

Classical Wigner model based on a Feynman path integral open polymer

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The classical Wigner model is a way of accounting for quantum mechanical effects when studying the dynamics of molecular systems. In this model you initially have a quantum mechanical phase space distribution, called a Wigner function, and propagate it forward in time by classical mechanics.

A possibly difficult part of a practical implementation of the classical Wigner model is the sampling of the initial quantum mechanical distribution.

In this project small systems are studied, and the initial Wigner function is sampled by the use of Monte Carlo on an imaginary time Feynman path integral open polymer, and correlation functions are calculated.

An aim with this project is to based on this methodology calculate reaction rate constants for real systems.