Appunti di Fisica '18
&
Dottorato di Ricerca in Fisica

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Modeling heat transfer at the nanoscale: A mixed quantum-classical approach

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The Molecular junctions (MJs) are of great experimental and theoretical interest due to their heat conductance and thermoelectric properties. Gaining mechanistic insight into the vibrational energy transport through an MJ is important for designing efficient and robust molecular electronics devices. To date, fully quantum mechanical approaches have been used to study the steady-state heat current in MJs, but their use has been mainly limited to relatively small model systems that are weakly coupled to thermal reservoirs. In this work, we simulate the heat current dynamics of a non-equilibrium spin-boson model [1, 2] using mixed quantum-classical dynamics, whereby the two-level spin system (representing the MJ) is treated quantum mechanically and the two bosonic heat baths (which couple independently to the MJ) are treated in a classical-like fashion. Starting from the quantum-classical Liouville equation [3], an expression for the heat current is derived and then used to simulate the heat current dynamics through the model MJ for different MJ-bath coupling strengths and tunneling frequencies. We investigate the ability of this approach to capture the expected turnover behaviour in the steady-state heat current with increasing coupling strength. Our results demonstrate the viability of studying heat current dynamics in more realistic models via this mixed quantum-classical approach.

[1] A. J. Leggett *et al,* Rev. Mod. Phys. **59**, 1 (1987).
[2] N. Boudjada and D. Segal, J. Phys. Chem. A **118**, 11323 (2014).
[3] R. Kapral and G. Ciccotti, J. Chem. Phys. Chem. **110**, 8919 (1999).