# The KLEIN - paradox

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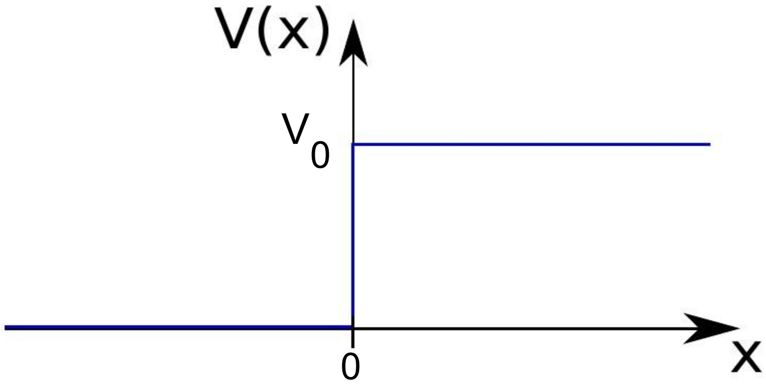
# The KLEIN - Paradox

Schrödinger equation:

$$\mathcal{H}\Psi = E\Psi$$ with the spinor $$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Dirac-like Hamiltonian:

$$\mathcal{H} = -i\hbar c \boldsymbol{\sigma}\boldsymbol{\nabla} + V(x,y) + mc^2\boldsymbol{\sigma}_z$$




solutions:

$$\Psi_L(x) = \begin{pmatrix} 1 \\ \alpha \end{pmatrix} \cdot e^{ikx} + r \begin{pmatrix} 1 \\ -\alpha \end{pmatrix} \cdot e^{-ikx}$$

$$|E| = \sqrt{\hbar^2 c^2 k^2 + m^2 c^4}$$

$$|E - V| = \sqrt{\hbar^2 c^2 q^2 + m^2 c^4}$$

$$\Psi_R(x) = t \begin{pmatrix} 1 \\ -\frac{1}{\beta} \end{pmatrix} \cdot e^{iqx}$$

$$\alpha = \sqrt{\frac{E - mc^2}{E + mc^2}} \qquad \beta = \sqrt{\frac{V_0 - E - mc^2}{V_0 - E + mc^2}}$$

# The KLEIN - Paradox

matching condition: $\Psi_L(x=0) = \Psi_R(x=0)$

reflection: $r = \frac{\alpha\beta + 1}{\alpha\beta - 1}$

assuming: $V_0 > E + mc^2$

$$R = |r|^2 > 1$$

the KLEIN - paradox

observing the group velocitiy inside the barrier:

$$v_g = \hbar^{-1}\frac{dE}{dq} = -\frac{\hbar q c^2}{V_0 - E}$$

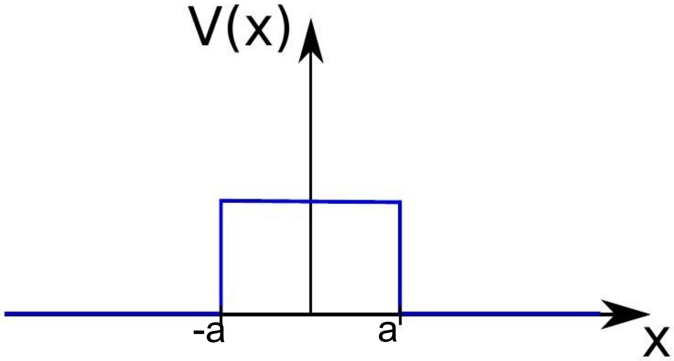
holes inside the barrier

creation of electron-hole pairs at the barrier edge

no paradox anymore

# The KLEIN - Paradox

assuming another potential:




doing exactly the same calculation leads to:

$$R = \frac{(1-\alpha^2\beta^2)^2 \cdot sin^2(2qa)}{4\alpha^2\beta^2 + (1-\alpha^2\beta^2)^2 \cdot sin^2(2qa)}$$

$$T = \frac{4\alpha^2\beta^2}{4\alpha^2\beta^2 + (1-\alpha^2\beta^2)^2 \cdot sin^2(2qa)}$$

the infinite case:

$$R_\infty = \frac{(1-\alpha^2\beta^2)^2}{8\alpha^2\beta^2 + (1-\alpha^2\beta^2)^2}$$

$$T_\infty = \frac{8\alpha^2\beta^2}{8\alpha^2\beta^2 + (1-\alpha^2\beta^2)^2}$$

$\Rightarrow$ Paradox!

# Role of Chirality

Regarding the massless case: $m = 0$

chirality $\propto \boldsymbol{\sigma} \cdot \boldsymbol{p}$

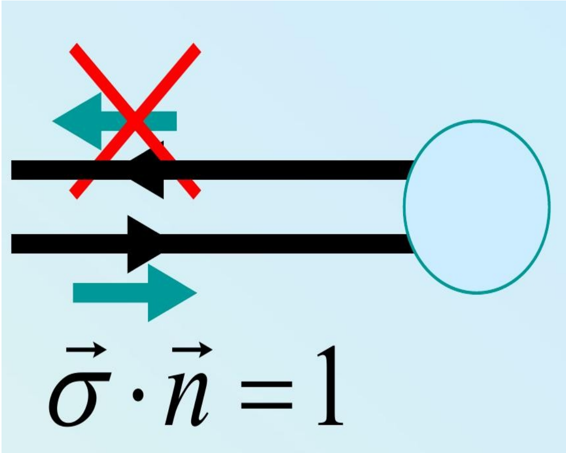
Dirac Hamiltonian: $\mathcal{H} = -i\hbar c \boldsymbol{\sigma} \nabla = c \boldsymbol{\sigma} \cdot \boldsymbol{p} = c p \boldsymbol{\sigma} \cdot \boldsymbol{n}$

with $\boldsymbol{n} = \frac{\boldsymbol{p}}{p}$ and its eigenfunctions $\Psi_{\pm} = \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} e^{i\boldsymbol{k} \cdot \boldsymbol{r}}$

→ chirality operator $\xi = \boldsymbol{\sigma} \cdot \boldsymbol{n}$ with eigenvalues $\pm 1$

→ $$\boldsymbol{\sigma} \cdot \boldsymbol{n} \Psi_{\pm} = \pm \Psi_{\pm}$$

→ Pseudospin is directly linked with the direction of the momentum of the electron



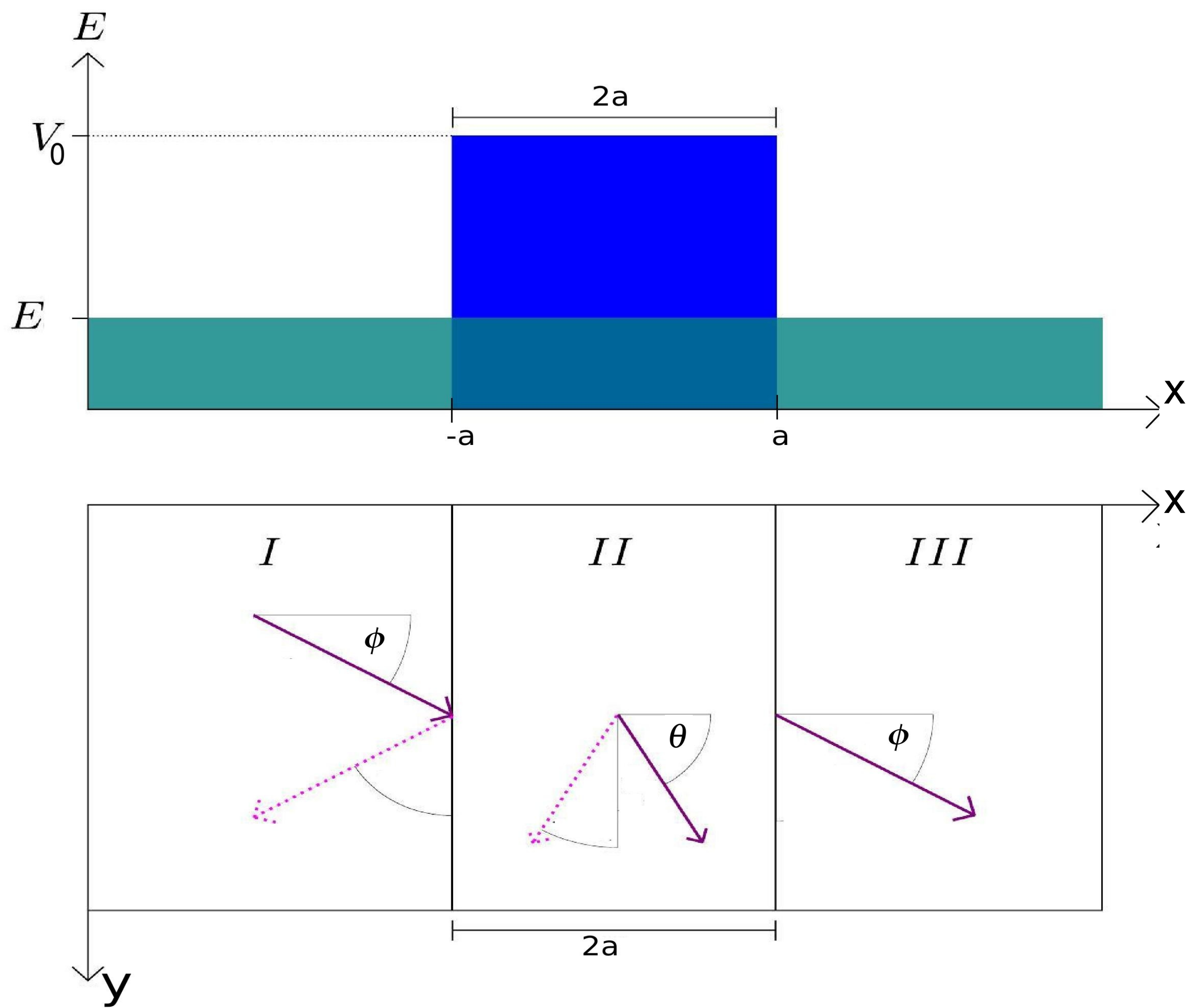

from [5]

conservation of the pseudospin

→ no backscattering

# KLEIN – Tunneling in Single-layer Graphene

Regarding the following potential shape:




from [4]

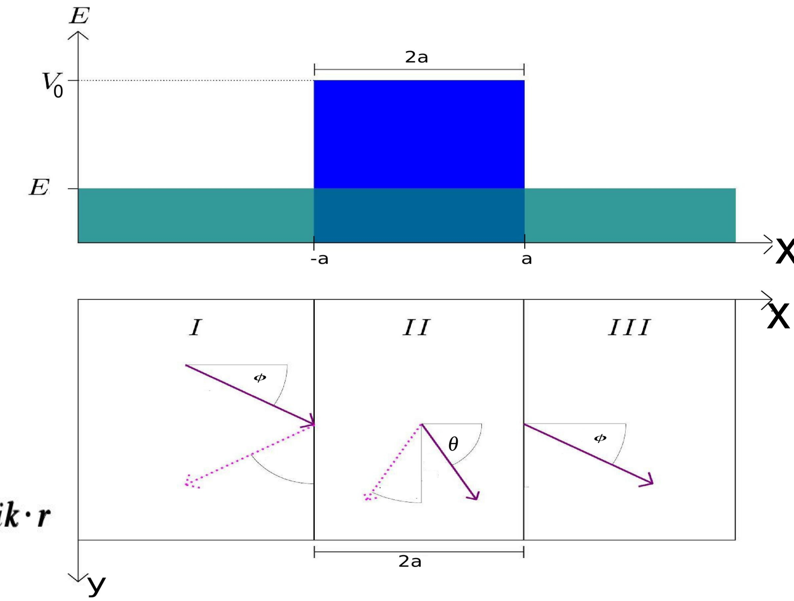
# KLEIN – Tunneling in Single-layer Graphene

momentum conservation:

$$k_y = k\sin\phi = q_y = q\sin\theta$$

Ansatz:

$$\psi_1(x,y) = \psi_1(x)e^{ik_y y}$$
$$\psi_2(x,y) = \psi_2(x)e^{ik_y y}$$




Dirac equation:

$$-i\hbar\frac{\mathrm{d}\psi_2(x)}{\mathrm{d}x} = (E - V(x))\,\psi_1(x)$$
$$-i\hbar\frac{\mathrm{d}\psi_1(x)}{\mathrm{d}x} = (E - V(x))\,\psi_2(x)$$

Solution:

$$\Psi_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}}$$

We can build up the whole wave function

$$\psi_1(x,y) = \begin{cases} \left[e^{ik_x x} + re^{-ik_x x}\right] e^{ik_y y} & x < -a \\ \left[Ae^{iq_x x} + Be^{-iq_x x}\right] e^{ik_y y} & -a < x < a \\ te^{ik_x x + ik_y y} & x > a \end{cases}$$

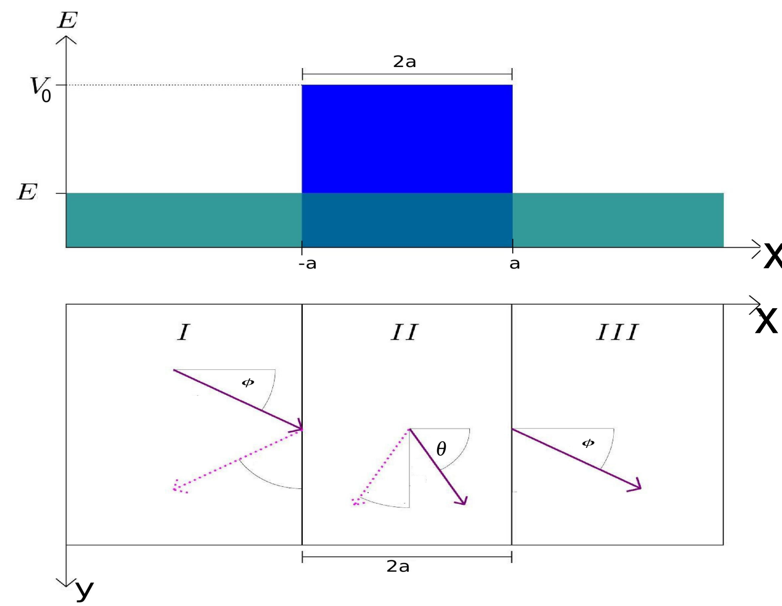
$$\psi_2(x,y) = \begin{cases} s\left[e^{ik_x x + i\phi} + re^{-ik_x x - i\phi}\right] e^{ik_y y} & x < -a \\ s'\left[Ae^{iq_x x + i\theta} + Be^{-iq_x x - i\theta}\right] e^{ik_y y} & -a < x < a \\ ste^{ik_x x + ik_y y + i\phi} & x > a \end{cases}$$

$$s = \mathrm{sign}(E)$$
$$s' = \mathrm{sign}(E - V_0)$$

# KLEIN – Tunneling in Single-layer Graphene

Using the matching condition:

$$
\begin{aligned}
e^{-ik_xa}+re^{ik_xa} &= Ae^{-iq_xa}+Be^{iq_xa}\\
s\left[e^{-ik_xa+i\phi}+re^{ik_xa-i\phi}\right] &= s'\left[Ae^{-iq_xa+i\theta}+Be^{iq_xa-i\theta}\right]\\
Ae^{iq_xa}+Be^{-iq_xa} &= te^{ik_xa}\\
s'\left[Ae^{iq_xa+i\theta}+Be^{-iq_xa-i\theta}\right] &= ste^{ik_xa+i\phi}
\end{aligned}
$$




4 equations for 4 unknown parameters

reflexion coefficient:

$$
\begin{aligned}
r &= 2e^{i\phi-2ik_xa}\sin(2q_xa)\\
&\times \frac{\sin\phi - ss'\sin\theta}{ss'\left[e^{-2iq_xa}\cos(\phi+\theta)+e^{2iq_xa}\cos(\phi-\theta)\right]-2i\sin(2q_xa)}
\end{aligned}
$$

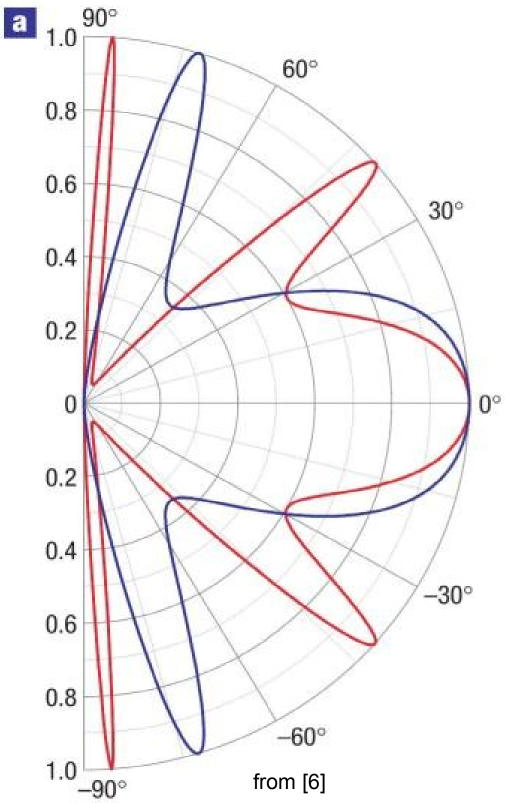
momentum conservation for monolayer graphene:

$$\sin(\phi)=\frac{V_0-E}{E}\sin(\theta)$$

transmission: $T=|t|^2=1-|r|^2$

$$\boxed{T=\frac{\cos^2(\phi)\cos^2(\theta)}{\cos^2(2q_xa)\cos^2(\phi)\cos^2(\theta)+(1-ss'\sin(\phi)\sin(\theta))^2\sin^2(2q_xa)}}$$

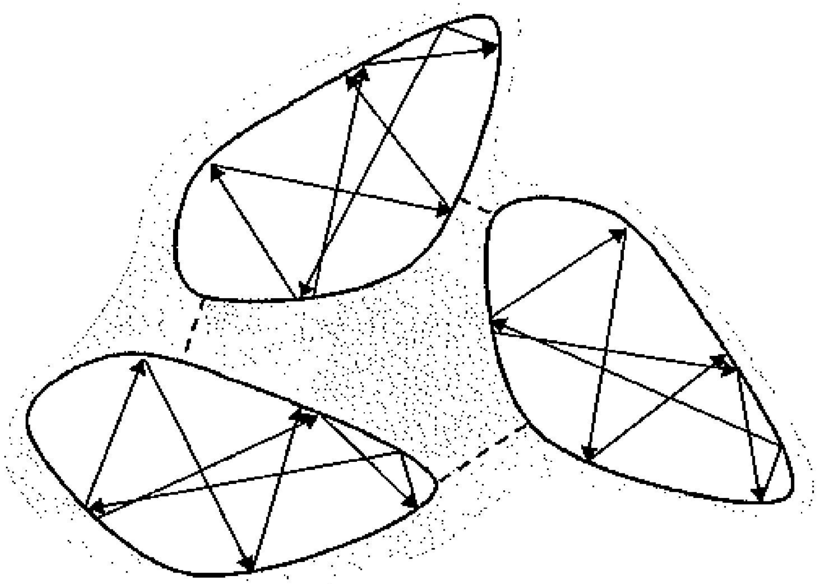
# KLEIN – Tunneling in Single-layer Graphene



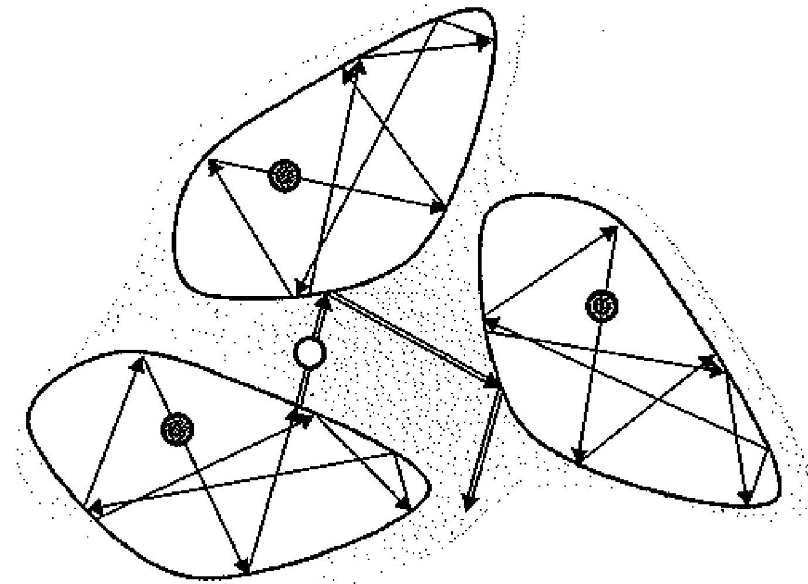

from [6]

„Transmission probabilities through a 100-nm-wide barrier as a function of the angle of incidence for single layer grahene. The elecron concentration n outside the barrier is chosen as 0.5x10^(12) 1/cm for all cases. Inside the barrier, hole concentration p are 10^(12) 1/cm for the red and 3x10^(12) 1/cm for the blue curve (typical values for experiments). This corresponds to a Fermi-energy of ca. 80 meV. The barrier height is chosen 200 meV for the red and 285 meV for the blue curve“. ( from [2])

# KLEIN – Tunneling and Conductivity



Electronic states in a conventional semiconductor (from [2])



Electronic states in graphene (from [2])

$\mu$ - chemical potential
$v$ - velocity
$\tau$ - sattering time

Einsteins relation for conductivity: $\sigma = e^2 \dfrac{\partial n}{\partial \mu} D$

with $\dfrac{\partial n}{\partial \mu} = N(E_F) = \dfrac{2|E_F|}{\pi \hbar^2 v^2} = \dfrac{2k_f}{\pi \hbar v}$ (for graphene), and the diffusion coefficient $D = \dfrac{1}{2} v^2 \tau$

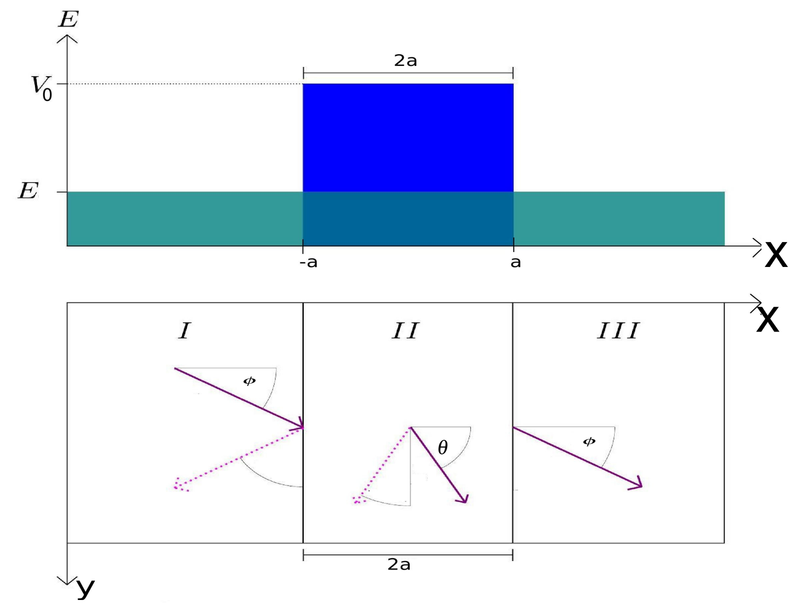
conductivity: $\sigma = \dfrac{e^2}{\pi \hbar} k_F l = \dfrac{2e^2}{h} k_F l$

# Chiral Tunneling in Bilayer Graphene

Assumptions: $|E|, |E - V_0| \ll 2|\gamma_1|$ → energies smaller than interlayer hopping

$ka, qa > |\frac{\gamma_3 \gamma_1}{\gamma_0^2}|$ → no trigonal warping effects

Potential:




$$k = \sqrt{\frac{2m^*|E|}{\hbar^2}}$$

$$q = \sqrt{\frac{2m^*|E - V_0|}{\hbar^2}}$$

Ansatz:

$$\psi_1(x,y) = \psi_1(x) e^{ik_y y}$$

$$\psi_2(x,y) = \psi_2(x) e^{ik_y y}$$

# Chiral Tunneling in Bilayer Graphene

Second order equations:
$$\left(\frac{d^2}{dx^2}-k_y^2\right)^2\psi_i=k^4\psi_i$$ outside the barrier

$$\left(\frac{d^2}{dx^2}-k_y^2\right)^2\psi_i=q^4\psi_i$$ inside the barrier

Solutions:
$$\begin{aligned}
\psi_1^I(x) &= \alpha_1 e^{ik_x x}+\beta_1 e^{-ik_x x}+\gamma_1 e^{\chi_x x}\\
\psi_2^I(x) &= s\left[\alpha_1 e^{ik_x x+2i\phi}+\beta_1 e^{-ik_x x-2i\phi}+\gamma_1 h_1 e^{\chi_x x}\right]\\
\psi_1^{II} &= \alpha_2 e^{iq_x x}+\beta_2 e^{-iq_x x}+\gamma_2 e^{\chi_x' x}+\delta_2 e^{-\chi_x' x}\\
\psi_2^{II} &= s'\left[\alpha_2 e^{iq_x x+2i\theta}+\beta_2 e^{-iq_x x-2i\theta}-\gamma_2 h_2 e^{\chi_x' x}-\frac{\delta_2}{h_2}e^{-\chi_x' x}\right]\\
\psi_1^{III} &= \alpha_3 e^{ik_x x}+\delta_3 e^{-\chi_x x}\\
\psi_2^{III} &= s\left[\alpha_3 e^{ik_x x+2i\phi}-\frac{\delta_3}{h_1}e^{-\chi_x x}\right]
\end{aligned}$$

with

$$\chi_x=\sqrt{k_x^2+2k_y^2}=k\sqrt{1+sin^2\phi} \qquad \chi_x'=q\sqrt{1+sin^2\theta}$$

$$h_1=\left(\sqrt{1+sin^2\phi}-sin\phi\right)^2 \qquad h_2=\left(\sqrt{1+sin^2\theta}-sin\theta\right)^2$$

# Chiral Tunneling in Bilayer Graphene

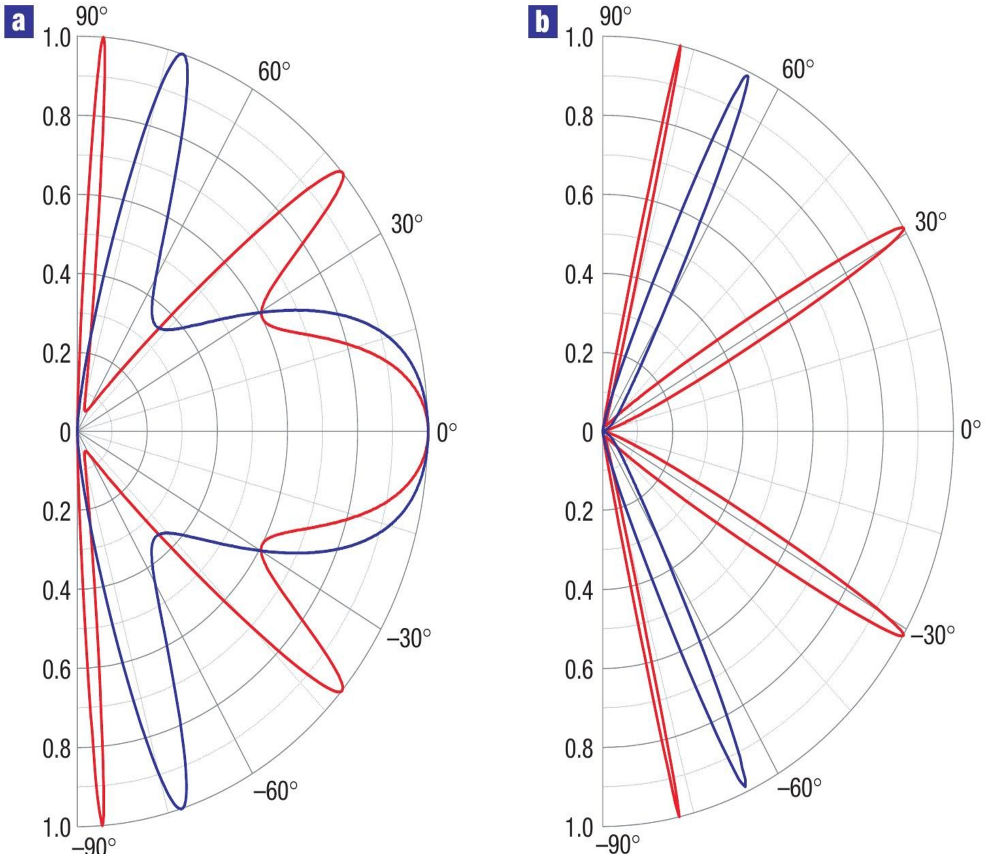
- Continuity conditions
  - eight equations for eight unknown parameters
  - Only numerical solution possible

- transmission coefficient for the special case $\phi = \theta = 0$

$$t = \frac{\alpha_3}{\alpha_1} = \frac{4ikqe^{2ika}}{(q+ik)^2 e^{-2qa} - (q-ik)^2 e^{2qa}}$$

  - exponential decay!!

# Chiral Tunneling in Bilayer Graphene

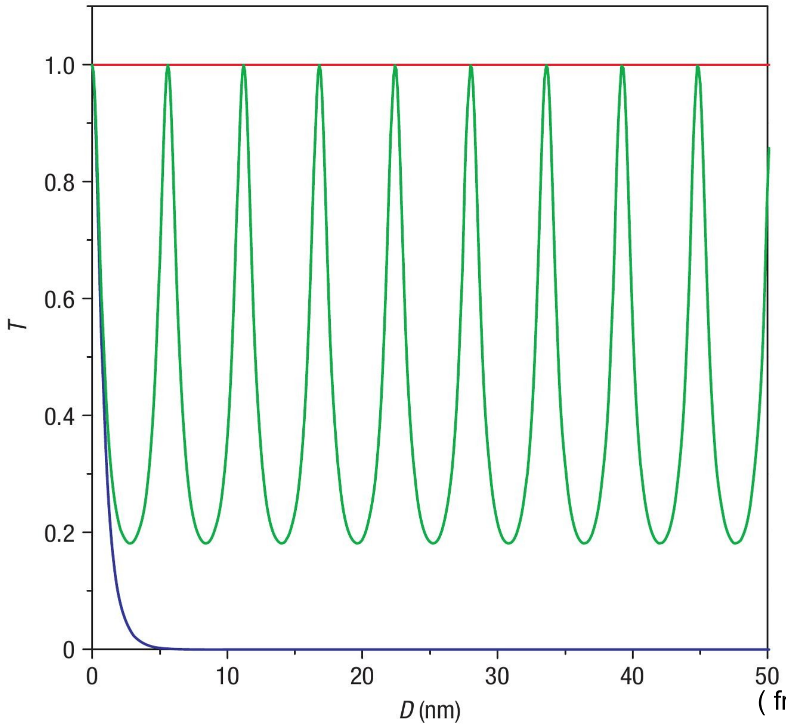



- no perfect transmission for perpendicular incidence in bilayer graphene, but in monolayer graphene
- magic angles with perfect transmission in monolayer and bilayer graphene
- sharper peaks (magic angles) in bilayer graphene than in monolayer graphene → less transmission for most angles

**Figure 2 Klein-like quantum tunnelling in graphene systems. a**,**b**, Transmission probability $T$ through a 100-nm-wide barrier as a function of the incident angle for single- (**a**) and bi-layer (**b**) graphene. The electron concentration $n$ outside the barrier is chosen as $0.5 \times 10^{12}$ cm$^{-2}$ for all cases. Inside the barrier, hole concentrations $p$ are $1 \times 10^{12}$ and $3 \times 10^{12}$ cm$^{-2}$ for red and blue curves, respectively (such concentrations are most typical in experiments with graphene). This corresponds to the Fermi energy $E$ of incident electrons ≈80 and 17 meV for single- and bi-layer graphene, respectively, and $\lambda \approx 50$ nm. The barrier heights $V_0$ are (**a**) 200 and (**b**) 50 meV (red curves) and (**a**) 285 and (**b**) 100 meV (blue curves). ( from [6])

# KLEIN – Tunneling

perpendicular incidence:




( from [6])

Fig. 4.10. The transmission probability $T$ for normally incident electrons in single-layer and bilayer graphene and in a nonchiral zero-gap semiconductor as a function of the width $D$ of the tunnel barrier. The concentrations of charge carriers are chosen as $n = 0.5 \times 10^{12}$ cm$^{-2}$ and $p = 1 \times 10^{13}$ cm$^{-2}$ outside and inside the barrier, respectively, for all three cases. The transmission probability for bilayer graphene (the lowest line) decays exponentially with the barrier width, even though there are plenty of electronic states inside the barrier. For single-layer graphene it is always 1 (the upper line). For the nonchiral semiconductor it oscillates with the width of the barrier (the intermediate curve). (Reproduced with permission from Katsnelson, Novoselov & Geim, 2006.) ( from [2])

- perfect transmission for monolayer graphene for arbitary width of the tunnel barrier
- transmission decays exponentially for bilayer graphene
  → semiclassical behaviour
- oscillating transmission for nonchiral semiconductor
- even though the dispersion for both bilayer graphene and conventional semiconductor are parabolic, there is a difference in their tuneling behaviour
  → chirality

# Conclusion

Due to Klein tunneling one cannot confine electrons by electrostatic gates in monolayer graphene

→ not very useful for applications (e.g. quantum dots)

In bilayer graphene for the case of $\phi = \theta = 0$ the tunneling disappears

→ higher capability for application

# Literature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[6] Kartnelson, Geim et al.: Chiral tunnelling and the Klein paradox in graphene, Published online: 20 August 2006; doi:10.1038/nphys384