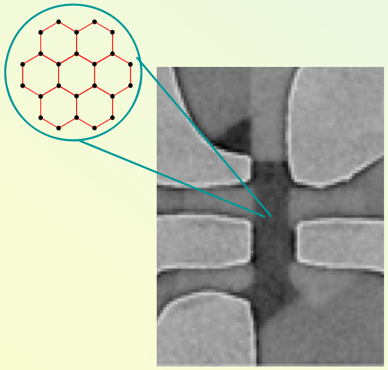
Electronic properties of graphene, from ‘high’ to ‘low’ energies.

Vladimir Falko, Lancaster University

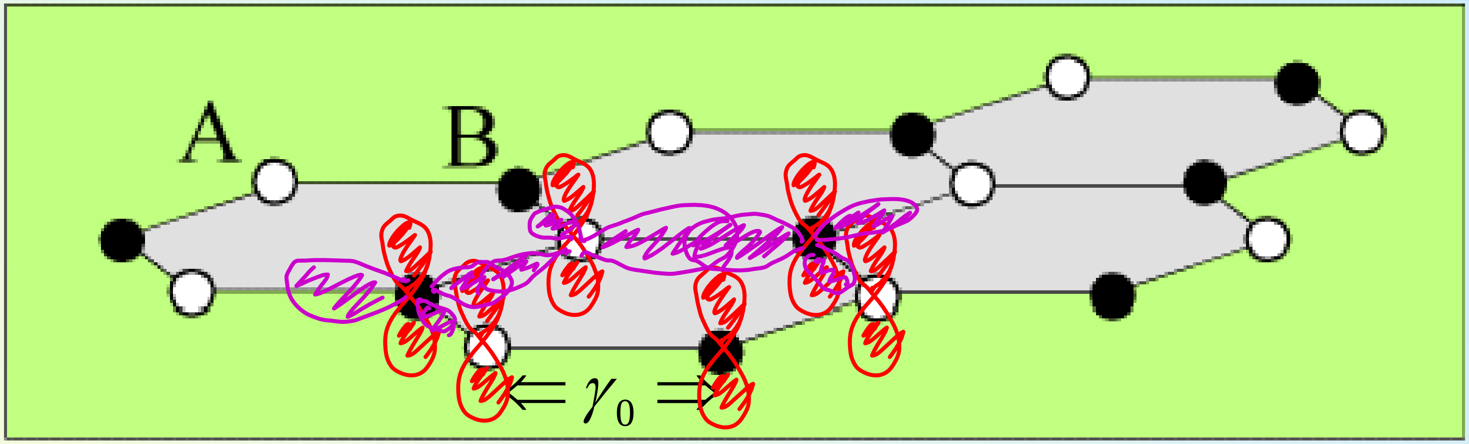


Graphene for beginners: tight-binding model.
Berry phase π electrons in monolayers.
Trigonal warping. Stretched graphene.
PN junction in graphene.

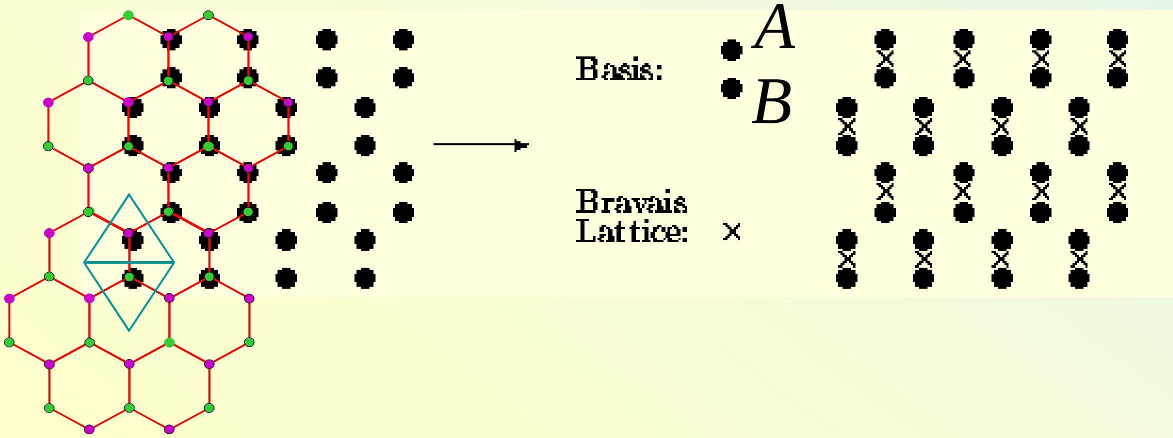
Berry phase 2π electrons in bilayer graphene.
Landau levels & QHE. Interlayer asymmetry gap.
Lifshitz transition and magnetic breakdown in BLG. Stretched BLG.
Renormalisation group theory for interaction and spontaneous symmetry breaking in BLG.

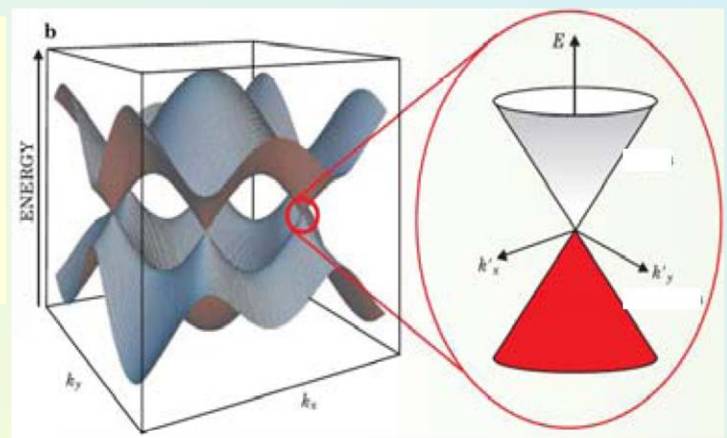
4 electrons in the outer s-p shell of carbon

sp^2 hybridisation forms strong directed bonds which determine a honeycomb lattice structure.



$P^z(\pi)$ orbitals determine conduction properties of graphite





Graphene: gapless semiconductor

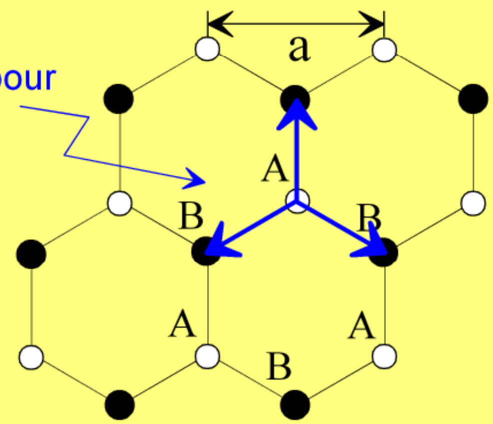
Wallace, Phys. Rev. 71, 622 (1947)
Slonczewski, Weiss, Phys. Rev. 109, 272 (1958)

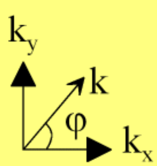
Transfer integral on a hexagonal lattice

$$\mathcal{H}_{AB} = \langle \Phi_A | H | \Phi_B \rangle$$

$$\mathcal{H}_{AB} = \frac{1}{N} \sum_{\mathbf{R}_A}^{N} \sum_{\mathbf{R}_B}^{N} e^{i\mathbf{k}.(\mathbf{R}_B - \mathbf{R}_A)} \underbrace{\langle \phi_A(\mathbf{r}-\mathbf{R}_A) | H | \phi_B(\mathbf{r}-\mathbf{R}_B) \rangle}_{\gamma_0}$$

sum over 3 nearest neighbour positions





$$\mathcal{H}_{AB} = \gamma_0 f(\mathbf{k}) \; ; \quad \mathcal{H}_{BA} = \gamma_0 f^*(\mathbf{k})$$

$$f(\mathbf{k}) = e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}} \cos(k_x a/2)$$

Tight binding model of a monolayer

Saito *et al*, "Physical Properties of Carbon Nanotubes" (Imperial College Press, London, 1998): Chapter 2.

Bloch function
$$\Phi_j(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j}^{N} e^{i\mathbf{k}.\mathbf{R}_j} \phi_j(\mathbf{r}-\mathbf{R}_j)$$

sum over N atomic positions

j^{th} atomic orbital: j = A or B

Eigenfunction
$$\Psi_j(\mathbf{k}, \mathbf{r}) = \sum_{i=1}^{2} C_{ji}(\mathbf{k}) \Phi_i(\mathbf{k}, \mathbf{r})$$

Transfer integral matrix $\quad \mathcal{H}_{ij} = \langle \Phi_i | H | \Phi_j \rangle$

Overlap integral matrix $\quad S_{ij} = \langle \Phi_i | \Phi_j \rangle$

Column vector $\quad C_j = \begin{pmatrix} C_{j1} \\ C_{j2} \end{pmatrix}$

Eigenvalue equation
$$\mathcal{H} C_j = \varepsilon_j S C_j$$

Wallace, Phys. Rev. 71, 622 (1947)
Slonczewski, Weiss, Phys. Rev. 109, 272 (1958)

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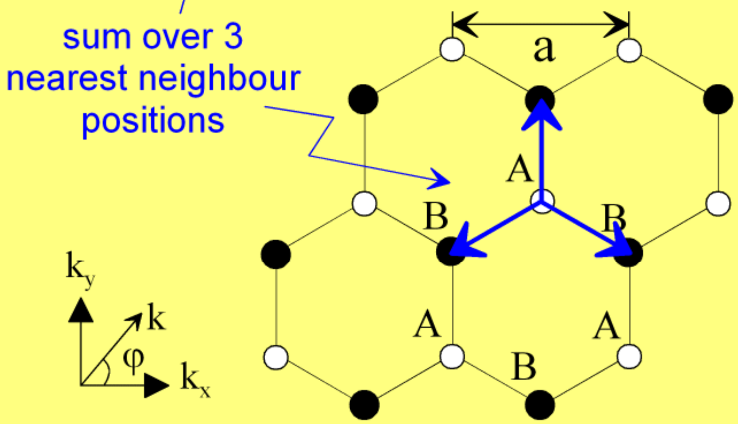
$$\mathcal{H}_{AB} = \frac{1}{N} \sum_{\mathbf{R}_A}^{N} \sum_{\mathbf{R}_B}^{N} e^{i\mathbf{k}.(\mathbf{R}_B - \mathbf{R}_A)} \underbrace{\langle \phi_A(\mathbf{r}-\mathbf{R}_A) | H | \phi_B(\mathbf{r}-\mathbf{R}_B) \rangle}_{\gamma_0}$$



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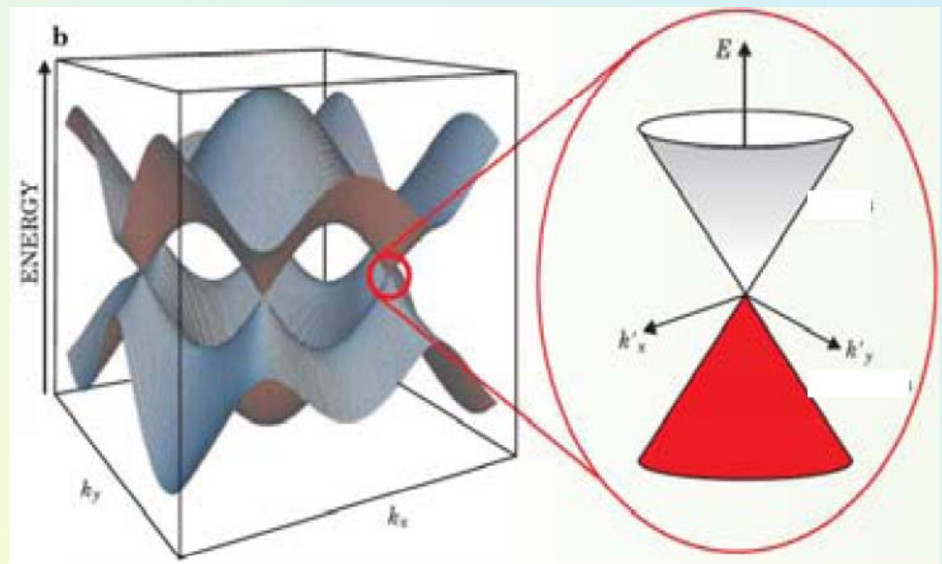
$$f(\mathbf{k}) = e^{i k_y a/\sqrt{3}} + 2e^{-i k_y a/2\sqrt{3}} \cos(k_x a/2)$$

Tight binding model of a monolayer

Saito *et al*, "Physical Properties of Carbon Nanotubes"

$$\hat{H} \approx \begin{pmatrix} 0 & \gamma_0 f(\vec{k}) \\ \gamma_0 f^*(\vec{k}) & 0 \end{pmatrix}$$

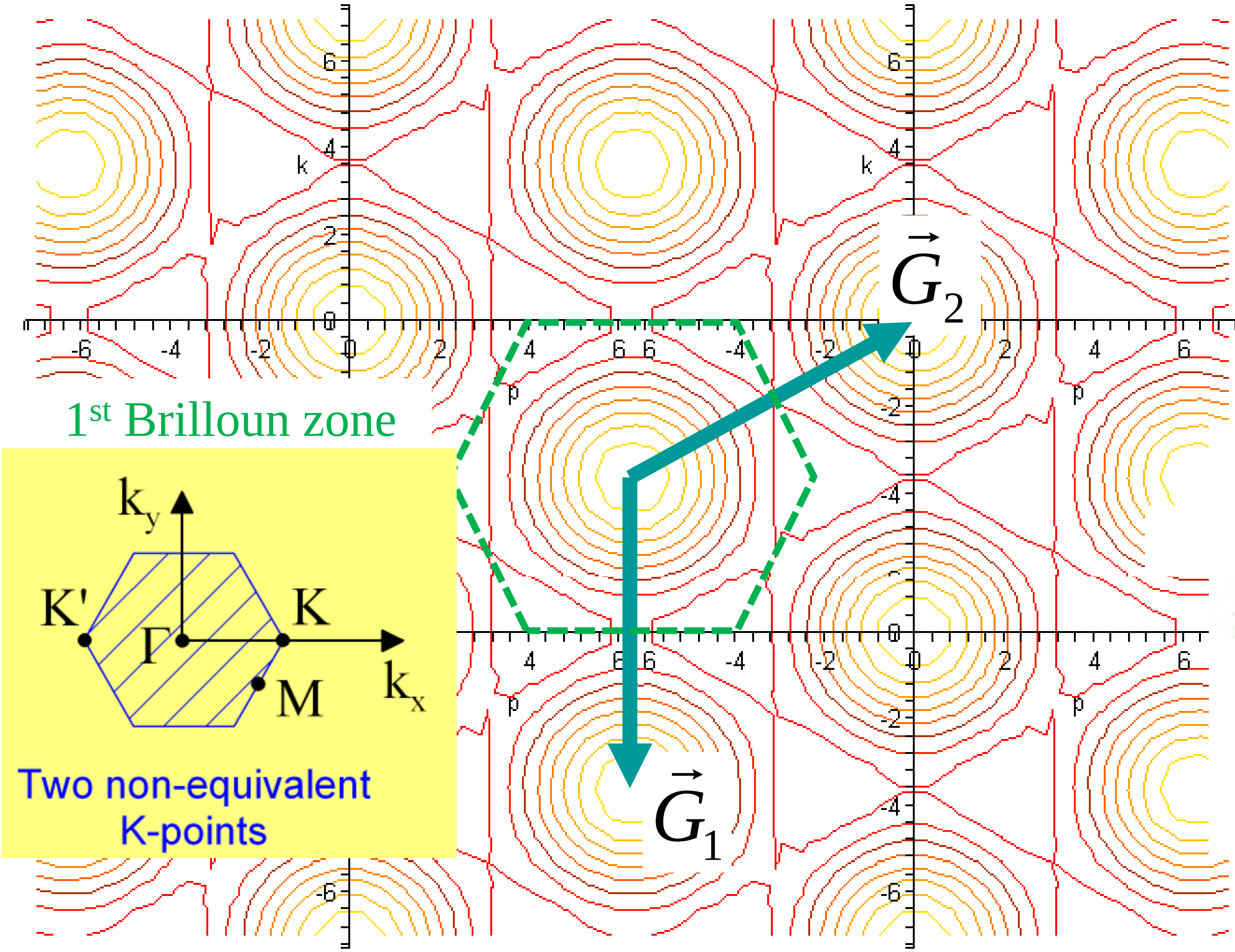
$$\varepsilon = \pm | \gamma_0 f |$$



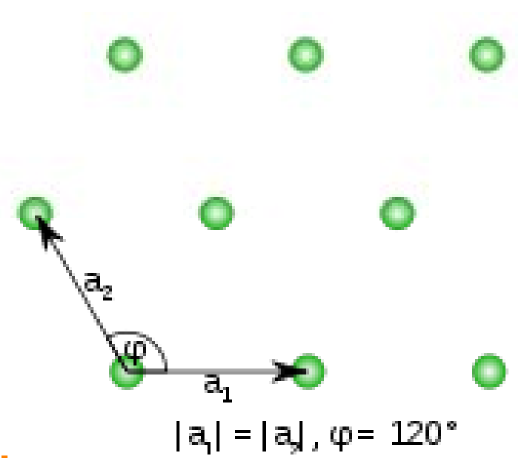
Reciprocal lattice

$$\varepsilon(\vec{k} + \vec{G}_{N_1 N_2}) = \varepsilon(\vec{k})$$

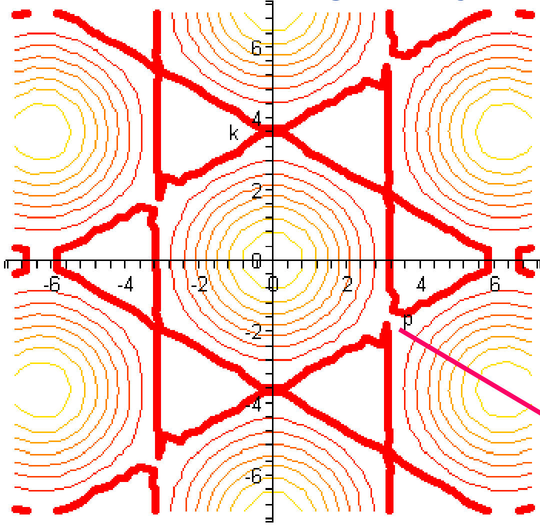
$$\vec{G}_{N_1 N_2} = N_1 \vec{G}_1 + N_2 \vec{G}_2$$

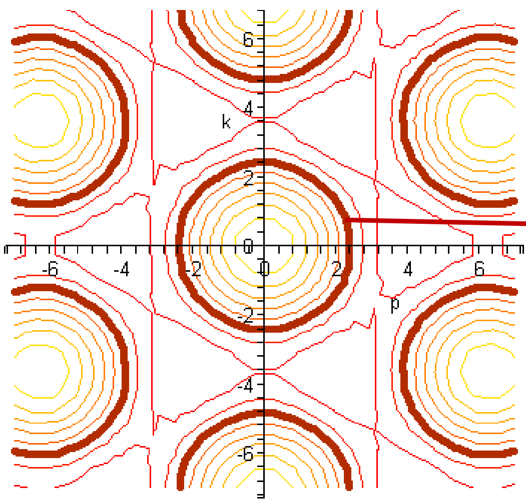


Hexagonal reciprocal lattice corresponding to the hexagonal Bravais lattice

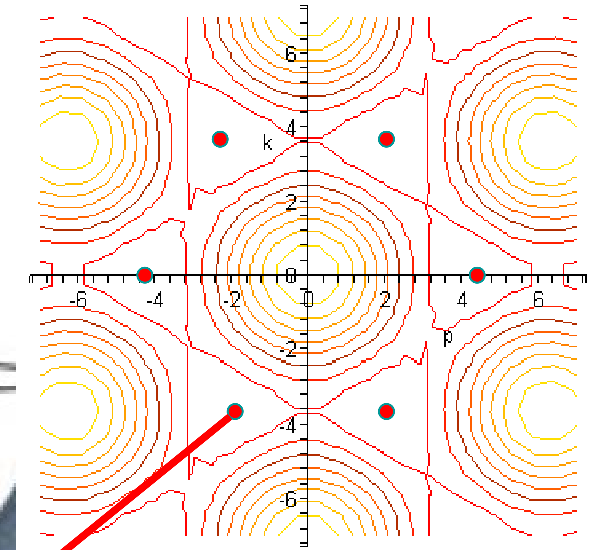


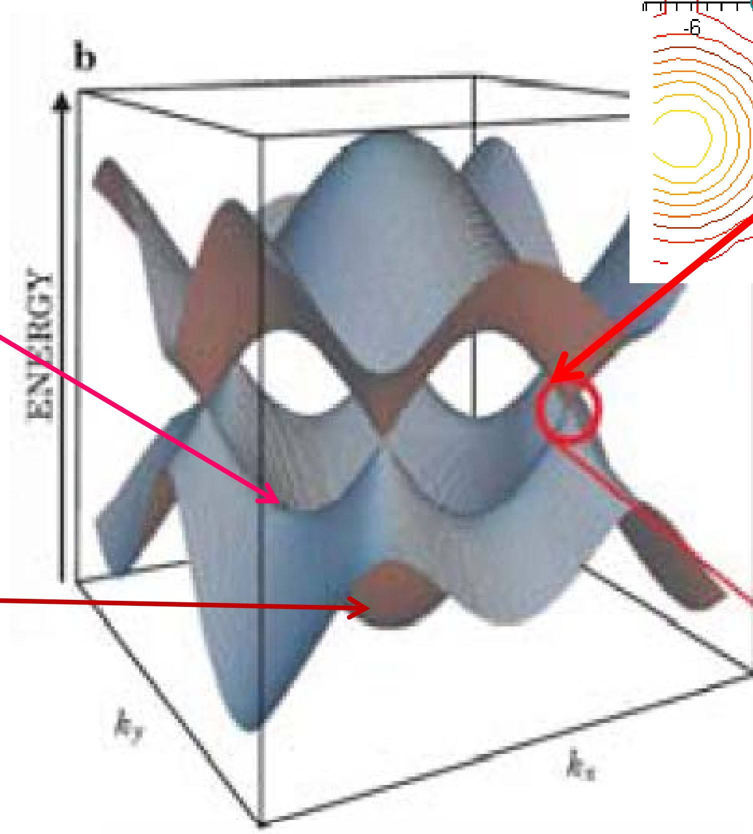
M-point,
van Hove singularity



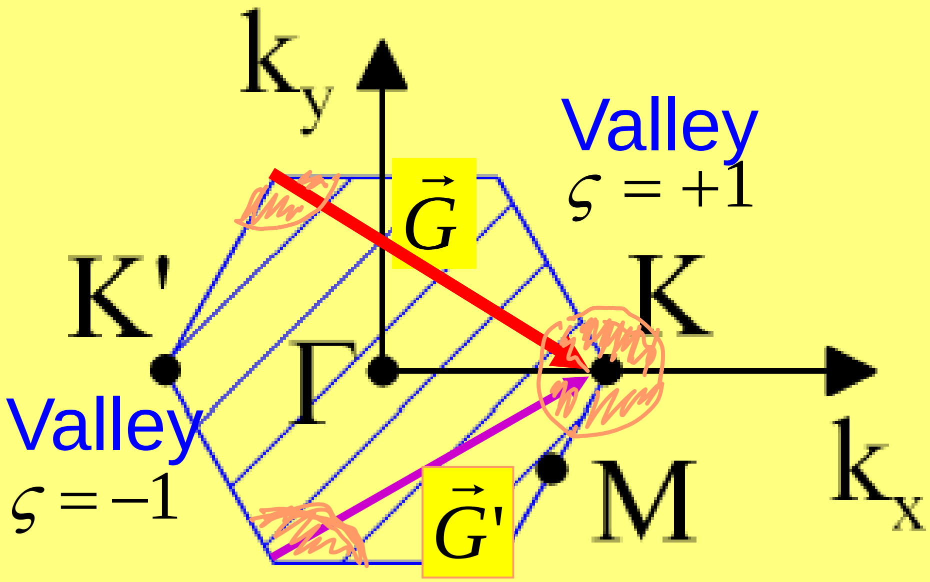


Fermi ‘point’ in undoped Graphene: K(K’) point



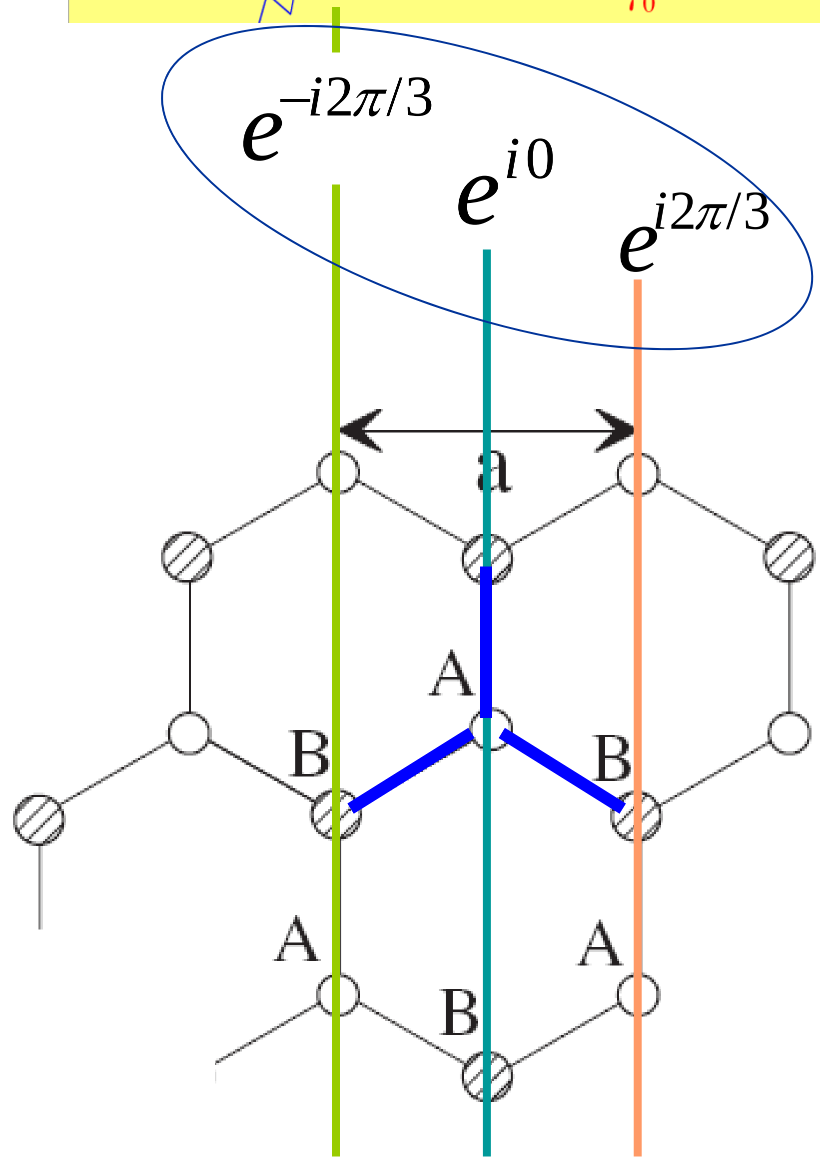


First Brillouin zone



Two non-equivalent K-points

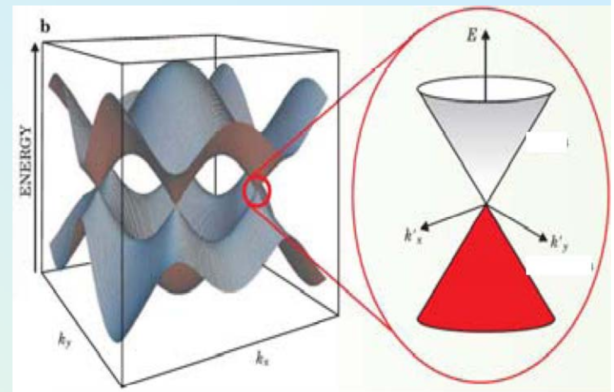
$$\mathcal{H}_{AB} = \frac{1}{N}\sum_{\mathbf{R}_A}^{N}\sum_{\mathbf{R}_B}^{N} e^{i\mathbf{k}.(\mathbf{R}_B - \mathbf{R}_A)} \underbrace{<\phi_A(\mathbf{r}-\mathbf{R}_A)|H|\phi_B(\mathbf{r}-\mathbf{R}_B)>}_{\gamma_0}$$



$$H_{AB,K} = \gamma_0 \left[e^{-i\frac{2\pi}{3}} e^{-i\left(\frac{a}{2}p_x + \frac{a}{2\sqrt{3}}p_y\right)} + e^{i\frac{a}{\sqrt{3}}p_y} + e^{i\frac{2\pi}{3}} e^{i\left(\frac{a}{2}p_x - \frac{a}{2\sqrt{3}}p_y\right)} \right]$$

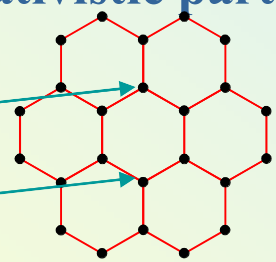
$$\approx \frac{\sqrt{3}}{2}\gamma_0 a(p_x - ip_y)$$

$$H_{BA,K} \approx \frac{\sqrt{3}}{2}\gamma_0 a(\underline{p_x + ip_y}) \equiv v\underline{\pi}$$



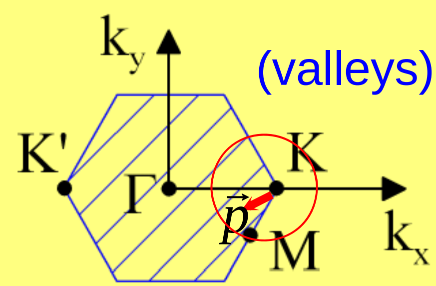
Bloch function amplitudes (e.g., in the valley K) on the AB sites ('isospin') mimic spin components of a massless relativistic particle.

$$\psi = \begin{pmatrix} \varphi_A \\ \varphi_B \end{pmatrix}$$



$$\hat{H} = v \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} = v\vec{\sigma}\cdot\vec{p}$$

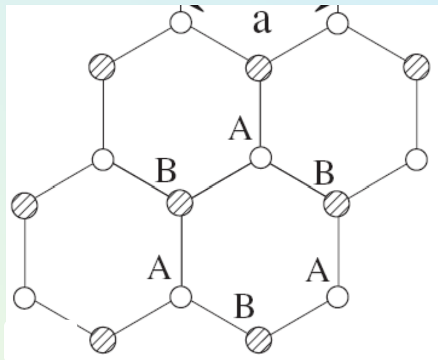
Brillouin zone



Two non-equivalent K-points

McClure, PR 104, 666 (1956)

$$v = \frac{\sqrt{3}}{2}\gamma_0 a \sim 10^8 \frac{cm}{sec}$$

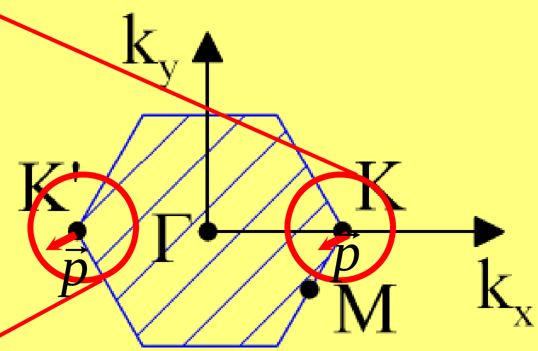


valley index
'pseudospin'

$$\varsigma = \pm 1$$

$$\hat{H} = v \begin{pmatrix} 0 & \pi^{+} & & \\ \pi & 0 & & \\ & & 0 & -\pi^{+} \\ & & -\pi & 0 \end{pmatrix} \begin{pmatrix} \varphi_{A,+} \\ \varphi_{B+} \\ \varphi_{B-} \\ \varphi_{A-} \end{pmatrix}$$

Brillouin
zone



Two non-equivalent
K-points

$$\pi = p_x + ip_y$$

$$\pi^{+} = p_x - ip_y$$

sublattice index
'isospin'

Also, one may need to take into account an additional real spin degeneracy of all states

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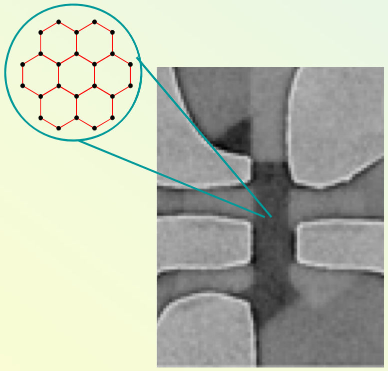

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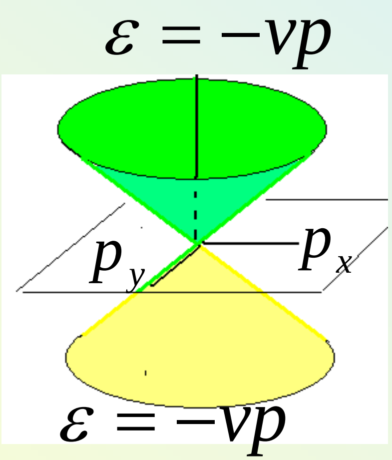


$$H = v\begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} = v\vec{\sigma}\cdot\vec{p}$$

$$\vec{p} = (p\cos\vartheta,\, p\sin\vartheta)$$

$$\pi = p_x + ip_y = pe^{i\vartheta}$$

$$\pi^+ = p_x - ip_y = pe^{-i\vartheta}$$

sublattice 'isospin' $\vec{\sigma}$ is linked to the direction of the electron momentum

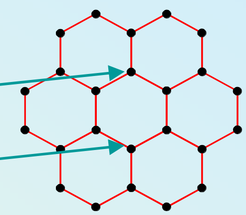
conduction band $\vec{p}$

$\vec{\sigma}\cdot\vec{n} = 1, \varepsilon = vp$

$\vec{\sigma}\cdot\vec{n} = -1, \varepsilon = -vp$

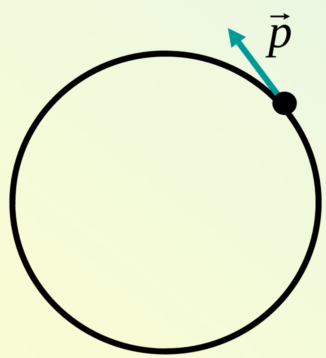
valence band $\vec{p}$

$$\psi_{\vec{p}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{-i\vartheta} \end{pmatrix}$$



Berry phase

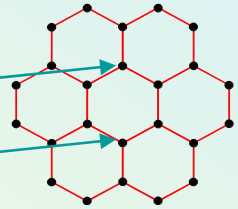
$$\pi = i\int_0^{2\pi} d\vartheta\, \psi^+ \frac{d}{d\vartheta}\psi$$

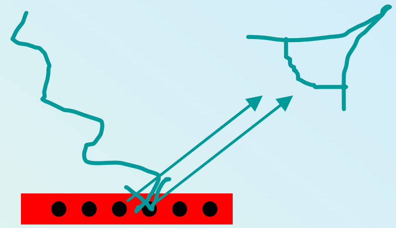


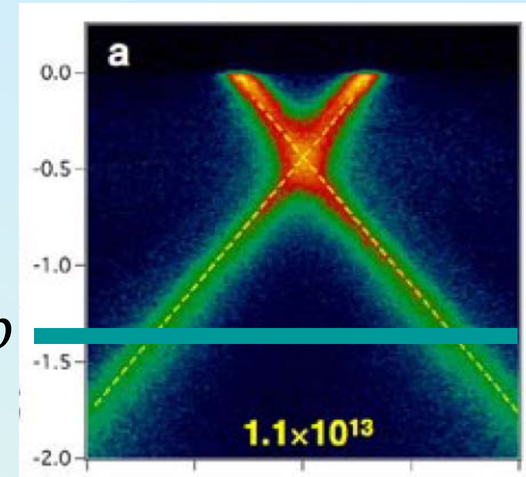
$$\psi \to e^{2\pi\frac{i}{2}\sigma_3}\psi = e^{i\pi\sigma_3}\psi = -\psi$$

Electronic states in graphene observed using ARPES

$$\psi_{\vec{p}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -e^{-i\vartheta} \end{pmatrix}$$





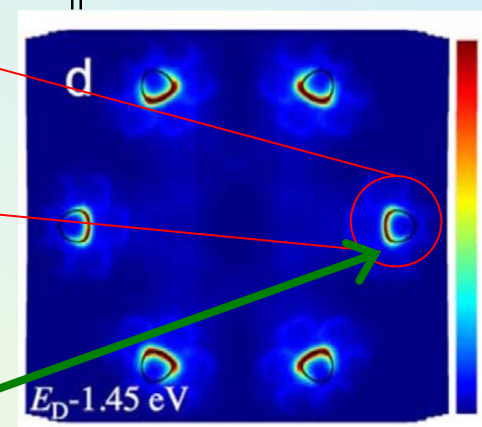


$$\varepsilon = -vp$$

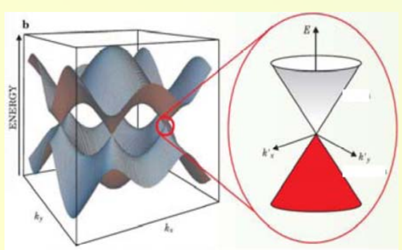
$$I_{ARPES} \sim |\varphi_A + \varphi_B|^2$$

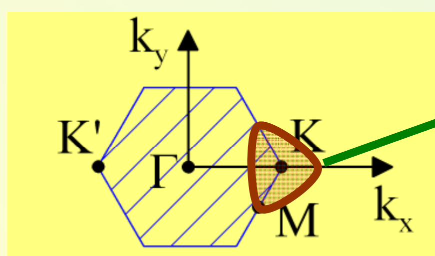
$$\sim \sin^2\left(\frac{\vec{k}\cdot\vec{R}_{BA}}{2} + \frac{\vartheta}{2}\right)$$

$$\vec{k}_{\parallel} = \vec{G} \pm \vec{K} + \vec{p}$$



Mucha-Kruczynski, Tsyplyatyev, Grishin, McCann, VF, Boswick, Rotenberg - PRB 77, 195403 (2008)





ARPES of heavily doped graphene synthesized on silicon carbide

Bostwick *et al* - Nature Physics, 3, 36 (2007)

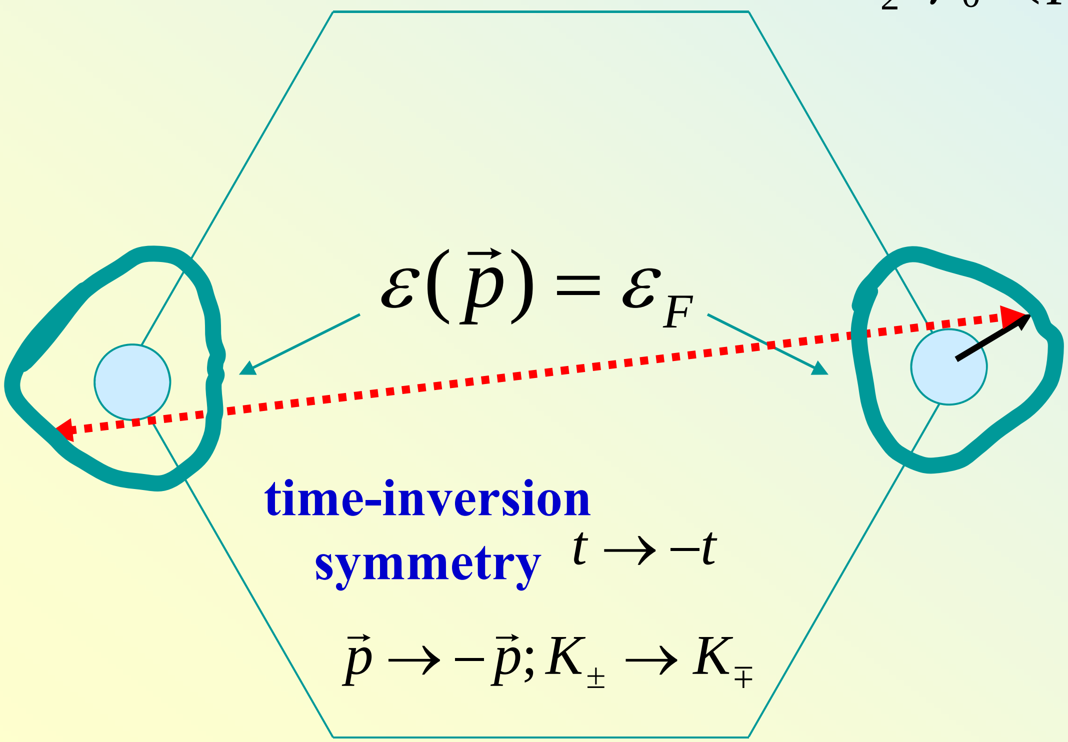
$$\hat{H} = \varsigma v \begin{pmatrix} 0 & \pi^+ \\ \pi & 0 \end{pmatrix} + \boxed{\mu \begin{pmatrix} 0 & \pi^2 \\ (\pi^+)^2 & 0 \end{pmatrix}}$$

weak trigonal warping

valley

$\varsigma = \pm 1$

$$H_{AB,K_+} = \gamma_0 \left[e^{-i\frac{2\pi}{3}} e^{-i(\frac{a}{2}p_x + \frac{a}{2\sqrt{3}}p_y)} + e^{i\frac{a}{\sqrt{3}}p_y} + e^{i\frac{2\pi}{3}} e^{i(\frac{a}{2}p_x - \frac{a}{2\sqrt{3}}p_y)} \right]$$
$$\approx \frac{\sqrt{3}}{2}\gamma_0 a(p_x - ip_y) - \frac{\gamma_0 a^2}{8}(p_x + ip_y)^2$$



$$\pi = p_x + ip_y = pe^{i\vartheta}$$
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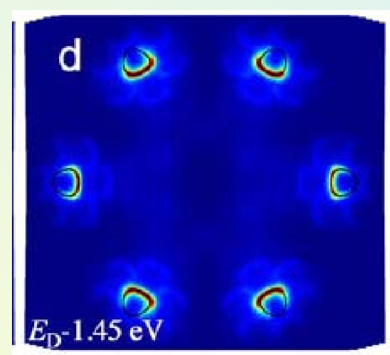
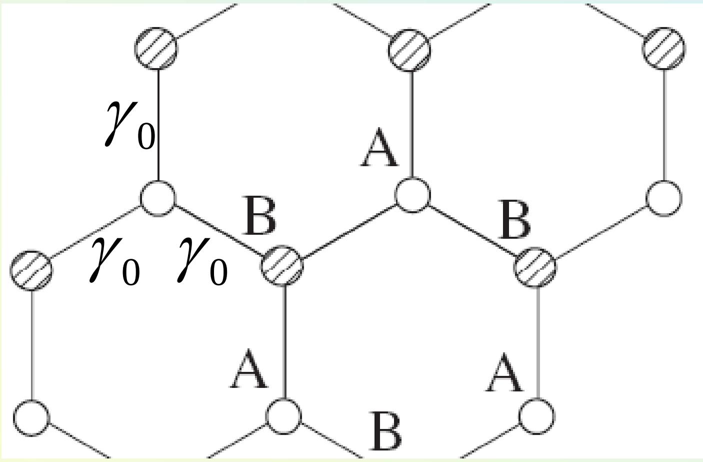
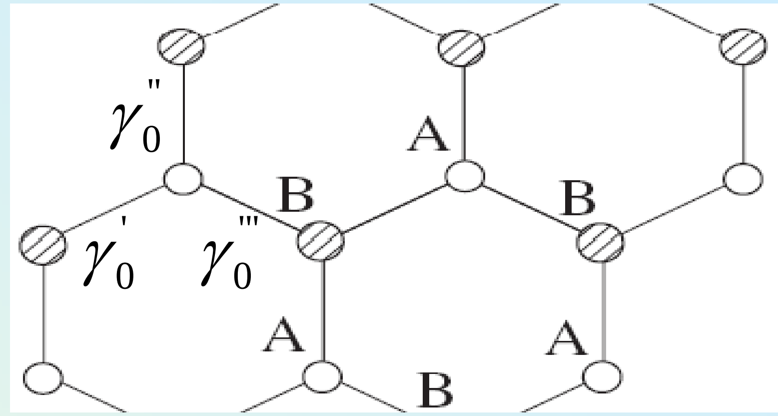
$$\vec{p} = (p\cos\vartheta, p\sin\vartheta)$$



A. Bostwick *et al* – Nature Physics 3, 36 (2007)

Slightly stretched monolayer graphene





$$\gamma_0 e^{-i\frac{2\pi}{3}} + \gamma_0 + \gamma_0 e^{i\frac{2\pi}{3}} = 0$$

$$\gamma_0' e^{-i\frac{2\pi}{3}} + \gamma_0'' + \gamma_0''' e^{i\frac{2\pi}{3}} = u_x + iu_y \neq 0$$

$$\hat{H} = \zeta v \vec{p}\cdot\vec{\sigma} + \vec{u}\cdot\vec{\sigma} \equiv \zeta v[\vec{p} + \frac{\zeta}{v}\vec{u}]\cdot\vec{\sigma}$$

shift of the Dirac point in the momentum space, opposite in K/K' valleys, like a vector potential

Ando - J. Phys. Soc. Jpn. 75, 124701 (2006)

$$B_{eff} = \zeta[\nabla \times \vec{u}(\vec{r})]_z$$

Foster, Ludwig - PRB 73, 155104 (2006)
Morpurgo, Guinea - PRL 97, 196804 (2006)

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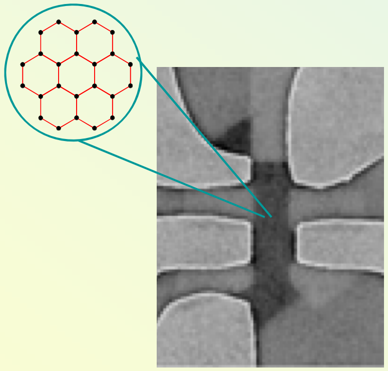

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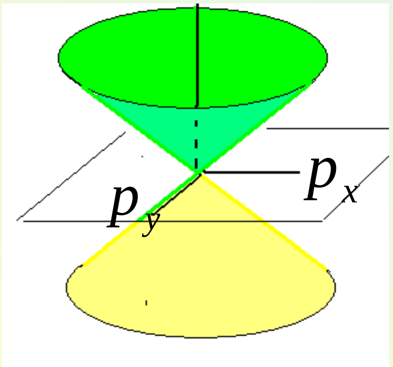
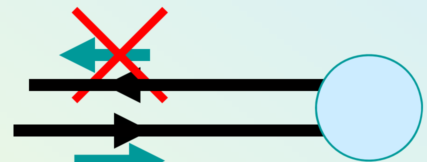
Monolayer graphene: two-dimensional gapless semiconductor with Berry phase $\boldsymbol{\pi}$ electrons

$$\varepsilon = vp$$



$$H = v\vec{\sigma}\cdot\vec{p} + \hat{1}\cdot U(\vec{r})$$



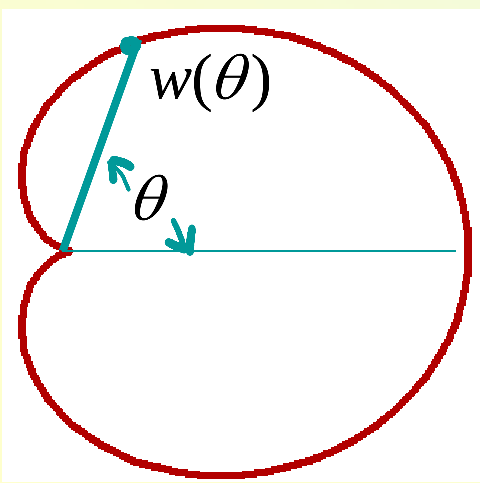
$$\vec{\sigma}\cdot\vec{n} = 1$$

$$\psi_{\vec{p}} = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{-i\vartheta} \end{pmatrix} e^{i\vec{p}\vec{r}}$$

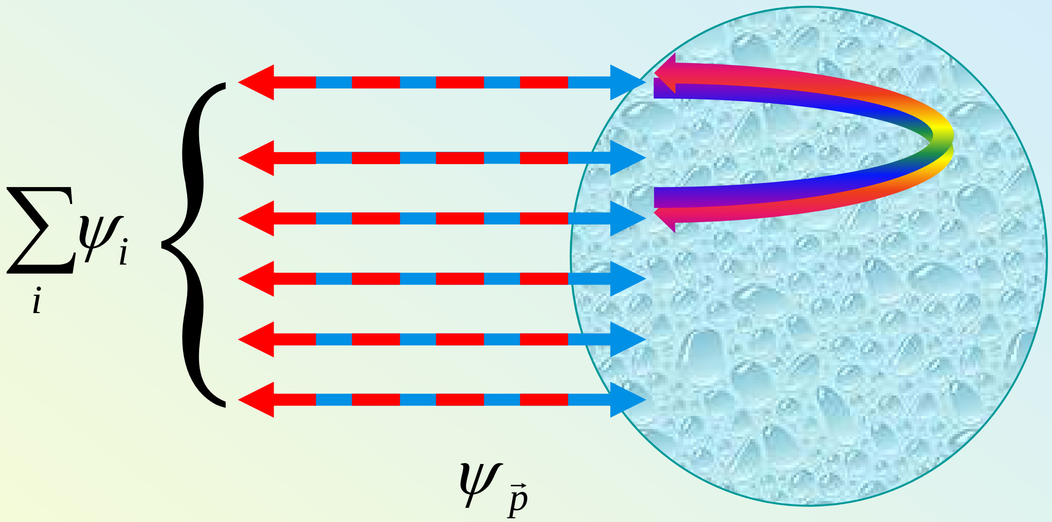
$$\left\langle \psi_{-\vec{p}} \middle| \hat{1}\cdot U(x) \middle| \psi_{\vec{p}} \right\rangle = 0$$

Due to the 'isospin' conservation, A-B symmetric perturbation does not backward scatter electrons,

Ando, Nakanishi, Saito
J. Phys. Soc. Jpn 67, 2857 (1998)



$$w(\theta) \sim \cos^2\tfrac{\theta}{2}\,|U_{\vec{p}-\vec{p}'}|^2$$



$$H = v\vec{\sigma}\cdot\vec{p} + \hat{1}\cdot U(x)$$

Potential which is smooth at the scale of lattice constant (A-B symmetric) cannot scatter Berry phase **π** electrons in exactly backward direction.

$$\boxed{w_{\vec{p}\to-\vec{p}} = \left|\sum_i \psi_i\right|^2 = \left|\sum_{(a,b)} [\psi_{a\to b} + \psi_{b\to a}]\right|^2 = \left|\sum_{(a,b)} 0\right|^2 = 0}$$

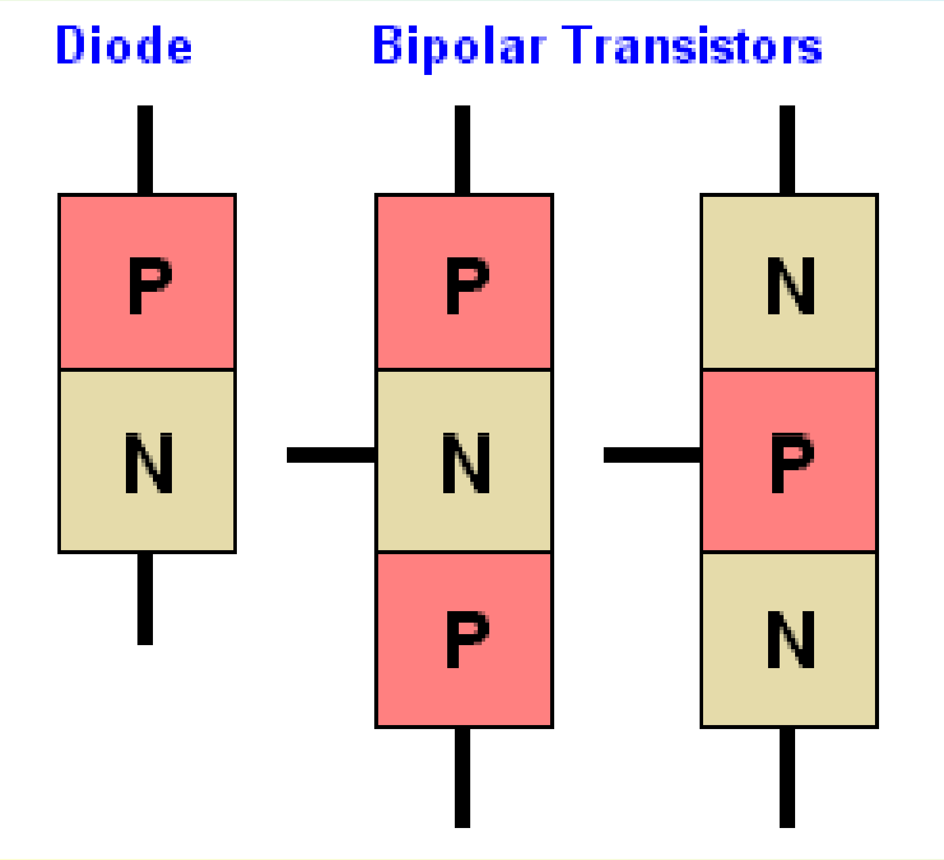
$$\psi_{a\to b} = Ae^{i\frac{\pi}{2}\sigma_z}\psi_{\vec{p}}$$

$$\psi_{b\to a} = Ae^{i\frac{-\pi}{2}\sigma_z}\psi_{\vec{p}}$$

$$\Rightarrow \quad \psi_{a\to b} = e^{i\pi\sigma_z}\psi_{b\to a} = -\psi_{b\to a}$$

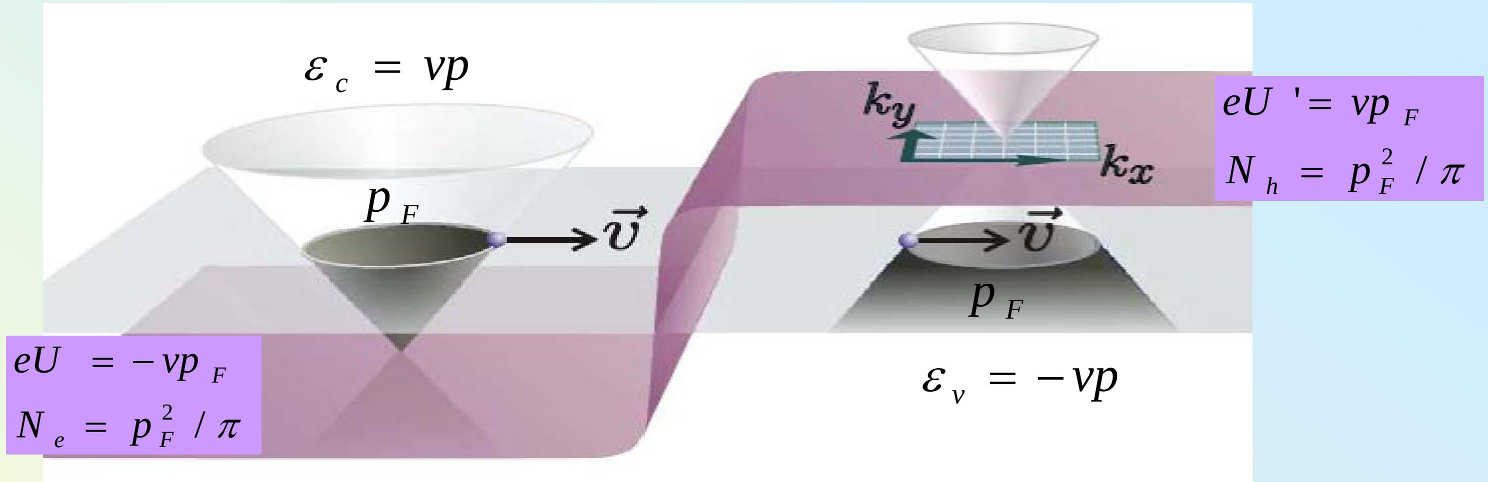
Berry phase **π** electrons

PN junctions in the usual gap-full semiconductors are non-transparent for incident electrons, therefore, they are highly resistive.

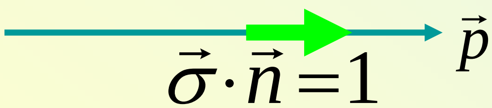


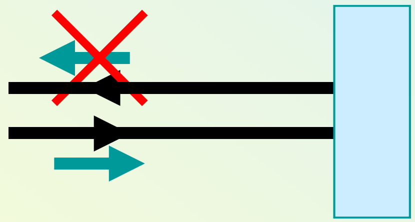
PN junctions in in graphene are different.

Transmission of chiral electrons through the PN junction in graphene



conduction band electrons





$$H = v\vec{\sigma}\cdot\vec{p} + \hat{1}\cdot U(\vec{r})$$

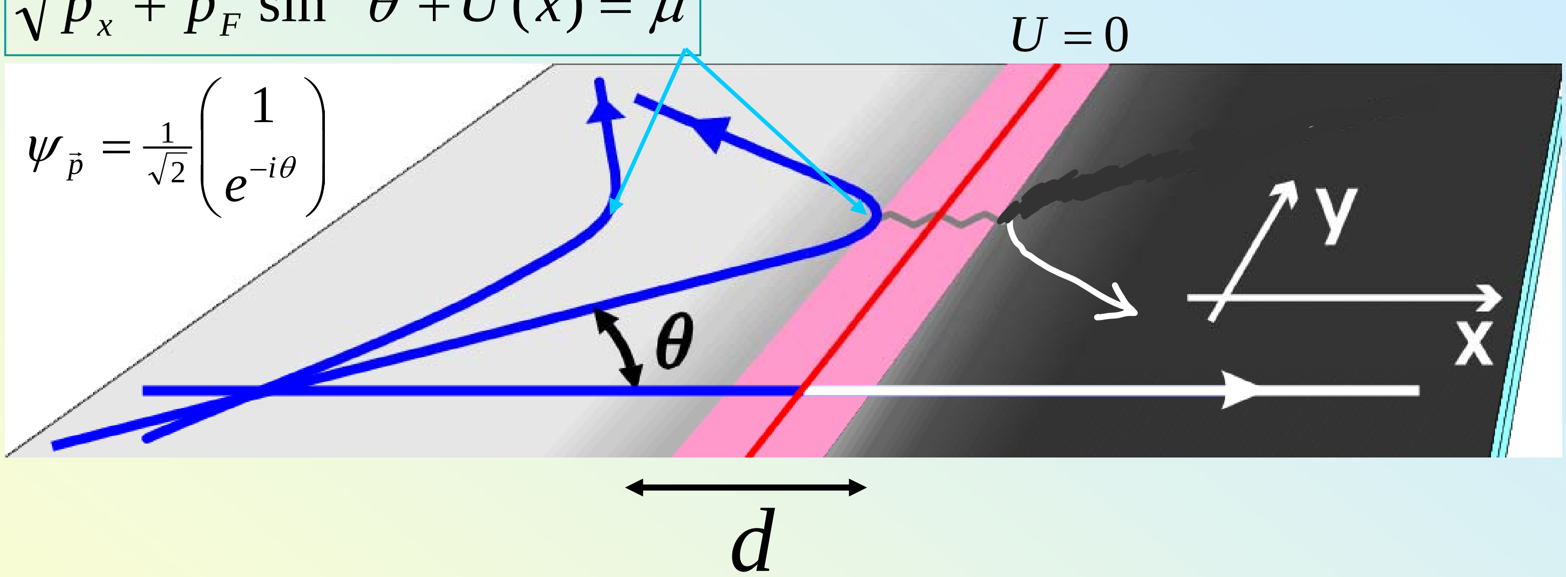
Due to the isospin conservation, A-B symmetric potential cannot backward scatter electrons in monolayer graphene.

For graphene PN junctions: Cheianov, VF - PR B 74, 041403 (2006)

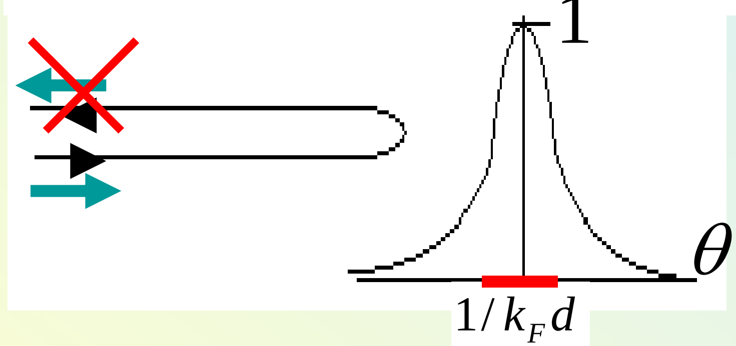
'Klein paradox': Katsnelson, Novoselov, Geim, Nature Physics 2, 620 (2006)

Transmission of chiral electrons through the PN junction in graphene

$$\sqrt{p_x^2 + p_F^2 \sin^2\theta} + U(x) = \mu$$

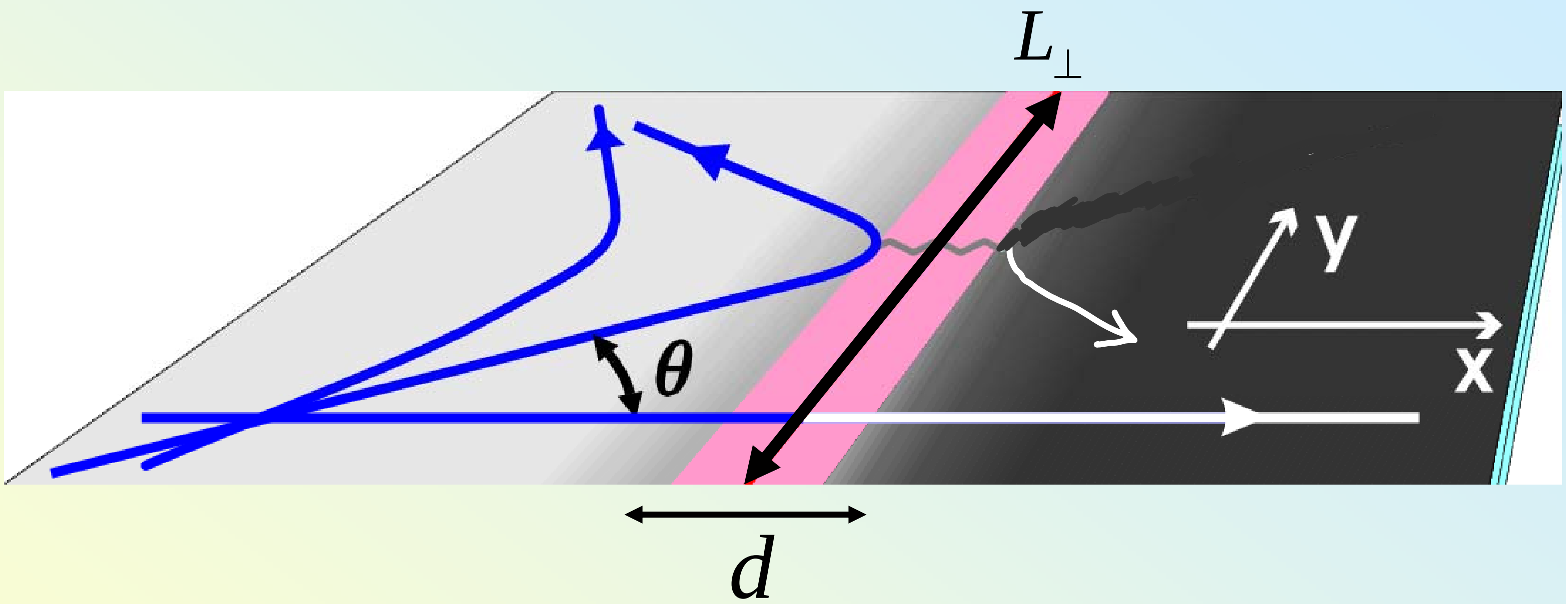


$$w(\theta) = e^{-\pi p_F d \sin^2\theta} \cos^2\theta$$



Due to the 'isospin' conservation, electrostatic potential ***U(x)*** which smooth on atomic distances cannot scatter electrons in the exactly backward direction.

Transmission of chiral electrons through the PN junction in graphene



Due to transmission of electrons with a small incidence angle, $\theta<1/p_F d$, a PN junction in graphene should display a finite conductance (no pinch-off).

$$\boxed{\frac{g_{np}}{L_\perp} = \frac{2e^2}{\pi h}\sqrt{\frac{p_F}{d}}}$$

A characteristic Fano factor in the shot noise:

$$\langle I \cdot I \rangle = (1-\sqrt{\tfrac{1}{2}})\ eI$$

Cheianov, VF - PR B 74, 041403 (2006)

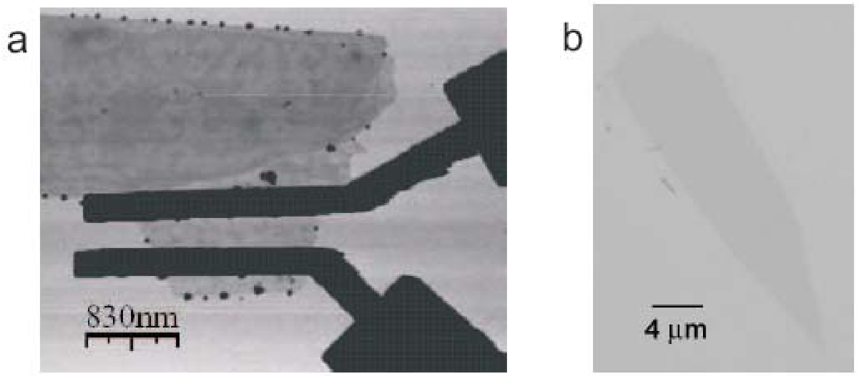
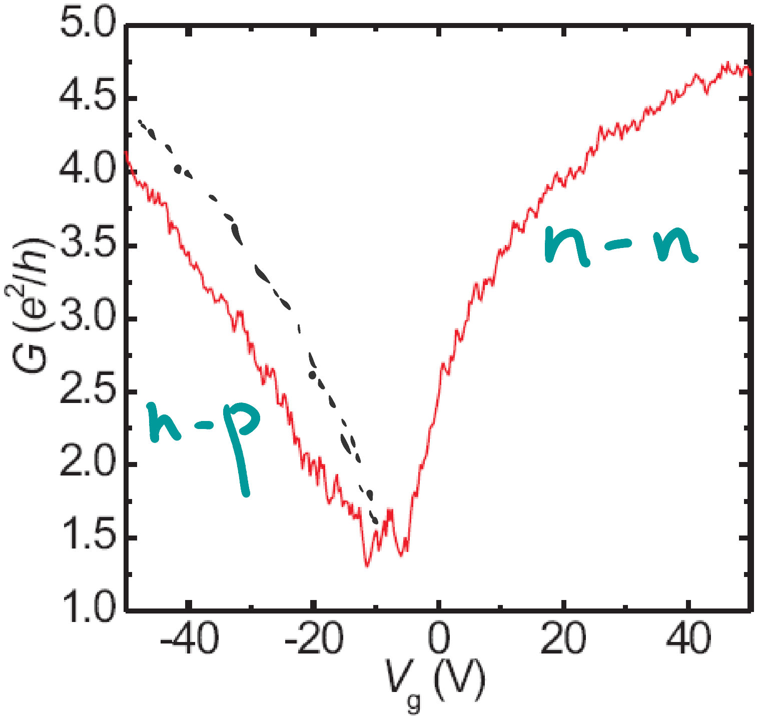
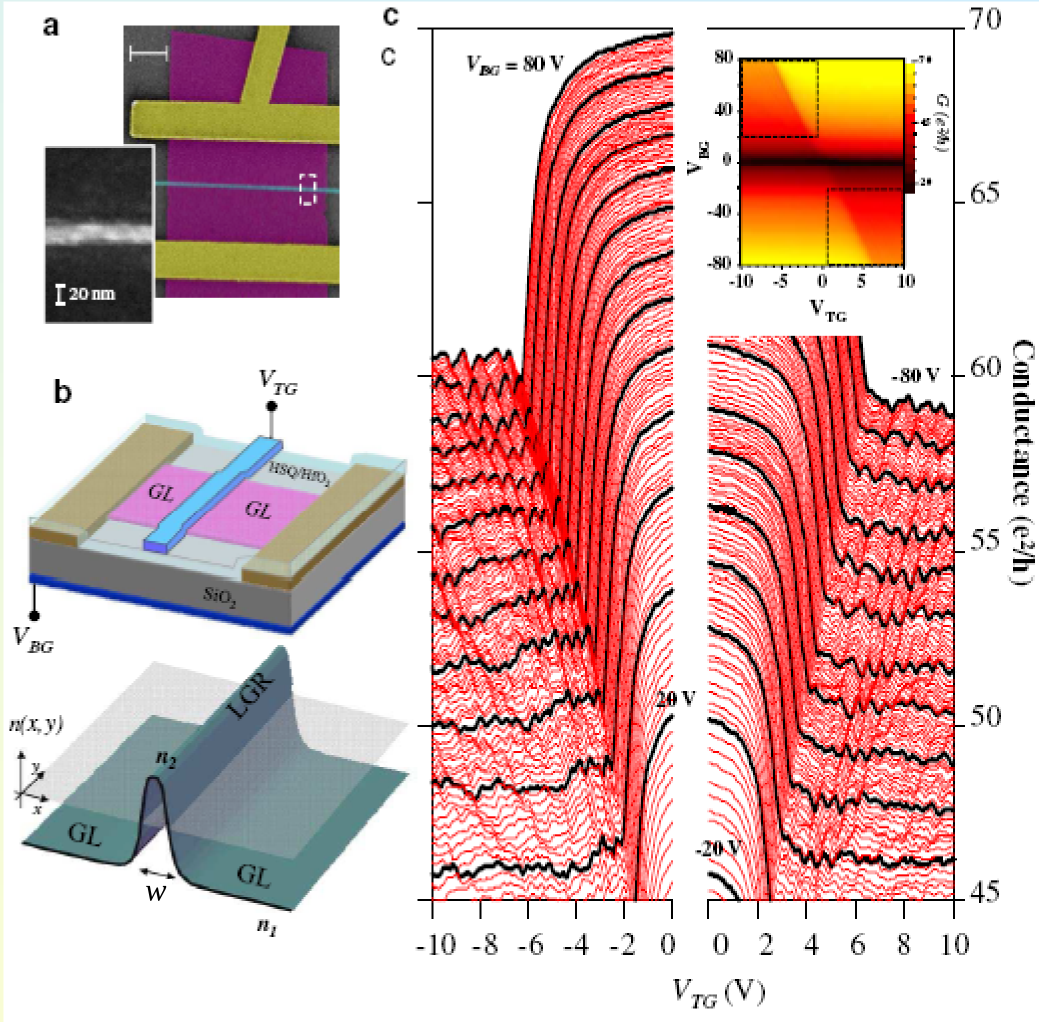


Fig. 2. (a) Atomic force microscopy image of a single-layer graphene Josephson junction used in our experiments. The electrodes consist of a Ti/Al bilayer, with the Tutatnium in contact with graphen.(b) Large graphene layer deposited on top of a Si/SiO_2 substrate by controlled exfoliation of a single graphite crystal. graphe



PN junctions should be taken into consideration in two-terminal devices, since metallic contacts dope graphene, due to the work function difference.

Heersche *et al* - Nature Physics (2007)



PNP junction with a suspended gate: an almost ballistic regime: ***w~l***.

A Young and P Kim - Nature Physics 5, 222 (2009)

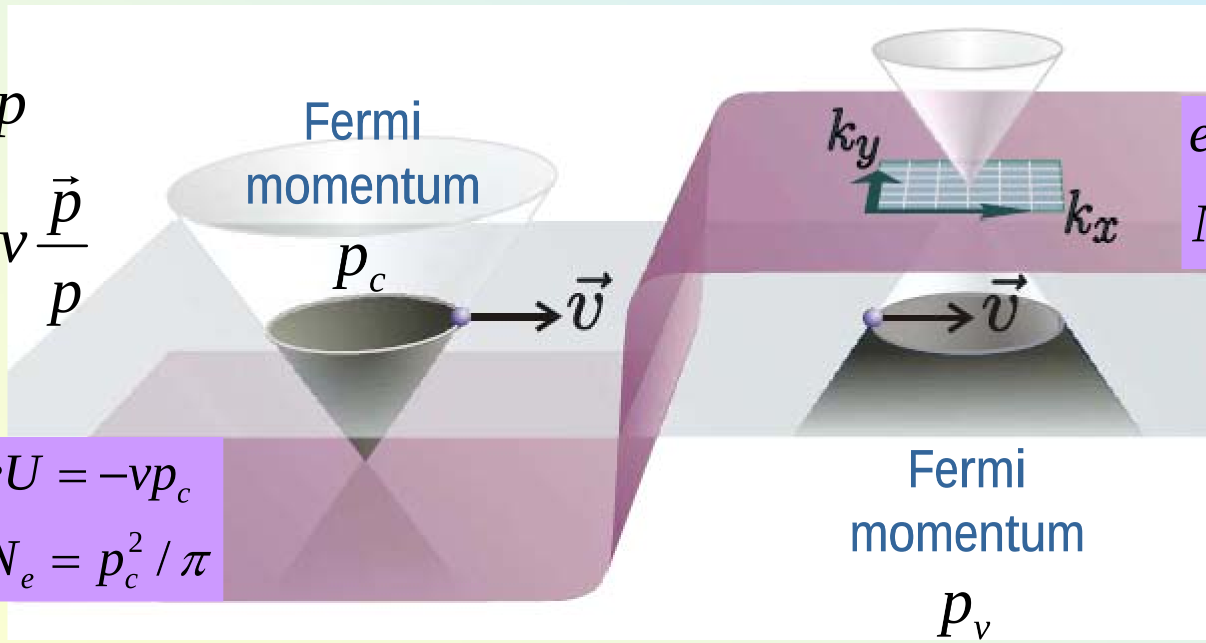
Wishful thinking about graphene microstructures

Focusing and Veselago lens for electrons in ballistic graphene

Cheianov, VF, Altshuler - Science 315, 1252 (2007)

$$\varepsilon_c(\vec{p}) = vp$$

$$\vec{v} = \frac{\partial \varepsilon}{\partial \vec{p}} = v\frac{\vec{p}}{p}$$



$$eU = -vp_c$$

$$N_e = p_c^2/\pi$$

$$eU' = vp_v$$

$$N_h = p_v^2/\pi$$

$$\varepsilon_v(\vec{p}) = -vp$$

$$\vec{v} = \frac{\partial \varepsilon}{\partial \vec{p}} = -v\frac{\vec{p}}{p}$$

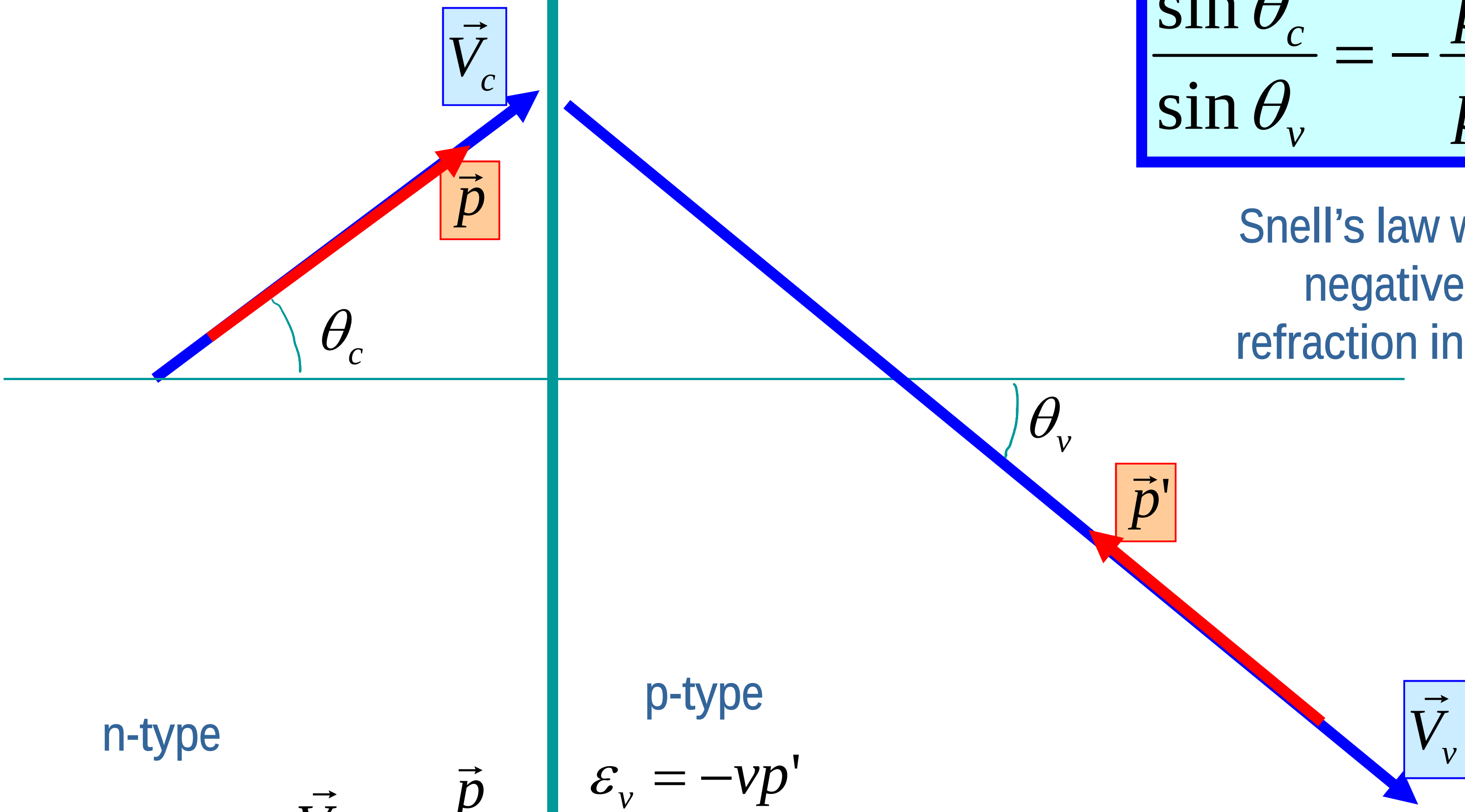
The effect we'll discuss would be the strongest in sharp PN junction, with $d \sim \lambda_F$.

PN junction

$$p_y = p_y^{'} \;\Rightarrow\; p_c \sin\theta_c = -p_v \sin\theta_v$$

$$\boxed{\frac{\sin\theta_c}{\sin\theta_v} = -\frac{p_v}{p_c} = n}$$

Snell's law with negative refraction index



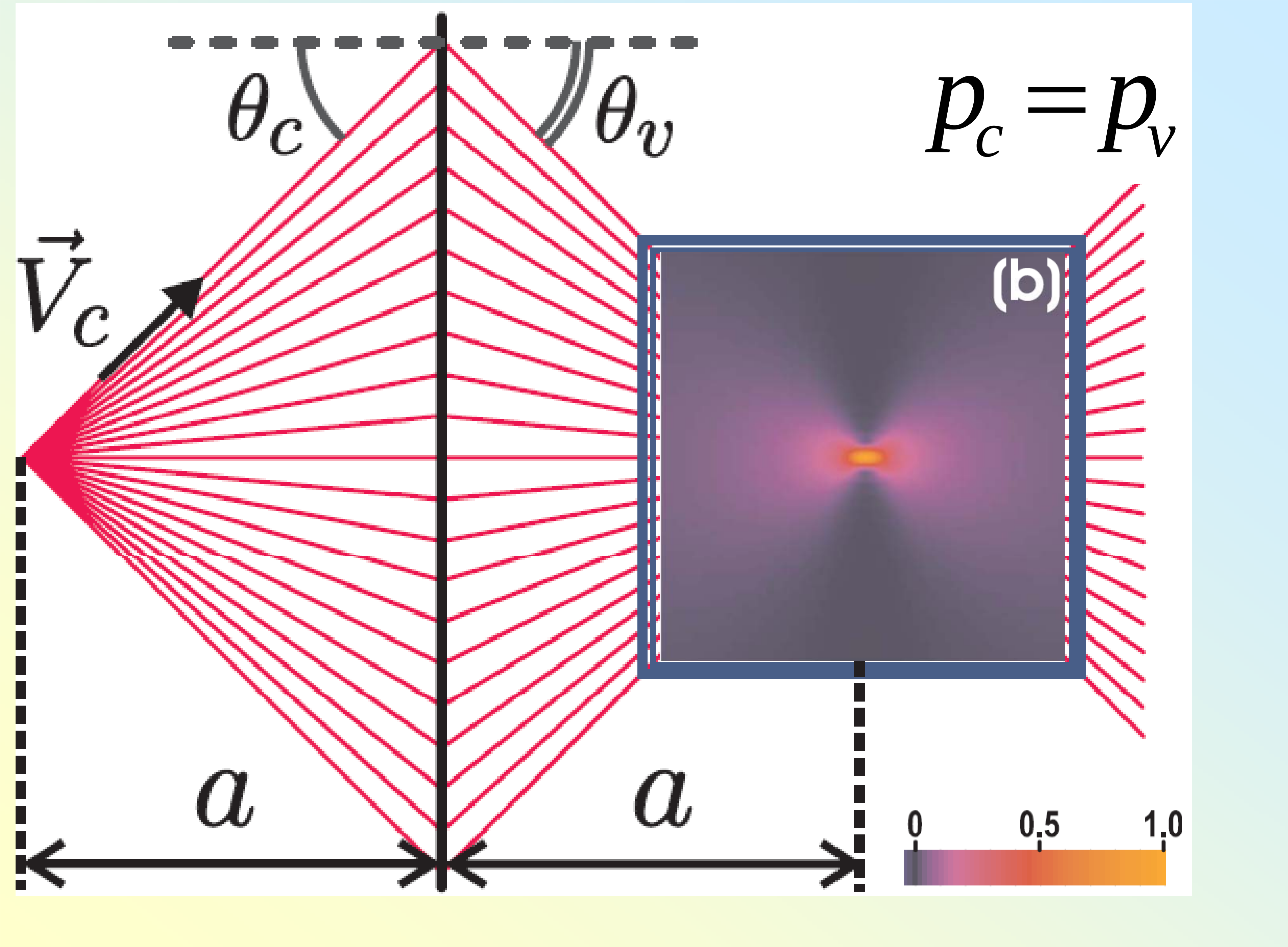
n-type

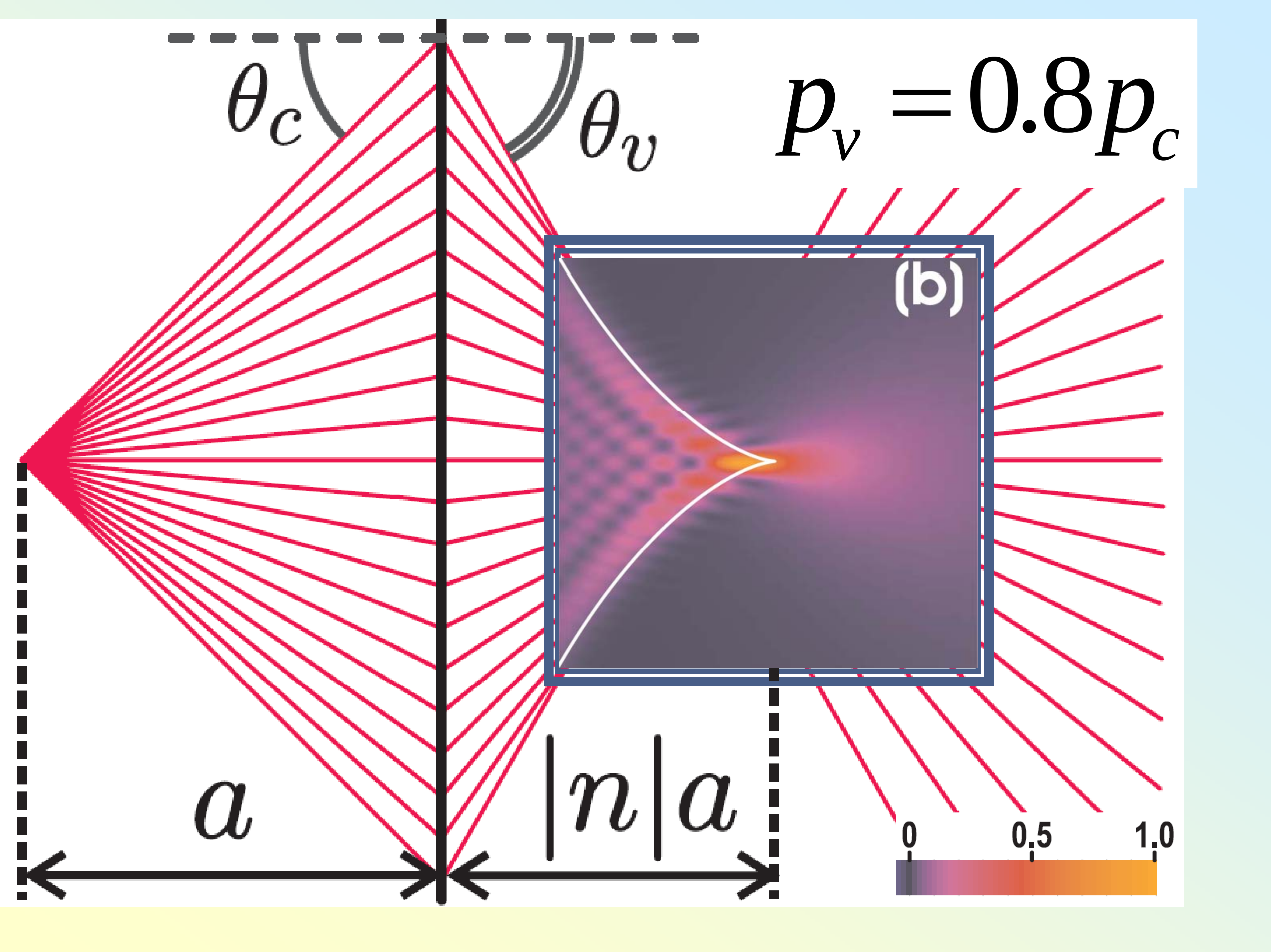
$$\varepsilon_c = vp; \quad \vec{V}_c = v\frac{\vec{p}}{p}$$

p-type

$$\varepsilon_v = -vp'$$

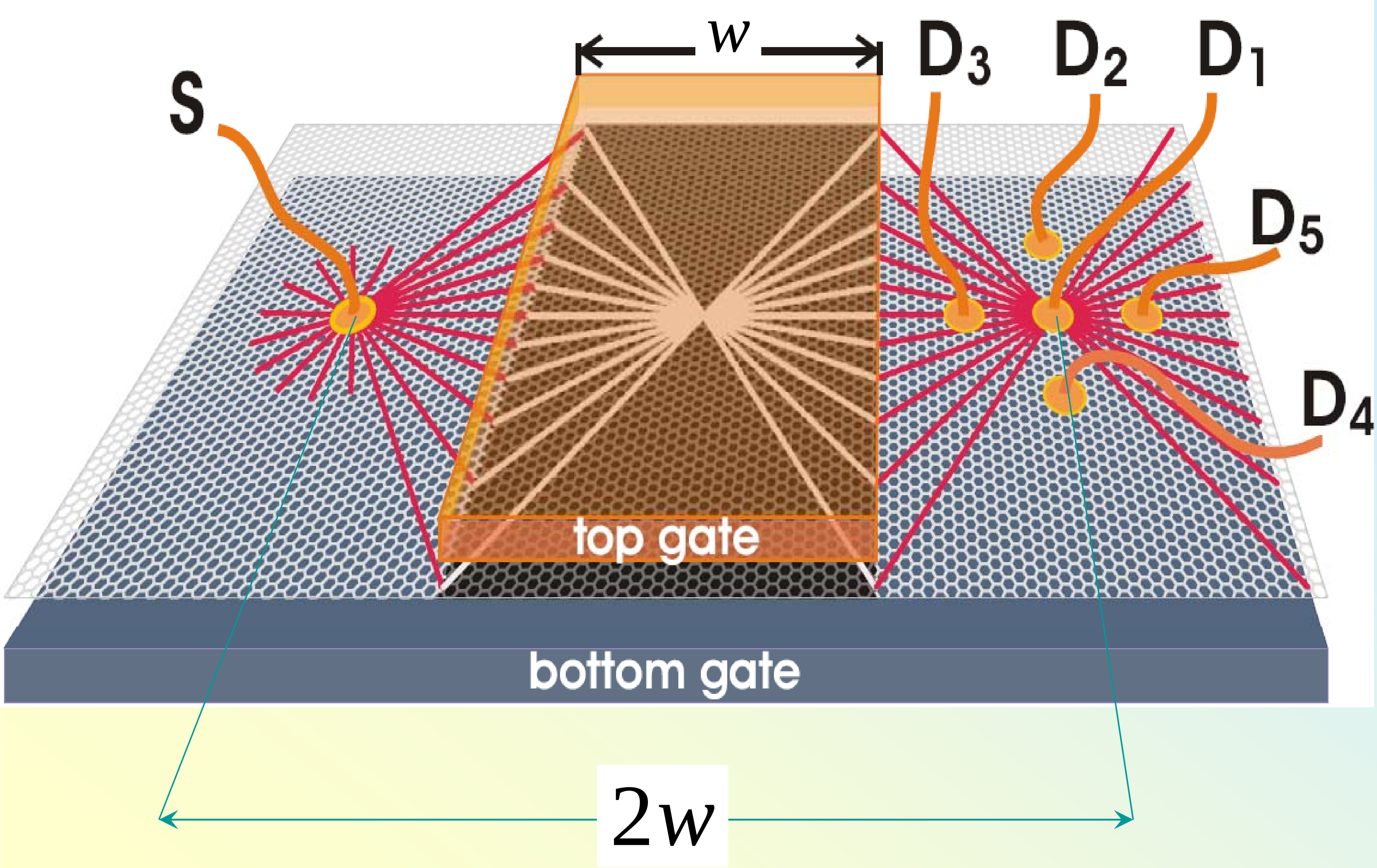
$$\vec{V}_v = -v\frac{\vec{p}'}{p'}$$


θ_c
θ_v
$p_c = p_v$
$\vec{V}_c$
(b)
a
a
0
0.5
1.0

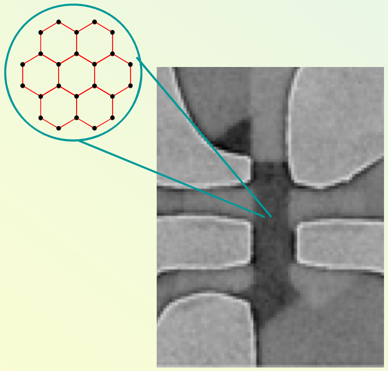


θ_c
θ_v
$p_v = 0.8 p_c$
(b)
a
$|n|a$
0
0.5
1.0

Graphene bipolar transistor: Veselago lens for electrons



Electronic properties of graphene, from 'high' to 'low' energies.



Graphene for beginners: tight-binding model.
Berry phase π electrons in monolayers.
Trigonal warping. Stretched graphene.
PN junction in graphene.

Berry phase 2π electrons in bilayer graphene.
Landau levels & QHE. Interlayer asymmetry gap.
Lifshitz transition and magnetic breakdown in BLG. Stretched BLG.
Renormalisation group theory for interaction and spontaneous symmetry breaking in BLG.