Bridging Non-Equilibrium Green's Function and Scattering Formalism: Electronic Transport Across Silicene

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Abstract. The generalized Fisher-Lee relation in non-orthogonal localized basis set was implemented within the framework of TRANSIESTA package in order to bridge the non-eqilibrium Green's function theory (NEGF) and scattering formalism. The implementation is divided into two phases. Firstly, the complex band structures of leads are solved, from which transverse wave-functions and group velocities for propagating states can be calculated. Secondly, Green's functions and spectral functions from NEGF and propagating states from the first step are used to calculate the tranmission and reflection coefficients in terms of Bloch waves from leads.

With the help of the Fisher-Lee relation, one can transform the results from *de facto* standard NEGF method to scattering formalism which is more physically transparent and easiler to understand. More importantly, this enables us to use NEGF together with semiclassical Boltzmann equation.

Although the Landauer formula were routinely employed to study the phase-coherent electronic transport, one should turn to semiclassical Boltzmann equation when electronic scattering cannot be neglected. In order to solve the semiclassical Boltzmann equation in multilayered systems, transmission and reflection coefficients for each interface in terms of Bloch waves can be obtained from TRANSIESTA and the Fisher-Lee relation from our implementation.

Details in the implementation and illustrative results on Ag(111)/silicene/Ag (silicene: silicon analog of monolayer graphene) junctions will be presented.