

Transition State Theory Rate in Nonlinear Environment: the Under-damping Case

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Abstract: We investigate the escape behavior of systems governed by the one-dimensional nonlinear Kramers' equation $\frac{\partial W}{\partial t} = -v \frac{\partial W}{\partial x} + (f'(x)/m) (\frac{\partial W}{\partial v}) + \gamma \frac{\partial (vW)}{\partial v} + (\frac{\gamma k_{BT}}{m}) (\frac{\partial^2 W}{\partial v^2})$, where $f(x)$ is a metastable potential and μ an anomalous exponent. We obtain an expression for the transition state theory escape rate, whose predictions are in good agreement with numerical simulations. The results exhibit the anomalies due to the nonlinearity in W that the TST rate grows with T and drops as μ becomes large at a fixed T . Indeed, particles in the subdiffusive media ($\mu > 1$) can escape over the barrier only when T is above a critical value, while there does not exist this confinement in the superdiffusive media ($\mu < 1$).

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Key words: Kramers' escape rate, nonlinear Fokker-Planck equation, anomalous diffusion

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