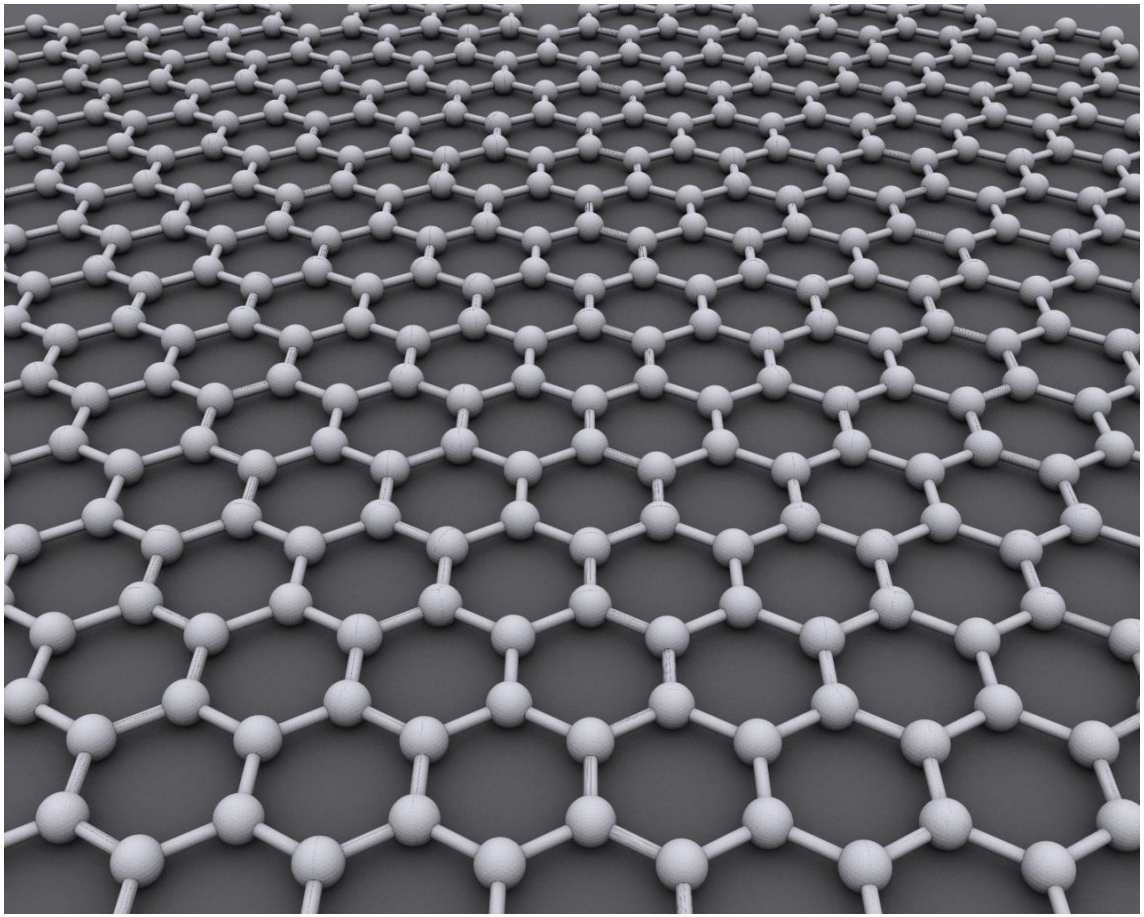
**Triangular lattice**

**Graphene**

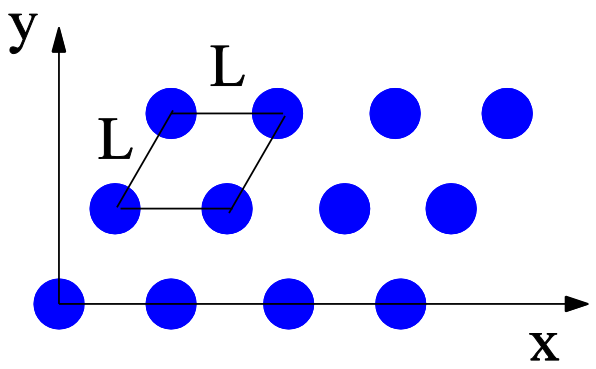
Graphene is an atomic-scale honeycomb lattice carbon atoms monolayer.
Conduction via $\pi$-orbitals of carbon. Tight binding.



# Artificial Graphene

## Weak coupling

Consider a 2D electron gas in a potential U(r) with hexagonal (triangular) symmetry and spacing L.



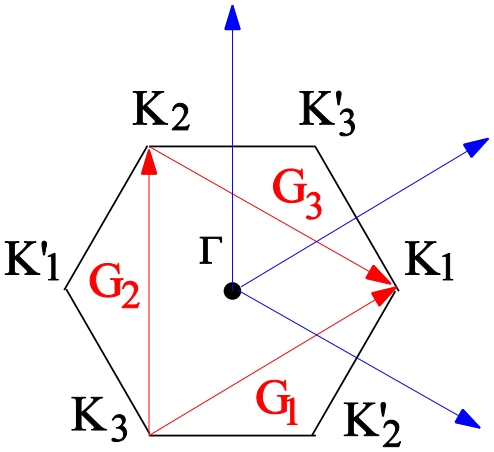

$$H = \frac{p^2}{2m} + U(r)$$

The lattice translation vectors are

$\mathbf{L}_1$ = (L, 0)

$\mathbf{L}_2$ = (L/2,√3L/2)

There are two independent reciprocal lattice vectors in the Brillouin zone

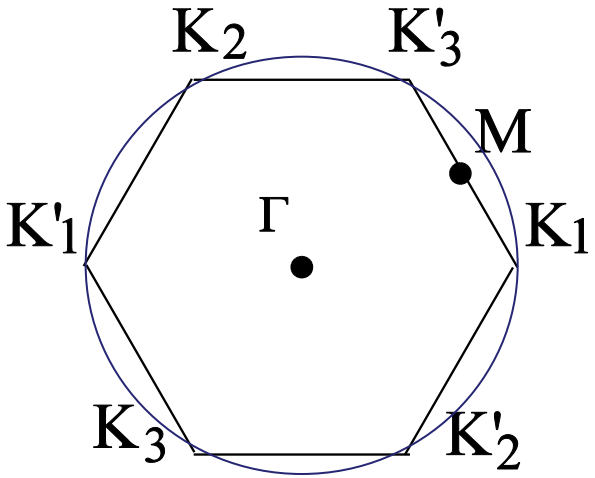



$$G_1 = \frac{2\pi}{3L}(3,\sqrt{3}), \quad G_2 = \frac{2\pi}{3L}(0,2\sqrt{3}), \quad G_3 = G_1 - G_2$$

The points $K_1$, $K_2$, $K_3$ are connected by vectors $G_i$
$K'_i$ are obtained from the $K_i$ by reflection.

$$\vec{G}_1 \cdot \vec{L}_1 = 2\pi$$
$$\vec{G}_1 \cdot \vec{L}_2 = 2\pi$$
$$\vec{G}_1 \cdot \vec{L}_1 = 0$$
$$\vec{G}_2 \cdot \vec{L}_2 = 2\pi$$

$$\vec{K}_1 = \frac{4\pi}{3L}(1,0)$$
$$\vec{K}_2 = \frac{4\pi}{3L}\left(-1/2, \sqrt{3}/2\right)$$
$$\vec{K}_3 = \frac{4\pi}{3L}\left(-1/2, -\sqrt{3}/2\right)$$




Below I measure energy in units of the bandwidth:

$$E_0 = \frac{K^2}{2m} = \frac{(4\pi/3L)^2}{2m}$$

We assume a periodic potential with a single Fourier component

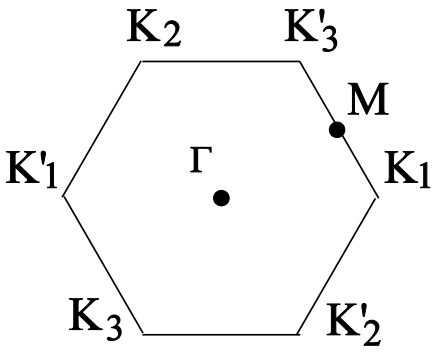
$$U(r) = 2W\left[\cos\left(G_1 \cdot r\right) + \cos\left(G_2 \cdot r\right) + \cos\left(G_3 \cdot r\right)\right]$$

This potential has nonzero matrix elements only between states |k> and $|k \pm G_i>$ with matrix elements given by W.

# Perturbation Theory. Practically works up to $\mathcal{W} = W/E_0 = 2$



A state close to the Dirac point, q ≪ 1, is described by degenerate perturbation theory as




$$\psi_{\mathbf{q}} = c_1 |1> + c_2 |2> + c_3 |3>$$

$$|j> = e^{i(\mathbf{K}_j + \mathbf{q})\cdot\mathbf{r}}$$

Kinetic energy:

$$\frac{p^2}{2m} \to \frac{(\mathbf{K}_i + \mathbf{q})^2}{2\mathbf{m}} \delta_{ik} \approx \left( E_0 + \frac{\mathbf{K}_i \cdot \mathbf{q}}{\mathbf{m}} \right) \delta_{ik}$$

Potential energy:

$$U(r) \to W \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Kinetic energy is a weak perturbation on the potential energy.

# Diagonalize potential energy

$$|U-\varepsilon| = \begin{vmatrix} -\varepsilon & W & W \\ W & -\varepsilon & W \\ W & W & -\varepsilon \end{vmatrix} = -(\varepsilon+W)^2(\varepsilon-2W)$$

The eigen-energies of the U-matrix are (-W, -W, 2W).

## There is the double degenerate subspace!!!!

In order to project in the double degenerate subspace of U we define:

$$|a\rangle = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \qquad |b\rangle = \begin{pmatrix} \sqrt{2/3} \\ -1/\sqrt{6} \\ -1/\sqrt{6} \end{pmatrix}$$

Projecting the kinetic energy to this basis and shifting the zero energy level to $E_0$ one finds:

$$<a|H|a>=\frac{(\mathbf{K}_2+\mathbf{K}_3)\cdot\mathbf{q}}{2m}=-vq_x$$

$$<b|H|b>=\frac{(4\mathbf{K}_1+\mathbf{K}_2+\mathbf{K}_3)\cdot\mathbf{q}}{2m}=+vq_x$$

$$<b|H|a>=\frac{(\mathbf{K}_3-\mathbf{K}_2)\cdot\mathbf{q}}{2\sqrt{3}m}=-vq_y$$

$$v=\frac{K}{2m}=\frac{2\pi}{3Lm}$$

is the Fermi-Dirac velocity

$$\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Hence, in the Pauli matrix (pseudo-spin) representation the effective low energy Hamiltonian reads:

$$H=v(-\sigma_z q_x-\sigma_x q_y)$$

One can perform the unitary transformation $H \rightarrow T^{\dagger} H T$ , where T represents two subsequent π/2 rotations around x- and y-axes in the pseudo-spin space:

$$T^{+}\sigma_x T = -\sigma_y$$
$$T^{+}\sigma_y T = +\sigma_z$$
$$T^{+}\sigma_z T = -\sigma_x$$

$$T = \frac{1}{2}\begin{pmatrix} 1+i & -1-i \\ -1+i & -1+i \end{pmatrix}$$

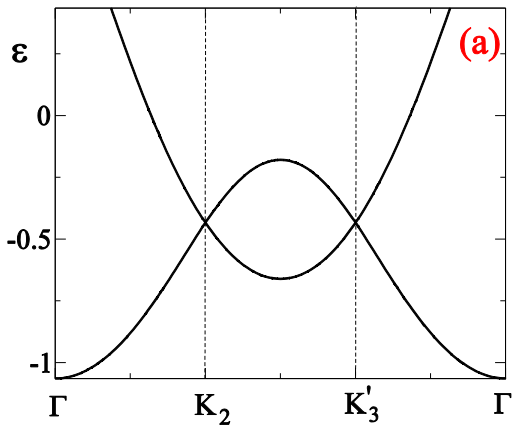
This transforms the Hamiltonian to the conventional form of a 2D Dirac Hamiltonian

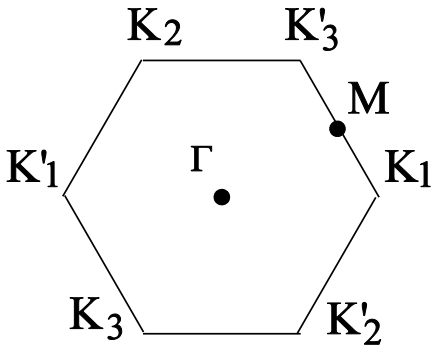
$$H = v\boldsymbol{\sigma}\cdot\mathbf{q}$$

However, in what follows we will use the “blue” form as it is slightly more convenient for the study of the edge states.

$$H = v(-\sigma_z q_x - \sigma_x q_y)$$

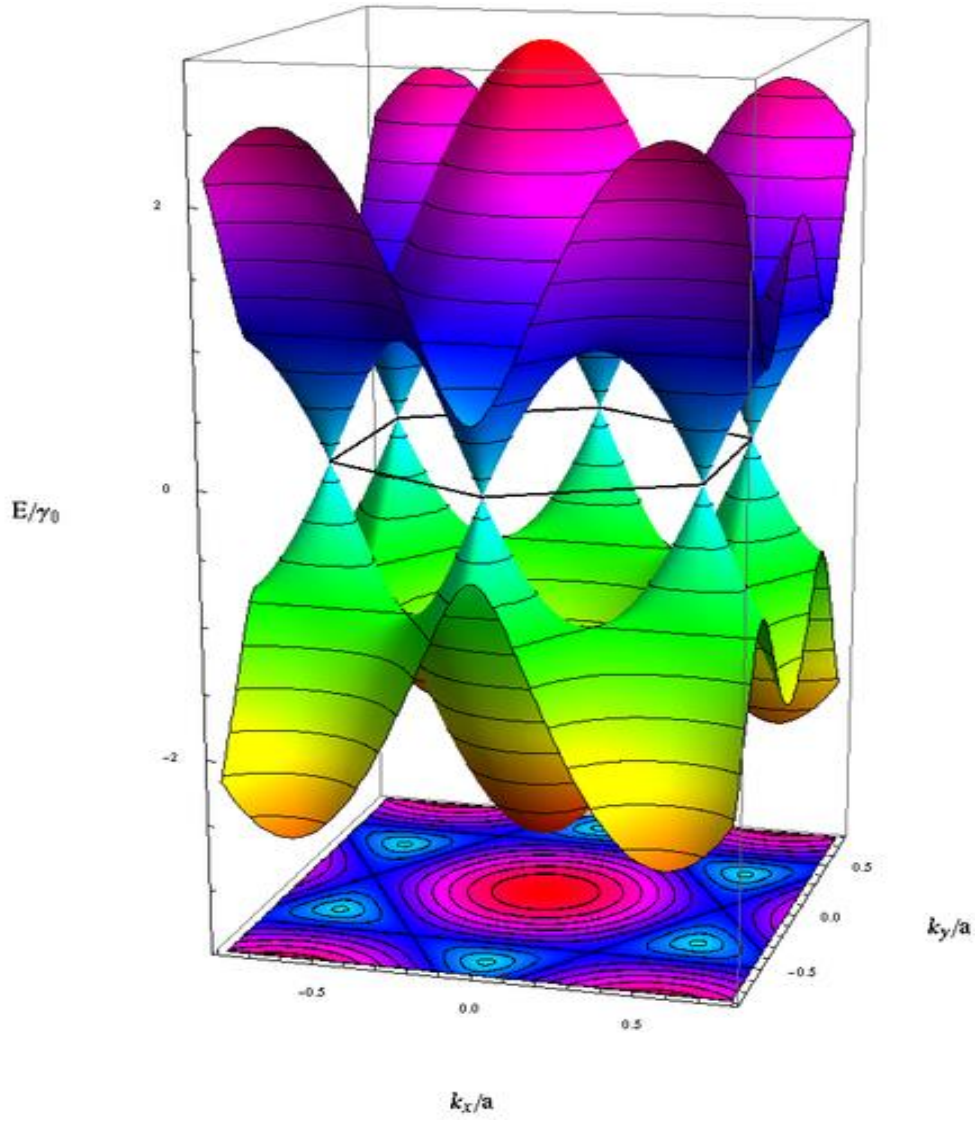
Numerical diagonalization of the Hamiltonian is straightforward.

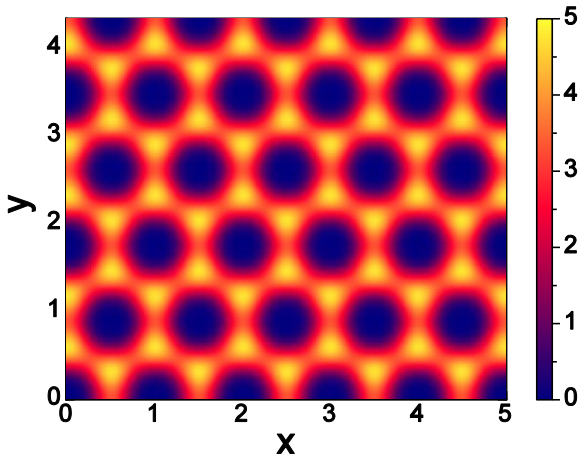



The hole dispersion along a particular contour in the BZ, $\mathcal{W}=W/E_0=1$

Two Dirac points of opposite parity.


E/γ0
2
0
-2
-0.5
0.0
0.5
kx/a
0.5
0.0
-0.5
ky/a




Map of the total charge density (in units $1/L^2$) at the chemical potential tuned to the Dirac point.
The average hole density is $\langle n \rangle = 8/3L^2$.
At L = 50nm the average density is $1.1 \times 10^{11} cm^{-2}$.

Even when the potential is strong, namely $w = W/E_0 = 1-2$, the dispersion is rather close to the result obtained by perturbation theory. The charge density plot is fully connected with empty spots at positions of the potential maximums. So, in clear contrast to natural graphene at $w < 2$ the system is much closer to the nearly free electron regime than to the tight-binding one.

# Chiral edge states in toplogical insulator

# Topological insulator

Let us switch on the spin orbit interaction $\mathbf{H_{so}}$.
Whatever is the microscopic mechanism of the interaction the interaction must satisfy the following conditions

1)The interaction depends on spin s. This is true spin, not pseudospin.
2)The interaction is time reversal invariant.
3) The intercation is space inversion invariant

Therefore matrix element of $H_{so}$ between two plane wave must be of the following form

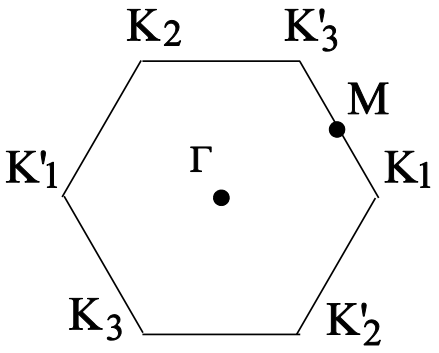
$$<\mathbf{p}_2|H_{so}|\mathbf{p}_1> \;\propto\; i([\mathbf{p}_1\times\mathbf{p}_2]\cdot\mathbf{s})$$

An additional condition follows from the Bloch's theorem.
Since the spin-orbit interaction has period of the lattice the matrix element of $H_{so}$ is nonzero only if

$$\mathbf{p}_2-\mathbf{p}_1=\pm\mathbf{G}_i$$

Near the Dirac cone

$$<2|H_{so}|1> \propto i[\mathbf{K}_1 \times \mathbf{K}_2]\cdot \mathbf{s} \propto i s_z$$




Hence the effective 3x3 spin-orbit Hamiltonian reads

$$H_{so} \propto \begin{pmatrix} 0 & i & -i \\ -i & 0 & i \\ i & -i & 0 \end{pmatrix}$$

Projecting this to the degenerate pseudospin states |a> and |b> we find

$$H_{so} \rightarrow -2\eta s_z \sigma_y$$

Total Hamiltonian

$$H = v(-\sigma_z q_x - \sigma_x q_y) - 2\eta s_z \sigma_y$$

This is the K-Dirac cone, for the K'-Dirac cone we have to replace v→-v (opposite parity).

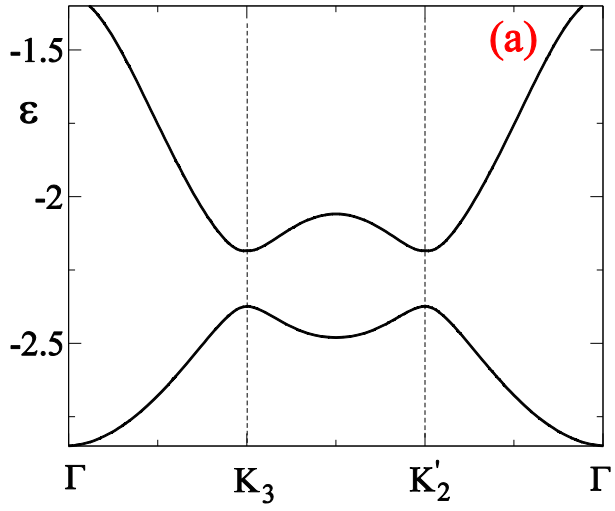
One can perform the unitary transformation H → T †HT to transform to the conventional form

$$H = v\boldsymbol{\sigma}\cdot\mathbf{q}\text{-}2\eta s_z \sigma_z$$

The energy is

$$\varepsilon^2 = v^2 q^2 + (2\eta s_z)^2$$

$$\varepsilon = \pm\sqrt{v^2 q^2 + \eta^2}$$



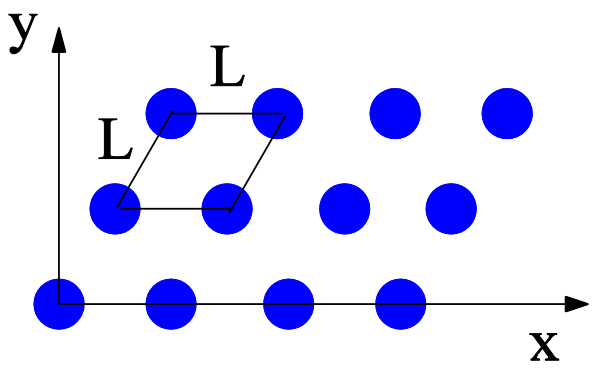

Due to η the gap is opened at Dirac points

If chemical potential is inside the gap this is insulator
What is topological about this?
Why this is different from usual band insulator?

# Topological chiral edge states

Lateral confinement: let us limit the 2D crystal by the infinite wall potential

$$U_{conf} = \begin{cases} 0 & \text{if} \quad y > y_0 \\ \infty & \text{if} \quad y < y_0 \end{cases}$$




The envelope wave function of the edge state at $y > y_0$

$$\psi = A\begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{iq_x x} e^{-\lambda y}$$

Solution of Dirac Eq. $H\psi=\varepsilon\psi$ gives

$$H = v(-\sigma_z q_x - \sigma_x q_y) - 2\eta s_z \sigma_y$$

$$\varepsilon = \pm\sqrt{\eta^2 + v^2 q_x^2 - v^2\lambda^2}$$

$$\alpha = 1$$

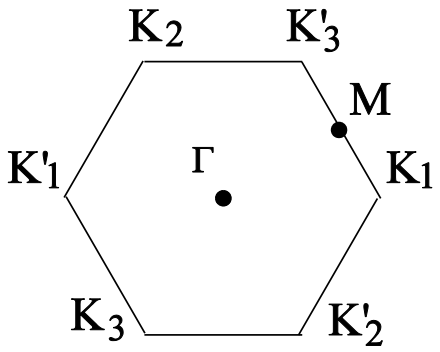
$$\beta = i\frac{v\lambda + 2\eta s_z}{vq_x - \varepsilon}$$

In the explicit coordinate form this is

$$\psi \propto e^{iq_x x} e^{-\lambda y} \{\alpha \,|\, a> + \beta \,|\, b>\}$$

$$|\, a> = \frac{1}{\sqrt{2}} \left( e^{iK_2 \cdot r} - e^{iK_3 \cdot r} \right)$$

$$|\, b> = \frac{1}{\sqrt{6}} \left( 2e^{iK_1 \cdot r} - e^{iK_2 \cdot r} - e^{iK_3 \cdot r} \right)$$




Let us tune the position of the wall

$$|\, a> \;\propto \left( e^{iK_2 \cdot r} - e^{iK_3 \cdot r} \right) \propto \sin\left( \frac{2\pi}{\sqrt{3}L} y_0 \right) \to 0$$

$$\frac{2\pi}{\sqrt{3}L} y_0 = \pi n, \quad \text{n is integer}$$

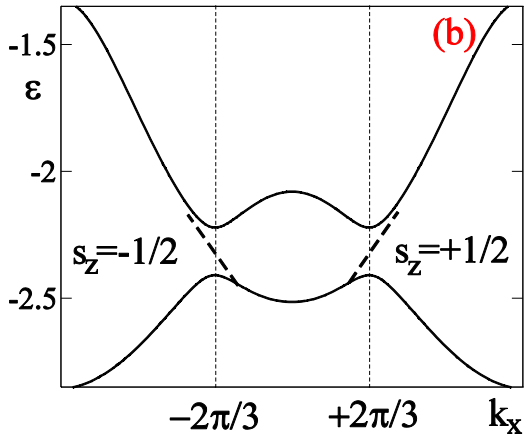
Hence, to satisfy $\psi(x,y_0)=0$ we need only to impose

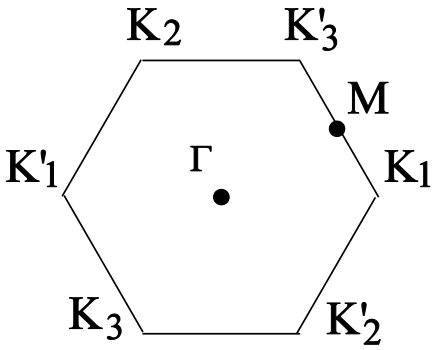
$$\beta = i \frac{v\lambda + 2\eta s_z}{v q_x - \varepsilon} = 0$$

$$s_z = -1/2, \;\; \lambda = \eta/v, \;\; \varepsilon = -vq_x$$

For the opposite parity Dirac cone the edge solution has different chirality

$$s_z = +1/2,\ \lambda = \eta/\mathrm{v},\ \varepsilon = +\mathrm{v}q_x$$




**Topological protection:**

The edge states are found at a special position of the confining wall. An explicit calculation at a different wall position/shape is more involved since the calculation must include admixture of high momentum states to the wave function. However, it is obvious that a variation of the wall position/shape does not influence the edge states since they are topologically protected.

The edge states support the spin polarized  current at the edge of system.