DMRG Study of the S = 1 quantum Heisenberg antiferromagnet on a Kagome-like lattice without loops

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Motivation

- **The Kagome Heisenberg Antiferromagnet (K HAFM), S>1/2**
  - Prime candidate for the realization of a quantum spin liquid (QSL) for small S, but large S is known to be ordered
  - Experimental realizations have $S > 1/2$ (e.g. $S = 5/2$ (jarosites), 3/2 BSZCGO)
  - Numerics (QMC, ED, cluster series expansion) limited by Hilbert space size, undeveloped variational wavefunctions
- **Husimi Cactus**
  - Locally Kagome-like, but no loops!
  - Has been used before to approximate the K HAFM (Elser & Zeng, '93)
  - Replicates: coplanar order (Simon & Douçot '98), spin disorder, VBS
  - Misses: coloring selection, spin-loop tunneling effects (von Delft & Henley '93), spin liquid flux patterns

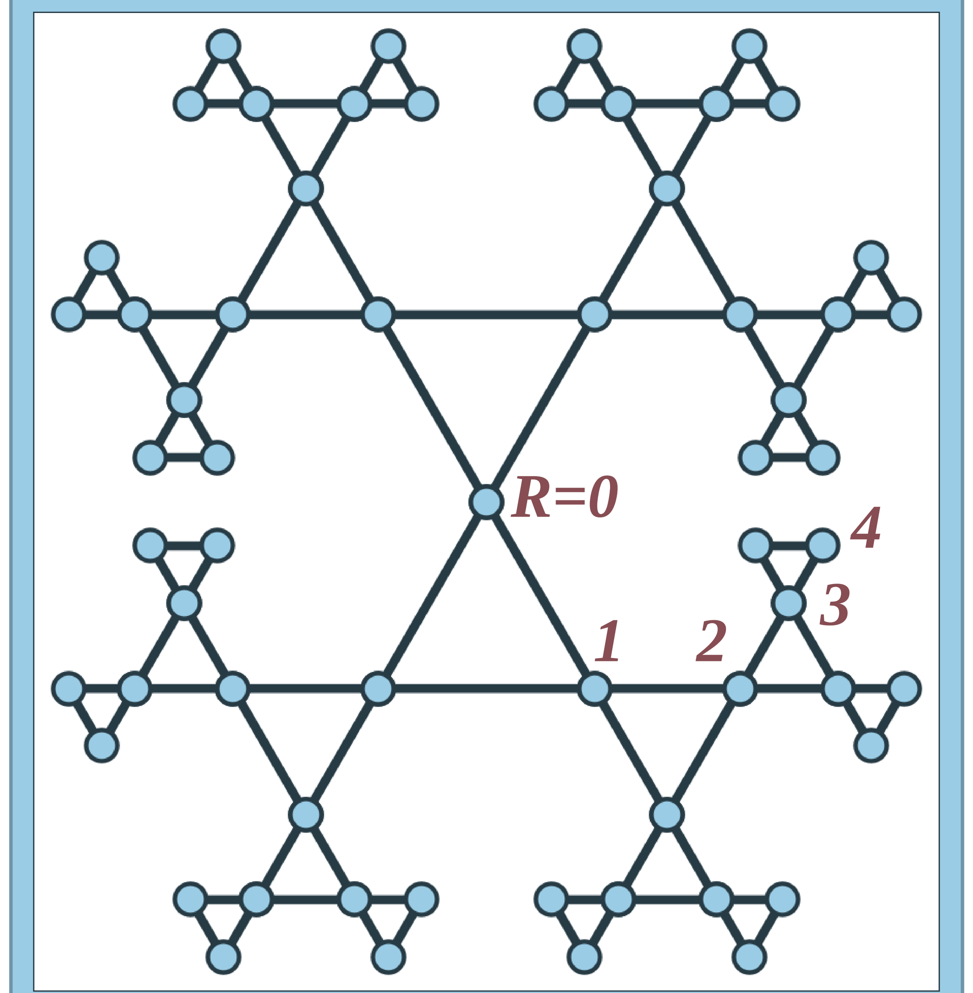


Figure 1: The vertex-centered Husimi Cactus at the fourth generation. The distance from the central node is listed for a few representative points.

- **Density Matrix Renormalization Group**
  - Why: Truncation of the exp. growing Hilbert space makes large S easier
  - May be able to study the transition from the predicted quantum spin liquid (QSL) at $S = 1/2$ (Chandra & Douçot '93) to the ordered state for large S (Douçot & Simon '98)
  - Why not: K lattice loops limit simulation sizes (Yan, Huse, & White, '11)

Method

- **DMRG**
  - Standard DMRG algorithms (White '92) works for recursively built lattices
  - Complexity: keeping M states on an individual block $\Rightarrow O(M^4)$

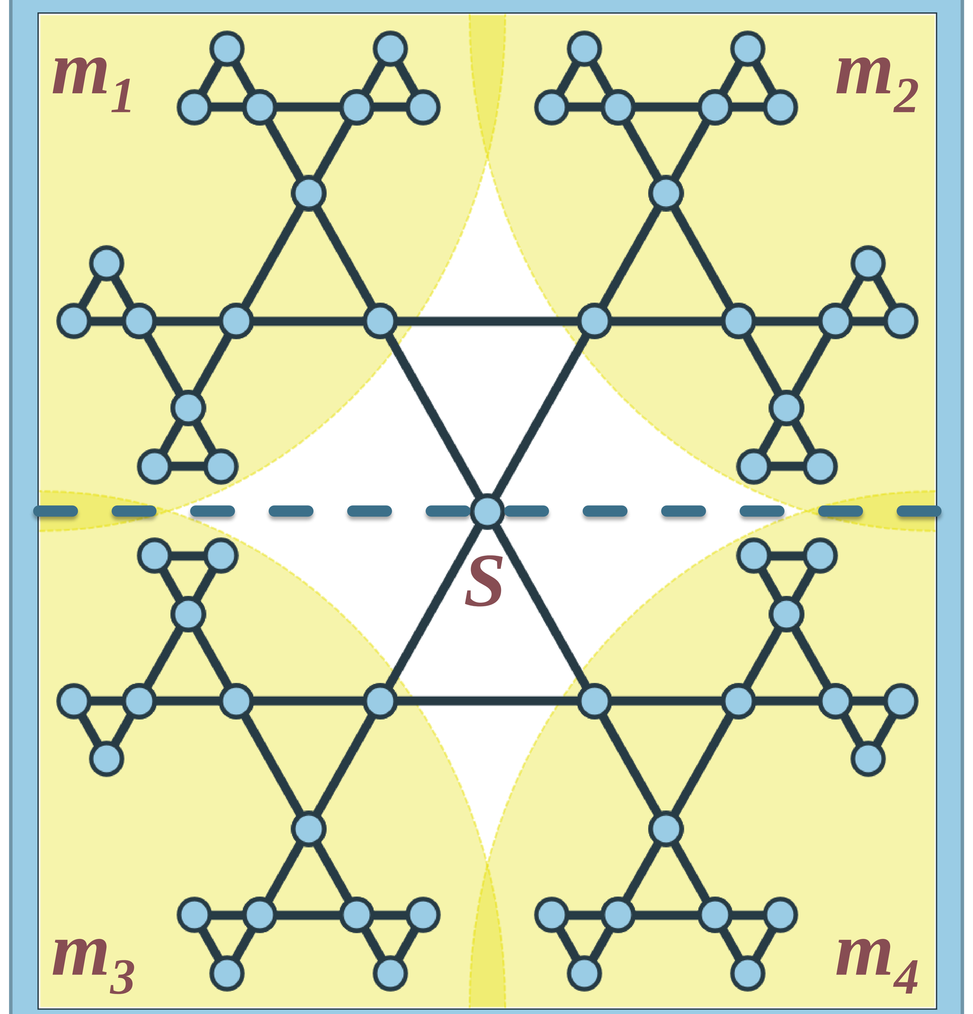


Figure 2: Blocks m_i from the previous generation interact with a single spin S; half the degrees of freedom ($m_{3,4}$) are traced out.

- **Correlations**
  - Our primary diagnostic tools are spin-spin correlation functions

$$\langle S_i \cdot S_{i+R}\rangle \quad \langle S_i^z S_{i+R}^z\rangle \quad \langle S_i^{\pm} S_{i+R}^{\mp}\rangle$$

$$C(i, i+r) \propto \begin{cases} 1/R^0, & \text{ferromagnet} \\ \left(-\frac{1}{2}\right)^R, & \text{3-coloring} \end{cases}$$

- **Expected Phase Diagram**

$$H = \sum_{\langle i,j\rangle}\left[\frac{1}{2}J_x\left(S_i^+ S_j^- + S_i^- S_j^+\right) + J_z S_i^z S_j^z\right] + \sum_i d(S_i^z)^2$$

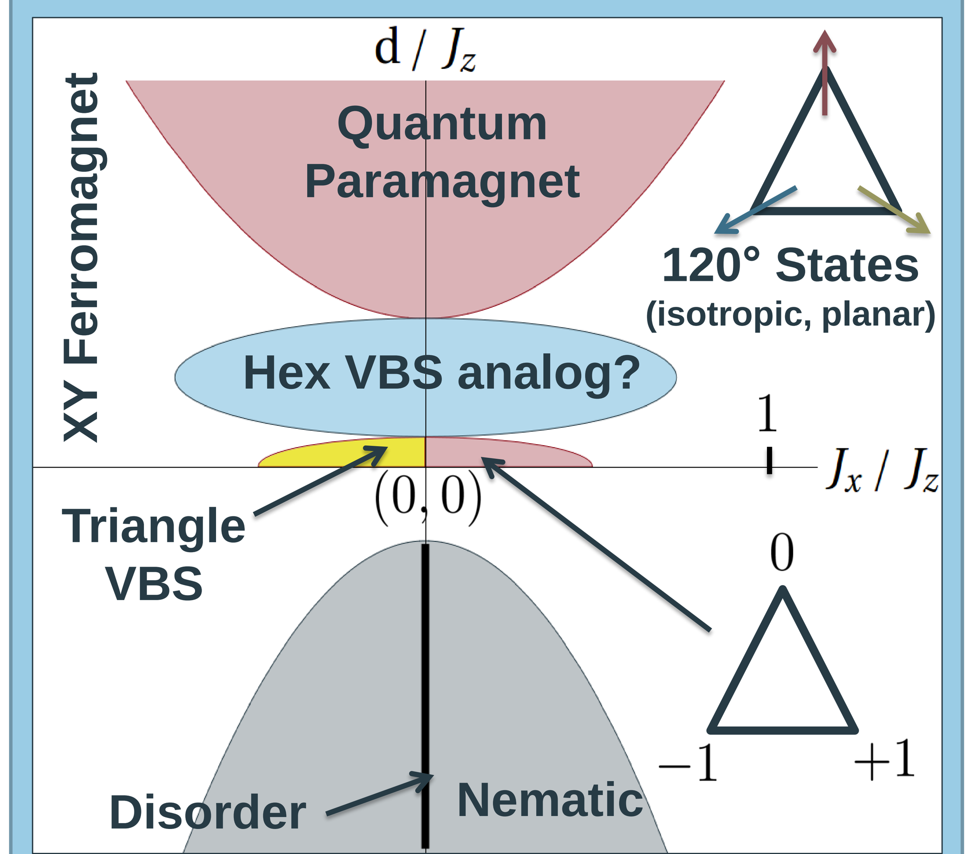


Figure 3: Hypothesized phase diagram, based in part on calculated Kagome phase diagrams (Isakov & Kim '09, Xu & Moore '07)

Results: On-Site Anisotropy, $S = 1$

- **Easy-axis on-site Anisotropy**
  - By including the on-site Hamiltonian

$$H_d = d\,\Sigma_i \left(S_i^z\right)^2$$

we can look at ground states in several interesting parameter regions (see fig 3)

- **XY Ferromagnet (as a test)**

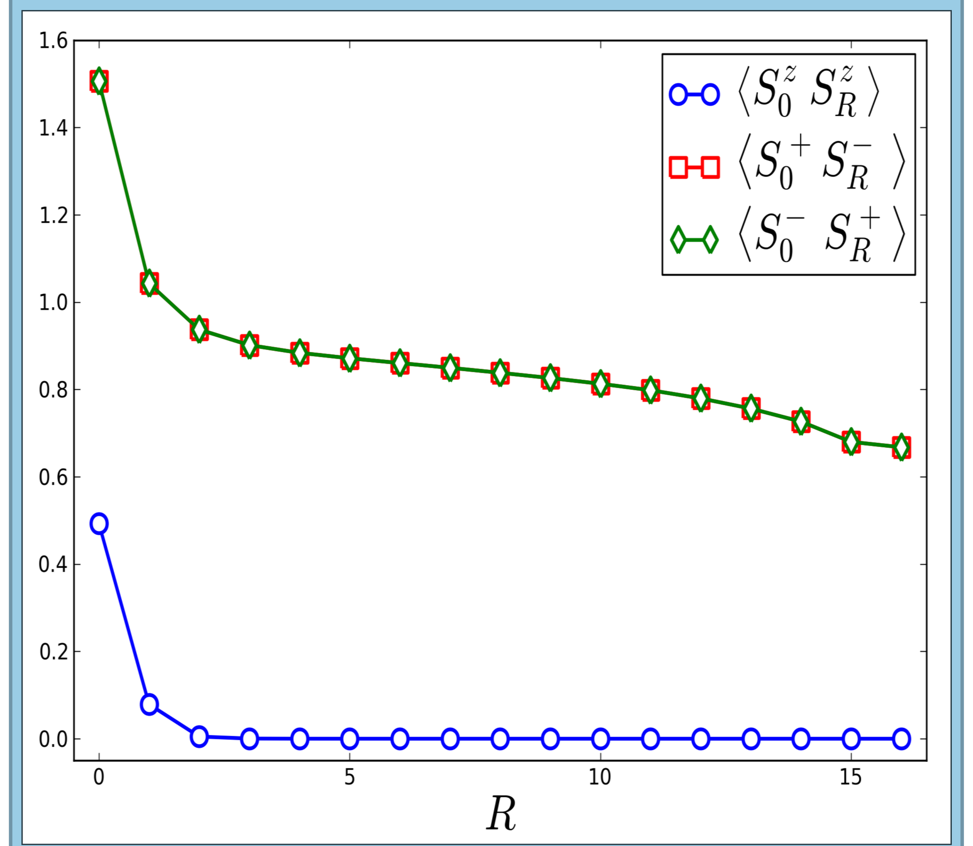


Figure 4: When $d = 0$, large anisotropic ferromagnetic J_x interactions will result in an XY ferromagnetic state. Here we show three correlation functions, $\langle S_i^z S_{i+R}^z\rangle$, $\langle S_i^+ S_{i+R}^-\rangle$, and $\langle S_i^- S_{i+R}^+\rangle$, for $J_x = -10.0 J_z$. The first correlation function should decay to zero exponentially, and the later two should be equal and non-zero, as is observed here.

- **Disordered Quantum Paramagnet**

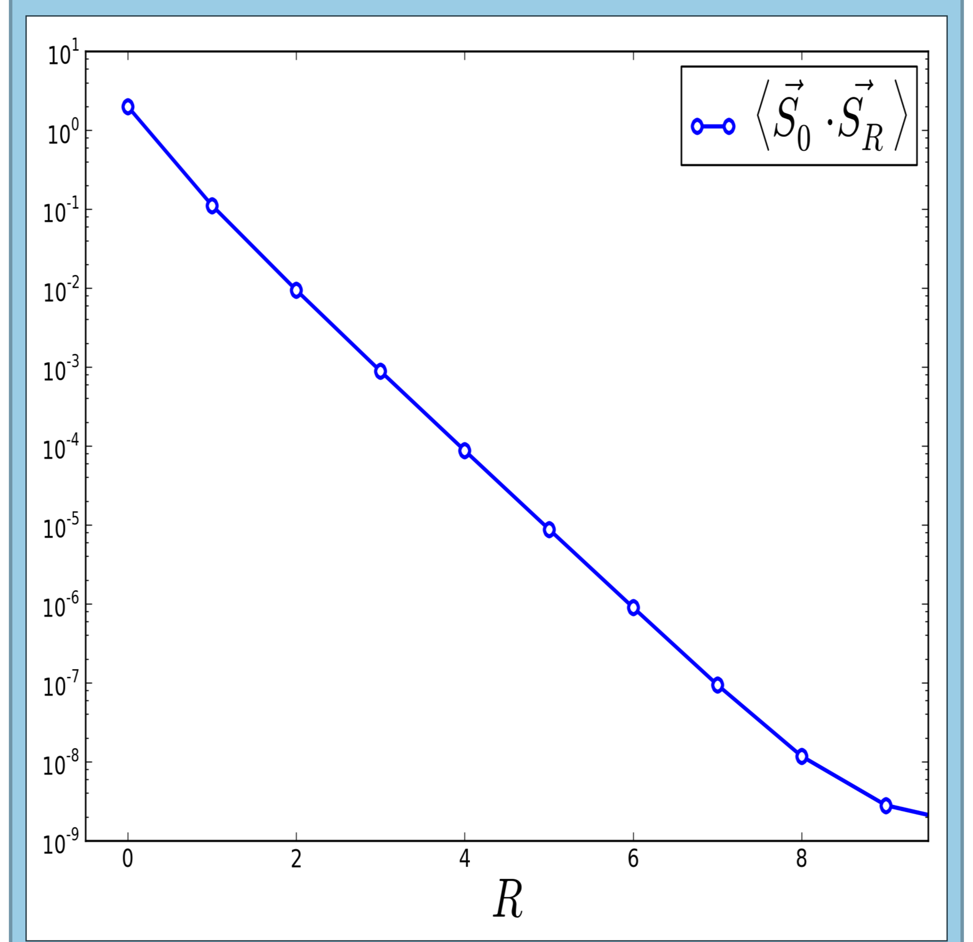


Figure 5: For very large positive values of d, we obtain a disordered quantum paramagnet, evidenced here by exponentially decaying spin-spin correlations for $d = 10 J_z,\ J_x = 0 J_z$.

Results: Correlation Scaling

- **Correlation Function Scaling**
  - As mentioned before, the scaling behavior of a correlation function is indicative of certain types of order
- **120 deg States and 3-color ordering**

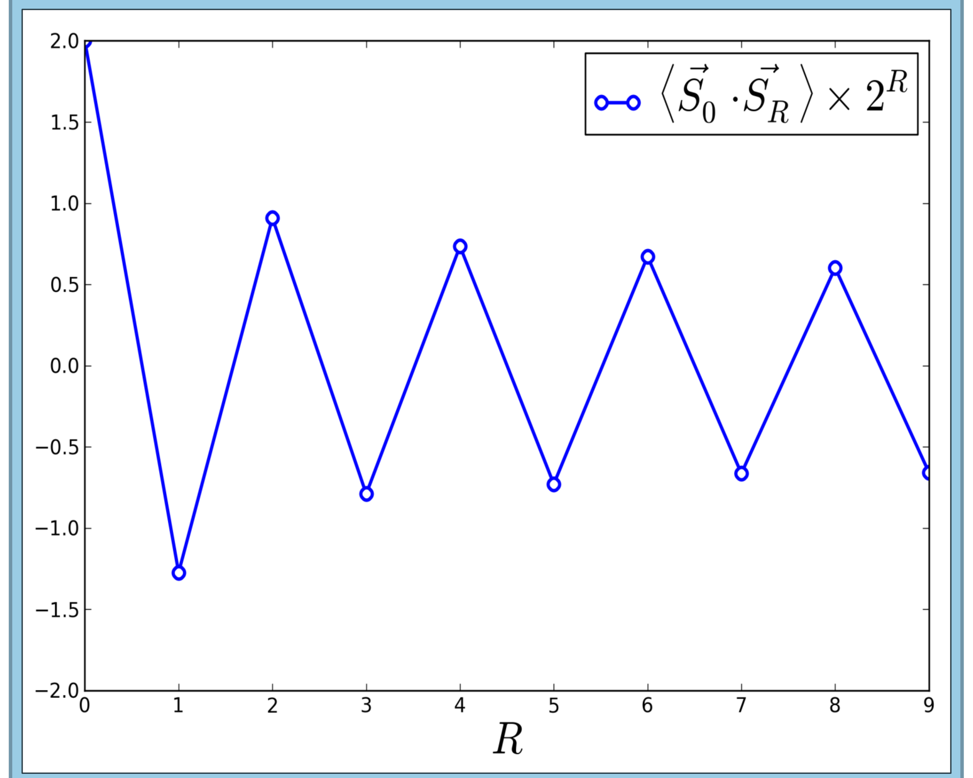


Figure 6: While 3-coloring states do not strictly possess long range order, they do possess a different type of constraining order. This leads to correlations which decay as $(-1/2)^R$. In this trial, $d = 0,\ J_x = 20 J_z$. This is nearly a 120 degree state, as evidenced by correlations decaying as $(-1/a)^R$ for $a \approx 2$

Scaling at the Heisenberg Point

- ***S = 1* and beyond**

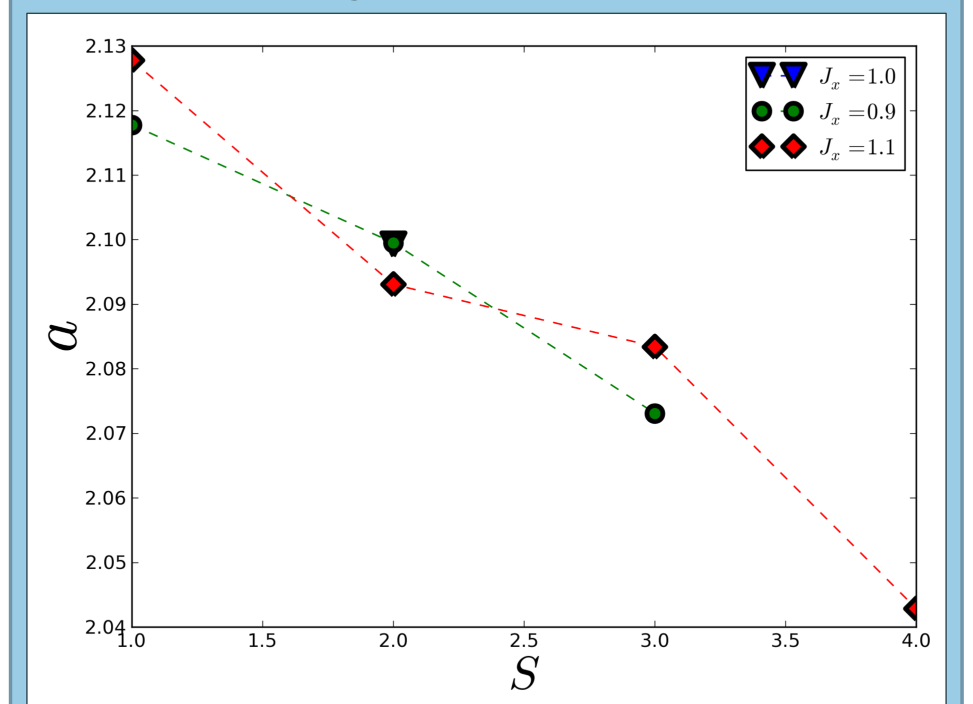
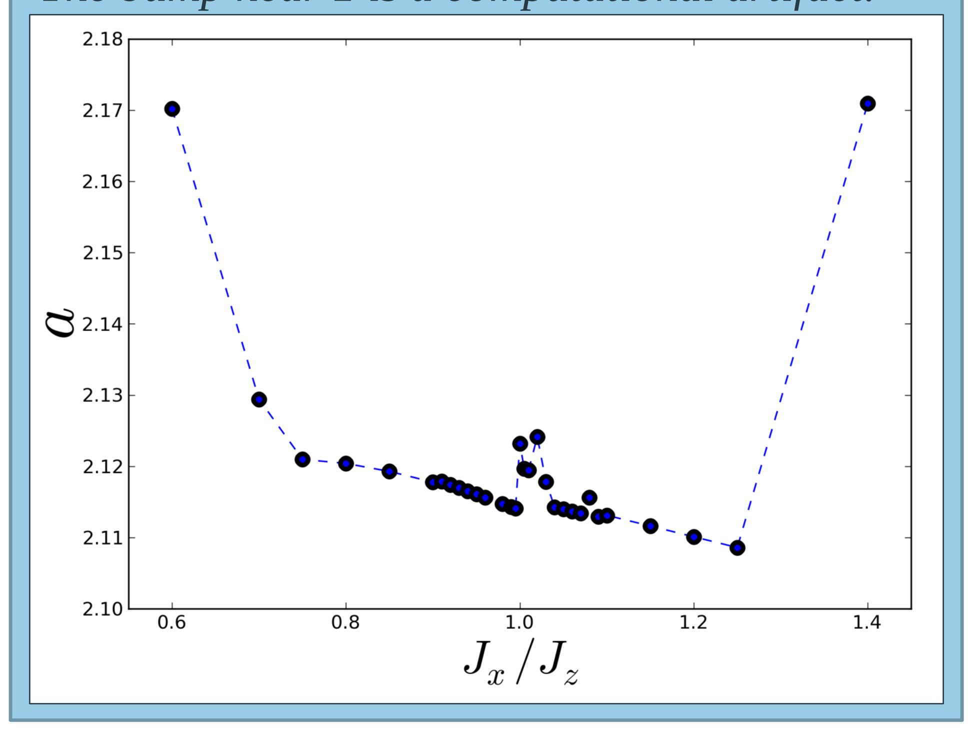


Figure 7/8: Above we see how the value of a in $C(R) = (-1/a)^R$ changes as a function of S. Below we see the same constant a near $J_x = J_z$. The bump near 1 is a computational artifact.



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