Quantum dissipative dynamics and quantum transport with path integral methods

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Iterative influence functional path integral techniques were recently generalized to follow the dynamics of a subsystem coupled to multiple bosonic and fermionic environments [1]. This was achieved by combining two powerful tools: QUAPI, a path integral approach which has been developed to treat the dynamics of a subsystem in contact with a harmonic bath [2], and INFPI, able to follow dissipative dynamics with fermionic baths and electron transfer between metal terminals [3]. Using this new tool, I will describe several problems that we have recently tackled: charge transport and vibrational instability in molecular electronic rectifiers [1], thermal energy transfer in nanojunctions [4], and driven dynamics induced by the application of time dependent fields [5].

[1] L. Simine and D. Segal, J. Chem. Phys. 138, 214111 (2013).
[2] N. Makri and D. E. Makarov, J. Chem. Phys. 102, 4600 (1995).
[3] D. Segal, A.J. Millis, and D. R. Reichman, Phys. Rev. B 82, 205323 (2010).
[4] N. Boudjada and D. Segal, arxiv:1409.3201
[5] A. Dodin, S. Garmon, L. Simine, and D. Segal, J. Chem. Phys. 140, 124709 (2014).