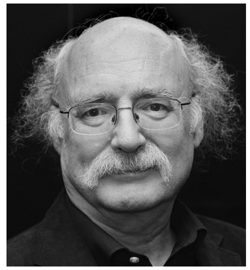
Dirac points are Berry curvature monopoles

$$\Omega(k) = \nabla \times \mathcal{A}$$

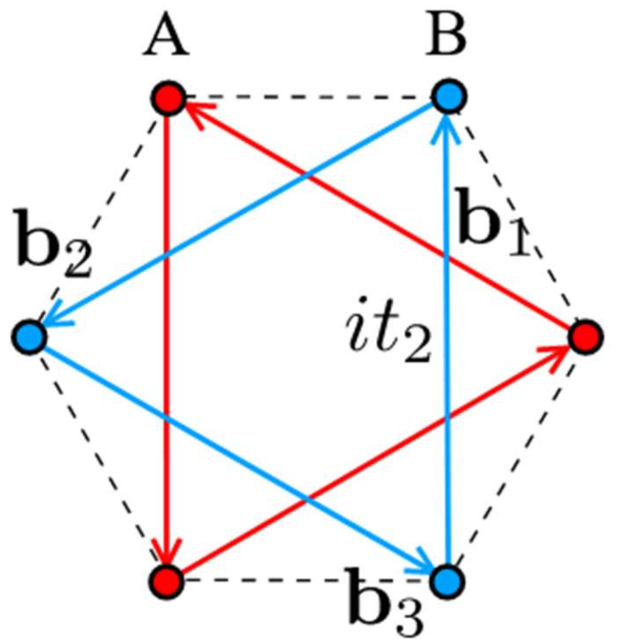
$$C = \frac{1}{2\pi} \oint_{BZ} \Omega dk^2 = \nu$$

Haldane model - Topology

2016



Duncan Haldane



- Next-nearest neighbor hopping induces gap opening
- Berry curvature loops
- Topological Chern bands