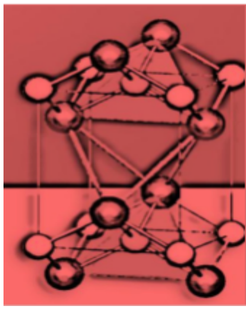

X Workshop on Novel Methods for Electronic Structure Calculations

04th – 06th December 2023
La Plata – Argentina

Generalized Quantum Langevin Equation for Transport: The Case for Interband Coherences in the Electrical Conductivity

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Decoherence, dissipation, and thermalization are key ingredients for a quantum theory of transport processes. To go beyond the semiclassical description given by the quantum Boltzmann equation, we explore the use of the generalized, quantum Langevin equation. A single memory-function approximation, appropriate for the hydrodynamical regime, allows the inclusion of interband coherences that are neglected in the semiclassical description. These interband coherences are relevant even in the limit of weak scattering, where the Boltzmann description is deemed appropriate. As an example, we discuss the case of narrow band gap semiconductors at low doping that are commonly used in thermoelectric applications. In these materials, Boltzmann wrongly predicts zero conductivity at zero temperature, while we obtain a finite residual conductivity. This improvement in the description of transport coefficients is achieved without extra computational cost and can be easily implemented in current electronic structure codes and is already implemented in Exciting and PAOFLOW. The memory-function approach to quantum dynamics has a long history of development. I will review the basics of this approach and provide a perspective on possible applications in the description of decoherence and dissipation in materials.