# Dirac equation: chirality, Klein-paradox

Theory seminar on the electronic properties of graphene

04.05.09,
Theorie Seminar
Graphen

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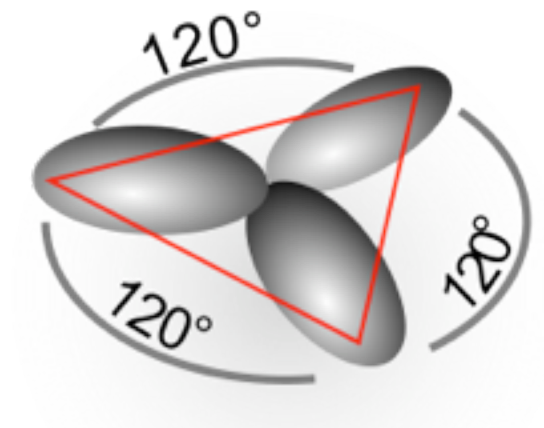
# Outline

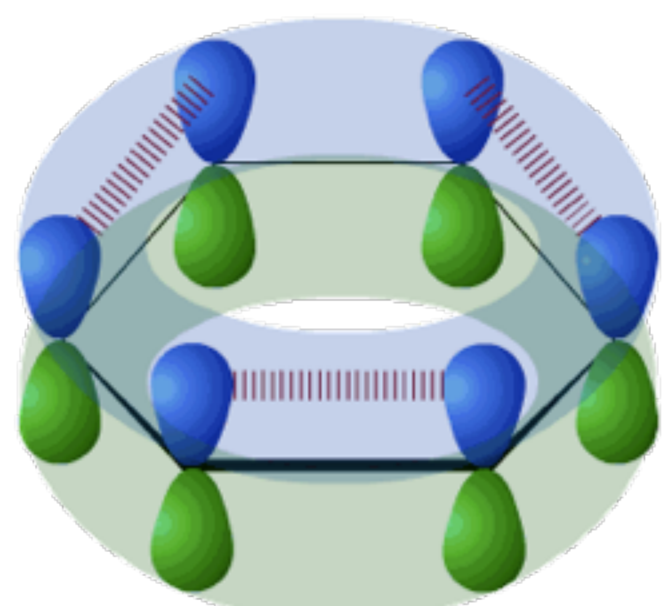
- Review: tight-binding, lattice
- Dirac equation
- Klein-tunneling

# Carbon

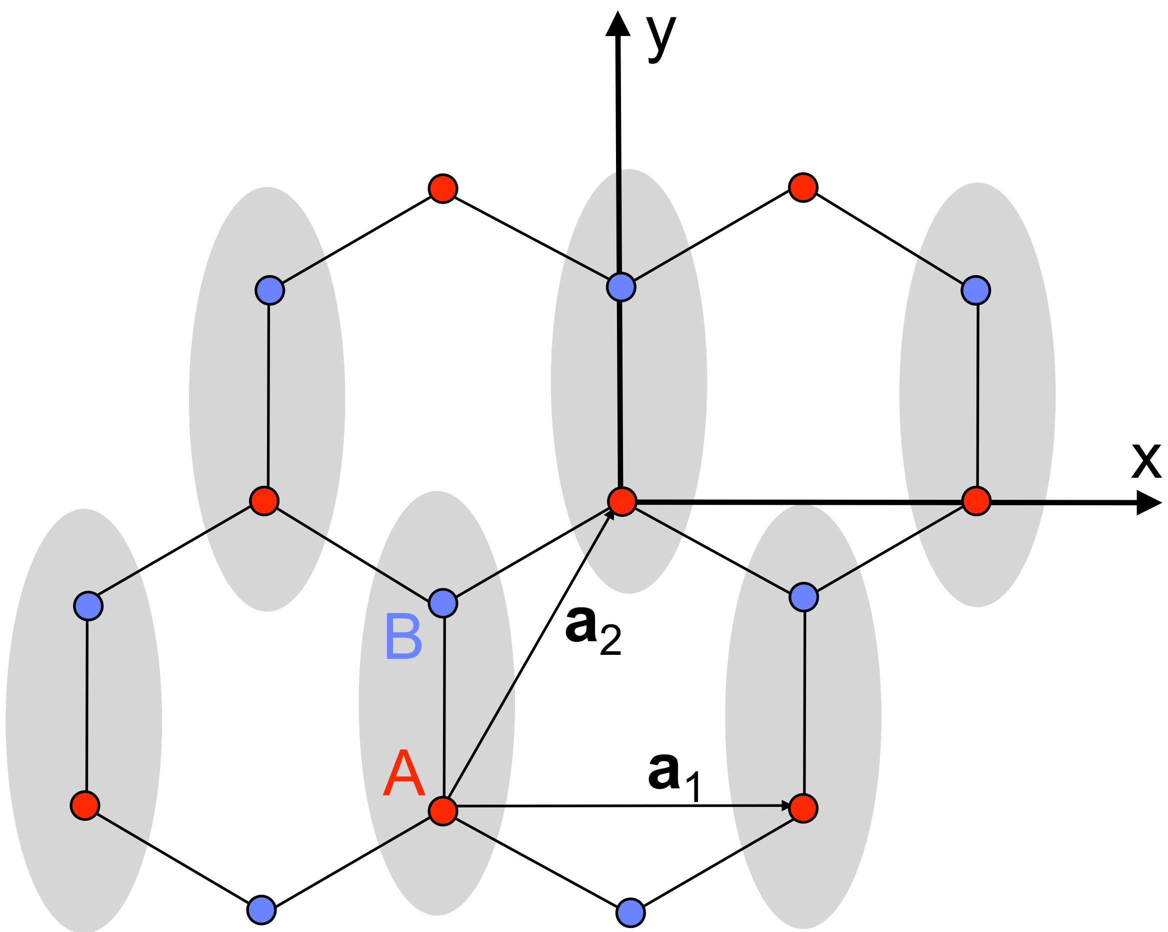
- in graphen atoms $sp^2$-hybridised
  - $\underbrace{1s^2 \; 2s^2 \; 2p_x^1 \; 2p_y^1}_{\text{valence electrons}} \rightarrow 1s^2 \; 2sp^2 \; 2sp^2 \; 2sp^2 \; 2\pi^1$
  - bonding angle 120°

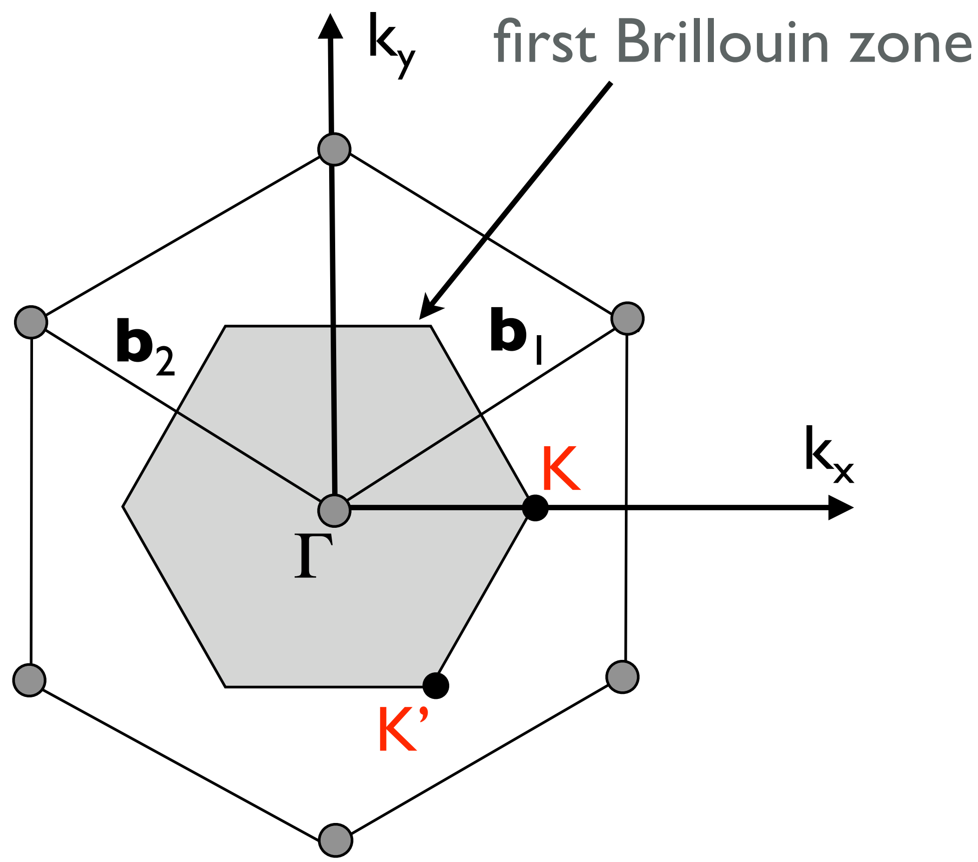



- π-orbitals
  - are weakly bound
  - are delocalised



# Hexagonal Lattice




real lattice

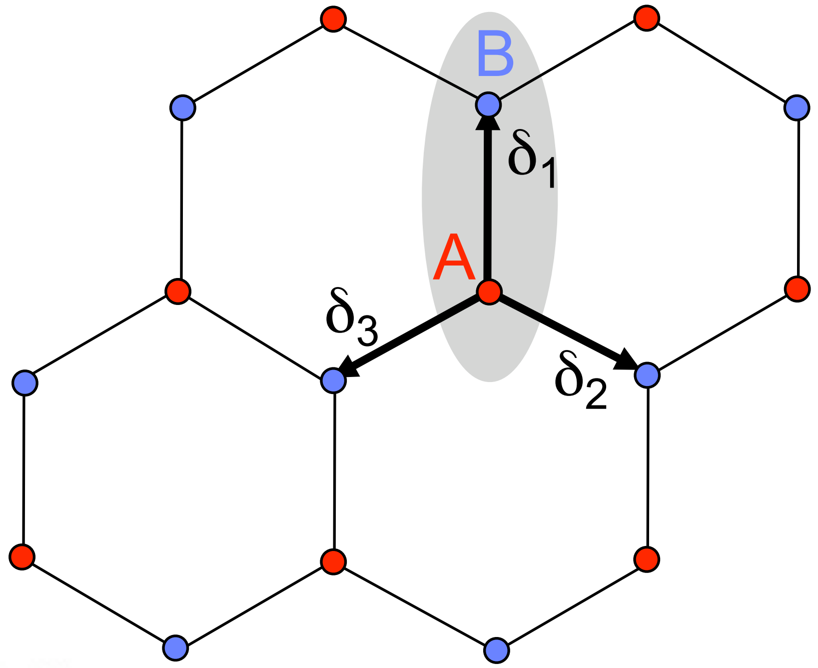
2 atoms (A and B) per unit cell

lattice constant a=|$\mathbf{a}_i$|=0.24 nm

reciprocal lattice

first Brillouin zone

# Tight-Binding Model




- nearest-neighbour hopping

$$H = t\sum_{i,j}\left(a^\dagger_{\vec{R}_i} b_{\vec{R}_i+\vec{\delta}_j} + b^\dagger_{\vec{R}_i+\vec{\delta}_j} a_{\vec{R}_i}\right)$$

- Bloch states

$$|\psi_k\rangle = \sum_i e^{i\vec{k}\cdot\vec{R}_i}\left(\alpha_k a^\dagger_{\vec{R}_i} + \beta_k b^\dagger_{\vec{R}_i+\delta_1}\right)|0\rangle$$

- pseudo-spin representation

$$|\psi_k\rangle = \sum_i e^{i\vec{k}\cdot\vec{R}_i}\underbrace{\begin{pmatrix}\alpha_k \\ \beta_k\end{pmatrix}}_{\psi_k}\cdot\begin{pmatrix}a^\dagger_{\vec{R}_i} \\ b^\dagger_{\vec{R}_i+\delta_1}\end{pmatrix}|0\rangle$$

# Band Structure

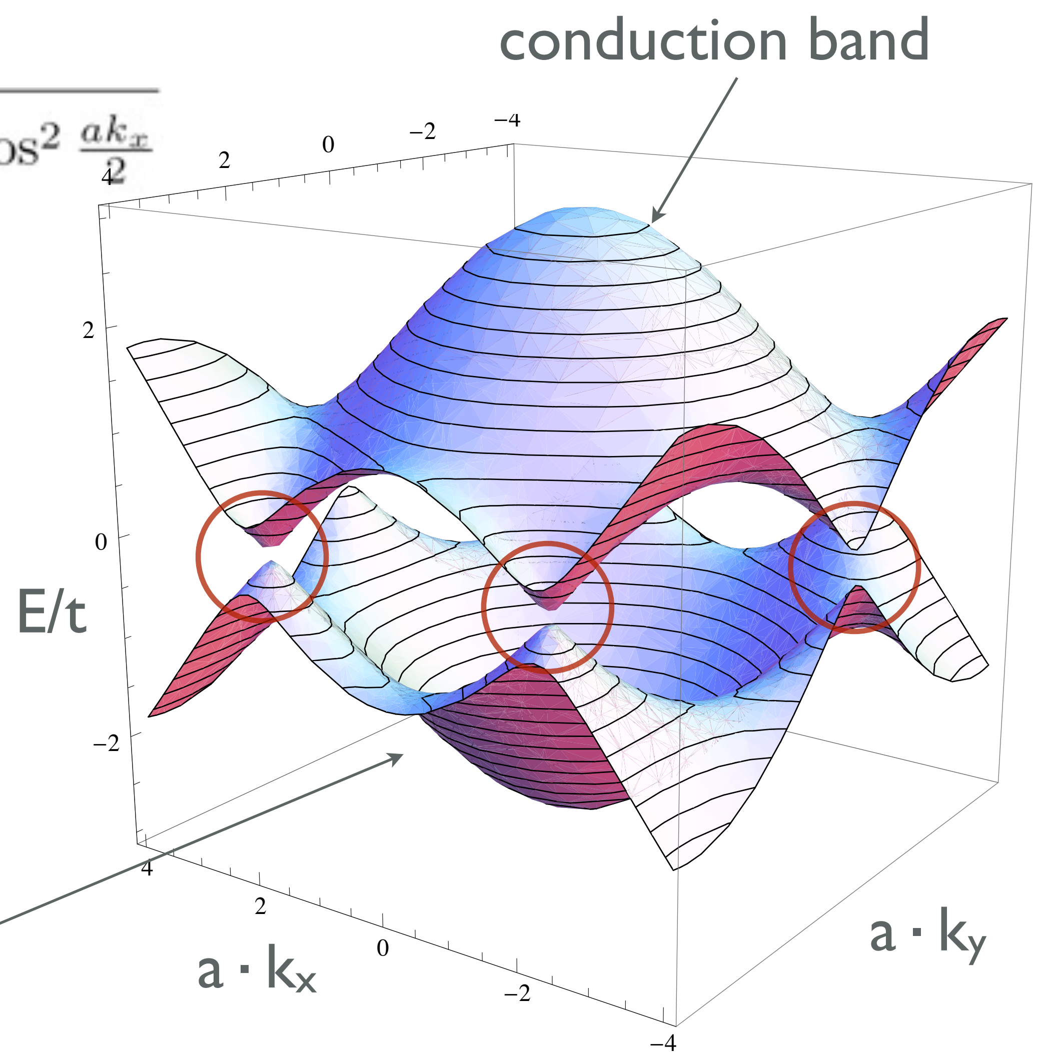
- Schrödinger equation for pseudo-spin $\psi_{\vec{k}} = \begin{pmatrix} \alpha_{\vec{k}} \\ \beta_{\vec{k}} \end{pmatrix}$

$$\begin{pmatrix} 0 & \gamma_{\vec{k}} \\ \gamma^*_{\vec{k}} & 0 \end{pmatrix} \psi_{\vec{k}} = E(\vec{k})\psi_{\vec{k}}$$

$$\gamma_{\vec{k}} = t\left(1 + e^{-i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot(\vec{a}_1-\vec{a}_2)}\right)$$

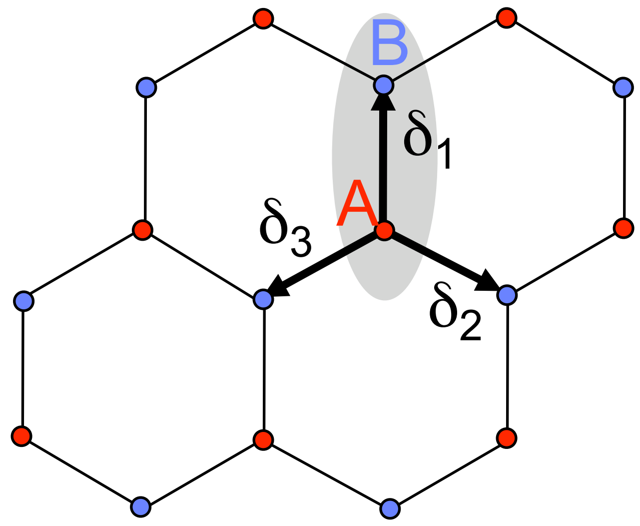
$$E(\vec{k}) = \pm|\gamma_{\vec{k}}| = \pm t\sqrt{1 + 4\cos\frac{\sqrt{3}ak_y}{2}\cos\frac{ak_x}{2} + 4\cos^2\frac{ak_x}{2}}$$

- conduction (+) and valence (-) bands touch at six K points: corners of the 1BZ



# Dirac fermions

- The graphene Hamiltonian is equivalent to the Dirac Hamiltonian!




- Start with tight binding Hamiltonian

$$H = t \sum_{i,j} \left( a^\dagger_{\vec{R}_i} b_{\vec{R}_i + \vec{\delta}_j} + a_{\vec{R}_i} b^\dagger_{\vec{R}_i + \vec{\delta}_j} \right)$$

- Use Fourier transformation of operators

$$a_{\vec{R}_i} = \int \frac{\mathrm{d}^2 k}{(w\pi)^2} e^{i\vec{k}\cdot\vec{R}_n} a(\vec{k})$$

# Dirac Hamiltonian

$$H = t \sum_{i,j} \left( a^\dagger_{\vec{R}_i} b_{\vec{R}_i + \vec{\delta}_j} + a_{\vec{R}_i} b^\dagger_{\vec{R}_i + \vec{\delta}_j} \right)$$

$$a_{\vec{R}_i} = \int \frac{\mathrm{d}^2 k}{(w\pi)^2} e^{i\vec{k}\cdot\vec{R}_n} a(\vec{k})$$

- plug in Fourier transform, write in spinor-form

$$H = t \int \frac{\mathrm{d}^2 k}{(w\pi)^2} \begin{pmatrix} a^\dagger(\vec{k}) \\ b^\dagger(\vec{k}) \end{pmatrix} \begin{pmatrix} 0 & e^{i\vec{k}\cdot\vec{\delta}_1} + e^{i\vec{k}\cdot\vec{\delta}_2} + e^{i\vec{k}\cdot\vec{\delta}_3} \\ e^{-i\vec{k}\cdot\vec{\delta}_1} + e^{-i\vec{k}\cdot\vec{\delta}_2} + e^{-i\vec{k}\cdot\vec{\delta}_3} & 0 \end{pmatrix} \begin{pmatrix} a(\vec{k}) \\ b(\vec{k}) \end{pmatrix}$$

- expand around K, K' , plug in $\delta_1$, $\delta_2$, $\delta_3$

# Dirac Hamiltonian

$$\begin{aligned} H &= \int \frac{\mathrm{d}^2 k}{(w\pi)^2} \psi_1^\dagger(\vec{k}) \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \psi_1(\vec{k}) \\ &\quad + \psi_2^\dagger(\vec{k}) \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \psi_2(\vec{k}) \\ &= \int \frac{\mathrm{d}^2 k}{(w\pi)^2} \psi_1^\dagger(\vec{k})(\vec{\sigma}\cdot\vec{k})\psi_1(\vec{k}) + \psi_2^\dagger(\vec{k})(\vec{\sigma}\cdot\vec{k})\psi_2(\vec{k}) \end{aligned}$$

$$\psi_1(\vec{k}) = t\frac{a\sqrt{3}}{2} e^{-i\frac{1}{3}\pi\sigma_z} \begin{pmatrix} a(\vec{k}-\vec{K}) \\ b(\vec{k}-\vec{K}) \end{pmatrix} \quad \psi_2(\vec{k}) = t\frac{a\sqrt{3}}{2} e^{-i\frac{1}{3}\pi\sigma_z} \sigma_x \begin{pmatrix} a(\vec{k}-\vec{K}') \\ b(\vec{k}-\vec{K}') \end{pmatrix}$$

Note: there are several different sign conventions for K and K'

# Wannier theorem

- Effective mass theory let's us treat particles in a periodic potential like free particles with an effective mass.

- Energy is periodic in k-space, so expand

$$E_n(\vec{k}) = \sum_m F_{nm} e^{i\vec{k}\cdot\vec{R}_m}$$

- Let operator $E_n(-i\nabla)$ act on a Bloch function

$$E_n(-i\nabla)\psi_n(\vec{k},\vec{r}) = \sum_m F_{nm}\psi_n(\vec{k},\vec{r}+\vec{R}_m)$$

- With Bloch's theorem

$$E_n(-i\nabla)\psi_n(\vec{k},\vec{r}) = E_n(\vec{k})\psi_n(\vec{k},\vec{r})$$

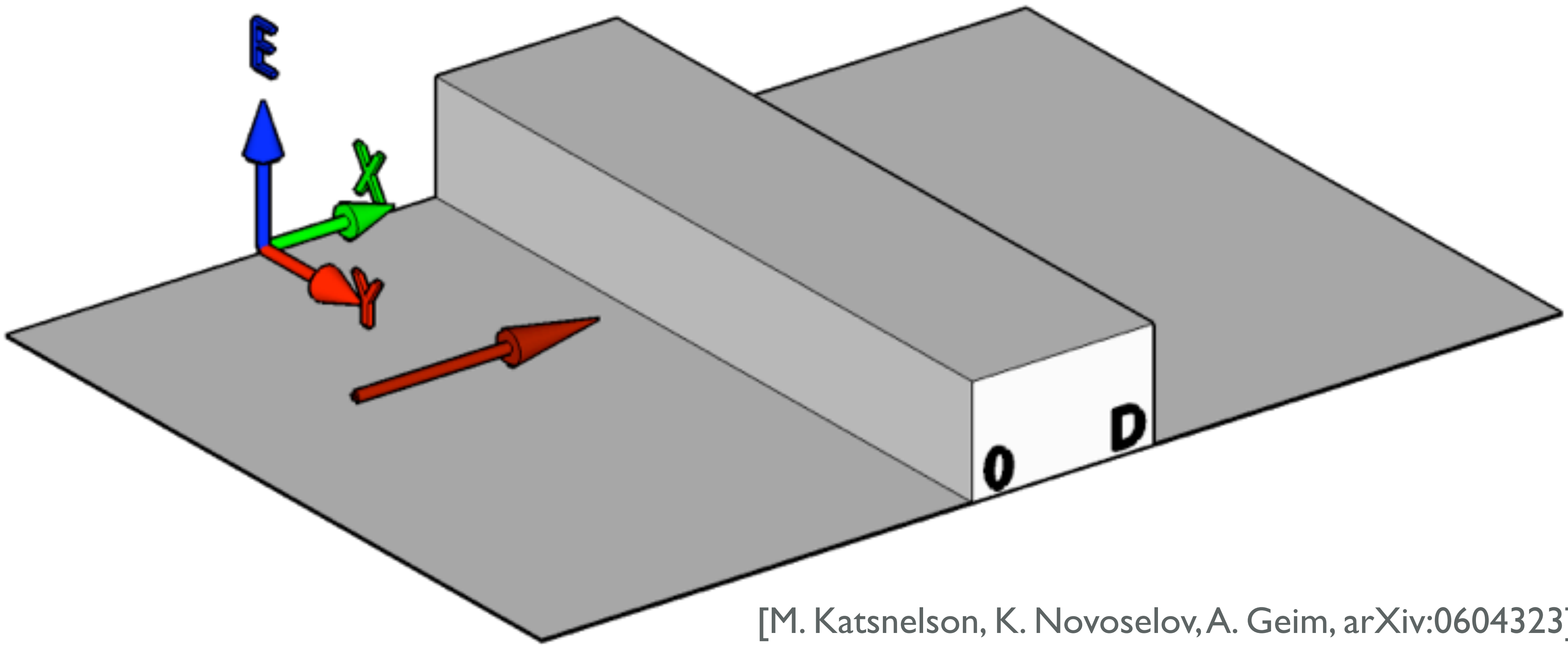
# Dirac equation

- With the Wannier theorem we obtain (in first quantised Landau gauge) a Dirac-like equation for the two spinors at K and K'

$$-i\hbar v_{\mathrm{F}} \vec{\sigma} \nabla \psi_i(\vec{r}) = E \psi_i(\vec{r})$$

- instead of c we have $v_F$ (≈c/300)

# Klein-paradoxon




[M. Katsnelson, K. Novoselov, A. Geim, arXiv:0604323]

- barrier height $V_0>0$
- barrier thickness D
- what's the transmission coefficient?

# Solving the eigensystem

- (free) graphene Hamiltonian

$$H_0\psi = -i\hbar v_{\rm F}\sigma^i\partial_i\psi = E\psi$$

- eigenenergies

$$E = s\hbar v_{\rm F}|\mathbf{k}|, \quad s = \pm 1$$ electron-like states, hole-like states

- eingenvectors

$$\psi(x,y) = \begin{pmatrix}\psi_1(x,y)\\ \psi_2(x,y)\end{pmatrix} = e^{ik_x x}e^{ik_y y}\begin{pmatrix}1\\ se^{i\phi}\end{pmatrix}$$

with $k_x = |\mathbf{k}|\cos\phi, \quad k_y = |\mathbf{k}|\sin\phi$

# Pseudo-spin

- How's the pseudo-spin orientated?

$$\langle\psi|\,\sigma_x\,|\psi\rangle = s\cos\phi = s\frac{k_x}{|\mathbf{k}|}$$

$$\langle\psi|\,\sigma_y\,|\psi\rangle = s\sin\phi = s\frac{k_y}{|\mathbf{k}|}$$

$$\Rightarrow \langle\psi|\,\sigma\,|\psi\rangle = s\frac{\mathbf{k}}{|\mathbf{k}|}$$

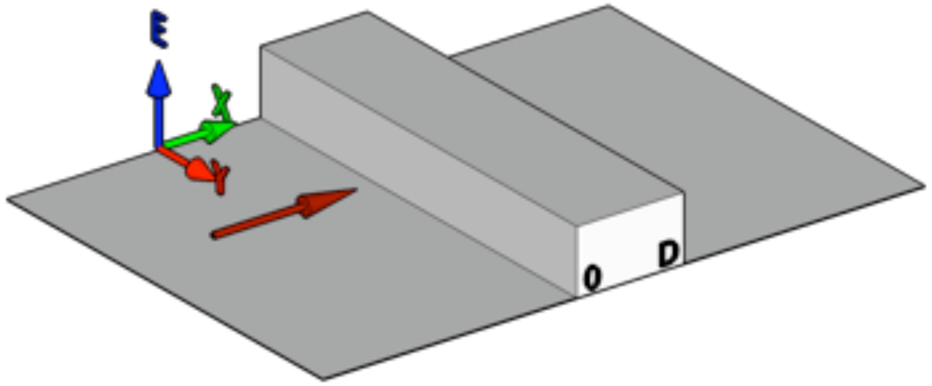
- just like for real phonons

# Hamiltonian

- The hamiltonian consists of two parts

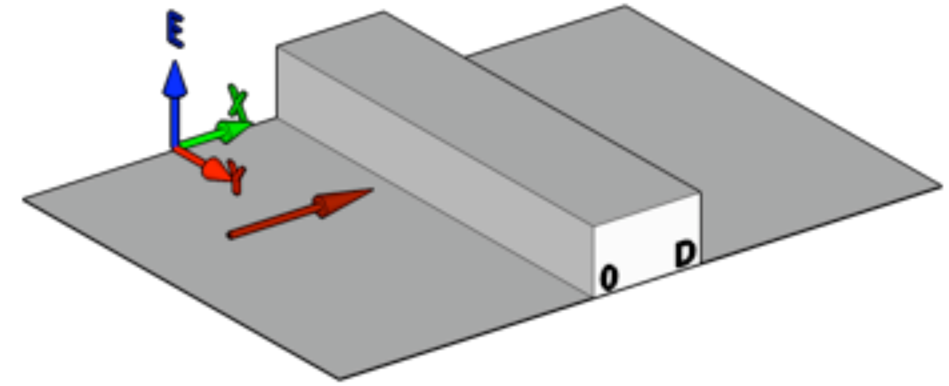
$$H_0 = -i\hbar v_{\mathrm{F}} \sigma^i \partial_i$$

$$V(x,y) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < D \\ 0 & x > D \end{cases}$$




- Note: V(x,y) does not couple to the pseudo-spin

# Ansatz




- Choose the following ansatz

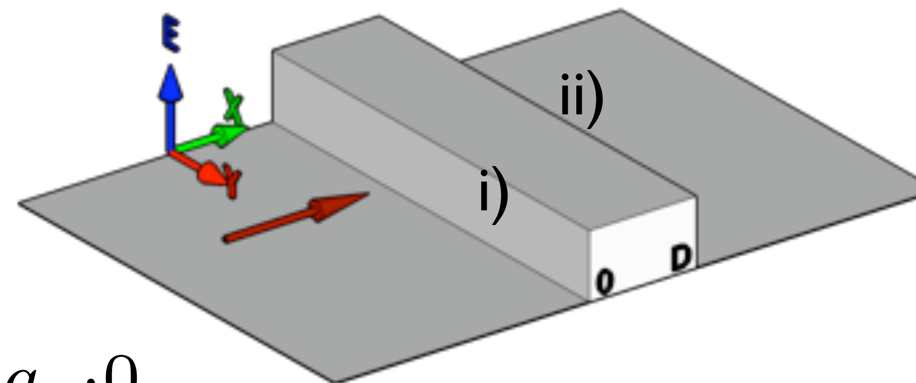
$$\psi_1(x,y) = \begin{cases} (e^{ik_x} + re^{-ik_x})e^{ik_y y} & x < 0 \\ (ae^{iq_x x} + be^{-iq_x x})e^{ik_y y} & 0 < x < D \\ te^{ik_x x + ik_y y} & x > D \end{cases}$$

$$\psi_2(x,y) = \begin{cases} s(e^{ik_x + i\phi} - re^{-ik_x - i\phi})e^{ik_y y} & x < 0 \\ s'(ae^{iq_x x + i\theta} - be^{-iq_x x - i\theta})e^{ik_y y} & 0 < x < D \\ ste^{ik_x x + ik_y y + i\phi} & x > D \end{cases}$$

- with $q_x = \sqrt{[(E-V)^2/\hbar^2 v_{\mathrm{F}}^2] - k_y^2}$ $\qquad \tan\theta = k_y/q_x$

$$s = \mathrm{sgn}(E) \qquad s' = \mathrm{sgn}(E-V)$$

# Requirements for continuity




i) $x < 0 \;\rightarrow\; 0 < x < D$

$$e^{ik_x \cdot 0} + re^{-ik_x \cdot 0} \stackrel{!}{=} ae^{iq_x \cdot 0} + be^{-iq_x \cdot 0}$$

$$s(e^{ik_x \cdot 0 + i\phi} - re^{-ik_x \cdot 0 - i\phi}) \stackrel{!}{=} s'(ae^{iq_x \cdot 0 + i\theta} - be^{-iq_x \cdot 0 + i\theta})$$

ii) $0 < x < D \;\rightarrow\; x > D$

$$ae^{iq_x D} + be^{-iq_x D} \stackrel{!}{=} te^{ik_x D}$$

$$s'(ae^{iq_x D + i\theta} - be^{-iq_x D - i\theta}) \stackrel{!}{=} ste^{ik_x D + i\phi}$$

- we have four unknowns $a, b, t, r$

# Side note

- We have

  i) four unknown variables

  ii) four equations from the continuity relations (matching of wave functions)

- No need to match the derivatives!
- Reason: Dirac(-like) equation: first order
  Schrödinger equation: second order
- Please refer to [Cohen-Tannoudji I, 1.12.1]

# Solving the equations

- set of inhomogeneous linear equations

$$e^{ik_x\cdot 0} + \underline{r}e^{-ik_x\cdot 0} \stackrel{!}{=} \underline{a}e^{iq_x\cdot 0} + \underline{b}e^{-iq_x\cdot 0}$$

$$s(e^{ik_x\cdot 0+i\phi} - \underline{r}e^{-ik_x\cdot 0-i\phi}) \stackrel{!}{=} s'(\underline{a}e^{iq_x\cdot 0+i\theta} - \underline{b}e^{-iq_x\cdot 0+i\theta})$$

$$\underline{a}e^{iq_xD} + \underline{b}e^{-iq_xD} \stackrel{!}{=} \underline{t}e^{ik_xD}$$

$$s'(\underline{a}e^{iq_xD+i\theta} - \underline{b}e^{-iq_xD-i\theta}) \stackrel{!}{=} s\underline{t}e^{ik_xD+i\phi}$$

- solution

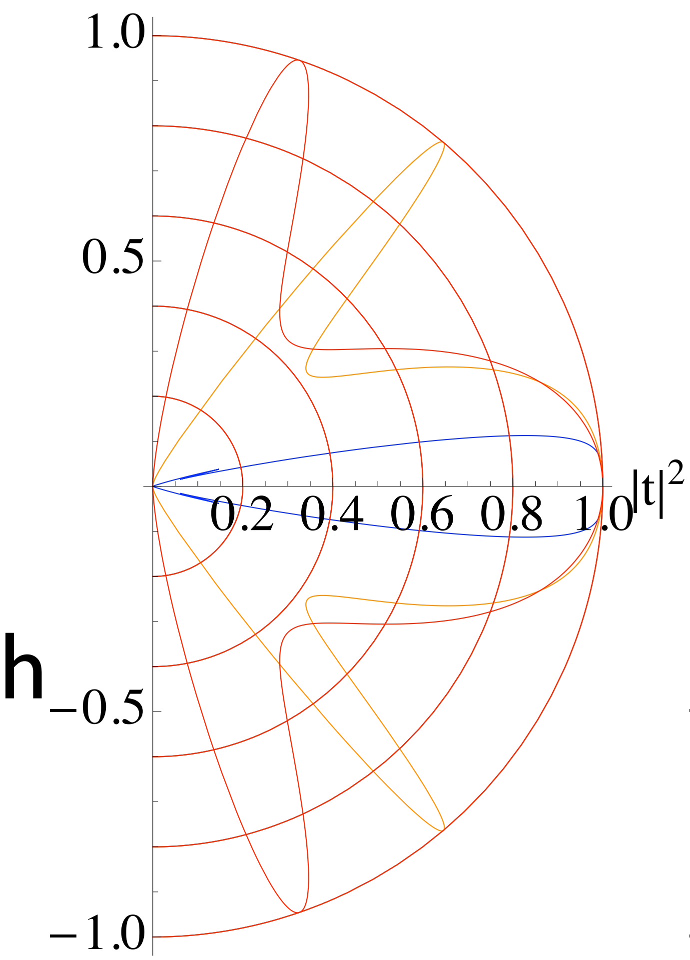
$$r = 2e^{i\phi}\sin(q_xD)\frac{\sin\phi - ss'\sin\theta}{ss'[e^{-iq_xD}\cos(\phi+\theta) + e^{iq_xD}\cos(\phi-\theta)] - 2i\sin(q_xD)}$$

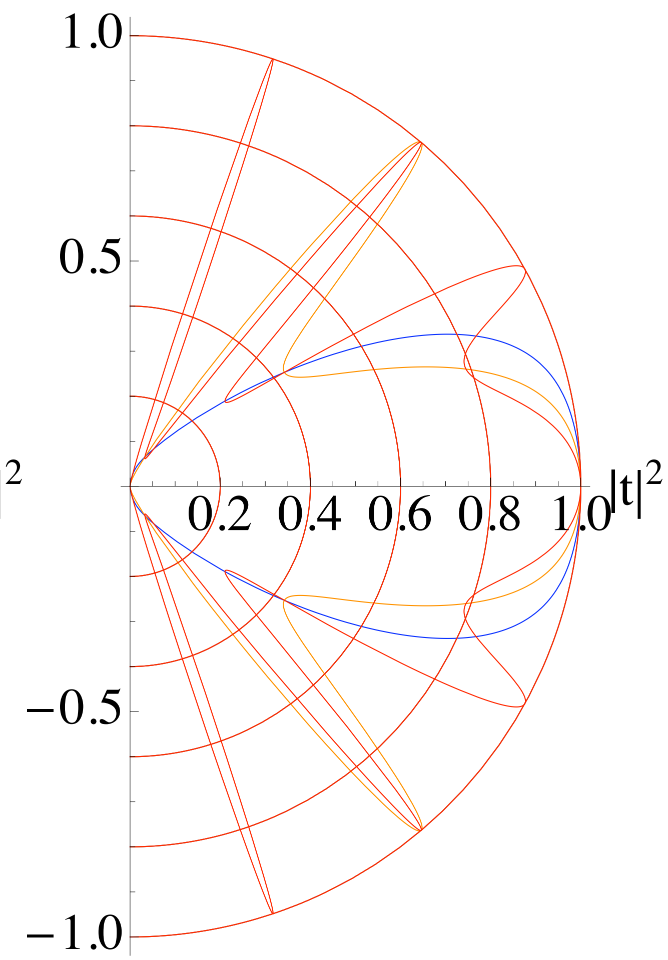
# Result

- transmission coefficient

  $|t|^2 = 1 - |r|^2$

- full transmission for φ=0
  - independent of barrier width
  - for arbitrarily high barrier




E=80meV
v=c/300

D=100nm
V=100meV
V=200meV
V=300meV

V=200meV
V=50nm
V=100nm
V=200nm

# Conclusion

- for massless particles: $v_F$ indepenent of E and (pseudo-)helicity is conserved
- carriers cannot backscatter
- transmition propability

$$T(p_y) = e^{-|p_y|\frac{\pi d_{\min}}{2\hbar}}$$