Lee-Yang Zeros at Quantum Phase Transitions with Quantum Network Algorithms

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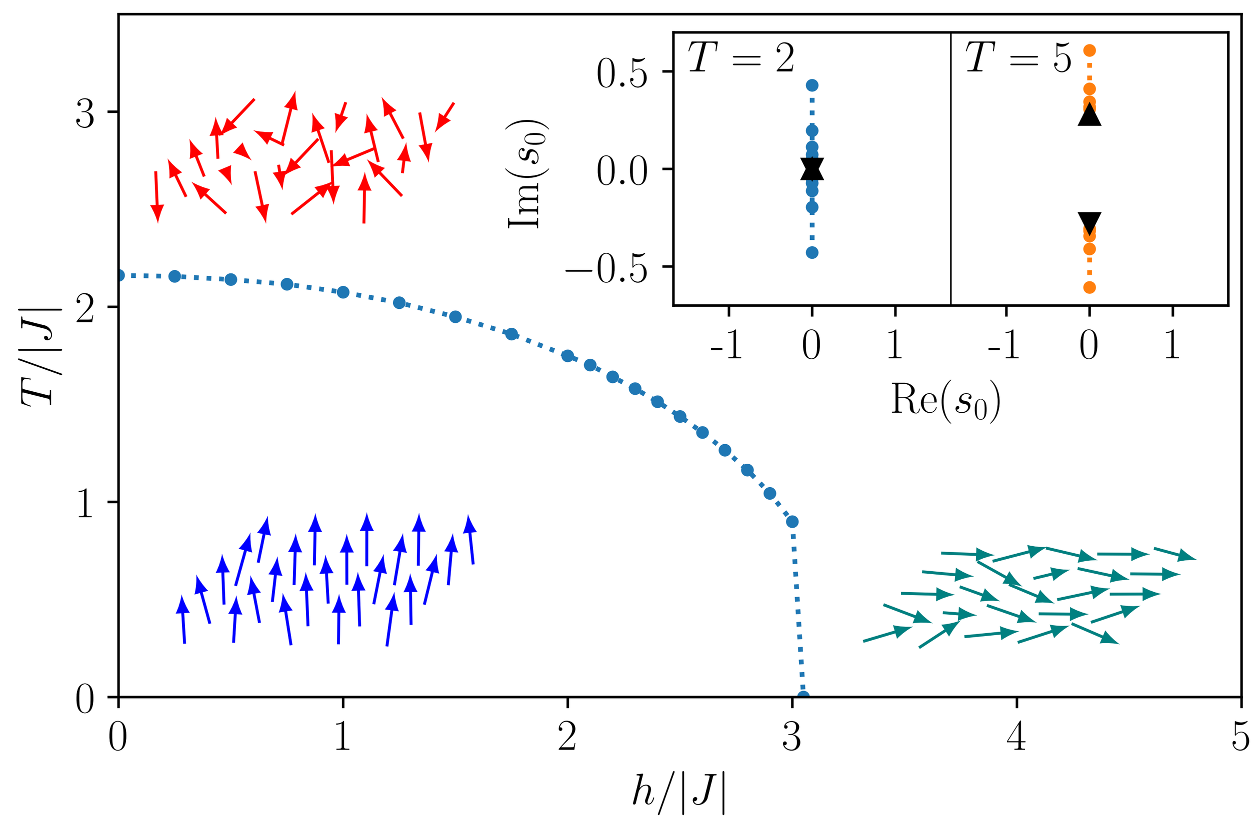
Abstract

- Prediction of phase diagrams of quantum many-body systems is hard, but useful to study for example superconductivity and spin liquids phases.
- We study zeros of a moment-generating function (Lee-Yang zeros) and their extrapolation to the thermodynamic limit to determine the position of the phase transition for the two-dimensional Quantum Ising model.
- A symmetry-broken phase is indicated by the convergence of the Lee-Yang zeros to the real axis in the thermodynamic limit.
- These Lee-Yang zeros are calculated from the high moments of the order parameter, the magnetization, determined using tensor-network methods.

Phase diagram of the quantum Ising model



Quantum Ising Model

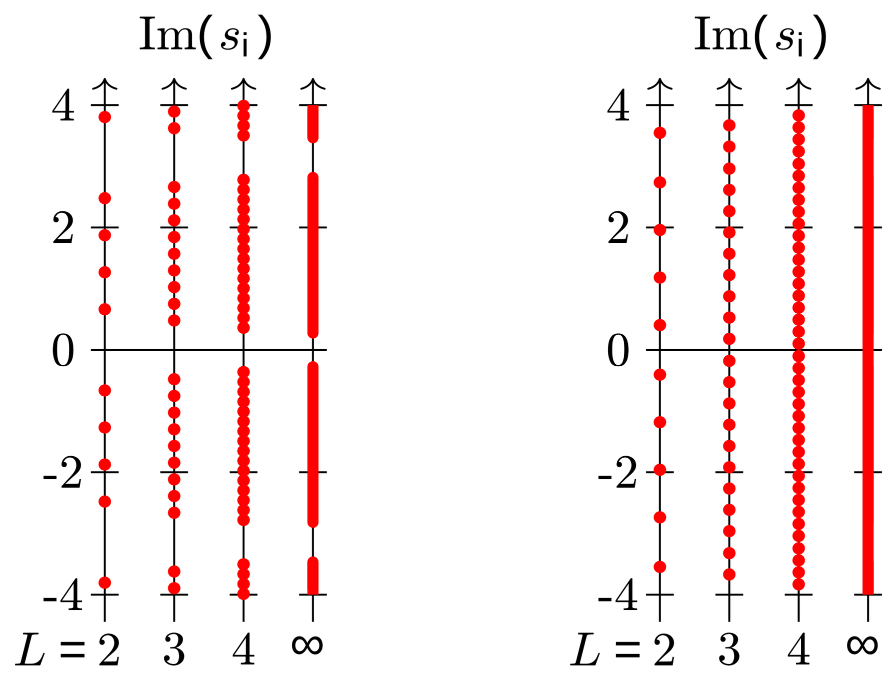
$$\hat{\mathcal{H}} = -J\sum_{\langle i,j\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z - h\sum_i \hat{\sigma}_i^x$$

- Spin-1/2 model on square lattice with nearest-neighbour coupling.
- $J<0$ ferromagnetic
- $J>0$ antiferromagnetic
- Order parameter $\hat{M}_z = \sum_i \hat{\sigma}_i^z$

Lee-Yang Zeros[2,4,5]

- Moment-generating function $\chi(s) = \dfrac{\mathrm{Tr}\left[e^{s\hat{M}_z}e^{-\beta\hat{\mathcal{H}}}\right]}{\mathrm{Tr}\left[e^{-\beta\hat{\mathcal{H}}}\right]}$
- $\langle \hat{M}_z^n\rangle = \partial_s^n \chi(s)|_{s=0}$
- Lee-Yang zeros s_i are defined by $\chi(s_i)=0$
- Away from the real axis for finite systems
- If the system is in a symmetry-broken phase, they converge towards the real axis towards the thermodynamic limit.
- Cumulant generating function $\Theta(s) = \ln\chi(s)$ for cumulants $\langle\langle \hat{M}_z^n\rangle\rangle = \partial_s^n\Theta(s)|_{s=0}$

Position of all the Lee-Yang zeros in the complex plane with increasing finite system size



The Lee-Yang zeros are purely imaginary.

The Cumulant Method[2,7]

- $\chi(s)$ can be expanded as

$$\chi(s) = e^{cs}\prod_i\left(1-\frac{s}{s_i}\right)$$

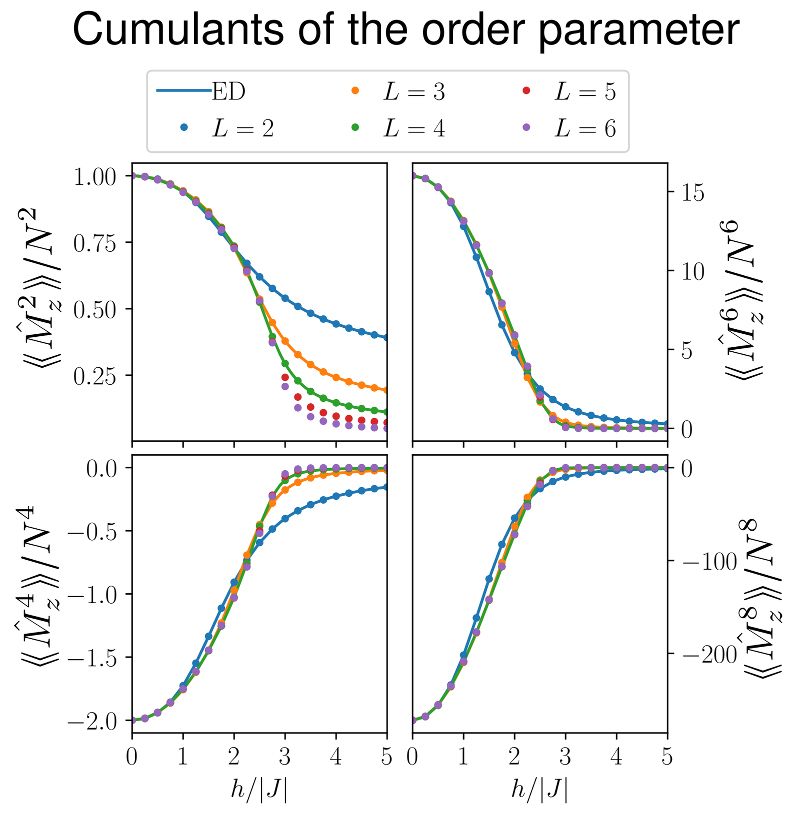
- $\langle\langle \hat{M}_z^n\rangle\rangle = -\sum_i \dfrac{(n-1)!}{s_i^n}$
- series dominated by first few few terms, drop $i>0$
- then

$$\mathrm{Im}[s_0] = \sqrt{2n(2n+1)|\langle\langle\hat{M}_z^{2n}\rangle\rangle/\langle\langle\hat{M}_z^{2n+2}\rangle\rangle|}$$

Numerics[6]

- Calculation of ground state and finite temperature moments
- Exact diagonalization for small systems
- Matrix product state-methods for larger systems
  → exact operator for $\langle\hat{M}_z^n\rangle$ with bond dimension $n+1$
- Neural network quantum states for even bigger systems at T=0
  → evaluation of $\langle\hat{M}_z^n\rangle$ by Monte carlo sampling

Cumulants of the order parameter



Numerics - Purification[3]

- For $T>0$
- Start with ∞ temperature state

$$|u_{\beta=0}\rangle = \bigotimes_{i=1}^{L^2}\left(|\uparrow\rangle_i|\uparrow\rangle_{i_{\mathrm{aux}}} + |\downarrow\rangle_i|\downarrow\rangle_{i_{\mathrm{aux}}}\right)$$

- Reach finite temperature state by time-evolution

$$|u_{\beta>0}\rangle = \left(e^{-\beta\hat{\mathcal{H}}}\otimes\mathbb{1}_{\mathrm{aux}}\right)|u_{\beta=0}\rangle$$

- calculate moments as

$$\langle\hat{M}_z^n\rangle = \frac{\langle u_{\beta/2}|\hat{M}_z^n|u_{\beta/2}\rangle}{\langle u_{\beta/2}|u_{\beta/2}\rangle}$$

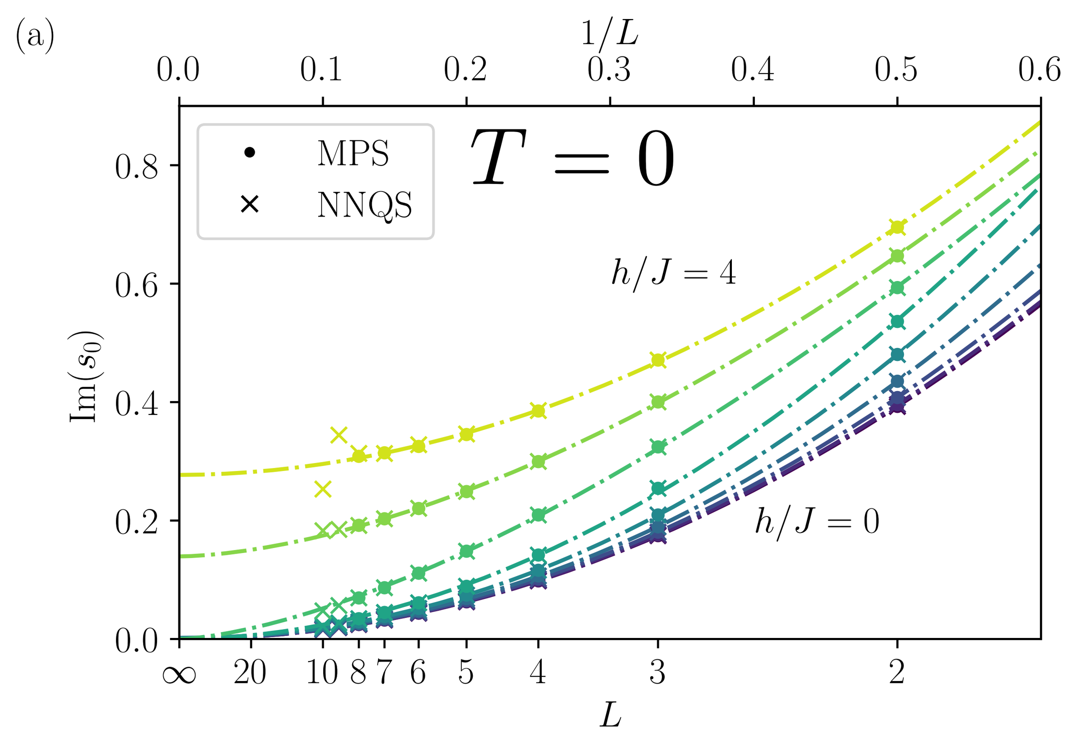
Results

- Obtain Lee-Yang zeros $\mathrm{Im}(s_0)$ as function of L for different values of h ($T=0$) or T (at fixed h, for $T>0$)
- Extrapolate to the thermodynamic limit using a simple scaling approach

$$\mathrm{Im}[s_0](L) = \mathrm{Im}[s_0](L=\infty) + \alpha L^{-\gamma}$$

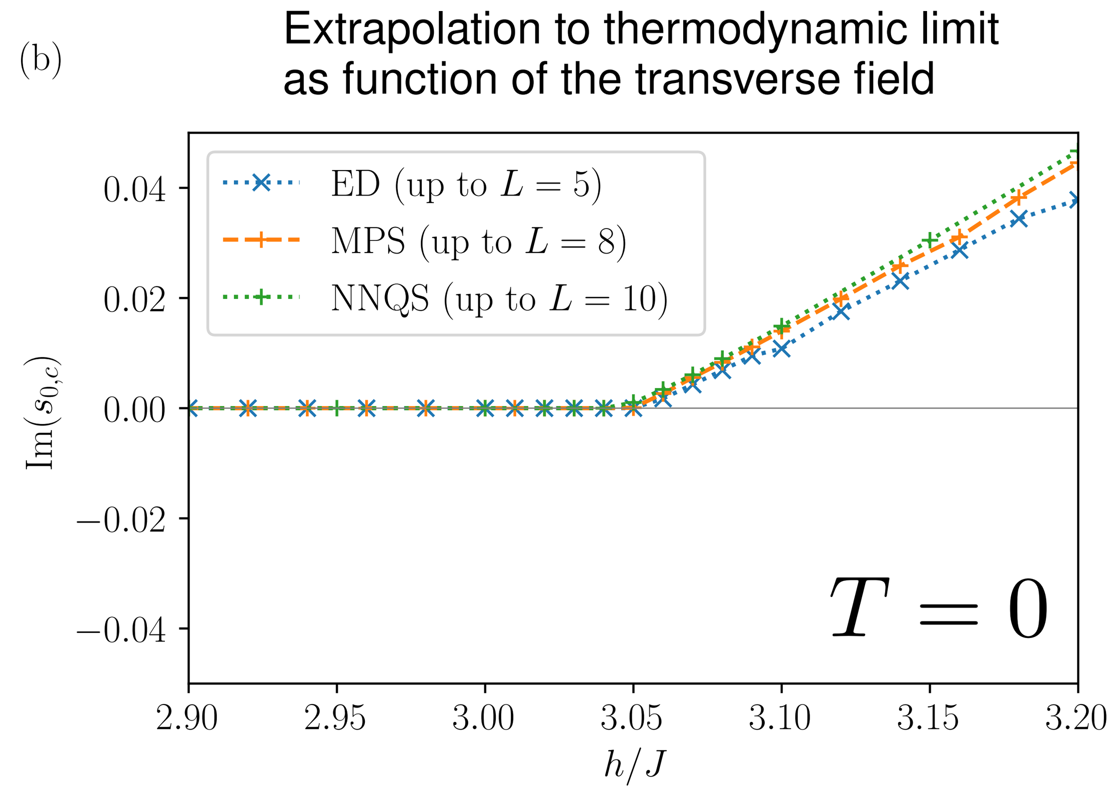
- Behaviour of extrapolation as function of varied parameter gives the point of the phase transition.

First Lee-Yang zeros as function of system size, transverse field



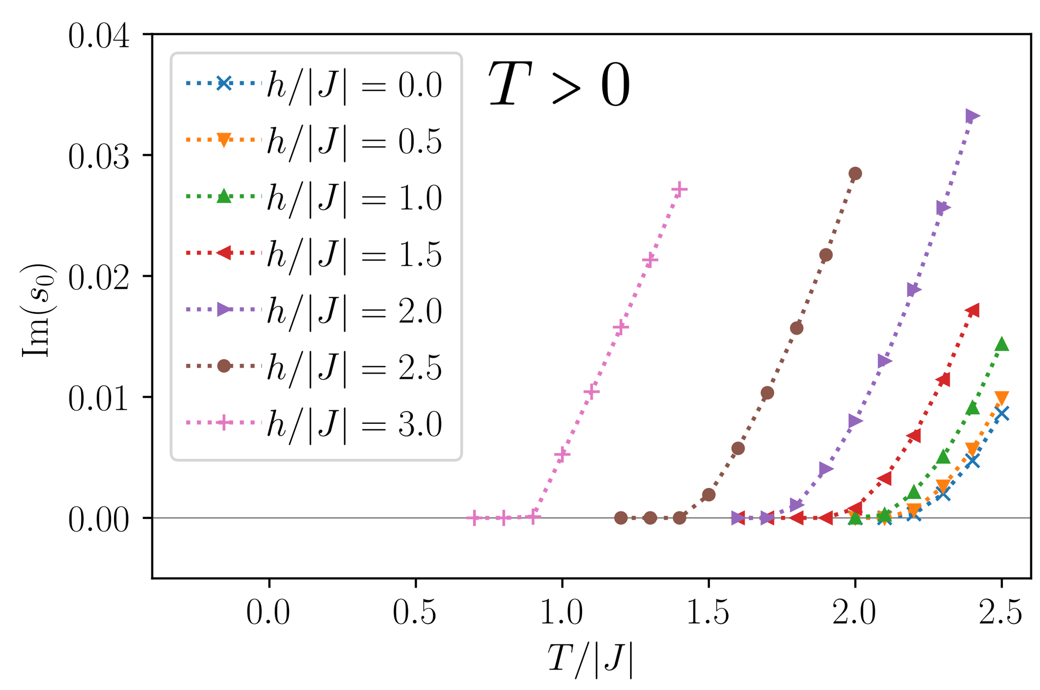
with a fitted extrapolation (scaling approach)

Extrapolation to thermodynamic limit as function of the transverse field



Phase transition at the kink

Extrapolation to thermodynamic limit as function of the temperature, transverse field



Phase transition where the extrapolation reaches 0

Conclusion

- Lee-Yang theory predicts phase diagram of the two-dimensional quantum Ising model
- The Lee-Yang methodology can potentially be employed to predict the phase diagrams of more complicated two- or three-dimensional quantum models, even at finite temperature.

References

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