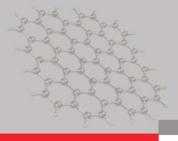
# Velocity-Modulation in Bilayer Graphene

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In memory of Prof. Malek Zareyan (1971-2014)

Workshop on "Quantum transport in graphene" Apr. 2014, IPM



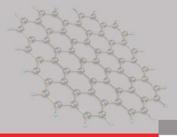
## Outline

### >Introduction:

- Bilayer Graphene: *Tight-binding model*
- ✤Fermi velocity modulation in graphene

### > Hamiltonian in presence of velocity modulation and gate bias:

- Spectrum and band gap behavior
- > Tunneling through velocity and electrostatic barriers:
- \*Optical analogous of MDFs, Wave guide designed bilayer graphene
- ≻Conclusion

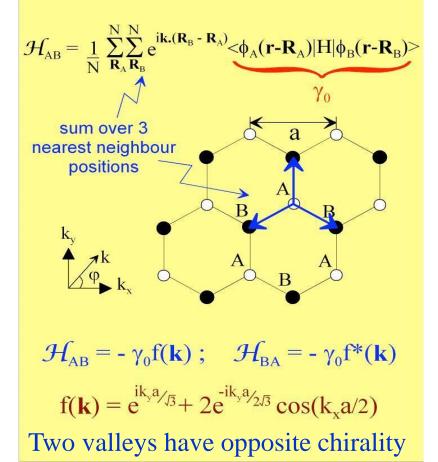


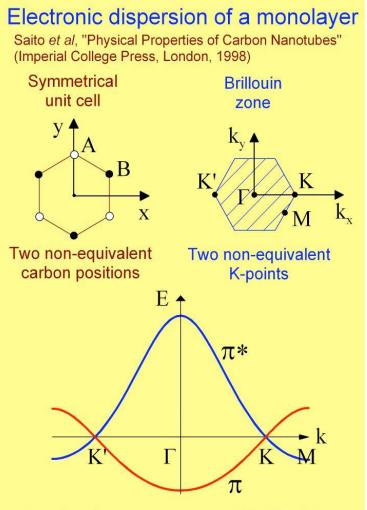
### **Monolayer Graphene**

#### In the Tight Binding Model:wallace1947

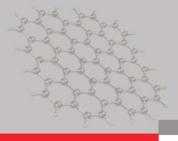
Transfer integral on a hexagonal lattice

 $\mathcal{H}_{AB} = <\!\!\Phi_A |H| \Phi_B \!>$ 

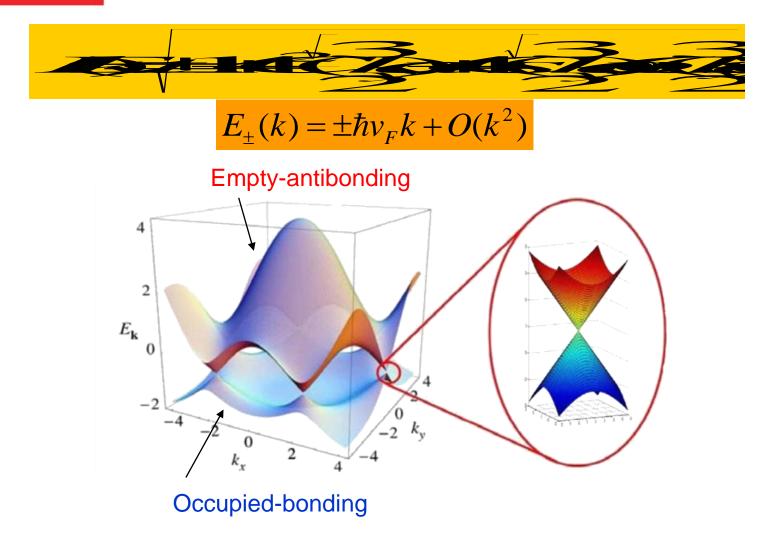




Two bands: no energy gap at the K-points

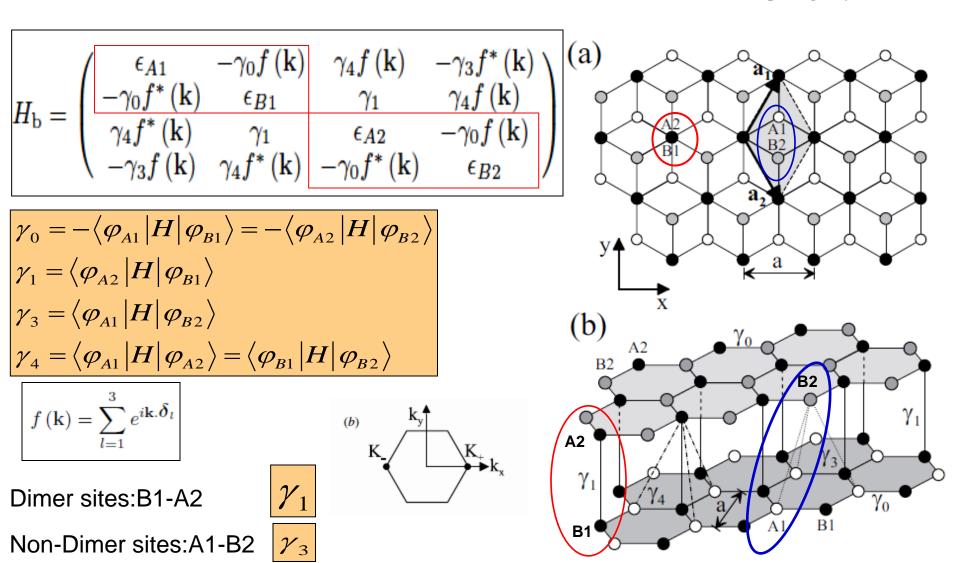


### **Spectrum of Monolayer Graphene**

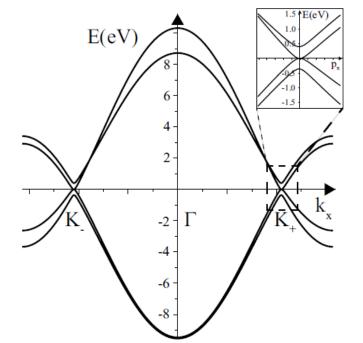


### Bilayer Graphene: the Tight Binding model

E. Mccann, et al. 2013 Rep. Prog. Phys. 76 056503



### Bilayer Graphene: the Tight Binding model



E. Mccann, et al. 2013 Rep. Prog. Phys. 76 056503

A bonding and anti-bonding pair arising from the strong coupling of the dimer B1 and A2 sites.
The '*low-energy*' bands arise from hopping between the non-dimer A1 and B2 sites.

$$\varepsilon \approx \frac{p^2}{2m} \quad m = \gamma_1/2v^2$$

 $\mathbf{p} = \hbar \mathbf{k} - \hbar \mathbf{K}_{\xi}$  $f(\mathbf{k}) \approx -\sqrt{3}a(\xi p_x - ip_y)/2\hbar$ 

Parameter	Graphite [48]	Bilayer [57]	Bilayer [36]	Bilayer [37]	Bilayer [61]	Trilayer [63]
$\gamma_{ m o}$	3.16(5)	2.9	$3.0^{a}$	-	3.16(3)	$3.1^{a}$
$\gamma_1$	0.39(1)	0.30	0.40(1)	0.404(10)	0.381(3)	$0.39^{a}$
$\gamma_2$	-0.020(2)	_	-	-	-	-0.028(4)
$\gamma_3$	0.315(15)	0.10	$0.3^{a}$	-	0.38(6)	$0.315^{a}$
$\gamma_4$	0.044(24)	0.12	0.15(4)	-	0.14(3)	0.041(10)

### Effective 4-band Hamiltonian at low energy

$$H_{\rm b} = \begin{pmatrix} \epsilon_{A1} & v\pi^{\dagger} & v_{3}\pi \\ v\pi & \epsilon_{B1} \\ -v_{4}\pi & \gamma_{1} \\ v_{3}\pi^{\dagger} & -v_{4}\pi \end{pmatrix} \xrightarrow{-v_{4}\pi^{\dagger}} v_{3}\pi \\ \epsilon_{A2} & v\pi^{\dagger} \\ v\pi & \epsilon_{B2} \end{pmatrix} \text{Neglecting } \underbrace{\gamma_{4} = 0}_{E} = \pm \epsilon_{\alpha}(p), \alpha = 1, 2$$

$$\epsilon_{\alpha}^{2} = \frac{\gamma_{1}^{2}}{2} + \frac{U^{2}}{4} + \left(v^{2} + \frac{v_{3}^{2}}{2}\right)p^{2} + (-1)^{\alpha}\sqrt{\Gamma},$$

$$\Gamma = \frac{1}{4}\left(\gamma_{1}^{2} - v_{3}^{2}p^{2}\right)^{2} + v^{2}p^{2}\left[\gamma_{1}^{2} + U^{2} + v_{3}^{2}p^{2}\right] \\ +2\xi\gamma_{1}v_{3}v^{2}p^{3}\cos 3\varphi,$$

$$\pi = \xi p_{x} + ip_{y}, \xi = \pm 1 \quad \& \quad v = \sqrt{3}a\gamma_{0}/2\hbar$$

$$v_{3} = \sqrt{3}a\gamma_{3}/2\hbar \quad \& \quad v_{4} = \sqrt{3}a\gamma_{4}/2\hbar$$

$$U = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{B1}) - (\epsilon_{A2} + \epsilon_{B2})\right] \\ \Delta' = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{B2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right]$$

$$\int_{A_{AB}}^{A_{AB}=0, U=0} \frac{\epsilon_{AB}}{\epsilon_{AB}} \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right]$$

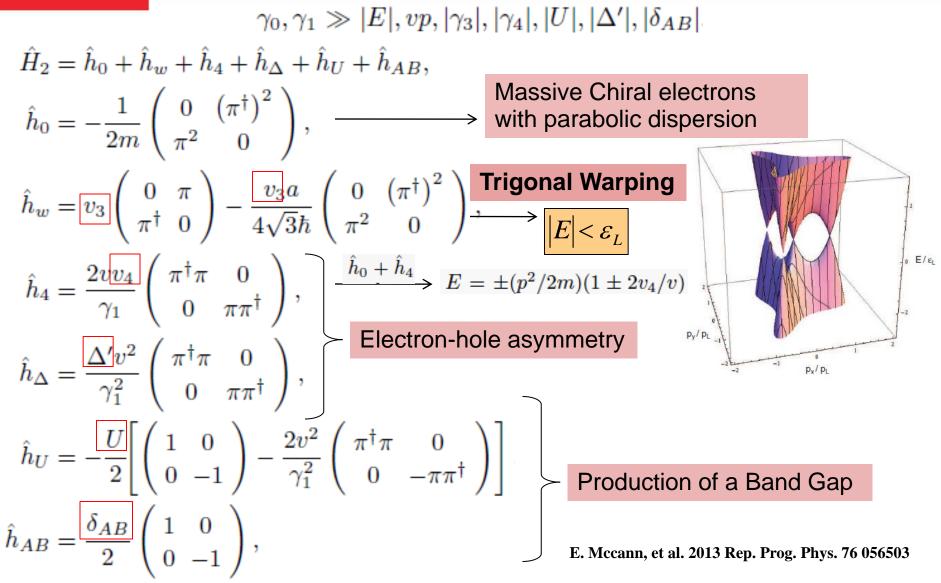
$$\int_{A_{AB}=0, U=0}^{A_{AB}=0, U=0, 2eV} \frac{\epsilon_{AB}}{\epsilon_{AB}} \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right]$$

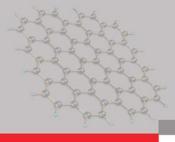
$$\int_{A_{AB}=0, U=0}^{A_{AB}=0, U=0, 2eV} \frac{\epsilon_{AB}}{\epsilon_{AB}} \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right]$$

$$\int_{A_{AB}=0, U=0}^{A_{AB}=0, U=0, 2eV} \frac{\epsilon_{AB}}{\epsilon_{AB}} \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{B1} + \epsilon_{B2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2}) - (\epsilon_{A1} + \epsilon_{A2})\right] \\ \delta_{AB} = \frac{1}{2}\left[(\epsilon_{A1} + \epsilon_{A2} + \epsilon_{A$$

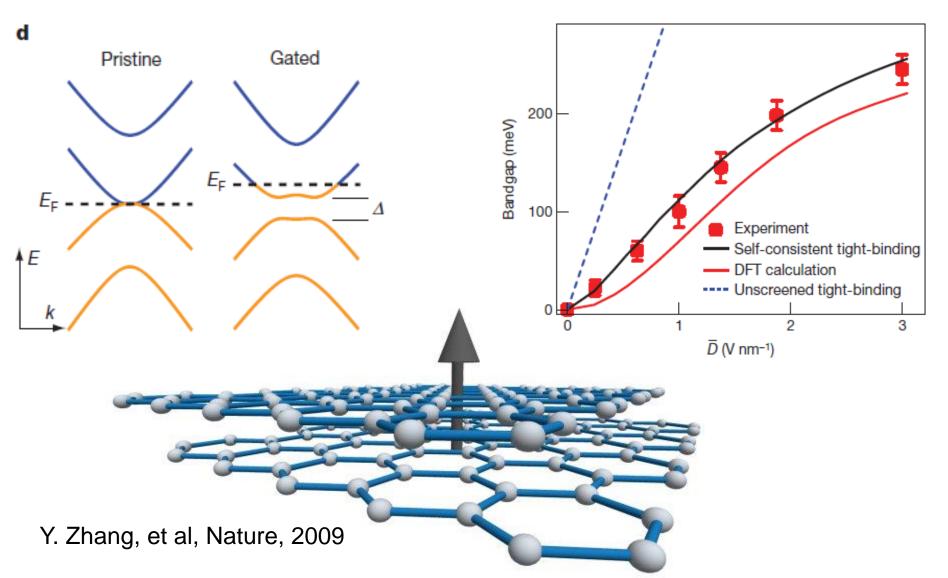


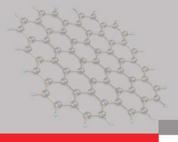
# Effective two band model for non-dimer sites





### Tunable Band gap in Bilayer Graphene

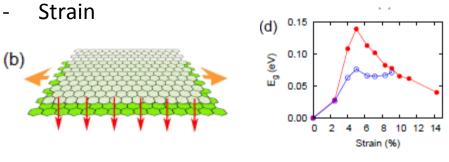




### Velocity Modulation in Graphene

### There are several ways to engineer Fermi velocity :

- e-e interaction
- Modifications in curvature of graphene sheet
- Periodic potential (Graphene superlattices)
- Appropriate doping
- Dielectric screening

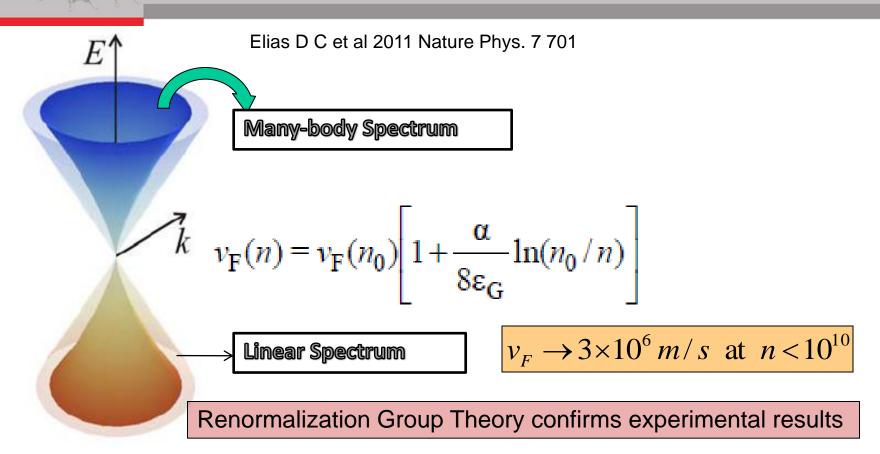


Nano Lett., 2010, 10 (9), pp 3486-3489

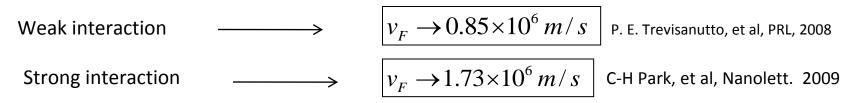
$$v_{ij} = v_0 \left[ \eta_{ij} + \frac{\beta}{4} (2u_{ij} + \eta_{ij} u_{kk}) \right],$$

Phys. Rev. Lett. 108, 227205 (2012)

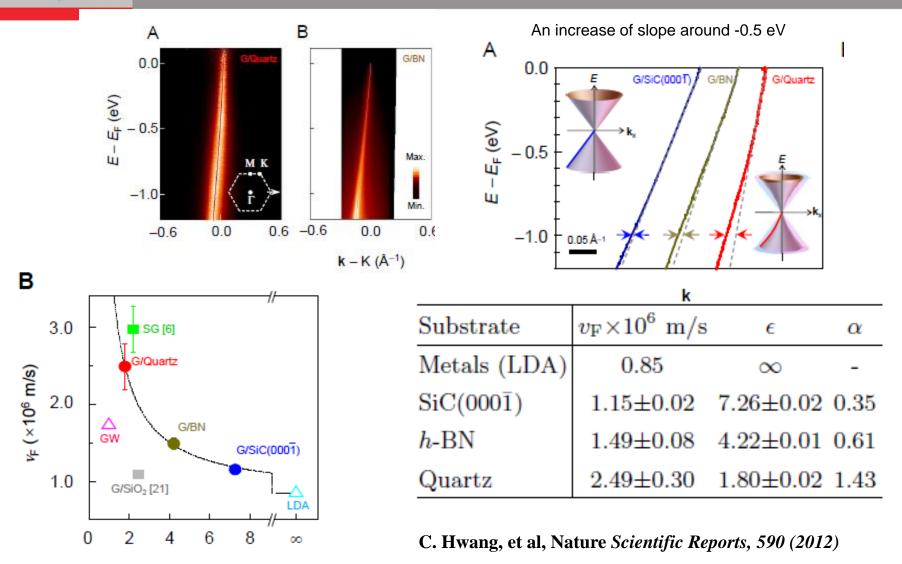
# Dirac cones reshaped by interaction effects in suspended graphene



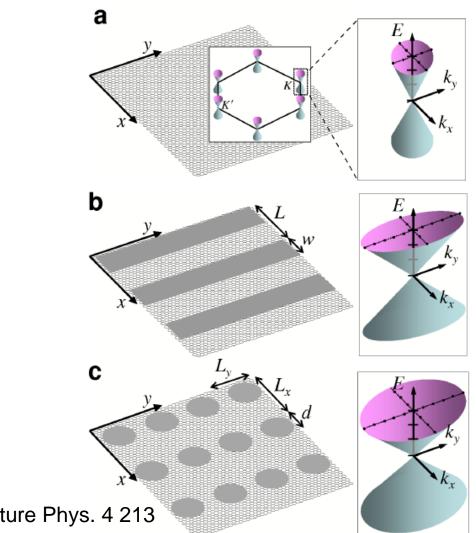
Non-local interband exchange leads to a renormalized Fermi velocity (G. Borghi, et al, SSC, 2009)



### Fermi velocity engineering by substrate modification



#### Anisotropic behaviors of massless Dirac fermions in graphene under periodic potential



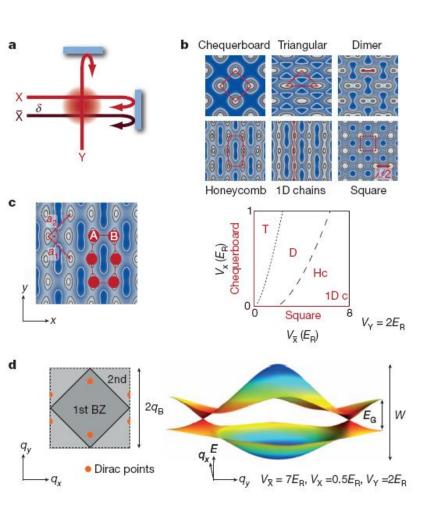
Park C H et al 2008 Nature Phys. 4 213

### LETTER

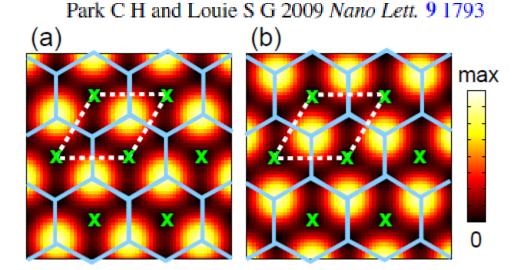
doi:10.1038/nature10871

## Creating, moving and merging Dirac points with a Fermi gas in a tunable honeycomb lattice

Leticia Tarruell<sup>1</sup>, Daniel Greif<sup>1</sup>, Thomas Uehlinger<sup>1</sup>, Gregor Jotzu<sup>1</sup> & Tilman Esslinger<sup>1</sup>



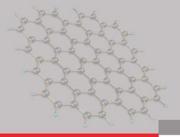
#### Making massless Dirac fermions from patterned 2DEG



$$M = \hbar \frac{v_0}{2} \left( k_x \sigma_x + k_y \sigma_y \right) .$$
$$v_g = v_0/2 = \frac{\hbar K}{2m^*} = \frac{2\pi\hbar}{3m^*L} .$$

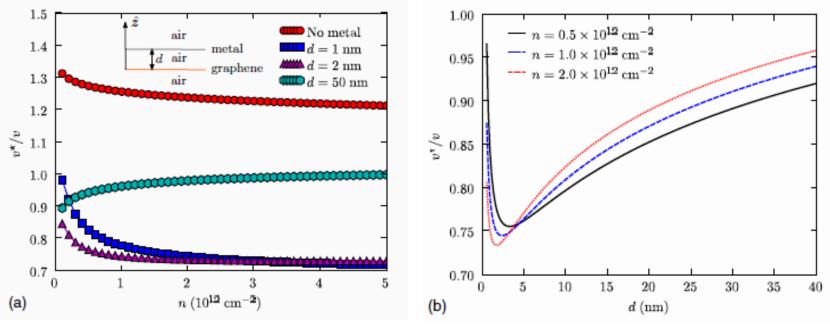
## Dirac Cone has been also observed in other honeycomb crystals:

- Acoustic surface waves (PRL2012)
- Photonic Crystals (nature 2012)



Many-body renormalized Fermi velocity induced by remote metallic gates

- Consider a grounded metal plane placed close to a graphene sheet.
- Quasiparticles under the screening plane move at a speed v\* that is smaller than in an isolated graphene sheet



A. Rauox, et al, PRB,81, 073407 (2010)

### Bilayer graphene in presence of effective velocity modulation: **Hamiltonian**

H.C, F. Adinehvand, JPCM, 26, 015302 (2014)

We consider the following dominant Four-band Hamiltonian:

$$H = \begin{pmatrix} -i\hbar v_{u}(\sigma \cdot \nabla)^{\dagger} + V_{u}I & F \\ F & -i\hbar v_{d}(\sigma \cdot \nabla) + V_{d}I \end{pmatrix}$$
where
$$F = \begin{pmatrix} t & 0 \\ 0 & 0 \end{pmatrix}, \quad -i\hbar v \sigma \cdot \nabla = \begin{pmatrix} 0 & \pi^{\dagger} \\ \pi & 0 \end{pmatrix}$$

$$\pi = -i\hbar v (\partial_{x} - k_{y}) \quad t=390 \text{ meV}$$

$$V_{u} = \xi_{u}V_{F}$$
are Fermi velocity in the upper and lower layers
$$V_{u} = \xi_{d}V_{F}$$
are electrostatic potential in the upper and lower layers
$$V_{u} = V_{0} + \delta$$

$$V_{d} = V_{0} - \delta$$

$$\overline{\Psi} = \begin{pmatrix} \psi_{A_{2}}^{u} & \psi_{B_{1}}^{u} & \psi_{A_{1}}^{d} \end{pmatrix}^{T}}$$
are eigen-function of Hamiltonian

# Bilayer graphene in presence of effective velocity modulation: **Spectrum**

$$\begin{split} k(E)^2 &= [a \pm \sqrt{a^2 - b}] / v_{\rm u}^2 \\ a(E, \eta, \delta) &= [\eta^2 (E - \delta)^2 + (E + \delta)^2] / 2 \\ b(E, \eta, \delta) &= \eta^2 (E^2 - \delta^2) (E^2 - \delta^2 - t^2) \\ \eta &= \xi_{\rm u} / \xi_{\rm d}. \end{split}$$

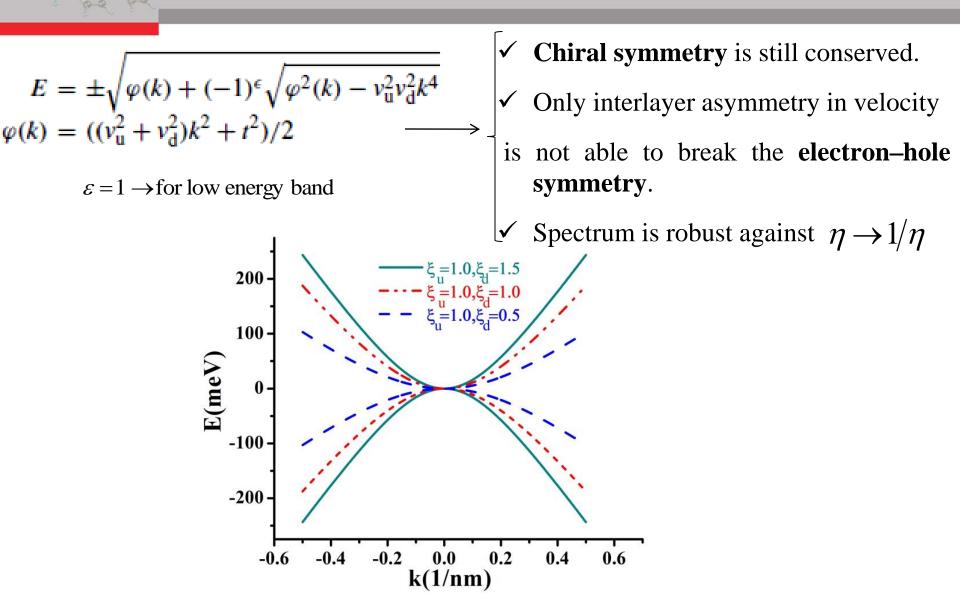
#### There are two extremum conditions: Band Gap Conditions

$$b = 0 \quad \forall \quad k = 0 \rightarrow E = \pm \delta, \pm (t + \delta)$$
$$b = a^2 \quad \forall \quad k_{c/v}(\xi_u, \xi_d) = \pm (v_u)^{-1} \sqrt{a(E_{c/v}, \eta, \delta)}$$

Results in the energy gap  $\implies E_g(\eta) = E_c(\eta) - E_v(\eta)$ 

At k=0, the gap is independent of the velocity ratio.

Gapless spectrum in presence of interlayer asymmetry in velocity but for  $\delta = 0$ 



Band structure in presence of interlayer asymmetry in potential but symmetry in velocity: **direct band gap** 

$$\eta = 1 , \ \delta \neq 0 , \ v_u = v_d = v$$

$$E^2 = (vk)^2 + \delta^2 + t^2/2 + (-1)^{\epsilon}$$

$$\times \sqrt{(vk)^2(4\delta^2 + t^2) + t^4/4 + k^2}.$$

$$\varepsilon = 1 \rightarrow \text{Mexican hat structure}$$

$$k_{gap} = \pm (2\delta/v_F) \sqrt{(t^2 + 2\delta^2)/(t^2 + 4\delta^2)} \frac{1}{\xi}$$

$$\int_{g} \delta < t \Rightarrow E_g \rightarrow t \quad (\text{Band Gap Saturation})$$
For both limit:
$$k_{gap} \propto 2\delta/v$$

$$k_{gap} \propto 2\delta/v$$

$$k_{gap} = \frac{1}{2} \delta = \frac{1}{$$

# Band structure in presence of interlayer asymmetry in potential and velocity: **e-h asymmetry**

 $\eta \! \neq \! 1$  ,  $\delta \! \neq \! 0$ 

✓e-h asymmetry:  $E_c ≠ -E_v \forall k ≠ 0$ ✓Indirect Band gap  $k_c ≠ k_v$ ✓The gap depends on η instead of velocities

e-h asymmetric factor:  $r = (|E_c| - |E_v|) / |E_c|$ 

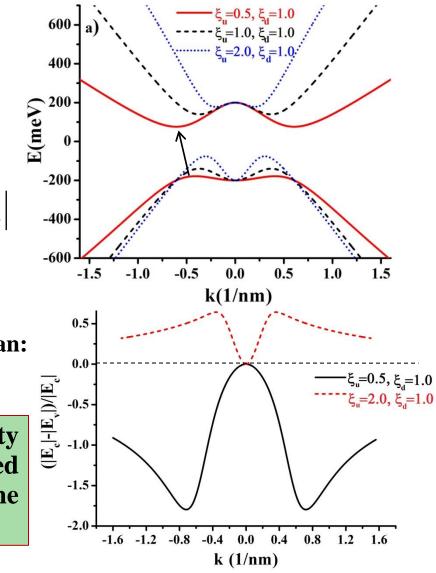
$$\eta \to \eta^{-1} \Longrightarrow r \to r^{-1}$$

Conduction band exchange with valence band

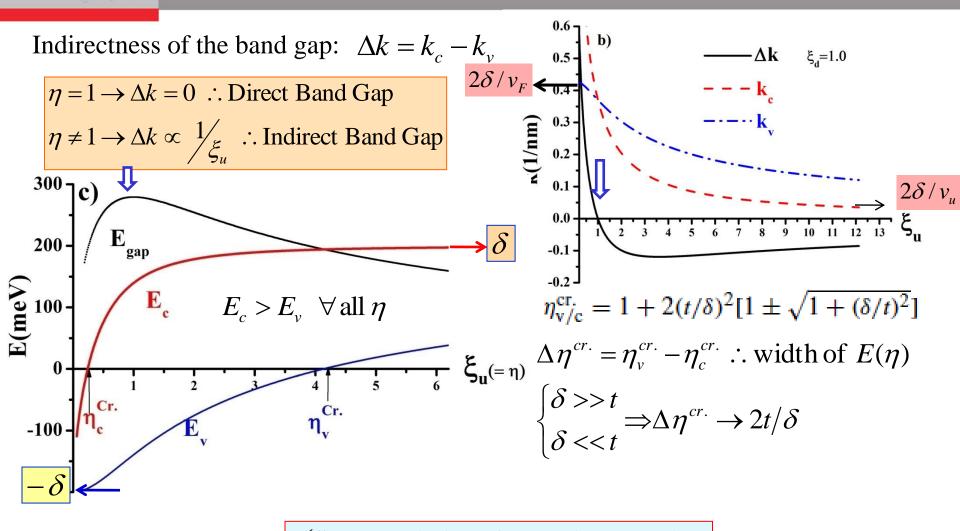
e-h asymmetric factor caused by Full Hamiltonian:

$$r = 4\gamma_4 / \gamma_0 \approx 0.1$$

the e-h asymmetry arising from the velocity engineering is a dominant factor compared with the e-h asymmetry caused by the parameter  $\gamma_4$ 

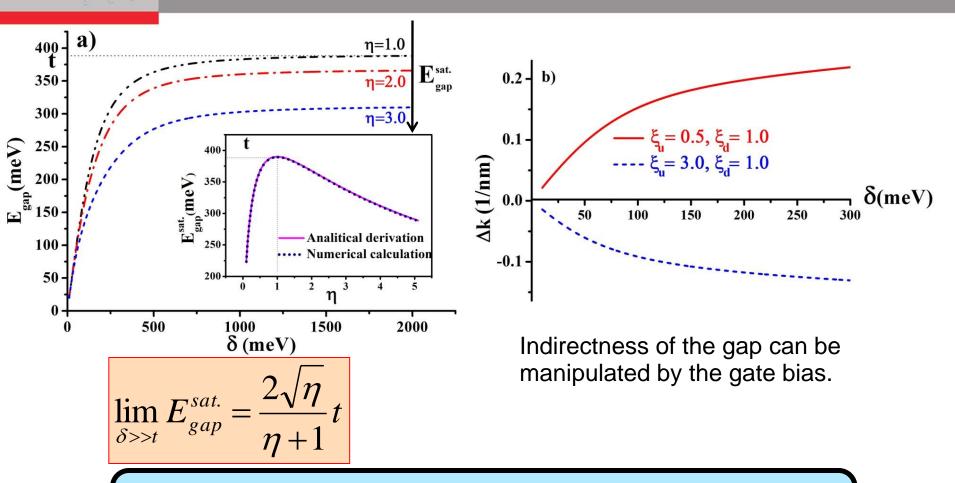


## Band structure in presence of interlayer asymmetry in potential and velocity: **indirect band gap**



**✓** Sharp variation of  $E(\eta)$  in large bias

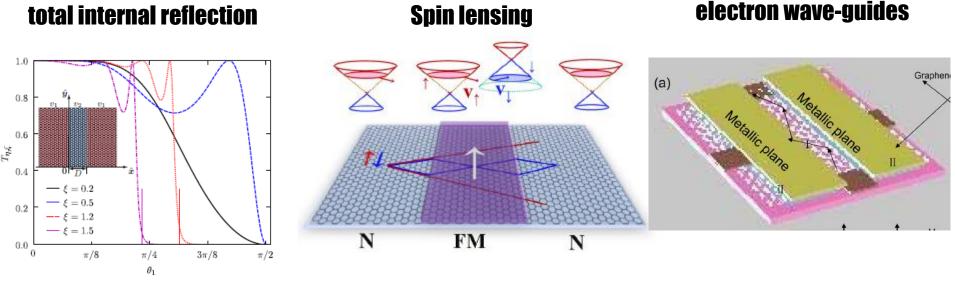
## Band structure in presence of interlayer asymmetry in potential and velocity: **Saturated indirect band gap**



the dependence of the energy gap on the velocity ratio can be manifested in transport properties through a velocity junction.

### Analogy between MDF transport and light propagation

- ✓ MDF's velocity is independent of the wavelength, the same as the speed of light.
- ✓ The optical-like behaviors of electron waves in graphene such as focusing, collimation, Bragg reflection, electron wave-guides, total internal reflection.



A. Rauox, et al, PRB2010 A. G. Moghaddam, M. Zareyan, PRL2010

J. Yuan, et al, APL2011

# Transport properties across non-uniform potential and velocity junctions: **transfer matrix method**

a)

- Current density operator
- Continuity equation:  $\vec{\nabla} \cdot \vec{j} = -\partial_t \rho$  $j_i = \Phi_i^T \sum \Phi_i$  $\Sigma = \begin{pmatrix} \sigma^T & 0 \\ 0 & \sigma \end{pmatrix} \qquad \widetilde{v}_i = \begin{pmatrix} \sqrt{v_u^i} & 0 \\ 0 & \sqrt{v_d^i} \end{pmatrix}$  $v_{\mu}, v_{d}$  $\Phi_{i} = \widetilde{v}_{i} \psi_{i} \qquad \psi_{i} = \begin{pmatrix} \psi_{u} \\ \psi_{u} \end{pmatrix} \stackrel{b)}{}_{\delta = 0} \uparrow$ Auxiliary Spinor **Transfer Matrix Method** c) AE(meV)Assuming a plane wave solution for  $\delta \neq 0$ the Hamiltonian:  $\psi(x) = P(x)A$ d) U(x)2δ΄ Coefficients matrix Plane wave matrix

# Transport properties across non-uniform potential and velocity junctions: **transfer matrix method**

Conservation of current density at the interfaces  $\longrightarrow$  Auxiliary spinor continuity

$$j_i = A_i^T P_i^T \widetilde{v}_i^T \sum \widetilde{v}_i P_i A_i \qquad \blacksquare \qquad \Rightarrow \Phi_1 = \Phi_2 \rightarrow \widetilde{v}_1 \psi_1 = \widetilde{v}_2 \psi_2$$

 $A_{1} = MA_{3}$  $M = P_{1}^{-1}(0)\tilde{v}_{1}^{-1}\tilde{v}_{2}P_{2}(0)P_{2}^{-1}(w)\tilde{v}_{2}^{-1}\tilde{v}_{3}P_{3}(w) \quad \longleftarrow \quad \text{Transfer matrix}$ 

$$A_1 = \begin{pmatrix} 1 \ r \ 0 \ e_g \end{pmatrix}^\top, \qquad A_3 = \begin{pmatrix} t \ 0 \ e_d \ 0 \end{pmatrix}^\top$$

**Transmission Probability** 

Conductance

Transport properties across non-uniform potential and velocity junctions: **Wave function** 

$$\psi(x) = P(x)A$$

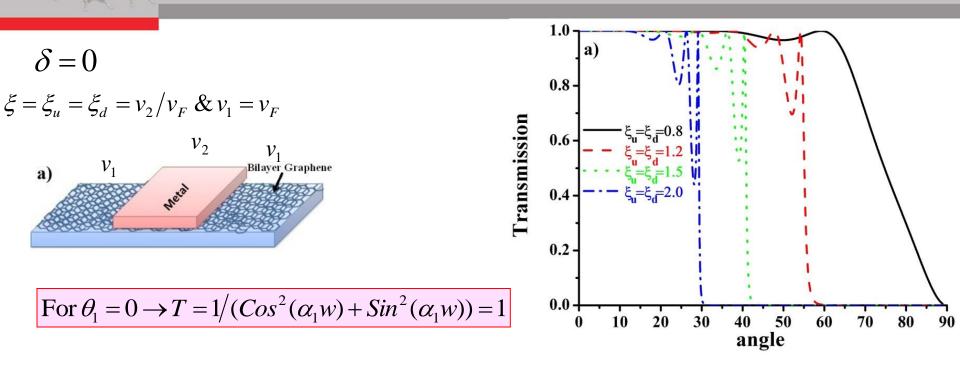
$$P(x) = \begin{pmatrix} e^{i\alpha_{+}x} & e^{-i\alpha_{+}x} & e^{i\alpha_{-}x} & e^{-i\alpha_{-}x} \\ f_{+}^{+}e^{i\alpha_{+}x} & f_{+}^{-}e^{-i\alpha_{+}x} & f_{-}^{+}e^{i\alpha_{-}x} & f_{-}^{-}e^{-i\alpha_{-}x} \\ s_{+}e^{i\alpha_{+}x} & s_{+}e^{-i\alpha_{+}x} & s_{-}e^{i\alpha_{-}x} & s_{-}e^{-i\alpha_{-}x} \\ g_{+}^{+}s_{+}e^{i\alpha_{+}x} & g_{+}^{-}s_{+}e^{-i\alpha_{+}x} & g_{-}^{+}s_{-}e^{i\alpha_{-}x} & g_{-}^{-}s_{-}e^{-i\alpha_{-}x} \end{pmatrix}$$

$$\alpha_{\pm} =$$

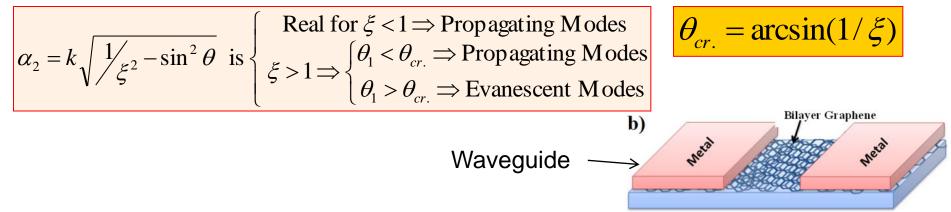
$$\sqrt{a(\varepsilon,\eta,\delta) - v_{u}^{2}k_{y}^{2} \pm \sqrt{a(\varepsilon,\eta,\delta)^{2} - b(\varepsilon,\eta,\delta)}/v_{u}}$$
$$A = \left(U_{A_{2}} U_{B_{2}} D_{B_{1}} D_{A_{1}}\right)^{\mathrm{T}}$$

### Transport across a single pure velocity barrier

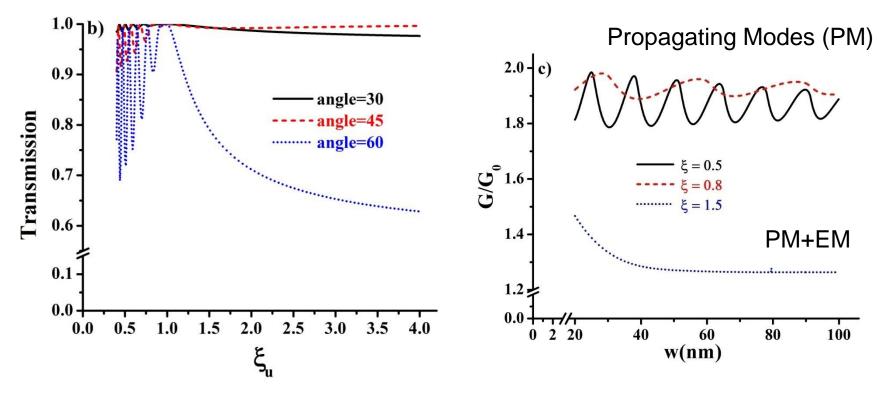
Total internal reflection



#### The wavevector inside the barrier



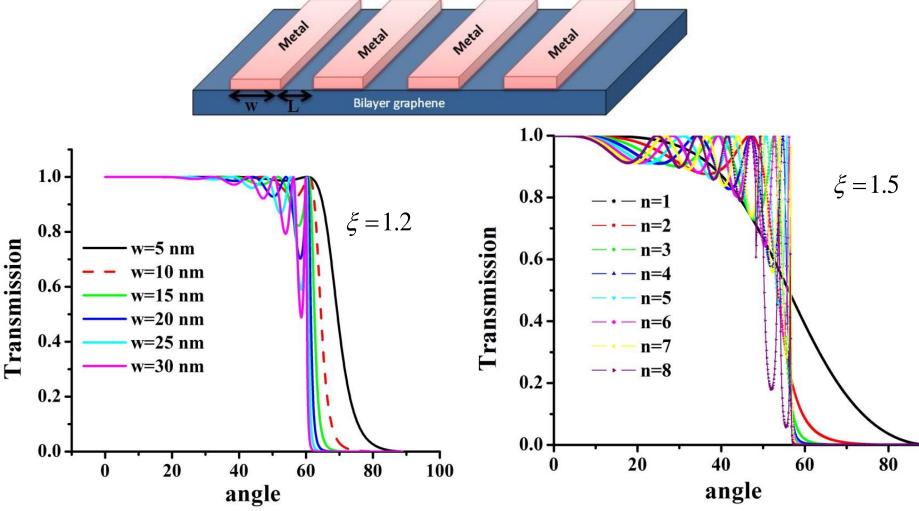
### Transport across a single pure velocity barrier



**Resonance Condition** 

 $\alpha_2 w = n\pi \ \forall \xi < 1$ 

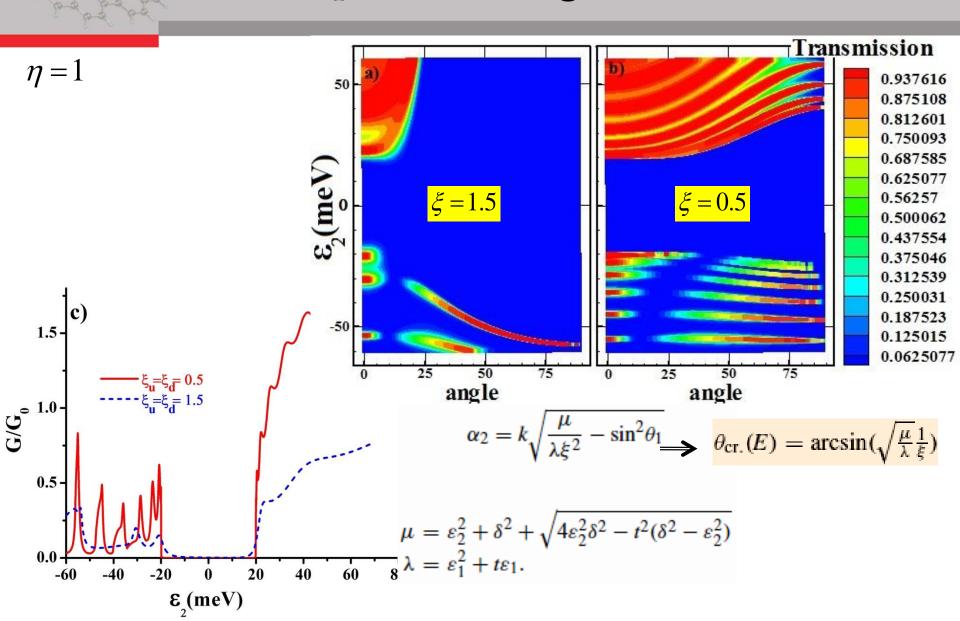
### Transport across multiple structure of pure velocity barriers



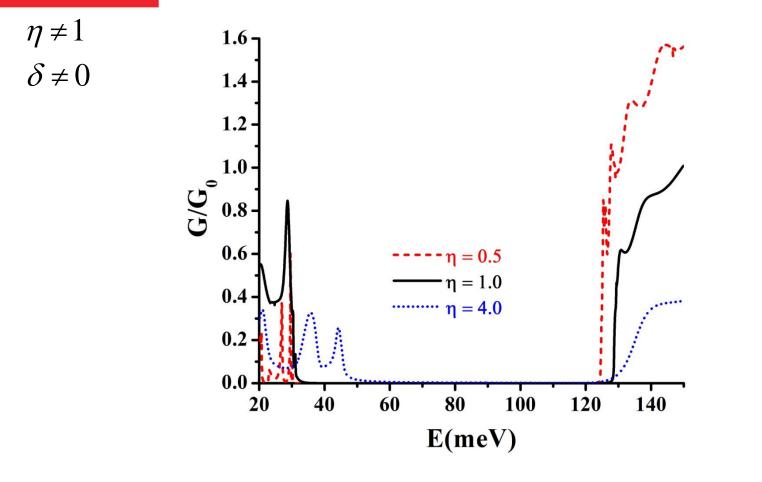
n=7

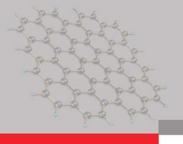
W=10 nm

Transport across velocity barrier in presence of a gate bias  $\delta \neq 0$ 



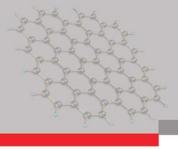
### Transport gap depends on the velocity ratio





## Conclusion

- The chiral symmetry is conserved for pure velocity modulation  $\delta = 0$  .
- In the broken-symmetry BLG, e-h symmetry preserved whenever the same velocity is modulated in both layers  $\eta = 1$ . In this case, the band gap is direct.
- In the broken-symmetry BLG and non-equal velocities in two layers η ≠ 1 result in a transition of the direct to indirect band gap. The electron–hole symmetry fails. Indirectness increases with the gate bias.
- In analogy with optics, we propose a total internal reflection angle.
- The transport gap which is induced by application of the gate bias in the barrier region depends on the velocity ratio.



- Collaboration: Fatemeh Adinehvand (PhD student)
- With special thanks:

### Dr. Reza Asgari

### Thank you for your attention

# Transmission through a barrier on bilayer graphene $\eta = 1 \& \xi = 1$

