

Diagrammatic and resummation algorithms for electron-magnon and electron-phonon interacting systems in nanojunctions far from equilibrium

Branislav K. Nikolić

University of Delaware, Department of Physics & Astronomy, 217 Sharp Lab, Newark, USA

The nanoelectronic and spintronic devices based on single-molecule or magnetic tunnel junctions are typically operated by finite bias voltage which can lead to highly nonequilibrium states of electrons and bosons (such as phonons or magnons). While nonequilibrium Green function (NEGF) formalism offers a rigorous theoretical and computational framework to describe the effect of their mutual interaction on charge and spin currents underlying the device functionality, the computational complexity of standard self-consistent diagrammatic many-body perturbation scheme for NEGFs has restricted simulations to very small junctions (containing few tens of atomic orbitals). Furthermore, magnons have small bandwidth meaning that weak interactions felt by electrons turns out to be strongly coupled regime for magnons, thereby requiring higher order diagrams in the expansion of magnonic NEGF. On the other hand, as the interactions strength increases, self-consistent diagrammatic series often converges to the unphysical branch. This talk will overview our recent NEGF-based approach [1] to nonequilibrium electron-magnon systems in magnetic tunnel junctions, where magnons become quasiparticles dressed by the cloud of virtual electron-hole pairs while electrons scattering of low frequency magnons experience anomaly in their current-voltage characteristics at small bias voltage. I will then use an example of a single molecule nanojunction [2] to show how self-consistent diagrammatic series for NEGFs describing electron-phonon (or electron-magnon) inelastic scattering can be evaded by evaluating only fourth-order bare diagrams [3] and subsequently performing very recently proposed [4] hypergeometric resummation of perturbative series for physical observables that preserves conservation laws and can make possible simulations of electron-boson coupled systems in devices containing very large number of atoms.

- [1] F. Mahfouzi and B. K. Nikolić, *Phys. Rev. B* 90, 045115 (2014).
- [2] K. K. Saha, B. K. Nikolić, V. Meunier, W. Lu, and J. Bernholc, *Phys. Rev. Lett.* 105, 236803 (2010).
- [3] H. Mera, T. G. Pedersen, and B. K. Nikolić, *Phys. Rev. Lett.* 115, 143001 (2015).
- [4] H. Mera, T. G. Pedersen, and B. K. Nikolić, *Phys. Rev. B* 94, 165429 (2016).