Minimal Tight-Binding Model for Quantum Transport in Graphene Heterojunctions

Ming-Hao Liu (劉明豪), Jan Bundesmann, Klaus Richter

Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

minghao.liu.taiwan@gmail.com

A real-space Green's function formalism based on a minimal tight-binding model (TBM) is adopted to efficiently simulate ballistic transport in graphene heterojunctions. The basic idea is to make use of the Bloch theorem along the transverse dimension of the bulk graphene (see Fig. 1), which greatly reduces the computation load and hence allows experimental sizes in the longitudinal dimension. Numerically, we will show [1]

(i) the consistency of our TBM calculations with the existing results based on the effective Dirac theory for chiral tunneling through pnp junctions in monolayer graphene (MLG) and in bilayer graphene (BLG) (see Fig. 2), and

(ii) spin-dependent tunneling through pn junctions in MLG with Rashba spin-orbit coupling (see Fig. 3).

Extending the length scale to the experimental size and taking into account the realistic charge density profile due to gating, we further show

(iii) good agreement of our minimal TBM, without free parameters, with the recent ballistic Klein tunneling experiment by Young and Kim [2].

[1] M.-H. Liu, J. Bundesmann, and K. Richter, Phys. Rev. B **85**, 085406 (2012).
[2] A. F. Young and P. Kim, Nat. Phys. **5**, 222 (2009).
[3] M. I. Katsnelson, K. S. Novoselov, and A. K. Geim, Nature Physics **2**, 620 (2006).

FIGURES

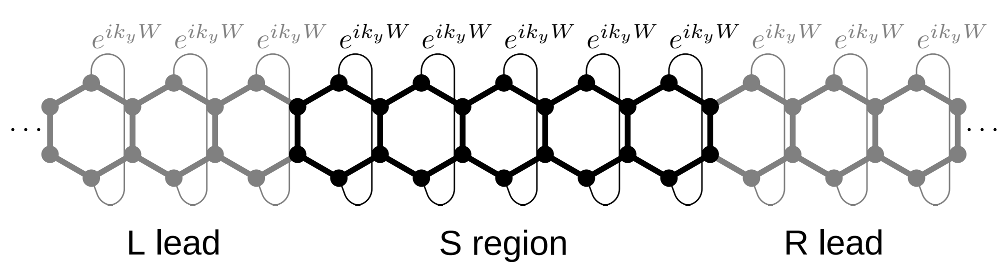

FIG 1. *Schematic of a minimal tight-binding model that simulates a bulk MLG up to the nearest neighbor hoppings.*

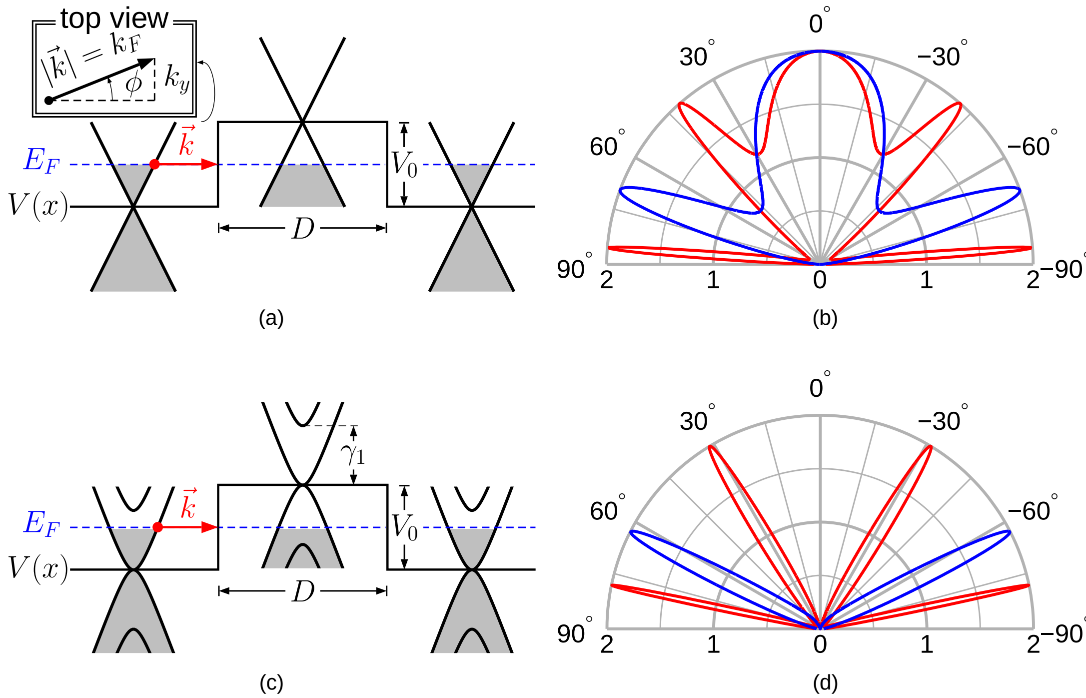

FIG 2. *Tunneling through a barrier for (a), (b) MLG with Fermi energy* E_F = 81.6 meV *and (c), (d) BLG with* E_F = 17.1 meV. *In (b), red (light gray) and blue (dark gray) curves correspond to* V_0 = 196.8 meV *and* V_0 = 280.3 meV, *respectively. In (d), red (light gray) and blue (dark gray) curves correspond to* V_0 = 48.7 meV *and* V_0 = 100.7 meV, *respectively. In both cases the barrier width is* D = 100 nm *and the incoming Fermi wave vector is* $k_F = 2\pi/50\,\text{nm}^{-1}$, *as considered in [3].*

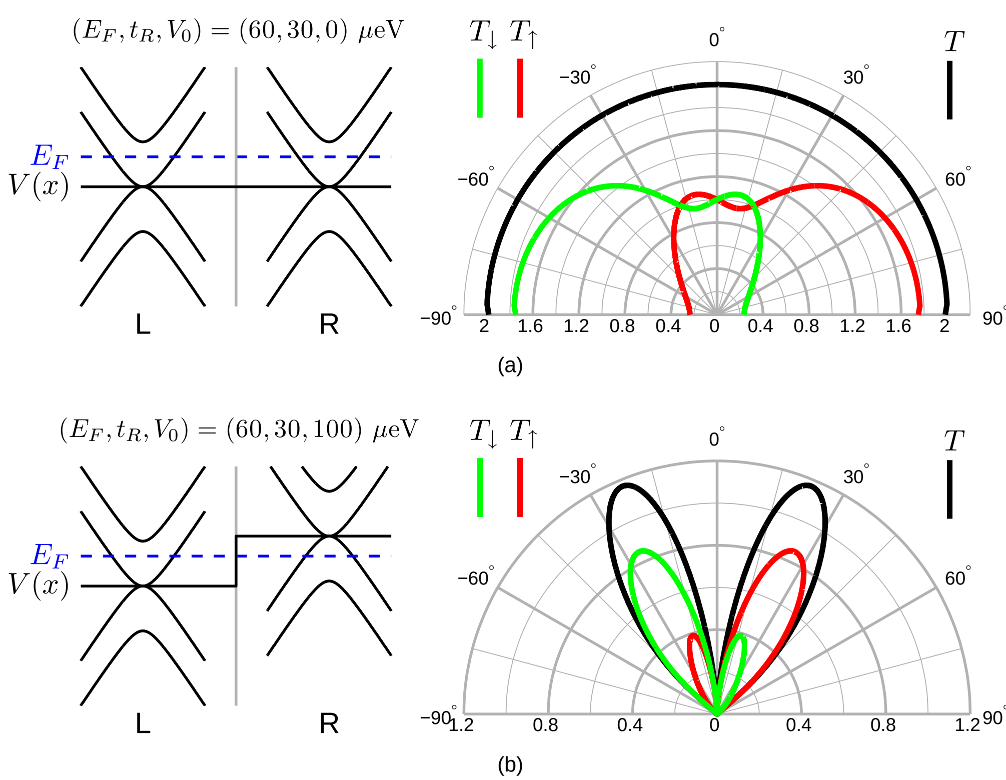

FIG 3. *Angular dependence of total and spin-resolved transmissions through a pn junction in MLG in the presence of the Rashba spin-orbit coupling with (a) zero potential and (b) finite potential.*