# Universal Approach to Dynamics of Finite and Extended Atomistic Systems in the Phase Space

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In our work, we propose and construct the theoretical framework for nonadiabatic dynamics under general non-equilibrium conditions based on the stochastic hierarchy of equations of motion (EoM) for various dynamical moments, combinations of positions and momenta. In principle, it unifies the thermalization and real-time evolution for finite atomic systems along the Konstantinov-Perel's contour, i.e. both electrons and nuclei are tackled under the same quantum-mechanical footing.

[1] L. K. Dash, H. Ness, and R. W. Godby. Nonequilibrium electronic structure of interacting single-molecule nanojunctions: Vertex corrections and polarization effects for the electron-vibration coupling. J. Chem. Phys.132 (2010) 104113

[2] Hong-Yi Fan. Operator ordering in quantum optics theory and the development of Dirac's symbolic method. J. Opt. B: Quantum Semiclass. 5 (2003) 147

[3] Per Hedegrd. Quantum diffusion in a metallic environment. Phys. Rev. B 35(1987) 6127.

[4] L. Kantorovich. Nonadiabatic dynamics of electrons and atoms under nonequilibrium conditions. Phys. Rev. B 98(2018) 14307

[5] Jing-Tao Lü, Mads Brandbyge, Per Hedegård, Tchavdar N. Todorov, and Daniel Dundas. Current-induced atomic dynamics, instabilities, and Raman signals: Quasiclassical langevin equation approach. Phys. Rev. B 85 (2012) 245444