DIFFUSION AND NONLINEAR DYNAMICS OF ADATOMS AND DIMERS ON PERIODIC SURFACES

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The motion of molecules on solid surfaces is of interest for technological applications such as catalysis, lubrication and coating, but it is also a theoretical challenge at a more fundamental level.
We study the simplest objects diffusing on a substrate at finite temperature T, namely an atom and a diatomic molecule (dimer), using the Langevin equation approach.
The Newtonian dynamics of the dimer is rather complex, displaying chaotic features, parametric resonances and nonlinear effects due to the coupling between the centre of mass and the intramolecular motion. Different dynamical regimes can be attained depending on the dimer initial velocity and on the strength of the intramolecular bonding. In the presence of thermal fluctuations we analyse the diffusive dynamics as a function of temperature.
Contrary to atomic diffusion, for the dimer it is not possible to define a single, temperature independent, activation barrier.
This reveals a complex behaviour determined by the interplay between vibrations and a temperature dependent intramolecular equilibrium length.
The relation between chaotic deterministic diffusion and stochastic thermal diffusion will be also briefly discussed.