Quantum Simulating Phase Transitions via Partition Function Zeros

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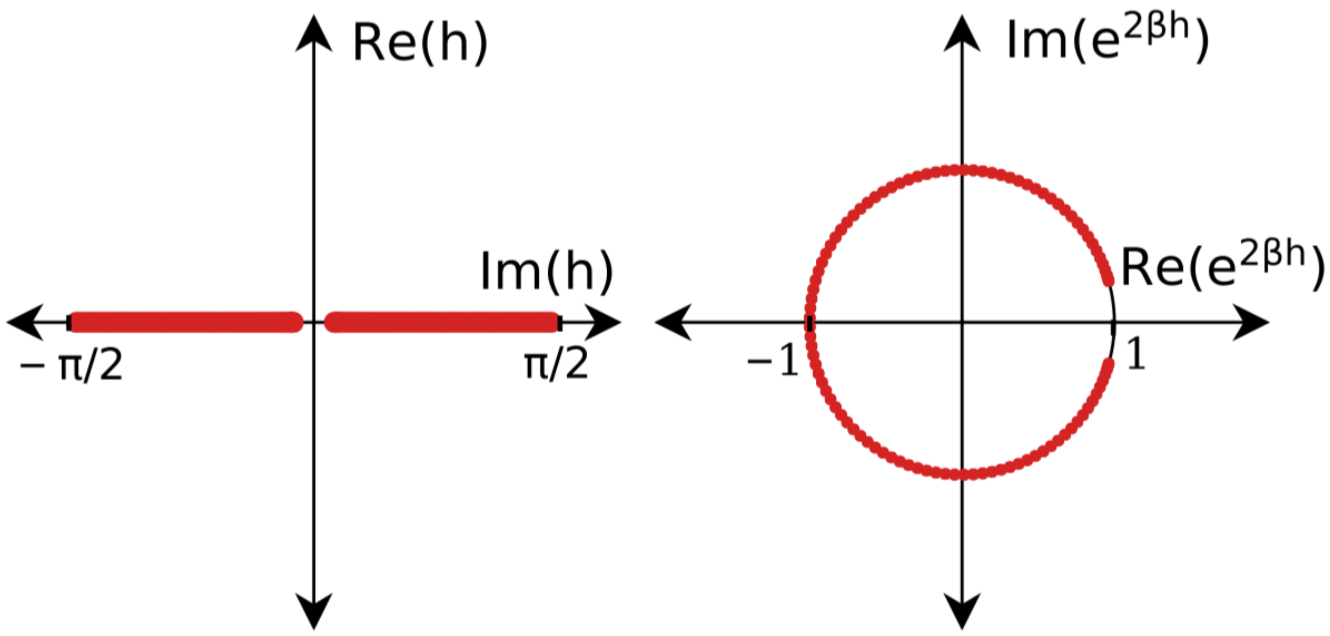
Phase transition from partition function

- In the thermodynamic limit, the free energy of a system becomes singular (non-analytic) at the critical point of a phase transition.

- Lee-Yang zeros: Through analytical continuation of free energy into the *complex* plane of control parameters, Yang and Lee showed that singularities of free energy, given as zeros of the partition function ($F = -k_B T \ln Z$), accumulate exactly at the transition point.

- Classical Ising model:

$$H = -\sum_{i,j} J_{ij} s_i s_j - h \sum_j s_j$$



Unit Circle Theorem (in complex fugacity plane)

Yang & Lee, Phys. Rev. 87, 404 (1952);
Yang & Lee, Phys. Rev. 87, 410 (1952);
Figure taken from Francis et al., Sci. Adv. 7, eabf2447 (2021)

Measuring partition function zeros - I

- Krishnan et al. proposed *two* ways of measuring the partition function for classical 2D Ising model on quantum computers Krishnan et al., PRA 100, 022125 (2019).

$$Z = \sum_{\vec{s}} \exp\left(-\sum_{i,j} K_{ij} s_i s_j - \sum_i H_i s_i \right),$$

$$\left| \langle + | \prod_{i,j} e^{-K_{ij}^R \sigma_i^z \sigma_j^z} e^{-iK_{ij}^I \sigma_i^z \sigma_j^z} e^{-H_i^R \sigma_i^z} e^{-iH_i^I \sigma_i^z} | + \rangle \right|^2 = \frac{|Z|^2}{2^{2N}}$$

$$e^{K_{ij}^R \sigma_i^z \sigma_j^z} |\psi\rangle = e^{|K_{ij}^R|} \langle + |_a U^{ZZ}_{i,a,\kappa_{ij}} U^{ZZ}_{j,a,\kappa'_{ij}} | + \rangle_a |\psi\rangle$$

$$e^{H_j^R \sigma_j^z} |\psi\rangle = e^{|H_j^R|} \langle + |_a U^{ZZ}_{j,a,\lambda_j} U^{Z}_{a,\mu_j} | + \rangle_a |\psi\rangle$$

Qubit scaling with cylindrical BC:

- $H = 0 : \ \ 3NL - N$
- $H \neq 0 : \ \ 4NL - N$

Measuring partition function zeros - II

- The second method is to map to a periodically kicked 1D transverse-field Ising model:

Krishnan et al., PRA 100, 022125 (2019).

$$P_{kicked} = \left| \langle + | e^{-k\sum_{\langle i,j \rangle}^{N} \sigma_i^z \sigma_j^z} \left(e^{-h\sum_i^N \sigma_i^x} e^{-k\sum_{\langle i,j \rangle}^{N} \sigma_i^z \sigma_j^z} \right)^L | + \rangle \right|^2 ,$$

$$P_{kicked} = \left| \frac{\sinh(-2h)^{N(L-1)}}{2^{N(L+1)}} \right| \left| Z_{2D}\left(k, \frac{\ln[\tanh(-h)]}{2}, N, L\right) \right|^2$$

$Z_{2D}(K_x, K_y, N, L)$: p.f. of the 2D Ising model with lattice size $N \times L$

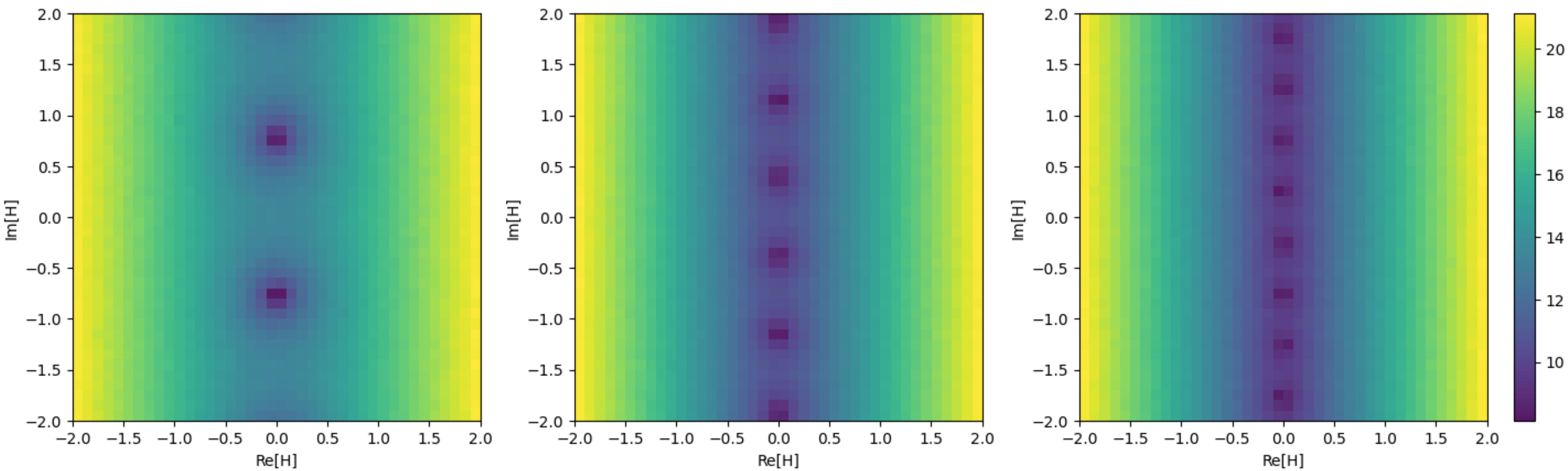
$$e^{h^R \sigma_j^x} |\psi\rangle = e^{|h^R|} \langle \uparrow |_a U^{XX}_{j,a,\lambda_j} U^{X}_{a,\mu_j} | \uparrow \rangle_a |\psi\rangle$$

Qubit scaling with cylindrical BC:

- $H = 0 : \ \ 2NL$
- $H \neq 0 : \ \ 3NL$

Qiskit simulations

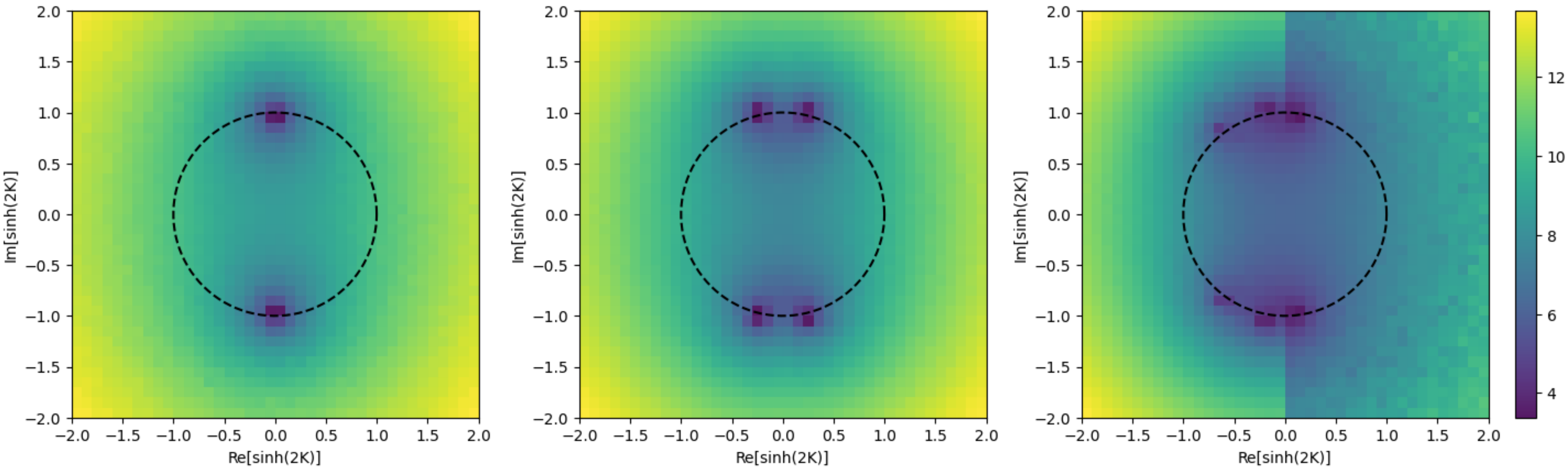
- Lee-Yang zeros (complex-H plane with $K_x = K_y = -1$): 5000 shots



2×1 $\quad$ 2×2 $\quad$ 3×2

Qiskit simulations

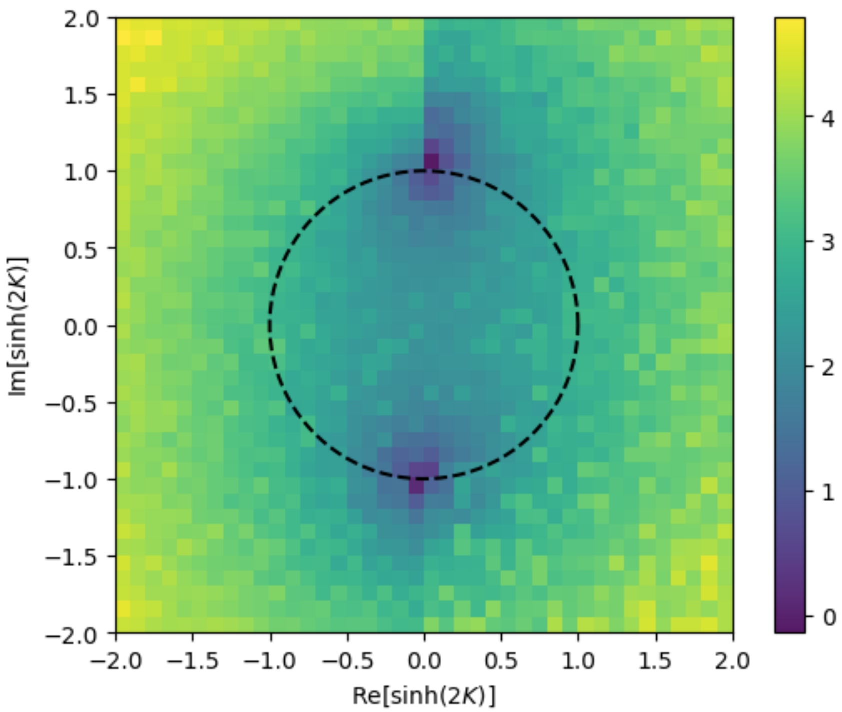
- Fisher zeros (complex-$\sinh(2K)$ plane with $H = 0$): 5000 shots; last one with 50000 shots



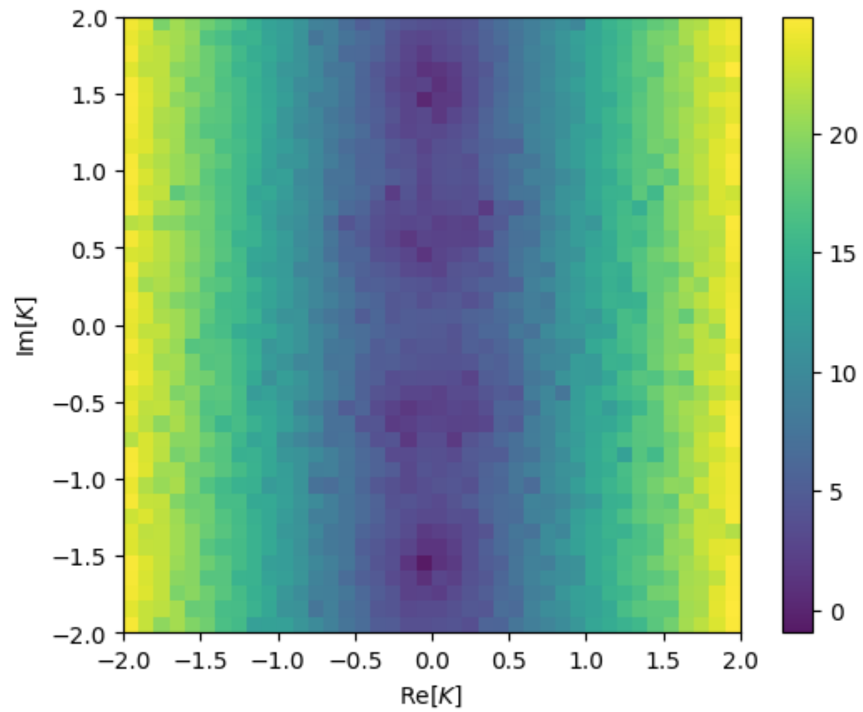
2×1 $\quad$ 2×2 $\quad$ 3×3

Preliminary hardware results

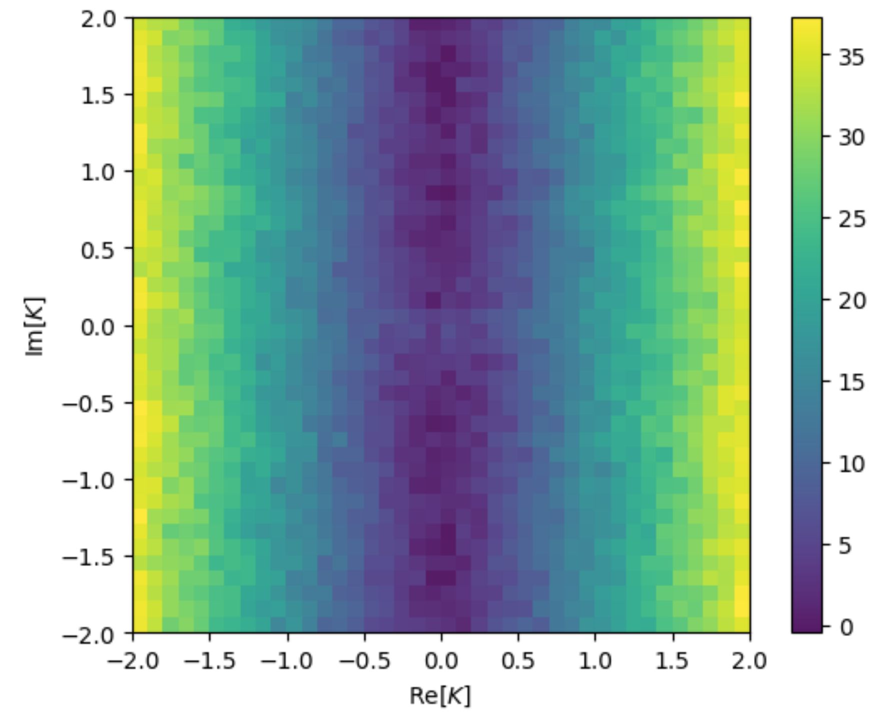
- Fisher zeros:



2×1; ibm_perth

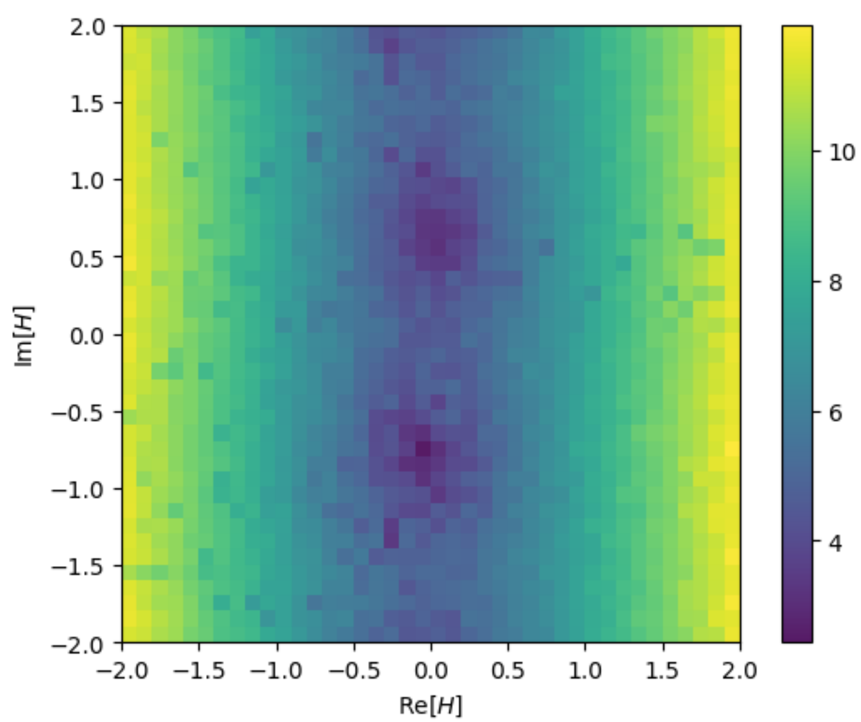


2×2; ibm_hanoi



3×2; ibm_cusco

- Lee-Yang zeros:



2×1; ibm_perth

Outlook

- Need to improve signal-to-noise ratio:
  - Improve qubit mapping on the heavy-hex topology to potentially reduce the number of SWAP gates & circuit depths
  - Employ error mitigation techniques
- Scale up to larger system sizes; will need to increase the number of samplings due to exponential suppression of the return probability
- Investigate spin glass models and their phases using this technique on QPUs