A PATH INTEGRAL APPROACH TO THE LACK-OF-FIT REDUCTION

Kateřina Mladá[1,2,*], Michal Pavelka[2]

[1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
[2]Faculty of Mathematics and Physics, Mathematical Institute, Charles University in Prague, Prague, Czech Republic
[*]mlada@fzu.cz

ABSTRACT

Even though microscopic dynamics is reversible in time, macroscopic systems show irreversible dynamics. The lack-of-fit reduction, as formulated by Kleeman in [1], gives macroscopic irreversible dynamics as the most probable trajectory, when minimizing the loss of information caused by the transition from a more detailed level of description. This trajectory is then given without any fitting constants, based purely on the minimizing principle.
In previous work [2], we focused only on the macroscopic trajectory, generalizing the lack-of-fit reduction for systems described by the GENERIC formalism (General Equation for Non-Equilibrium Reversible-Irreversible Coupling). In our current work, we add also the theory of fluctuations in the form of random noise. The reduction is tested on the Kac-Zwanzig model – large particle in an outside potential surrounded by a bath of N smaller particles. Detailed computer simulation is compared to the reduced dynamics found by the model. To show the emergence of damping from purely reversible dynamics as well as keep calculations explicit, we use harmonic potential as the outside potential.

REFERENCES

[1] R. Kleeman, A path integral formalism for non-equilibrium Hamiltonian statistical systems. *Journal of Statistical Physics*, 158(6): pp. 1271-1297, 2015
[2] K. Mladá, M. Šípka, M. Pavelka, Lack-of-fit reduction in non-equilibrium thermodynamics applied to the Kac–Zwanzig model, *Journal of Non-Equilibrium Thermodynamics*, vol. 49, no. 2, pp. 181-194., 2024