Shape-sensitive spectral asymptotics for quasi-stationary timescales.

Noé Blassel

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Abstract

So-called accelerated dynamics methods (Hyperdynamics, TAD, Parallel Replica) rely on local metastability to accelerate the sampling of long, asymptotically unbiased trajectories of molecular systems. These techniques rely on a separation of timescales assumption within well-chosen subsets of the configurational space called metastable states. Given a configurational domain Ω, this assumption states that the system started in Ω will quickly reach a local equilibrium inside Ω, much faster than the expected exit time from this local equilibrium. The validity of this assumption strongly relies on appropriate definitions of the state Ω.

In the dynamical setting of reversible elliptic diffusions, one can interpret this separation of timescales quantitatively, as a ratio of eigenvalues $\frac{\lambda_2(\Omega)-\lambda_1(\Omega)}{\lambda_1(\Omega)}$, where the eigenvalues are those of the infinitesimal generator of the evolution semigroup, endowed with Dirichlet boundary conditions on $\partial\Omega$. Motivated by the question of how to maximize the separation of timescales with respect to Ω, we study low-temperature asymptotics of these eigenvalues for families of domains $(\Omega_{\alpha,\beta})_{\beta>0}$, jointly parametrized by the inverse temperature parameter β, and a shape-design parameter α.

This study is equivalent to the semiclassical asymptotics of the Witten Laplacian in presence of a h-dependent Dirichlet boundary. In a suitable geometric framework, we compute previously unknown spectral asymptotics, which are only sensitive at first-order to β and the design parameter α. This allows to find asymptotically optimal choices of metastable state Ω with respect to the efficiency of the Parallel Replica algorithm within the class of domains satisfying our geometric assumptions.

This presentation is based on the recent preprint [1].

References

[1] N. Blassel, T. Lelièvre, and G. Stoltz. Quantitative low-temperature spectral asymptotics for reversible diffusions in temperature-dependent domains. *arXiv:2501.16082*, 2025.