Eigenmode following for direct entropy calculation and characterization of magnetic systems

S. von Malottki[1,2,3,4,*], M. A. Goerzen[1], H. Schrautzer[1,2], P. F. Bessarab[2,5] and S. Heinze[1,6]

[1] Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany, [2] Science Institute, University of Iceland, Iceland, [3]Thayer School of Engineering, Dartmouth College, USA, [4]UCLouvain, Institute of Condensed Matter and Nanosciences, Belgium, [5]CEMES, Université de Toulouse, France, [6]Department of Physics and Electrical Engineering, Sweden
*stephan.vonmalottki@uclouvain.be

Phase transitions and the stability of metastable states are key properties in many fields and applications. Typically described by an Arrhenius law, $\nu = \nu_0 e^{-\beta \Delta E}$, the average transition rate, ν, is given by the pre-exponential factor, ν_0, the thermal energy, $\beta = 1/(k_B T)$, and the energy barrier, ΔE, between the transition state and the initial state. In magnetism the optimisation of the thermal properties of magnetic skyrmions have been extensively studied over the last decade [1]. One of the key findings was the occurrence of an entropic barrier, i. e. the pre-exponential factor, to predominantly stabilise magnetic skyrmions [2].

The most common way to calculate transition rates is in the framework of transition state theory, in which the Boltzmann integral over all occupied states around the initial and transition states is determined. Due to the complexity of this integral, often, the harmonic approximation is applied to the energy, allowing to decouple the eigenmodes and analytically solve the integral. While the harmonic approximation is certainly powerful, it reaches its limitations when dealing with anharmonic potentials, i.e. potentials that do not follow the form of a parabola. For magnetic skyrmions, examples are the rotational mode of the chimera transition state [3,4] and the rotational mode of skyrmions in the presence of weak Dzyaloshinskii-Moriya interaction (DMI) [5].

In this presentation, we introduce the eigenmode following (EMF) method for direct entropy calculation. It explores the potential energy landscape by small displacements of the selected state along the eigenvectors of the chosen eigenmode. Since the eigenvectors change with the state along the displacements, we re-calculate them iteratively and ensure the application of the correct eigenvector by so-called mode tracking. The computational cost of EMF is larger than the application of the harmonic approximation due to the repeated (partial) diagonalization of the Hessian matrix. However, this can be mitigated by only applying EMF to the softest and most critical few eigenmodes of the state while modelling the rest of spectrum in harmonic approximation. This tailored combination of methods allows for an efficient yet accurate description of the individual entropy contributions and with that, of the total average transition rates. A preprint of the method is available at arXiv:2503.12109.

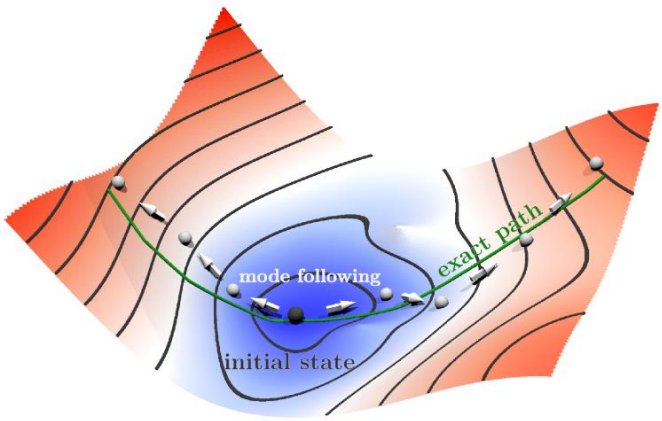

Figure 1. Scheme of the eigenmode following method. An initial state (black sphere) is displaced in positive or negative direction along the eigenvectors (white arrows) of the chosen eigenmode.

References

[1] B. Göbel, Physics Reports **895**, 1–28 (2021).
[2] J. Wild, Science advances **3**, e1701704 (2017).
[3] F. Muckel, Nature Physics **17**, 395–402 (2021).
[4] S. von Malottki, doctoral thesis, Christian-Albrechts-Universität zu Kiel (2021)
[5] M. A. Goerzen, npj Quantum Materials **8**, 54 (2023)