Asymptotic Analysis of Non-Equilibrium Chemical Reactions in the Thermodynamic Regime using WKB Method

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Non-equilibrium chemical reactions in the thermodynamic regime exhibit distinct asymptotic behavior, which can be comprehended through the reformulation and asymptotic analysis provided by the WKB method. The WKB asymptotic analysis uncovers the underlying structure of the chemical reaction network, revealing a first-order Hamiltonian-Jacobi equation and a Hamiltonian structure. These insights enable the exploration of phenomena such as the occurrence of law of large number type events and rare transitions among metastable states. I will also explain some rigorous asymptotic analysis techniques. The backward equation for the underlying stochastic process in the WKB reformulation corresponds to Varadhan's discrete nonlinear semigroup, acting as a monotone scheme that approximates the first-order Hamiltonian-Jacobi equations (HJE) in the limit. This convergence analysis justifies the application of large deviation principles and contributes to a comprehensive understanding of the asymptotic properties of non-equilibrium chemical reactions in the thermodynamic regime. Additionally, we will discuss a deconstruction of the general macroscopic reaction rate equation for species concentrations into a gradient flow and a Hamiltonian flow. This decomposition provides further insights into the behavior of the reaction system and enables the utilization of analytic tools for a more comprehensive analysis.