Open-system density matrix theory for surface science problems

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Molecules or atoms interacting with solid surfaces constitute typical "system-bath" type problems, in which a system (the molecule or atom) interacts with a bath of unobserved degrees of freedom (the surface), leading to energy and phase relaxation. Detailed insight into energy and phase flow during laser pulse-induced processes or scattering events, for example, can be gained by a time-dependent approach. One way to model the quantum dynamics for this kind of problems is by reduced (open-system) density matrix theory, another one by explicit solution of a multi-dimensional, time-dependent Schrödinger equation based on a system-bath Hamiltonian.

In the presentation, various flavours of open-system density matrix theory and its numerical realization will be presented. Where possible, the solutions are compared to those obtained from the full, albeit approximate, time-dependent Schrödinger equation.

Several examples for dissipative dynamics, all related to surface science will be presented to illustrate the concepts: (i) The selective laser-pulse control of vibrating adsorbates at surfaces, (ii) dissipative, laser-driven electron dynamics near surfaces, and (iii) dissipative molecule-surface scattering.