Ballistic Interferences in Suspended Graphene
—Theoretical Modeling from Contact to Contact—

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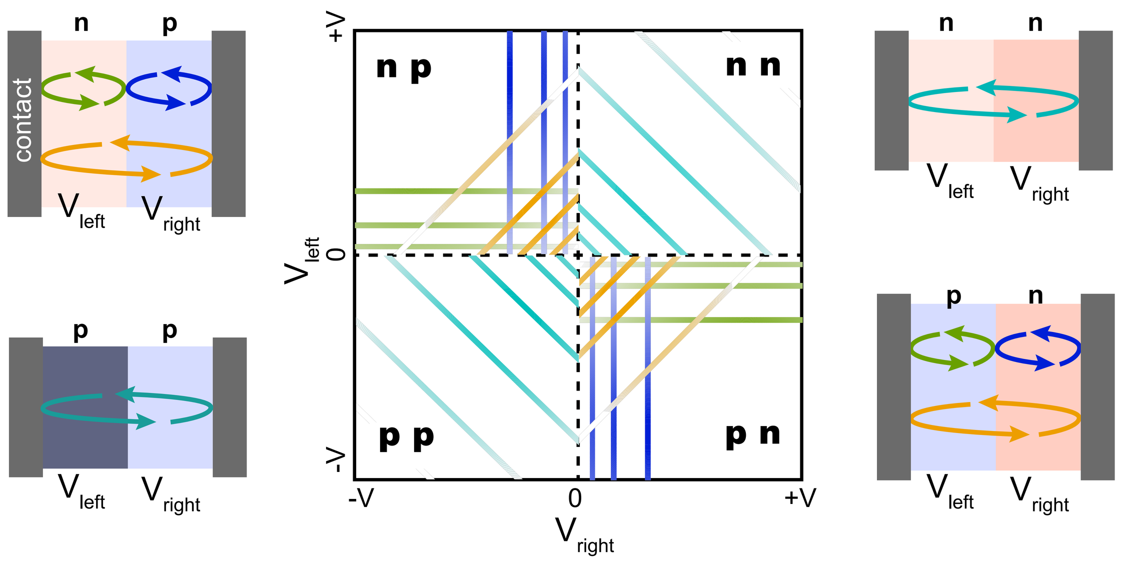
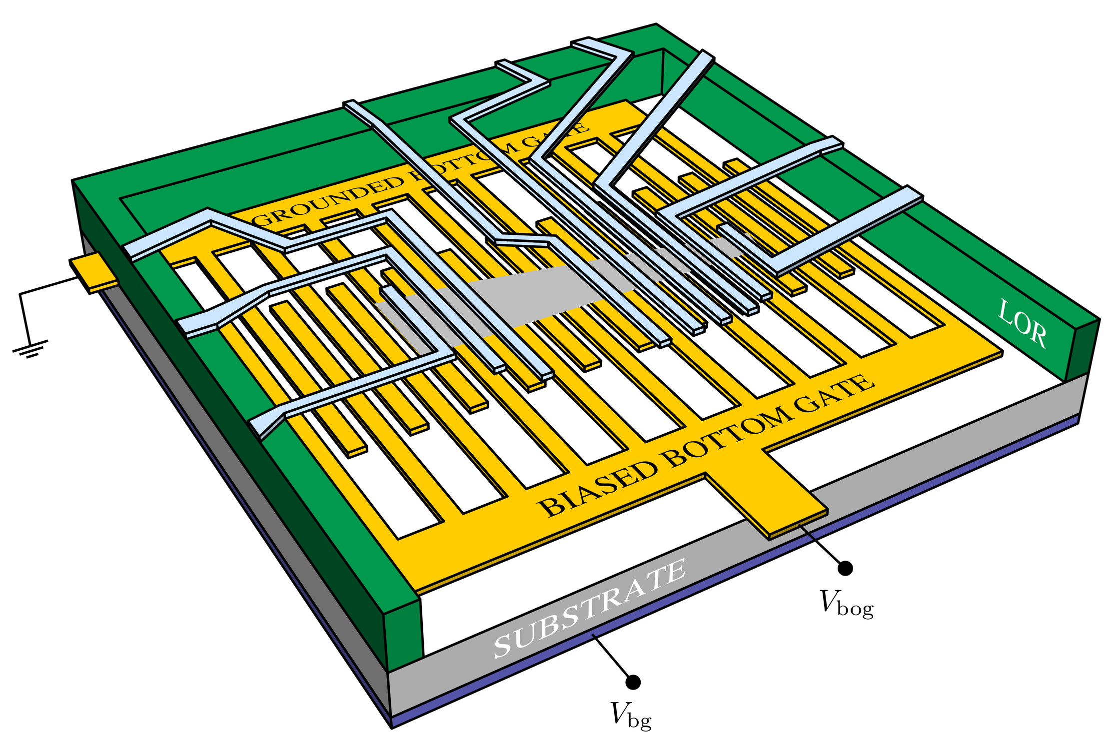
I. Motivation

I.1 Experimental: Can we measure these?

- For ideal control, one expects:



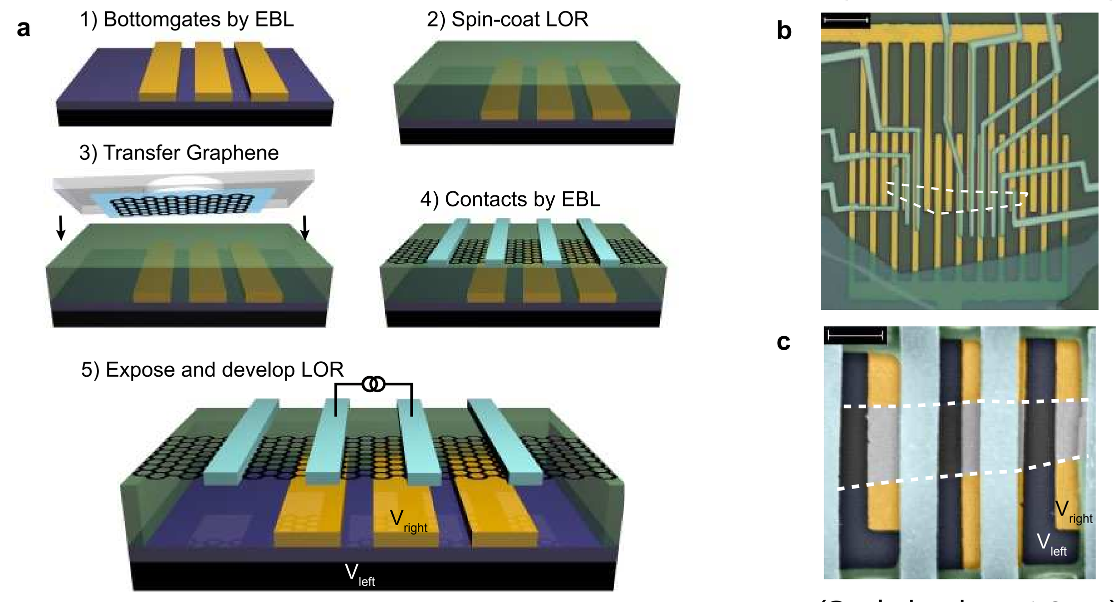
I.2 Theoretical: Can we model this?



II. Experiment

II.1 Device

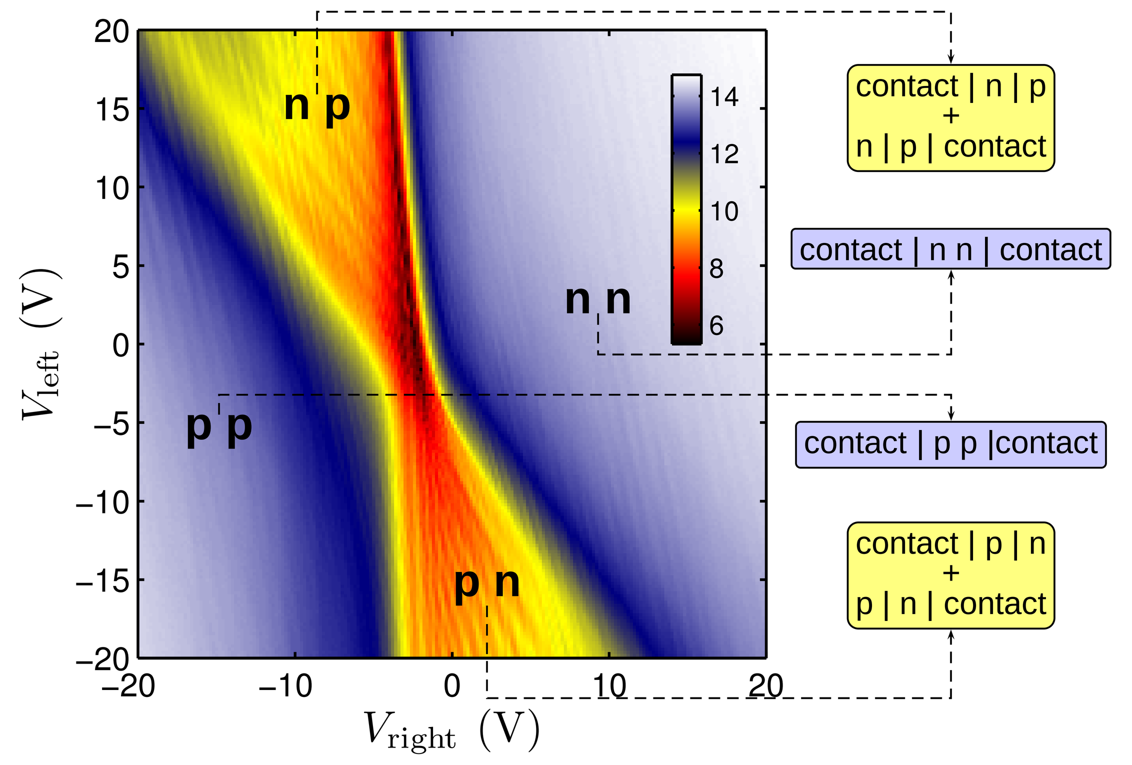
(Scale bar in **b**: 5 μm)



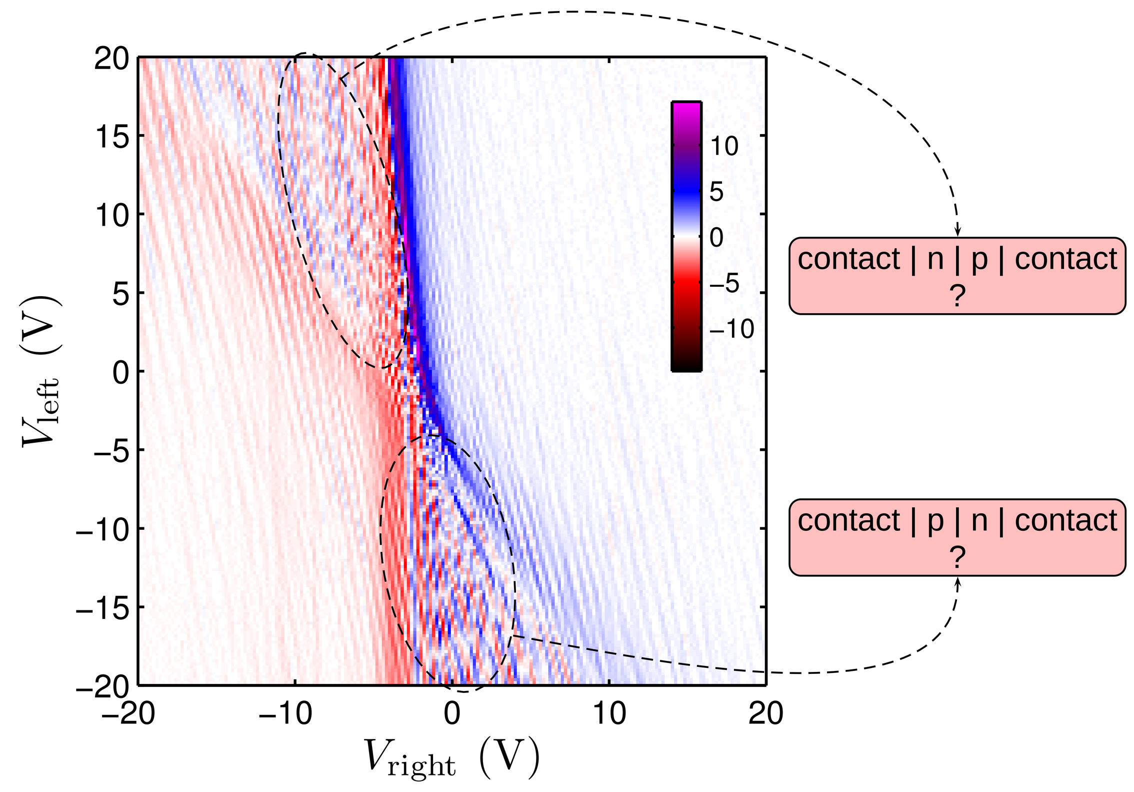
(Scale bar in **c**: 1.2 μm)

II.2 Conductance measurement

- Differential conductance measured at $T = 1.5$ K by standard lock-in techniques with a voltage bias of 100 μV at 77 Hz.
- Measured conductane map G (in e^2/h):

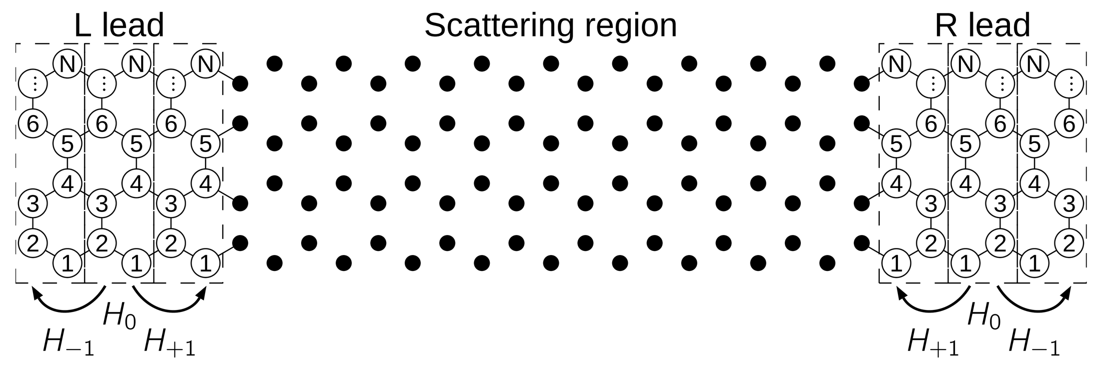


- Transconductance map dG/dV_{right}:



III. Theory

III.1 Real-space Green's function method



- Retarded Green's function of the scattering (S) region:

$$G_S^r(E) = \{E - [H_S + \textstyle\sum_{p=L,R}\Sigma_p(E)]\}^{-1}$$

  - H_S : Tight-binding model (TBM) Hamiltonian of the S region
  - Σ_p : self-energy of lead p, can be expressed in terms of H_0, $H_{\pm1}$ matrices[1]
- Transmission function (Fisher-Lee relation):

$$T = \mathrm{Tr}\left(\Gamma_R G_S^r \Gamma_L G_S^{r\dagger}\right), \quad \Gamma_{L|R} = i(\Sigma_{L|R} - \Sigma_{L|R}^\dagger)$$

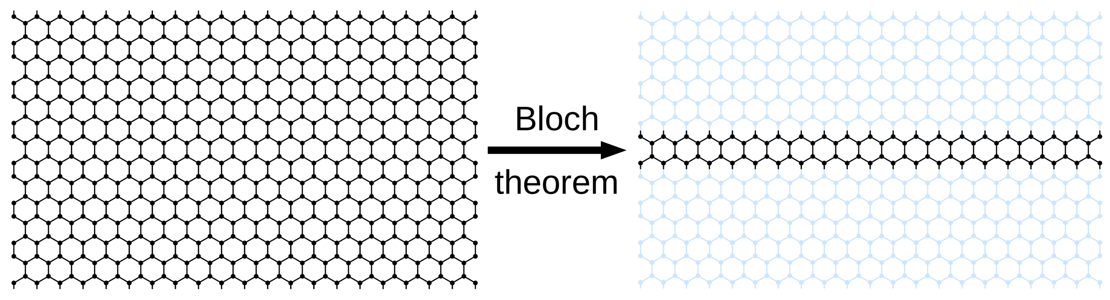
III.2 Model Hamiltonian

An efficient and accurate model Hamiltonian[2]

$$\boxed{\mathcal{H}_{model} = \mathcal{H}_{bulk} + \mathcal{V}_{real}}$$

requires:
- $\mathcal{H}_{bulk}$: Bloch-theorem-assisted TBM $\to$ efficient
- $\mathcal{V}_{real}$: Realistic on-site potential profiles $\to$ accurate

Minimal TBM for "bulk" graphene



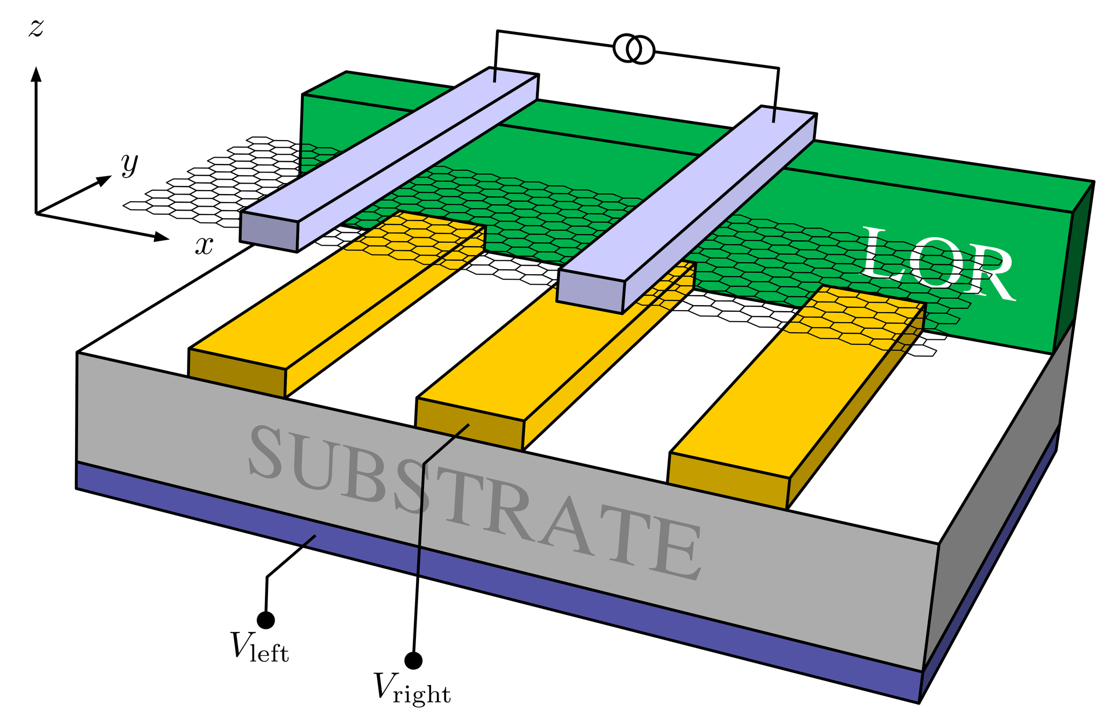
$$\mathcal{H}_{bulk} = \mathcal{H}_{GNR} + \left(-te^{ik_y w}\sum_n c^\dagger_{t,n} c_{b,n} + \text{H.c.}\right)$$

$t \sim 3$ eV : nearest neighbor (n.n.) hopping parameter
$\mathcal{H}_{GNR}$: standard TBM for $N_z = 2$ zigzag GNR up to n.n. hopping
$k_y \in [-\pi/w, \pi/w]$: Bloch momentum
$w = 3a$ for the present minimal TBM, bond length $a \sim 1.42$ Å

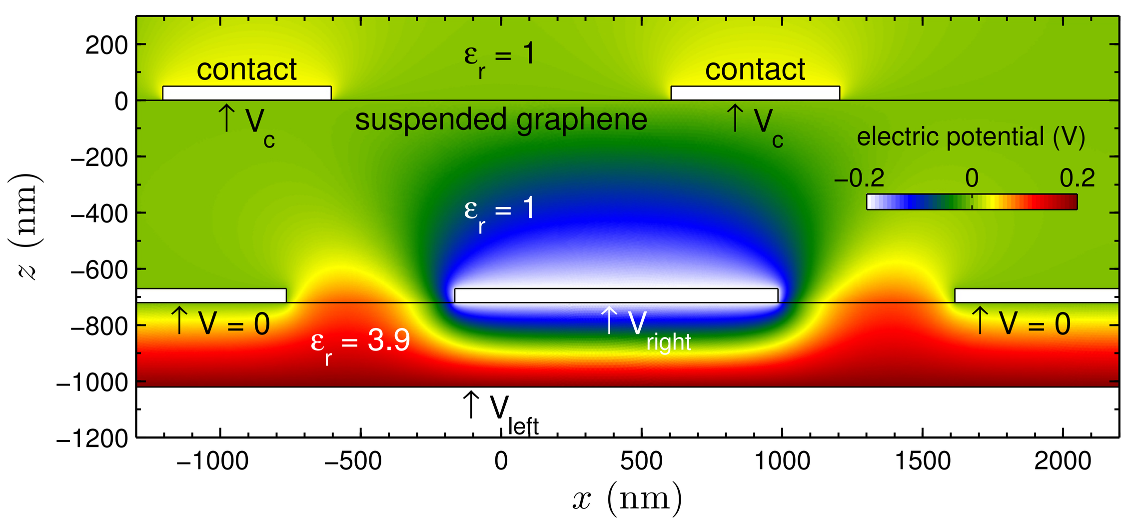
Realistic potential profile
- Realistic potential profile $\mathcal{V}_{real}$ needs to be extracted from carrier density.
- Computing carrier density profile $n(x)$:[3]
  - Without quantum correction—Classical capacitance model
  - With quantum correction
    - Self-consistent Poisson-Dirac iteration method
    - Exactly solvable quantum capacitance model[4,5]

III.3 Modeling the suspended graphene

Simplified device sketch for modeling



Electrostatic simulation
- Example with $V_c = 0.04$ V, $V_{left} = 0.2$ V, $V_{right} = -0.2$ V:



- Scattering region for transport calculation: $x_L \le x \le x_R$, $x_{L/R} = \mp 605$ nm.
- Contact potential for ideal Pd(111) based on first-principles[6] was estimated to be $V_c \approx 1.19$ V, but here $V_c = 0.04$ V fits better due to greatly reduced charge transfer [contacts are not (111), contact/graphene interface dirty, etc.].

Summary for computing conductance
- Electrostatic simulation (Esim) + quantum capacitance model (QCM) $\Longrightarrow V(x)$.
- Model Hamiltonian: $\mathcal{H}_{model} = \mathcal{H}_{bulk} + \sum_n V(x_n) c_n^\dagger c_n$.
- Slightly gapped graphene leads: $\Sigma_{L/R}(E = -V(x_{L/R}))$ with a phenomenological mass term to introduce a moderate reflection between contacted and suspended regions.
- Effective Hamiltonian: $\mathcal{H}_{eff} = \mathcal{H}_{model} + \Sigma_L + \Sigma_R$.
- Retarded Green's function at transport energy zero: $G^r = -\mathcal{H}_{eff}^{-1}$.
- Transmission function at a given incidence angle: $T(k_y) = \mathrm{Tr}[\Gamma_R G^r \Gamma_L G^a]$.
- Dimensionless single-moded conductance:

$$g = \frac{1}{2k_F}\int_{-k_F}^{k_F} T(k_y)\,dk_y.$$

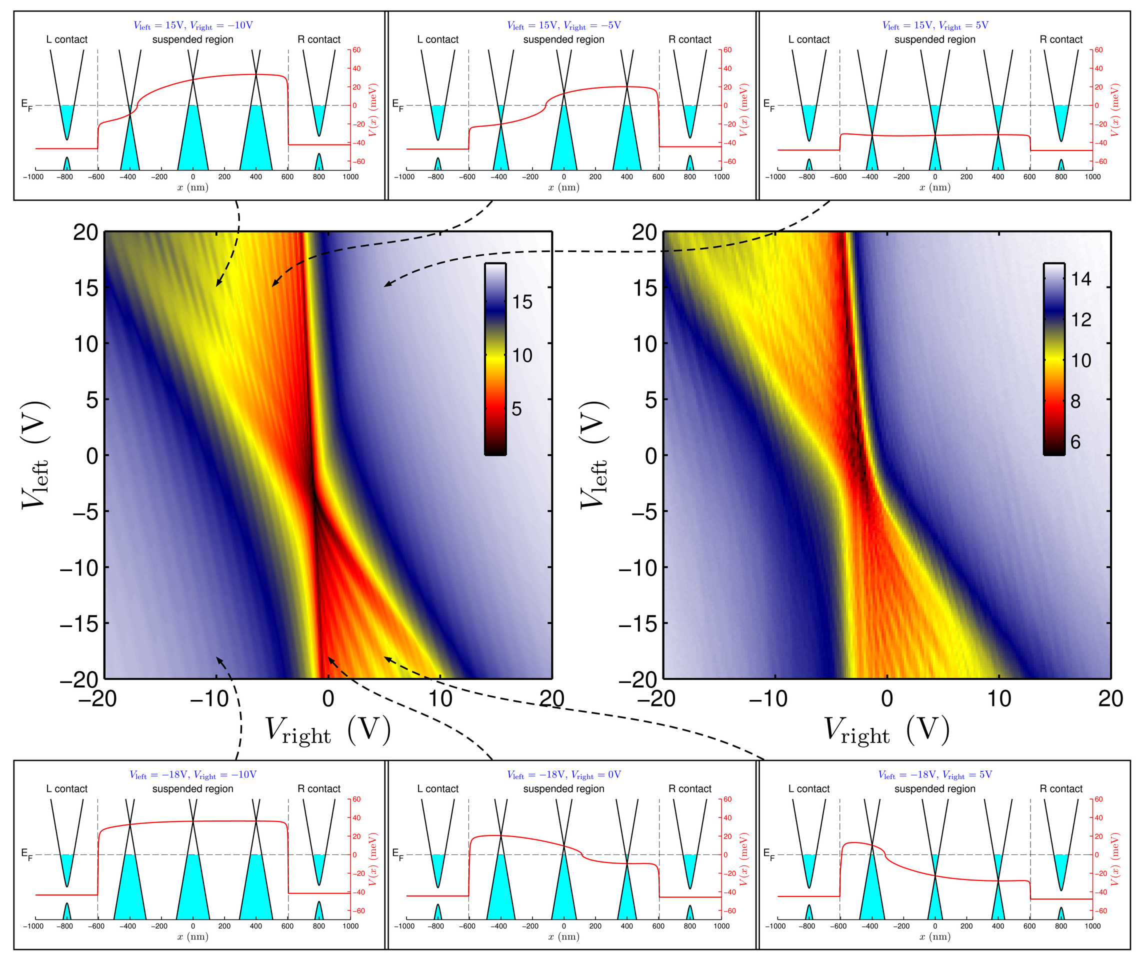
- Number of modes $M = W\sqrt{|n|/\pi}$; $W = 3.2\,\mu$m in the present experiment.
- Multi-moded conductance with mode counting and contact resistance

$$G = \frac{2e^2}{h}\left(\frac{1}{M\cdot g} + \frac{R_c}{h/2e^2}\right)^{-1}.$$

- $R_c = 1.27$ k$\Omega \approx 0.05 h/e^2$ deduced from experimetnal quantum Hall data.

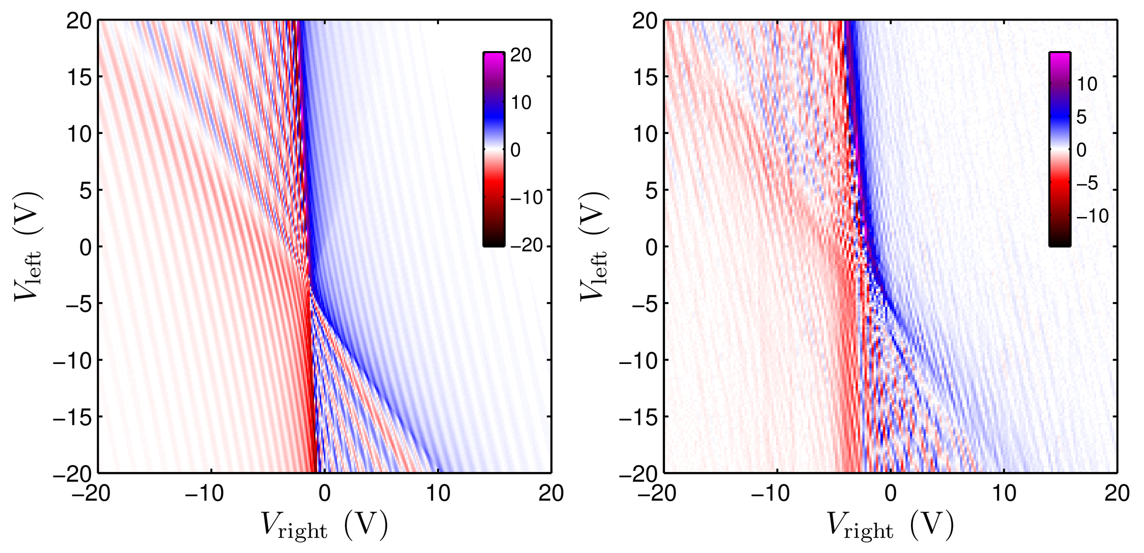
IV. Theory vs Experiment

Conductance maps

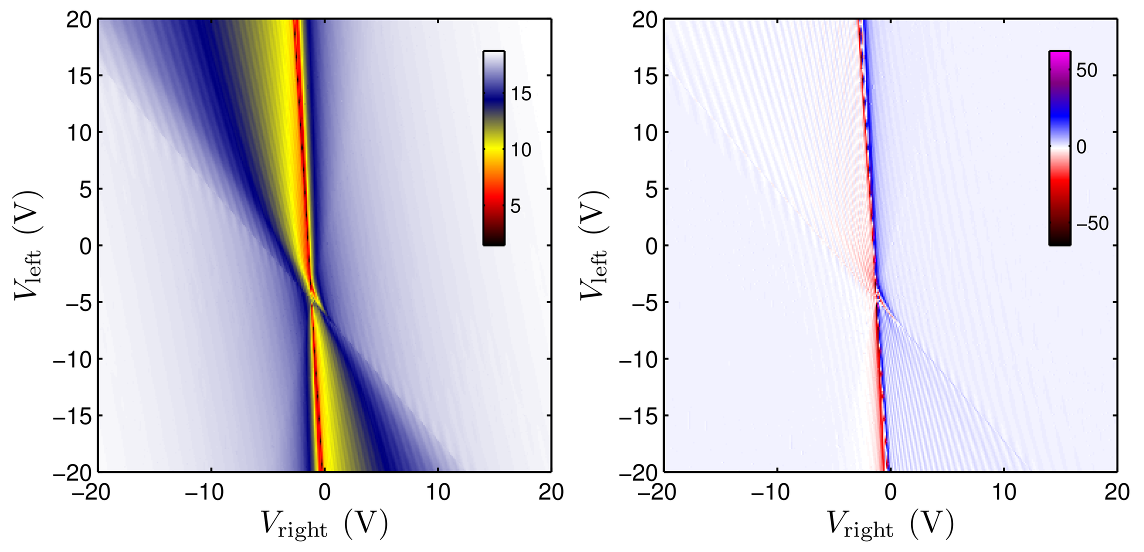


- $V_c = 0.04$ V, $n_0 = 1.5 \times 10^{10}$ cm^{-2} considered.
- Realistic potential profiles based on Esim+QCM.

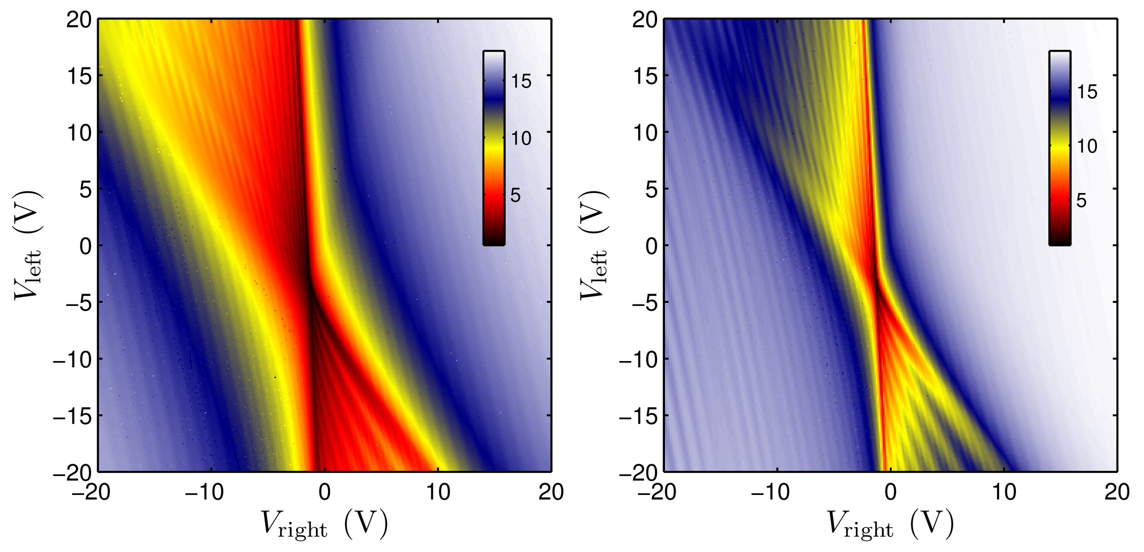
Transconductance maps



More tests for contact doping
- Without contacts:



- Higher contact doping ($V_c = 0.1$ V) vs lower contact doping ($V_c = 0.01$ V):



V. Summary

- Ballistic origin of the measured interference patterns in ultra-clean suspended graphene[7] are confirmed!
- Contact doping plays an important role in the present simulation.
- Simulation with $V_c = 0.04$ V fits best with the experimental data, implying that the charge transfer between contact and graphene is greatly reduced, as compared to the ideal case of Pd(111)[6] with predicted $V_c = 1.19$ V.
- The present simulation relies on the realistic carrier density profiles obtained by Esim+QCM[3,5] that can deal with electric, chemical, and contact-induced doping in a unified manner.

References

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[6] P. A. Khomyakov, G. Giovannetti, P. C. Rusu, G. Brocks, J. van den Brink, and P. J. Kelly, Phys. Rev. B **79**, 195425 (2009).
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