Griffiths-McCoy Singularities in the Dilute Transverse-Field Ising Model: A Numerical Linked Cluster Expansion Study

Foster Thompson
Case Western Reserve University, OH 44106, USA

Rajiv Singh
University of California Davis, CA 95616, USA
(Dated: August 2018)

We use Numerical Linked Cluster Expansions (NLCE) to study the site diluted transverse-field Ising model on the square-lattice at $T = 0$. NLCE with a self-consistent mean-field on the boundary of the clusters is used to obtain the ground state magnetization, susceptibility, and structure factor as a function of transverse field h and exchange constant J. Adding site-dilution to the model turns NLCE into a series expansion in the dilution parameter p. Studying the divergence of the structure factor allows us to establish the phase-diagram in the h/J and p plane. By studying the magnetization of the system in a longitudinal field, we investigate the Griffiths-McCoy (GM) singularities. We find that the magnetization develops non-linearities in the Griffiths phase with exponents that vary continuously with h. Additionally, the probability distribution of the local susceptibility in the Griffith's phase is studied in terms of its moments.

I. INTRODUCTION

Disorder occurs in physical systems for a plethora of reasons. We study a two-dimensional disordered version of the transverse field quantum Ising model–a classic statistical model of a magnet consisting of a lattice of 1/2 quantum spins constrained to orient along a single axis. The spins are typically taken to interact with those nearby, causing them to tend to point in the same direction as their neighbors. Additionally, the spins are coupled to an external "transverse" magnetic field which points in a direction perpendicular to the axis of their orientation. To introduce disorder into the model, we allowed the sites of the lattice to be randomly omitted, making the lattice "dilute." Physically this has the interpretation of a magnetic substance with a fixed concentration of non-magnetic impurities or alloyed with a non-magnetic substance. This model displays two noteworthy features: a discontinuity in the critical value of the transverse field as a function of a parameter controlling the strength of the dilution and Griffths-McCoy singularities.

In the pure system with no dilution the Ising model displays two phases. When the coupling to the transverse field is very large, the model possesses a single ground state in which the spins are mostly aligned with the direction of the transverse field. The model is said to be in a disordered phase; there is no long-range order and the overall magnetization of the system along the Ising axis is zero. When the coupling strength is tuned below a certain critical value the model changes phase and the spin-spin interactions take over. In this new, ordered phase, there are two degenerate ground states in which the spins point predominately in one of two directions along their naturally preferred axis and the system acquires nonzero magnetization.

When site dilution is introduced, this picture remains intact so long as the dilution is weak. When the lattice is highly dilute however, it is mostly composed of disconnected clusters of spins and so long-range order can never develop and the system never enters an ordered phase regardless of the strength of the transverse field. When the dilution parameter is brought above a certain critical value, the lattice exhibits a phase transition in its dilution, transitioning from predominately disconnected to a predominately connected. When this happens, the lattice is said to "percolate" and the point at which the phase transition occurs is referred to as the percolation threshold. As originally conjectured based on informal heuristic argument by Harris [1], this transition is not continuous in the critical value of the transverse field. Below the percolation threshold, the critical strength of the transverse field is zero as no long-range order can develop. As soon as the lattice percolates however, clusters of spins spanning the entire length of the lattice will dominate, permitting long range order with a critical transverse field strength of at least that of the one-dimensional pure system. This picture was later confirmed by Stinchcombe with analytic arguments using the renormalization group by [2].

Griffiths Singularities are nonanalyticities in statistical quantities of disordered models which arise due to the low but nontrivial impact of large non-dilute regions in an otherwise dilute lattice. These regions tend to magnetize, locally entering a ferromagnetic phase despite the disordered behavior of the bulk lattice, effectively behaving as embedded, finite-size copies of the pure system [3]. This has the effect of introducing weak "Griffiths" singularities in the low-concentration, low-field regime. In classical systems, the strength of these singularities scale inversely with the size of the region and consequently they are too weak to be detected either experimentally or numerically. However, in quantum systems, tunneling between the ground state and first excited states in the locally non-dilute regions causes the strength of the singularities to scale also with the difference in energy levels of the ground state and first excited state. This scales exponentially with region size, leading to a contribution of order unity. As a consequence, these quantum "Griffiths-McCoy" singularities are observable both in experiments and numerical calculations. For a more comprehensive discussion on Griffiths-McCoy singularities in a myriad of disordered models and on the role of disorder in general in quantum critical behavior,

see [4].

In this work, we study the critical behavior and Griffiths-McCoy singularities of the dilute quantum transverse-field Ising model using a computational technique for generating series expansions called numerical linked cluster expansions (NLCE). We focus specifically on the quantum critical behavior at zero temperature. We use NLCE to study the critical behavior of the susceptibility, magnetization, and structure factor to establish a numerical approximation of the location of the different phases and critical points of the dilute transversfield Ising model. We pay special attention to the existence of Griffiths singularities, finding numerical evidence for their existence in the behavior of the magnetization as a function of longitudinal field and the probability distribution of the local susceptibility.

II. OVERVIEW OF APPROACH

A. Model

We consider the zero temperature behavior of a site-diluted quantum transverse field Ising model on a two-dimensional square lattice. The model is parametrized by the three element set $\{J, h, p\}$, where J an exchange constant controlling the strength of nearest-neighbor spin-spin interactions, h is the coupling strength to a transverse field, and p is the dilution parameter. The Hamiltonian of the model is:

$$\mathscr{H} = J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \sigma_i^z \sigma_j^z + h \sum_i \epsilon_i \sigma_i^x, \tag{1}$$

where $\langle \cdot, \cdot \rangle$ denotes nearest-neighbor pairs of sites on the lattice and σ^z and σ^x are the pauli matrices. The ϵ_i terms are site dilution variables: random variables with bimodal distribution, taking values of 0 and 1 with probability p and $1-p$ respectively. These parameters are referred to as having "quenched" disorder, as they randomly take some fixed value and do not evolve with the system.

At zero temperature, thermal averages reduce to ground state expectation values. We denote the ground state by $|0\rangle$.

We will take $J < 0$ to study the ferromagnetic problem in which the nearest-neighbor interactions favor adjacent spins aligning along the same direction. Broadly speaking, the ratio h/J controls what phase the model is in. However, the magnitude of J does not change the qualitative behavior of the model. Subsequently, for convenience we constrain our analysis to a fixed $J = -1$.

B. Method

NLCE is a method of approximating an extensive property as a series with terms computed by exact diagonalization of small, finite size systems—'clusters'—which embed into the lattice of the full model as subgraphs. Specifically, given an extensive property P, its per-site value in the thermodynamic limit is given by subtracting sub-weights:

$$\lim_{N\to\infty} \frac{P}{N} = \sum_c L[c] W[c]. \tag{2}$$

The lattice constant $L[c]$ denotes the number of ways the cluster c can embed into the lattice. $W[c]$ is the weight of the cluster in the lattice, as determined recursively by:

$$W[c] = P[c] - \sum_{c' \subseteq c} W[c'], \tag{3}$$

where, $c' \subseteq c$ is a sub-cluster—a cluster which embeds into the cluster c—and $P[c]$ is the property computed on the cluster.

For disordered models, one is typically interested in quantities of the form $[P/N]_{\text{av}}$, where $[...]_{\text{av}}$ denotes the quenched average over the site dilution variables ϵ_i. NLCE can be generalized to a quenched average in a straightforward way by simply computing the quenched average of each cluster individually before summing up the total value of the property. In the case of the site diluted model we study this greatly simplifies the resulting series. For any cluster, any configuration of the site dilution variables ϵ_i in which any site is omitted will reduce the cluster to a collection of its sub-clusters, resulting in zero weight after the weights of sub-clusters are subtracted away. Only the single configuration with no dilution survives the sub-weight subtraction. Subsequently, the NLCE of the quenched average of a property P reduces to simply the NLCE of P for the pure system with an additional factor of $p^N[c]$, the probability of the non-dilute configuration:

$$\lim_{N\to\infty} \left[\frac{P}{N}\right]_{\text{av}} = \sum_c L[c] W[c] p^{N[c]} \equiv \sum_{n=1}^{\infty} a_n p^n, \tag{4}$$

where $N[c]$ denotes the number of sites in c. As a consequence, the NLCE becomes a power series in the dilution parameter p.

III. PURE SYSTEM ANALYSIS

To demonstrate the efficacy of this method, as an exercise we first considered the non-dilute Ising problem (that is, the $p = 1$ limit). We analyzed the susceptibility and structure factor, as both of these quantities are known to diverge strongly near the pure system's critical point of $h_c \simeq 3.044$. The structure factor S is defined by:

$$S = \sum_{i,j} \langle \sigma_i^z \sigma_j^z \rangle - \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle, \tag{5}$$

where we use the notation $\langle \sigma_i^z \rangle = \langle 0 | \sigma_z^i | 0 \rangle$. In order to compute the susceptibility, we add an additional longitudinal field term to the Hamiltonian:

$$\mathscr{H} = J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x + h_L \sum_i \sigma_i^z. \tag{6}$$

With this additional factor, letting E_0 denote the ground state energy, the susceptibility is given by:

$$\chi = \lim_{h_L \to 0} \frac{\partial^2 E_0}{\partial {h_L}^2}. \tag{7}$$

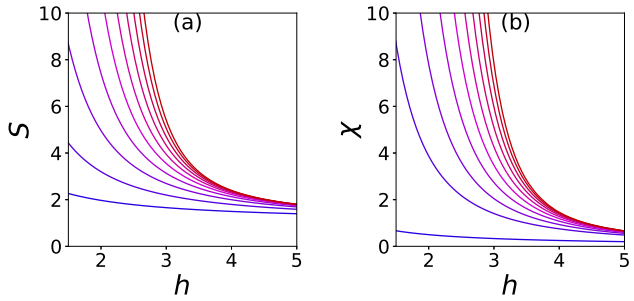

FIG. 1: (a) shows the structure factor S and (b), the susceptibility χ. In both plots. For both quantities, the NLCE is truncated to include only clusters with 10 or fewer bonds. Curves of order 1-10 in the number of bonds are shown simultaneously with increasing redness starting with blue at first order. The NLCE converge well for $h > h_c$ and increase sharply close to h_c before saturating for small values of h. The point at which divergence begins appropriately occurs closer to h_c the higher the order.

We used NLCE to compute the susceptibility χ and structure factor S for a range of values of h centering around h_c. The results of the computation are shown in fig. 1. Because convergence is poor in the ordered ($h \lesssim h_c$) phase, we sought a way of regulating both of these quantities. To achieve this, we included an additional term in the Hamiltonian of each cluster to account for the effects of the effect of the full lattice:

$$\mathscr{H} = J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x + m(h) \sum_i q_i[c] \sigma_i^z. \tag{8}$$

Specifically, this added term is a mean field acting on the boundary of the cluster: the quantity $q_i[c]$ represents the number of neighbors on the site i in the cluster c. Physically, we expect the h-dependent value of m to satisfy the self-consistency condition $m = M$, where M is the magnetization of the lattice, defined by:

$$M = \sum_i \langle \sigma_i^z \rangle. \tag{9}$$

We implemented this as a constraint numerically by computing M for a small number of guessed, constant values of m for each h, then interpolating to find the approximate value of m satisfying the constraint. Computed for a range of h, this gives an approximation for the magnetization M, which we used to regulate the convergence of the NLCE for both S and χ. The result of this computation is shown in fig. 2.

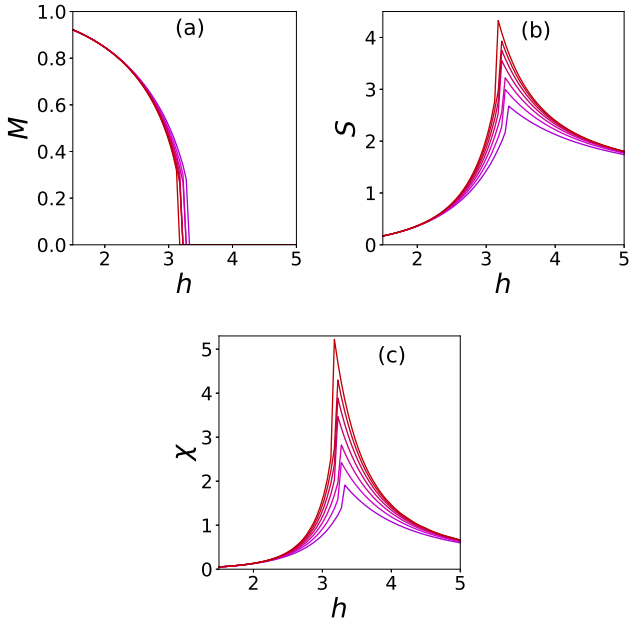

FIG. 2: In all three plots, orders 4-10 in the number of bonds are shown, with higher orders shown in redder colors. (a) shows the magnetization computed using the self-consistency constraint. Its shape is qualitatively typical for the magnetization of a ferromagnet, falling to zero near the critical point. (b) and (c) show curves of the structure factor S and susceptibility χ plotted using the magnetization self-consistent mean field. Both quantities now converge very well in both the ordered and disordered phases, peaking near the critical point.

IV. DILUTION PROBLEM

A. Phase Diagram

We now turn our attention to the dilute Ising problem. In the limit of $h \to 0$, this becomes a percolation problem with two phases controlled by the value of the percolation parameter p. At low values of p, highly dilute configurations dominate, the lattice becomes a collection of disconnected clusters, and no long-range order develops. Above the percolation threshold $p_c \simeq 0.59$, the lattice is said to percolate and non-dilute clusters play a larger role and long range order can develop. For small, nonzero values of h, it is believed that a flat phase boundary controlled by the change in typical geometry of the lattice at p_c independent of h extends into the $h - p$ plane to some value h_M with a lower bound of $h = 1$, the critical point of the one-dimensional model. Near the critical point h_c of the pure system, the phase boundary is believed the extend smoothly downward into the plane before meeting the flat boundary at the multi-critical point h_M. We used NLCE to confirm this picture of the phase diagram.

Due to the simplification of NLCE to a power series as given by eq. (4), we are able to use the ratio method to extrapolate how the critical point p_c varies as a function of h.

Specifically, for values of p near p_c, we expect the structure factor S to obey an asymptotic power law: $S \propto (p - p_c)^{-\gamma}$. Subsequently, we expect the coefficients of the power series for S from eq. (4) to obey (up to corrections of order $1/n^2$):

$$\frac{a_n}{a_{n-1}} = \frac{1}{p_c}\left(1 + \frac{\gamma - 1}{n}\right). \tag{10}$$

A plot of these ratios is shown in fig. 3 for a range of values of h. One can obtain an approximation of p_c at some h from

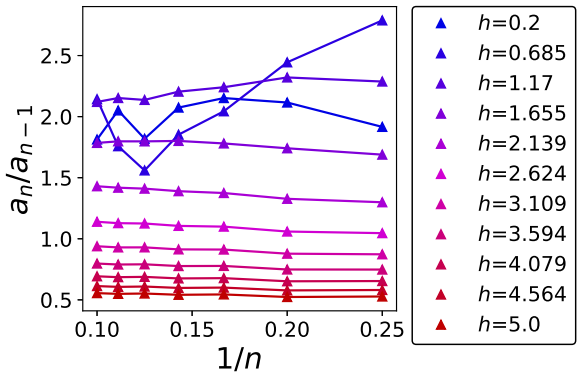

FIG. 3: Plot of ratios a_n/a_{n-1} as a function of $1/n$ for a representative range of h-values showing n taking values 2-10. For large values of h, these plots are all relatively flat. For values of $h \lesssim h_c$, it is clear from this plot that the intercept of a linear regression of the values shown here will yield a value of $1/p_c$ that is < 1. This is obviously nonphysical, corresponding to a probability greater than 1. Subsequently, the point at which the computed p_c becomes physical gives an approximation of the pure system critical point h_c. Additionally, for sufficiently small values of h, the plots here become very nonlinear, indicating the convergence of the NLCE to break down below some value close to h_M. We believe this is to be expected, as at the multi-critical point h_M, critical behavior switches from being governed by the value of h to being controlled by the geometry of the lattice, leading to the breakdown of the NLCE with h below h_M.

the intercept of a regression of these ratios computed at h. We used this method to compute p_c as a function of h and used the results to build an approximate phase diagram shown in fig. 4(a).

In addition to this, the slope of the linear regression ratios can be used to approximate the critical exponent γ. In the region where this method converges well and is physically meaningful, γ is approximately constant, with some fluctuation, as shown in fig. 4(b).

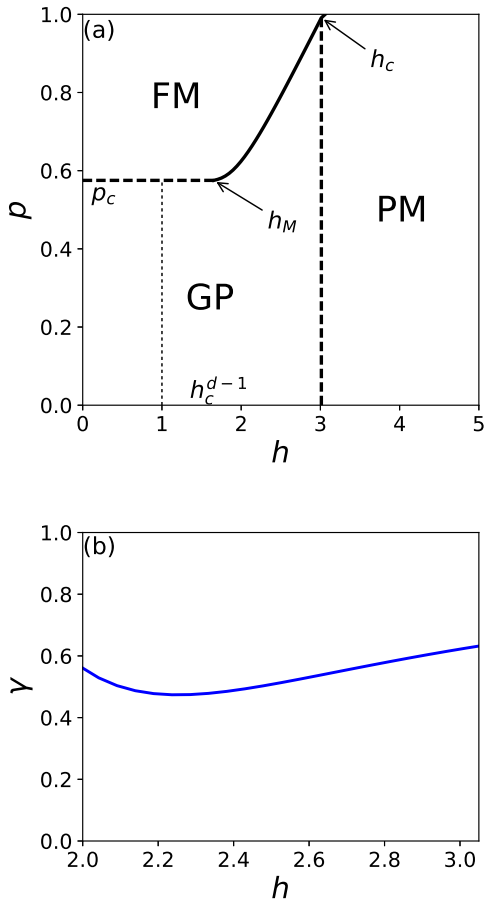

FIG. 4: (a) shows a complete phase diagram, showing distinct ferromagnetic (FM), paramagnetic (PM), and Griffiths (GP) phases. Using linear regression on data like that shown in fig. 4 for many values of h, we established the boundary shown by the full line. This line begins at the approximate h_c of the pure system, which we find to be 3.03, close to the known value of 3.04. The flat continuation of the phase boundary we expect after convergence of the NLCE breaks down for $h < h_M$ is shown by the horizontal dashed line. This point begins at $h_M \simeq 1.65$. This line intersects the p axis at the percolation probability p_c, which we find to be 0.58, also close to the known value of 0.59. The dotted line marked with h_c^{d-1} shows the value of the one-dimensional critical point, a lower bound on h_M. The vertical dashed line indicates a separation between the ordinary paramagnetic phase and the disordered Griffiths phase where we observe Griffiths-McCoy singularities to be present. (b) shows the value of γ computed from the slope of the same linear regression. This gives the rough bounds $0.47 \lesssim \gamma \lesssim 0.61$.

B. Griffiths-McCoy Singularities

Griffiths-McCoy (GM) singularities occur in disordered quantum models in their disordered phases. Rare, ordered regions can locally occupy a state which mimics the ordered phase of the pure system. In the context of the dilute Ising problem, these manifest in the low p and h regime—what we will refer to as the Griffiths phase—as non-dilute regions in an otherwise highly dilute lattice. This region is shown in fig. 4(a) labeled GP. For small values of h, these regions can occupy a ferromagnetic phase independent of the behavior of the rest of the lattice.

We expect GM singularities to manifest in the behavior of the magnetization M in a system with a longitudinal external

field h_L:

$$\mathscr{H} = J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \sigma_i^z \sigma_j^z + h \sum_i \epsilon_i \sigma_i^x + h_L \sum \epsilon_i \sigma_i^z. \quad (11)$$

The magnetization as a function of the longitudinal field of a pure ferromagnet is typically linear in the limit of small h_L. However, for our dilution model for values of p below p_c and values of h below h_c, we find curvature in the magnetization vs. h_L curve, as shown in fig. 5. Specifically, the magnetization obeys some nonlinear power law $M \sim {h_L}^a$. To quantify how the exponent varies with h, we used a linear fit of a log-log plot of M and h_L to compute the value of a for a range of values of h. As shown in fig. 6, for $h < h_c$, this varies continuously as a function of h.

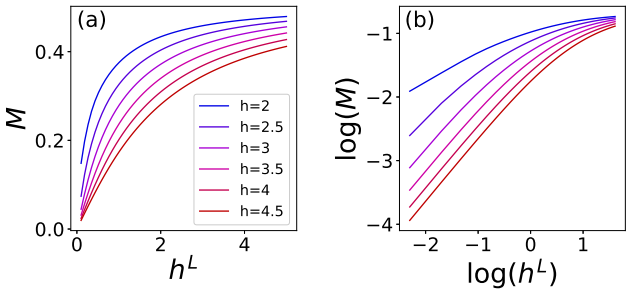

FIG. 5: Both plots show computations for $p = 0.5$, well below the percolation threshold p_c and in the Griffiths phase for small h. Computations were done to 10th order in the number of sites. (a) shows magnetization M plotted as a function of longitudinal field h_L for a for a representative range of h-values. Below the critical point h_c, curvature begins to develop in the small-h_L limit. This can be better visualized in (b), showing a log-log plot of the same quantities. For $h > h_c$, the slopes of the log-log plot are about 1, while for values $h < h_c$, they are noticeably less than 1.

As an additional indication of the influence of GM singularities, we considered the probability distribution of the local susceptibility $\chi_{\text{loc}} = \sum_i \chi_i$, with the one-site susceptibility defined by adding a one-site longitudinal term to the Hamiltonian:

$$\mathscr{H} = J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \sigma_i^z \sigma_j^z + h \sum_i \epsilon_i \sigma_i^x + h_L \epsilon_i \sigma_i^z. \quad (12)$$

The one-site susceptibility is then given by:

$$\chi_i = \frac{\partial^2 E_0}{\partial {h_L}^2}. \quad (13)$$

We study this probability distribution by examining the behavior of its moments $\chi_{\text{loc}}^n \equiv \sum_i \chi_i^n$. For small values of n, the value of h at which the moments begin to diverge is smaller than pure system h_c critical point, but as n is increased, the point moves closer to h_c. Curves for the moments plotted over a range of values of h and their points of divergence as a function of $1/n$ are shown in fig. 7(a) and (b) respectively.

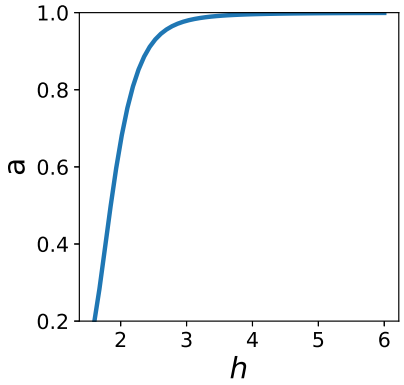

FIG. 6: Plot of the exponent a as a function of h for $p = 0.5$. For $h > h_c$, $a \simeq 1$ as is typical of the pure system. For $h < h_c$, a begins decreasing continuously with h, indicating the influence of GM singularities.

This movement of the divergence point is indicative of tails in the probability distribution of χ_{loc} induced by the presence of GM singularities.

V. CONCLUSION

In this work, we have used NLCE to compute the magnetization, structure factor, and susceptibility of the zero temperature dilute quantum transverse-field Ising model. In analyzing the pure system, we demonstrated the efficacy of the NLCE at computing the magnetization as a function of transverse field strength h by adding to the Hamiltonian a mean-field term coupled to the boundary of each cluster and imposing a self-consistency constraint between the strength of the coupling and the magnetization. We used this to regulate the convergence of the NLCE in the ordered phase of the structure factor and susceptibility, yielding an approximation that converged well in both the low and high h regimes. In the problem with dilution, we used the asymptotic behavior of the structure factor near the percolation threshold probability p_c to compute p_c as a function of h, leading to an approximate phase boundary. We found approximate values of the pure system critical point at $h_c \simeq 3.03$ and the percolation threshold and $p_c \simeq 0.58$, in reasonable agreement with known results of 3.04 and 0.59 resp. Additionally, we found the multi-critical point at which the phase boundary flattens to be at $h_M \simeq 1.65$, above the known lower bound of 1, and established bounds on the structure factor exponent γ of $0.47 \lesssim \gamma \lesssim 0.61$.

For small values of p and h, we found numerical evidence Griffiths-McCoy singularities in the behavior of the magnetization as a function of longitudinal field and moments of the local susceptibility. In low p regions of the paramagnetic phase, the slope a of the magnetization as a function of small h_L remains roughly constant at 1 for all values of h, but at values below h_c we found that a continuously diminished as a function of h. Additionally, in this region, the moments of the

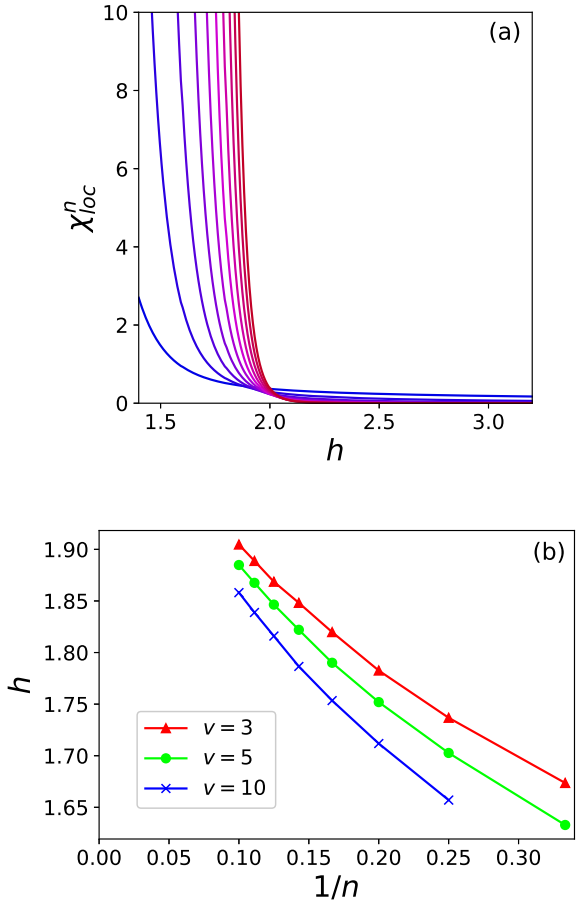

FIG. 7: (a) shows plots of the moments of the local susceptibility χ^n_{loc} shown for $p = 0.5$ for n ranging from 1 to 10, with smaller n values appearing in blue and larger n values in red. All values were computed to 10th order in the number of sites. (b) shows a series of points where each moment dips below a selection of fixed values v, indicating roughly where each moment begins to diverge, plotted as a function of $1/n$. As n is increased, these plots begin to curve closer to h_c.

susceptibility diverge at points $h < h_c$, with higher moments diverging for values of h closer to h_c, indicating the presence of tails in the probability distribution of the local susceptibility. Both of these effects evince the change in behavior when crossing below h_c in the low-p regime, demonstrating the existence of the Griffiths phase dominated by Griffiths-McCoy singularities.

Acknowledgements

This work was supported by the NSF and U.C. Davis through a physics REU program, NSF grant number PHY-1560482.

[1] Harris AB, "Diluted quantum transverse Ising model," *J. Phys. C: Solid State Phys.* **Vol. 7**, 3082 (1974).

[2] Stinchcombe RB , "Diluted quantum transverse Ising model," *J. Phys. C: Solid State Phys.* **Vol. 14**, L263 (1981).

[3] Griffiths RB, "Nonanalytic behavior of the critical behavior in a random Ising ferromagnet," *Phys. Rev. Lett.* **23**, 17 (1969).

[4] T. Vojta, J. Low Temp. Phys. **161**, 299 (2010).