Lee-Yang Zeros and Large-Deviation Statistics for a Molecular Zipper

A. Deger, K. Brandner, and C. Flindt

Department of Applied Physics, Aalto University, 00076 Aalto, Finland
email: aydin.deger@aalto.fi

Originally introduced to explain the behavior of a condensing gas [1], Lee-Yang zeros have nowadays become a universal and powerful tool for the unified description of phase transitions in equilibrium, non-equilibrium and dynamical systems, see for example [2, 3]. Here, we show that this concept can be developed even further by analyzing in detail a paradigmatic model for thermal phase transition in molecular systems [4].

For the most simple version of this model, we explicitly calculate the Lee-Yang zeros with respect to inverse temperature. Extrapolation then allows us to infer a phase transition in the macroscopic limit, from the analysis of systems containing only a few molecular units. In a second step, we increase the complexity of the model. The Lee-Yang zeros can still be obtained using a recently established relation involving high-order cumulants of the energy fluctuations. Finally, we show that, even for systems that do not undergo a phase-transition, the Lee-Yang zeros encode physical information. Specifically, they crucially determine the large-deviation statistics of energy fluctuations.

Our analysis reveals an interesting duality between the energy fluctuations of small-size systems in equilibrium and their phase-behavior in the thermodynamic limit [5]. To what extent this relation is valid in more complex systems, such as the two-dimensional Ising model, is a topic of future research.

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