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Classical and quantum mechanical calculations of adsorption/desorption and diffusion on surfaces
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An overview of classical and quantum mechanical rate theory will be given along with discussion of implementation techniques and applications to processes at surfaces of solids, such as adsorption/desorption of molecules and diffusion of atoms. The classical methodology is based on the two step WKE procedure where first a transition state is identified and classical trajectories then carried out starting from the transition state. Within the harmonic approximation the key issue is the identification of all relevant first order saddle points on the energy rim surrounding the local minimum corresponding to the initial state. The quantum mechanical methodology involves the use of statistical Feynman Path Integrals to identify a quantum mechanical transition state thereby including tunneling. Within a harmonic approximation this reduces to instanton theory. While the focus is on transitions involving atomic rearrangements, a brief mention of the formulation of these approaches to magnetic transitions will be given.