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Quantum transport in twisted bilayer graphene

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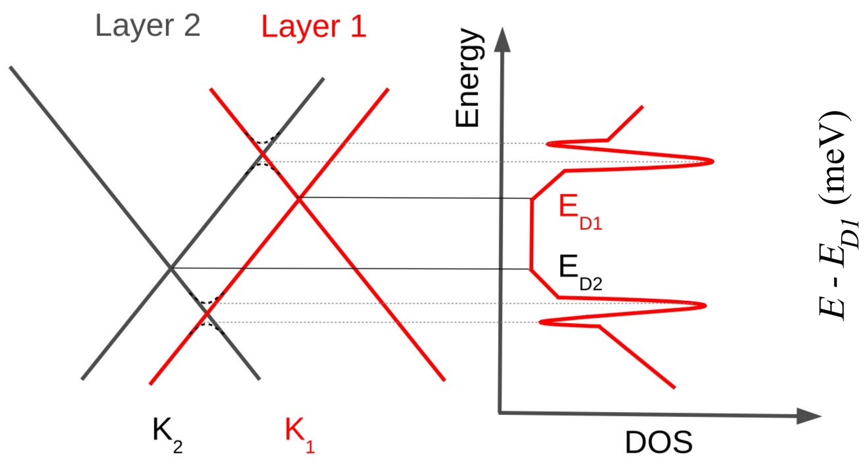
ABSTRACT: It has been shown theoretically and experimentally that twisted bilayer graphene (TBG), forming Moiré patterns, confine electrons in a tunable way as a function of the rotation angle [1-3]. The discovery of correlated insulators and superconductivity in 2018 [3] at so-called "magic angles" has stimulated an avalanche of experimental and theoretical activities. In the framework of the **Kubo-Greenwood formula for the conductivity**, we present **tight-binding (TB)** calculations of **quantum diffusion properties** in TBG at **various rotation angles θ** [4,5]. We analyze in particular the effect of **static defects**, the effect of and **electric bias**. One of the main results is that **flat-bands induce a breakdown of the standard Boltzmann theory of transport**.

This **anomalous quantum transport in flat-bands** can exist in other systems like **Quasicrystals** [6] and flat-bands induced by **defects in graphene** [7,8].

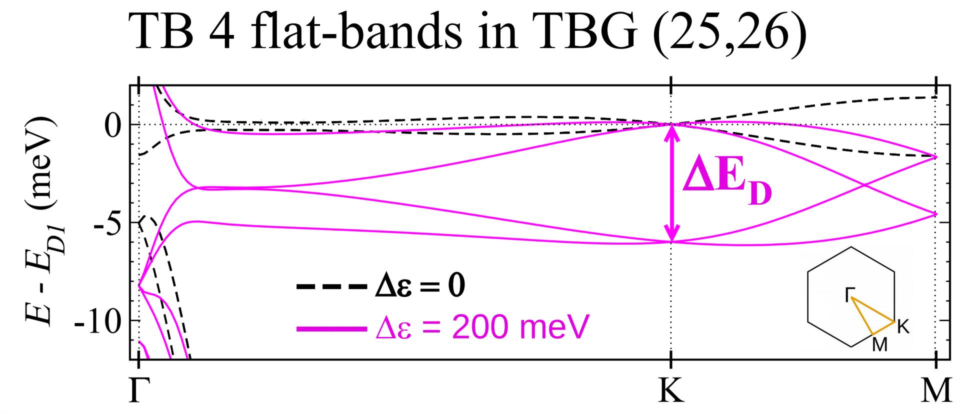
Effect of an electric bias on bands [4]

A difference Δε between the on-site energies of layer 1 and layer 2

⇒ **Difference ΔE_D** between the two corresponding Dirac energies



TB 4 flat-bands in TBG (25,26)

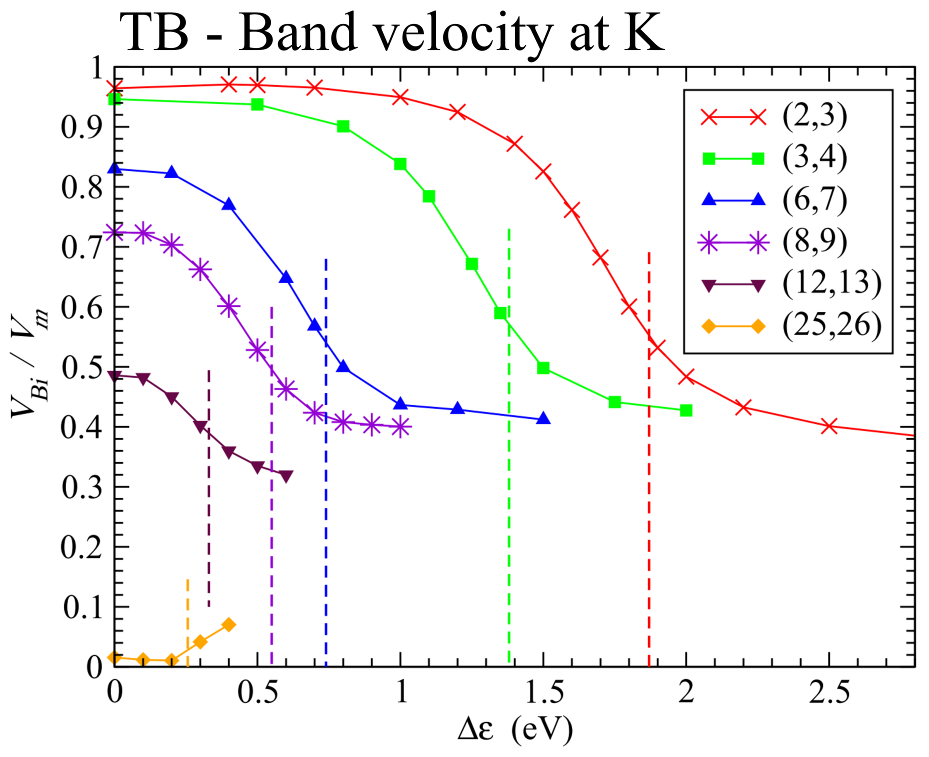


Twisted bilayer graphene (TBG) with varius rotation angle θ

(n,m)	θ (°)	N
(1,3)	32.20	52
(5,9)	18.73	604
(2,3)	13.17	76
(3,4)	9.43	148
(6,7)	5.08	508
(8,9)	3.89	868
(12,13)	2.65	1876
(15,16)	2.13	2884
(25,26)	1.30	7804
(33,34)	0.99	13468

N: number of atoms in a Moiré cell

TB - Band velocity at K



⇒ **Reduction of band velocity by bias potential**

Microscopic conductivity (static defects) [5]

Microscopic conductivity σ_M is a good estimation of **room temperature** conductivity (without quantum corrections)

With defects (vacancies) located in layer 2 only:

Continuous model:

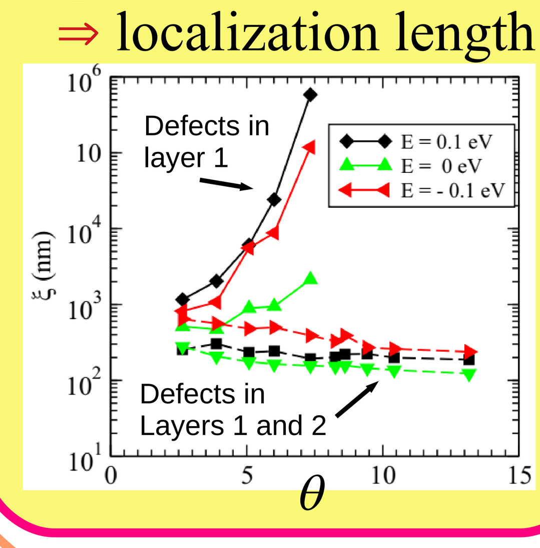
$$\sigma_M(E) \simeq \sigma_{M,\mathrm{MLG}}\left(1 + \frac{\rho_1(E)\,\theta^2}{\rho_2(E)\,\theta_0^2}\right)$$

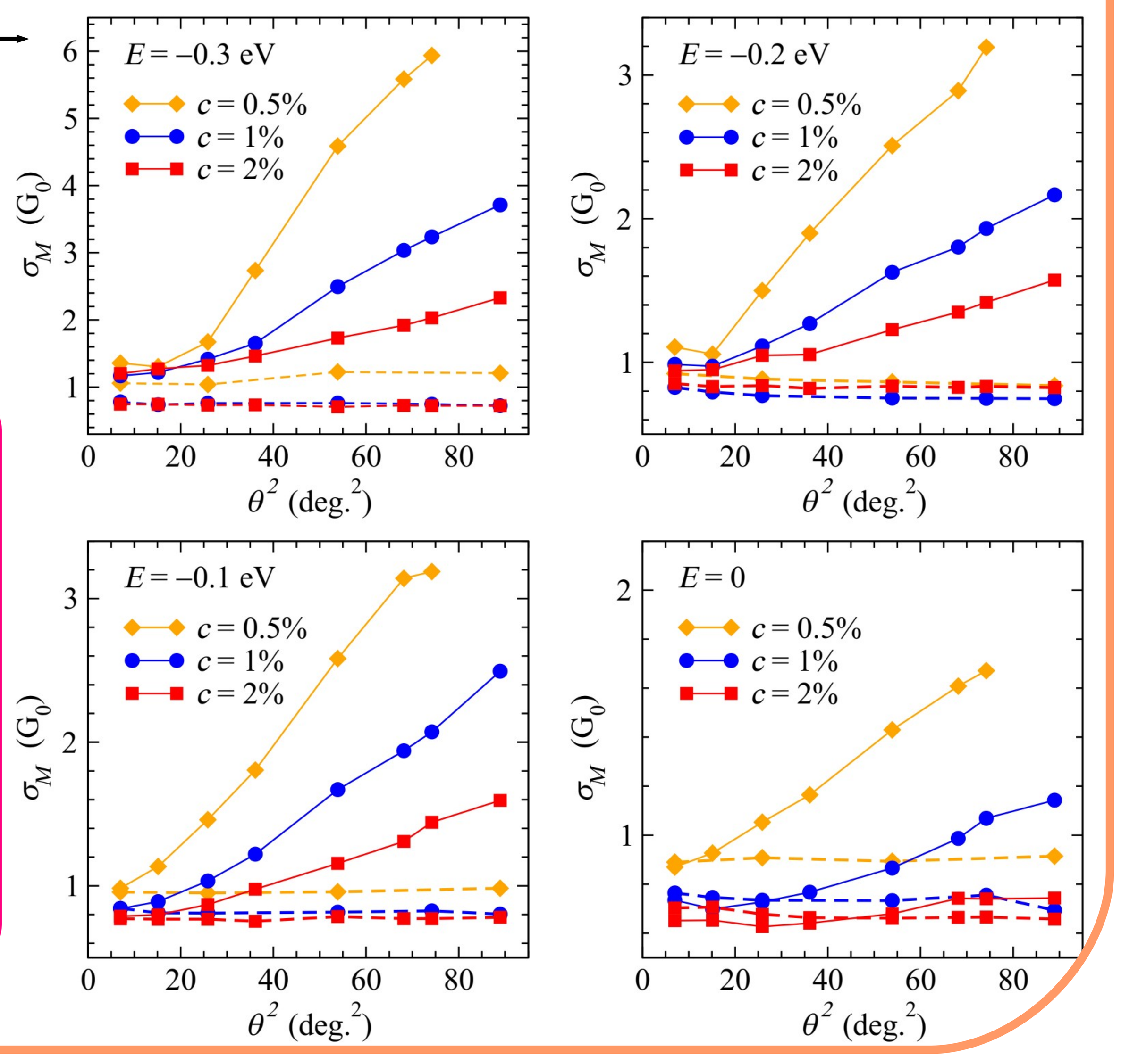
ρ_i DOS layer i, $\theta_0 \simeq 2°$

TB calculations:

For Fermi energy E closed to Dirac energy ($E_D = 0$), σ_M is almost linear with θ^2.

At **low temperature**: quantum corrections ⇒ localization length





Quantum diffusion: Boltzmann and non-Boltzmann terms [4]

Kubo-Greenwood dc-conductivity $\sigma_{xx}(E_F,\tau) = \frac{e^2}{S} n(E_F)\mathcal{D}(E_F,\tau)$

Diffusivity $D(E_F,\tau) = \frac{1}{2\tau^2}\int_0^\infty \Delta X^2(E_F,t)\, e^{-t/\tau}\, dt$

Relaxation time approximation: Scattering time (defect or phonon): τ

Mean square spreading: $\Delta X^2(E,t) = \left\langle (X(t) - X(0))^2 \right\rangle_E$

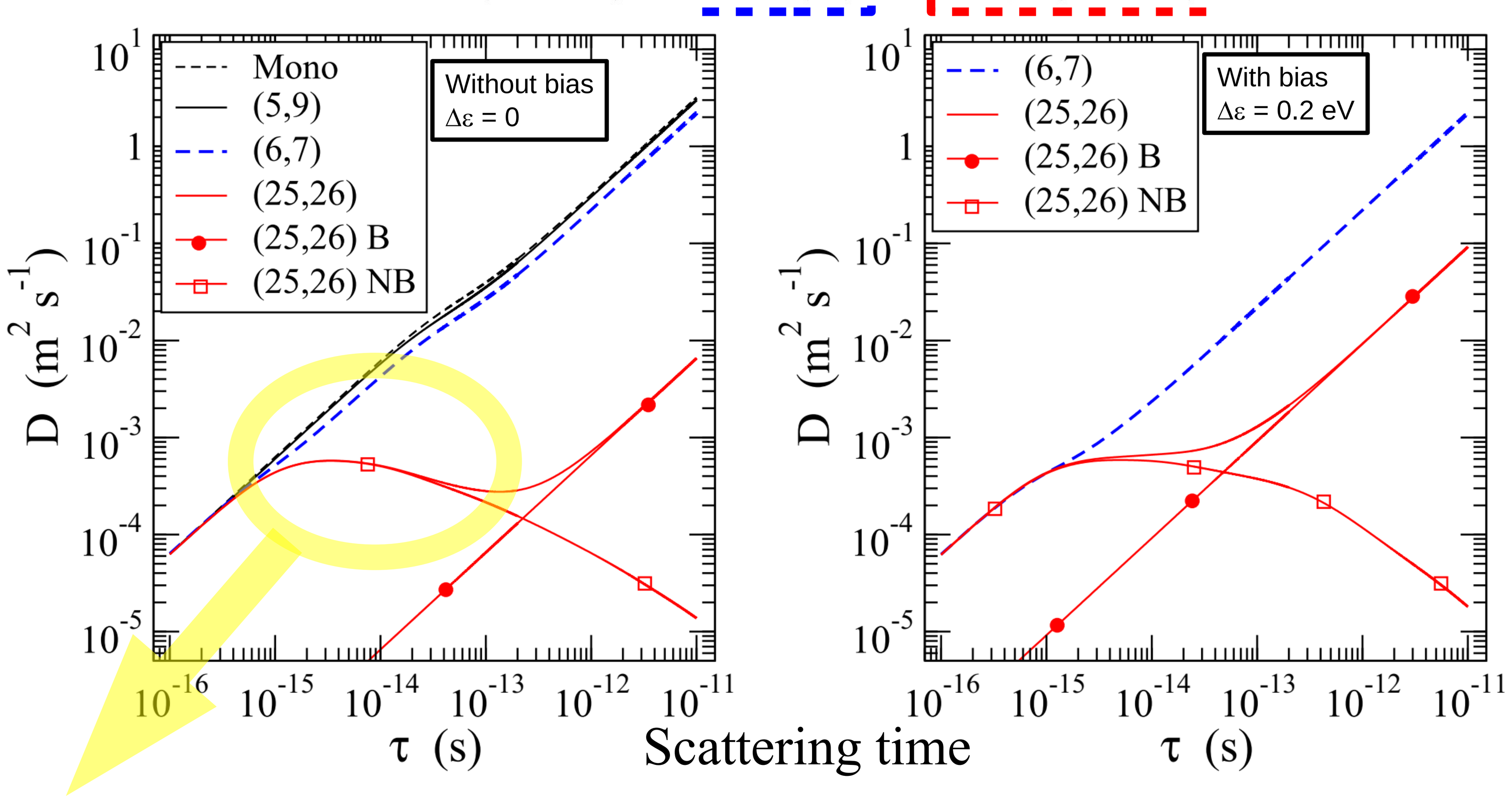
$$\Delta X^2(E,t) = 2\hbar^2 \left\langle \sum_{n'} \left[1 - \cos\left((E_n - E_{n'})\frac{t}{\hbar}\right)\right] \frac{\left|\langle n\vec{k}|V_x|n'\vec{k}\rangle\right|^2}{(E_n - E_{n'})^2} \right\rangle_{E_n = E} = V_B^2 t^2 + \Delta X_{NB}(E,t)$$

Velocity: $V_x = \frac{1}{i\hbar}[X,H]$

- Diagonal terms (**Boltzmann**): intra-bands
- Non diagonal terms (**Non Boltzmann**): inter-bands

Diffusivity of the 4 flat-bands of the Moiré (half-filling)

$$\mathcal{D}(E_F,\tau) = \mathcal{D}_B(\tau) + \mathcal{D}_{NB}(E_F,\tau)$$



⇒ **For Twisted Bilayer Graphene (25,26), θ = 1.3°, close to magic angle, Non-Boltzmann terms dominate in the conductivity**

SUMMARY:

- A applied **bias potential** –or and an asymmetric doping between the two layers– reduces the velocity of Dirac-bands in TBG
- **Conductivy** of TBG, with an asymmetric distribution of states defects between the two layers, **varies like θ^2**
- **Non-Bolzmann terms (inter-band hopping terms)** dominate in the quantum diffusion **in flat-bands** in TBG

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