Phase Transitions in a Molecular Zipper: Lee-Yang Zeros and Large Deviation Statistics

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Originally introduced to explain the behavior of a condensing gas, 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 [1, 2]. Here, we use Lee-Yang zeros to analyze a paradigmatic model for thermal phase transitions in molecular systems. 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. Finally, we show that, even when the system does not undergo a phase-transition, the Lee-Yang zeros still encode valuable physical information; they crucially determine the large deviation statistics of energy fluctuations. Specifically we show that the large deviation function generically has the form of an ellipse, whose tilt and width can be inferred from the complex Lee-Yang zeros. Our analysis reveals an interesting duality between the energy fluctuations of small-size systems in equilibrium and their phase-behavior in the thermodynamic limit [3]. To what extent this relation is valid in more complex systems, such as the two-dimensional Ising model, is a topic of future research.

References

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