Determination of χ_{xx} in the Transverse-Field Ising Model

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The transverse-field Ising model is a simple model of quantum phase transitions that can describe the quadrupolar behavior of Thulium Vanadate. To describe properties of this material it is important to calculate the transverse magnetic susceptibility (χ_{xx}). In this paper, we describe three methods for numerically determining χ_{xx}: mean-field theory, exact diagonalization, and numerical linked-cluster expansion (NLC). We found that the mean-field theory underestimates χ_{xx} close to the phase boundary. Numerical linked-cluster expansions provide accurate quantitative calculations of the transverse susceptibility in the paramagnetic phase. Using NLC, we find that, at the quantum critical point, χ_{zz} diverges as T^{-k} when $T \to 0$ where k is between 1.9 and 2.6.

I. INTRODUCTION

The transverse-field Ising model is a simple model of quantum phase transitions. However, the magnetic properties in the transverse direction has not been well studied for dimensions greater than 1. These properties, and the static χ_{xx} specifically, are useful in understanding NMR studies of Thulium Vanadate. [1]

In this paper, we will describe three different methods of calculating χ_{xx}: the single site mean-field approximation, exact diagonalization, and numerical linked-cluster expansion. Mean-field theory gives a qualitative picture for the susceptibility in the paramagnetic and the ferromagnetic phases. The numerical linked-cluster method converges in the paramagnetic phase but not in the ferromagnetic phase. In the paramagnetic phase it gives accurate calculations of the transverse susceptibility in the thermodynamic limit. We then show how numerical linked-cluster expansion is used to determine the divergence of susceptibility with temperature at the quantum critical point.

II. BACKGROUND

The classical Ising model consists of spins on a lattice with each spin site interacting with nearest neighbors. The transverse-field Ising model adds a magnetic field in the x direction in order to add quantum fluctuations to the model. The Hamiltonian for the transverse-field Ising model is given by

$$\hat{H} = -J \sum_{<i,j>} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^x \tag{1}$$

where $< i, j >$ denotes the sum over nearest neighbors in the lattice and $\hat{\sigma}_i^z$ refers to the Pauli spin operator in the z direction for site i. The interaction, J, is a constant which is set to 1 in subsequent calculations. When J is positive, aligned neighboring spins correspond to a lower energy state. The transverse-field term, h, corresponds to the strength of the magnetic field. Because the Hamiltonian contains non-commuting spin operators, we observe quantum fluctuations.

A useful quantity to measure is the average spin of the entire system in some direction, say $\hat{x}$. This is called the magnetization and is defined as

$$m_x = \frac{1}{N} M_x = \frac{1}{N} \sum_i^N \langle \sigma_i^x \rangle \tag{2}$$

where N is the total number of sites. We also define the susceptibility as

$$\chi_{xx} = \frac{\partial m_x}{\partial h} \tag{3}$$

where h is the transverse magnetic field from Eq. 1.

To calculate these quantities, we often use the partition function,

$$\mathcal{Z} = \sum_\alpha e^{-\beta E_\alpha} = \sum_\alpha \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \tag{4}$$

where α is a complete set of basis states for our system. The partition function can be thought of as a sum over all states of the system which is weighted by energy according to $e^{-E_\alpha \beta}$ where E_α is the energy of the state and $\beta = 1/T$ where T is the temperature of the environment (setting the Boltzmann constant to unity). Then, the magnetization can be written as

$$m_x = T \frac{\partial}{\partial h} \ln(\mathcal{Z}). \tag{5}$$

III. MEAN-FIELD THEORY

Mean-Field Theory approximates the interacting many-spin system with a single site problem where each spin interacts with an external field and the molecular field of the other spins. Using this approximation, we can estimate the phase boundary between the ferromagnetic and paramagnetic phases and an approximate expression for the magnetic susceptibility.

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A. Single Spin in Applied Field

First, let us consider the case of a single spin described by the Hamiltonian

$$\hat{H} = -h\hat{\sigma}^x. \tag{6}$$

Then, the magnetization in the x direction is

$$m_x = \langle \sigma^x \rangle = \frac{\sum_\alpha \langle \alpha | \hat{\sigma}^x e^{-\beta \hat{H}} | \alpha \rangle}{\sum_\alpha \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle} = \frac{\sum_\alpha \langle \alpha | \hat{\sigma}^x e^{\beta h \hat{\sigma}^x} | \alpha \rangle}{\sum_\alpha \langle \alpha | e^{\beta h \hat{\sigma}^x} | \alpha \rangle} \tag{7}$$

where we sum over basis states α. In the x basis, we have two states: $\sigma^x = \pm 1$. So,

$$m_x = \frac{\sum_{\sigma^x = \pm 1} \sigma^x e^{\beta h \sigma^x}}{\sum_{\sigma^x = \pm 1} e^{\beta h \sigma^x}} = \frac{e^{\beta h} - e^{-\beta h}}{e^{\beta h} + e^{-\beta h}}. \tag{8}$$

Thus, the magnetization in the x direction for a single site is

$$m_x = \tanh(\beta h) \tag{9}$$

and the transverse susceptibility is

$$\chi_{xx} = \frac{\partial m_x}{\partial h} = \beta \mathrm{sech}^2(\beta h). \tag{10}$$

B. Expanding to Multiple Sites

For the many spin problem, we can use the Mean-Field Approximation by assuming that each spin interacts with the average spin of the system instead of its nearest neighbors [2]. So, we average out local interactions and decouple the spins. The Hamiltonian becomes

$$\hat{H}_{\mathrm{MF}} = -Jqm_z \sum_i \hat{\sigma}_i^z - h \sum_i \hat{\sigma}_i^x \tag{11}$$

where q is the number of neighbors each spin site has. In a one-dimensional lattice, $q = 2$, and in a two-dimensional square lattice, $q = 4$. We have also added a new unknown variable, m_z, which is the magnetization in the z direction, which is to be determined self-consistently.

Since the spins are decoupled in this approximation, we can consider the contribution to the Hamiltonian of only spin i:

$$\hat{H}_{\mathrm{MF},i} = -Jqm_z\hat{\sigma}_i^z - h\hat{\sigma}_i^x. \tag{12}$$

Now, for a site i, we can define the operator

$$\hat{\sigma}_i^\gamma = \frac{1}{\gamma}\left(Jqm_z\hat{\sigma}_i^z + h\hat{\sigma}_i^x\right) \tag{13}$$

with a normalization term $\gamma^2 = (Jqm)^2 + h^2$ such that $\hat{\sigma}_i^\gamma$ has eigenvalues ± 1. This can be thought of the spin operator corresponding to the direction net magnetic moment

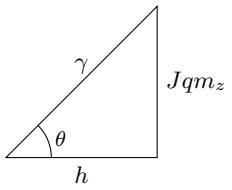

FIG. 1. Diagram of Effective Field in Mean-Field Approximation. A transverse field h is applied in the x direction. The Jqm_z component in the y direction comes from interactions with other spins on the lattice as calculated using the Mean-Field Approximation. The γ is defined to be the net moment with an associated spin operator defined in Eq. 13.

as shown in Fig. 1. Using the single spin results from earlier, we get that the magnetization in the γ direction for the entire system is

$$m_\gamma = \langle \sigma^\gamma \rangle = \tanh \beta\gamma. \tag{14}$$

To solve for m_z,

$$m_z = \sin\theta m_\gamma = \frac{Jqm_z}{\gamma}\tanh(\beta\gamma). \tag{15}$$

Now, we have two cases of m_z. In one case, $m_z = 0$ and the system is paramagnetic. In the other case, $m_z \neq 0$ and the system is ferromagnetic. In the ferromagnetic case, we can write Eq. 15 as

$$\frac{1}{Jq} = \frac{1}{\gamma}\tanh(\beta\gamma). \tag{16}$$

This equation is the self-consistency equation and it gives us allowed values of γ. Using this equation, we can now estimate the phase boundary. To do this, we take the limit as $m_z \to 0$ and we get that $\gamma \to h$. Then, Eq. 16 becomes

$$\frac{h}{Jq} = \tanh(\beta h). \tag{17}$$

Solving for critical temperature with $T = 1/\beta$ yields

$$T = \frac{h}{\mathrm{arctanh}(h/Jq)}. \tag{18}$$

At $T = 0$ we find that the critical field strength is $h_c = Jq$ and similarly at zero field strength the critical temperature is $T_c = Jq$. Substituting this into the previous equation,

$$\frac{T}{T_c} = \frac{h/h_c}{\mathrm{arctanh}(h/h_c)}. \tag{19}$$

This equation is graphed in Fig. 2 and we now have a qualitative picture of the phase boundary. The phase boundary extends to $T = 0$, indicating a quantum critical point (QCP). However, this result is just an approximation and does not correctly determine critical temperatures and transverse fields.

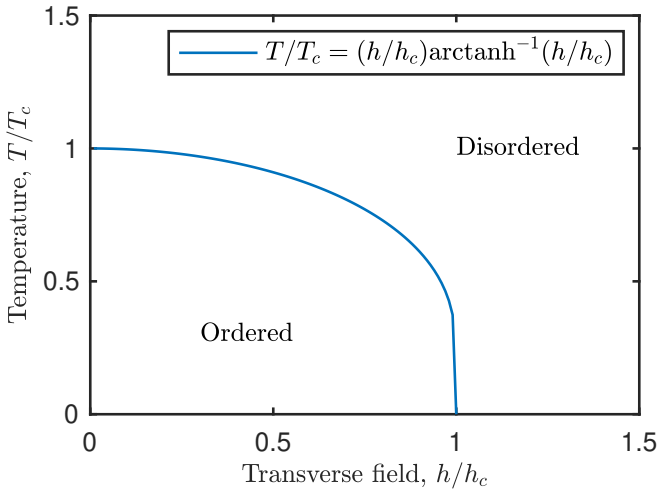

FIG. 2. Estimate of Phase Boundary from Mean-Field Approximation. For small temperatures and transverse fields, we expect to be in an ordered, ferromagnetic state with $m_z \neq 0$. For larger temperatures and transverse fields we expect to be in a disordered, paramagnetic state with $m_z = 0$.

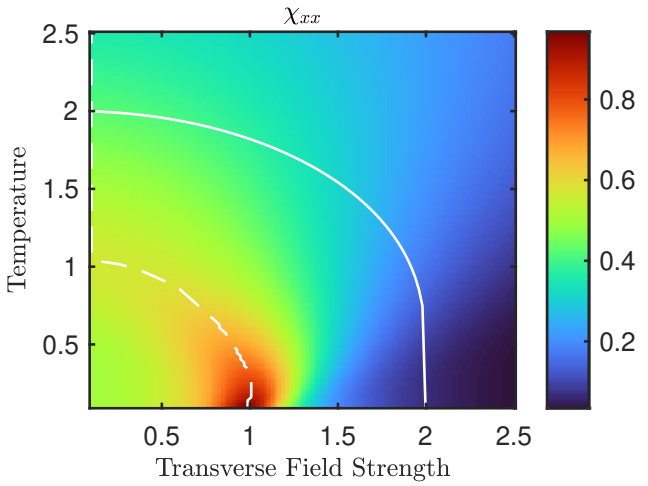

FIG. 3. Exact Diagonalization of χ_{xx} in One-Dimensional Lattice. The color of the heatmap corresponds to χ_{xx}. The dashed line traces a peak in the calculated χ_{xx} and the solid line is the mean-field theory estimate of the phase boundary with $q = 2$ in one dimension. The difference between mean-field theory and our calculation comes from mean-field theory erasing disorder in the system, leading to a larger range of values in the ordered phase. The lattice consists of 9 sites and has periodic boundary conditions with the Ising interaction, J, set to unity.

To calculate the transverse magnetic susceptibility in the paramagnetic phase, note that our single site Mean-Field Hamiltonian in Eq. 12 turns into the single spin Hamiltonian in Eq. 6. So, the susceptibility is the same as we calculated in Eq. 10.

To calculate the susceptibility in the ferromagnetic phase, we first calculate the magnetization as

$$m_x = \cos\theta m_\gamma = \frac{h}{\gamma}\tanh(\beta\gamma). \tag{20}$$

Then,

$$\chi_{xx} = \frac{\partial m_x}{\partial h} = \frac{1}{\gamma}\tanh(\beta\gamma). \tag{21}$$

However, we can substitute Eq. 16 into the equation above. Hence, the transverse magnetic susceptibility in the ferromagnetic phase is

$$\chi_{xx} = \frac{1}{Jq}. \tag{22}$$

Using mean-field theory, we can see how the applying a transverse magnetic field to the Ising model creates a phase boundary with a QCP at $T = 0$. However, this result is still an approximation and to get more accurate results, we must use numerical methods.

IV. EXACT DIAGONALIZATION

The method of exact diagonalization calculates properties of the system numerically. We start by representing the Hamiltonian as a matrix using the basis which consists of the Cartesian product, for each particle, of spin quantizations in the z direction. Then, the eigenvalues of the Hamiltonian are found numerically and the partition function is calculated according to Eq. 4 [3]. Then, numerical derivatives are taken according to Eq. 5 and

$$\chi_{xx} = T\frac{\partial^2}{\partial h^2}\ln(\mathcal{Z}). \tag{23}$$

Similarly, heat capacity can be calculated using

$$C = \frac{\partial^2}{\partial T^2}\left(T\ln(\mathcal{Z})\right). \tag{24}$$

We can also calculate the longitudinal susceptibility, χ_{zz}, using

$$\chi_{zz} = T\frac{\partial^2}{\partial h_z^2}\ln(\mathcal{Z}) \tag{25}$$

where we add an extra term to the Hamiltonian,

$$\hat{H} = -J\sum_{<i,j>}\hat{\sigma}_i^z\hat{\sigma}_j^z - h\sum_i\hat{\sigma}_i^x - h_z\sum_i\hat{\sigma}_i^z \tag{26}$$

with h_z corresponding to a magnetic field applied in the z-direction.

The results of exact diagonalization results for a one-dimensional lattice, shown in Fig. 3. There is a short-range order inside the region predicted to be ferromagnetic by the mean-field theory. However, there is no phase transition. So, the exact diagonalization results disagree with the mean-field theory, indicating that the mean-field theory is insufficient in describing χ_{xx}.

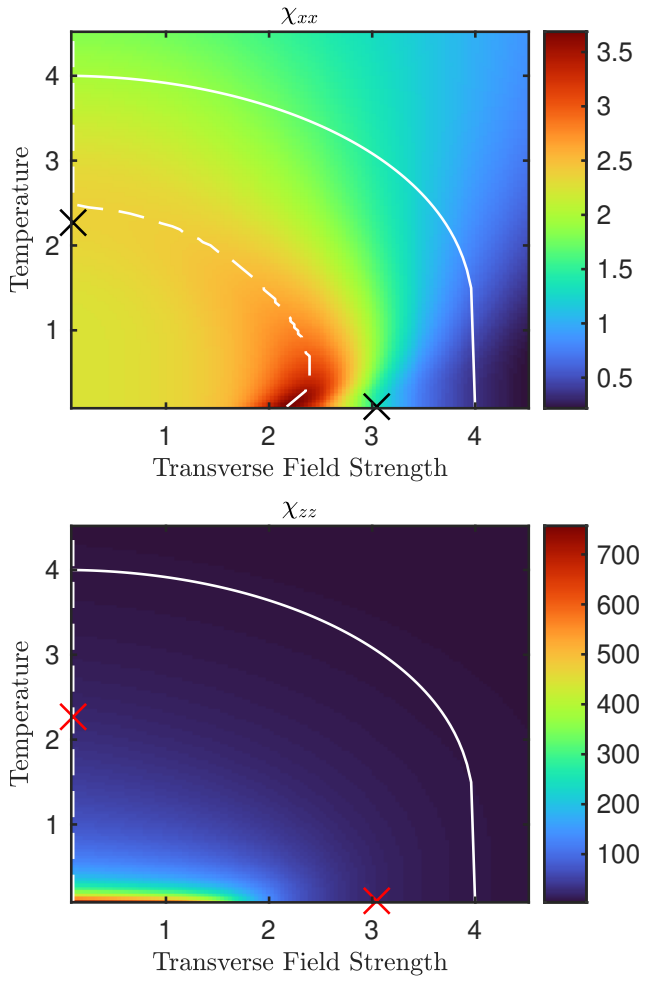

FIG. 4. Exact Diagonalization: χ_{xx} on a 3×3 Square Lattice. The Xs mark the quantum critical point at $h_c = 3.044$ and critical temperature at $T_c = 2.269$ for the 2D transverse-field Ising model. [4, 5] The solid white line is the mean-field theory estimate of the phase boundary. The dashed white line in χ_{xx} outlines the maximum susceptibility over various temperatures, indicating a phase boundary, but with h_c much lower than the true value. The χ_{zz} diverges as $T \to 0$ in the ferromagnetic phase, however, it converges for field strengths well below $h_c = 3.044$. A 3×3 lattice is too small to account for finite size effects.

The results of exact diagonalization on a two-dimensional square lattice is shown in figure 4. The χ_{xx} is qualitatively similar result to one dimension, but the calculated critical field strength of about 2 is smaller than the literature value of $h_c = 3.044$. Similarly, the χ_{zz} should diverge for field strengths less than 3.044, but we find convergence down to 2. However, a 3×3 lattice is not large enough to ensure that there are no finite size effects. Usually, measurements made for multiple system sizes are extrapolated to determine the properties of an infinite system. Because the size of the Hamiltonian is exponential with the number of particles, measuring properties for systems larger than 3×3 becomes computationally expensive.

V. NUMERICAL LINKED-CLUSTER EXPANSION

To work around the computational cost of exact diagonalization, we used the numerical linked-cluster expansion. This method involves using the principle of inclusion-exclusion to estimate the properties of an infinite lattice. To do this, we must calculate weights of various linked clusters. [6]

A linked cluster is a subgraph of a d dimensional lattice in which every site has at least one neighbor. A linked cluster has free boundary conditions and we calculate extensive properties of the cluster, like χ_{xx} using exact diagonalization. Then, the weights, W, are calculated recursively for a cluster c using

$$W(c) = F(c) - \sum_{s \in c} W(s) \tag{27}$$

where F is a property of the cluster and s is a subgraph of c.

After weights have been calculated for sufficiently clusters some number of bonds, we can estimate the intensive property of an infinite system as

$$f(c) = \sum_{\text{distinct } c} W(c)L(c) \tag{28}$$

where $L(c)$ is the number of distinct ways the cluster can be embedded in a lattice.

If we calculate the weights $W(c)$ up to clusters with a certain number of bonds n_c, we can calculate $f(c)$ efficiently. The number of bonds we calculate up to is called the order of the NLC expansion and results that agree for multiple orders have converged to the infinite-lattice solution.

Multiple orders of the NLC expansion for χ_{xx} are shown in Fig. 5 against exact diagonalization and the single-site mean-field approximation. For $h = 1$, the NLC calculation breaks down on approach to the phase transition. However, we can see that the NLC disagrees with the exact diagonalization below temperatures of 4, where the exact diagonalization predicts a near-constant χ_{xx} on approach to the phase transition. This is due to the finite-size effects when diagonalizing a 3×3 lattice. In the paramagnetic phase, the NLC calculation converges and is accurate.

VI. FUTURE WORK: SUSCEPTIBILITY DIVERGENCE AT QCP

Approaching the quantum critical point (QCP), we expect a divergence in the χ_{zz} to infinity as $T \to 0$ for an infinite lattice. In NLC, this divergence is characterized by

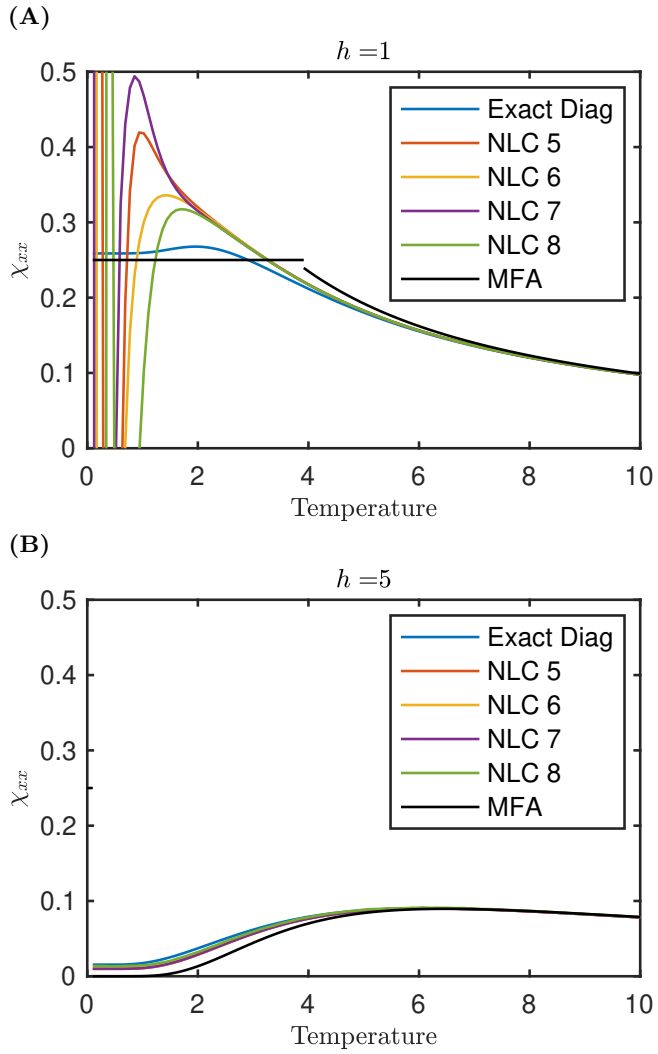

FIG. 5. Several Orders of Numerical Linked-Cluster Expansion Results for χ_{xx} with $h = 1$ in (A) and $h = 5$ in (B). NLC orders from 5 to 8 are graphed as indicated in the legend along with the exact diagonalization and the mean-field approximation (MFA). It converges, for large field strengths or temperatures, but breaks down on approach to the transition. In (A), NLC and exact diagonalization agree for all temperatures.

$$\chi = \mathcal{O}^{\alpha} f(T\mathcal{O}^{-\beta}) \tag{29}$$

or equivalently

$$\frac{\chi}{\mathcal{O}^{\alpha}} = f\left(\frac{T}{\mathcal{O}^{\beta}}\right)$$

where $\mathcal{O}$ is the order of the NLC, f is an arbitrary function, and α and β are constants. By comparing different orders of NLC, α and β can be determined. As $\mathcal{O} \to \infty$, we expect χ to be independent of $\mathcal{O}$. So, if f is a function with lowest power k, then $k = -\alpha/\beta$ in the limit as $\mathcal{O} \to \infty$. Therefore, the order of the temperature divergence is T^{-k} as $T \to 0$.

The χ_{zz} at the critical field strength is shown in panel (A) of Fig. 6 for orders of NLC from 8 to 11. Since χ_{zz} quickly converges to a constant value as $T \to 0$ for all orders of NLC, we take that value to be the zero-temperature χ_{zz} at a certain order and fit it against the order to determine $\alpha = 1.2625$ as shown in panel (B) of Fig. 6. Then, we normalize the χ_{zz} on the y-axis of Fig. 7 (A) and we similarly scale the x-axis of Fig. 7 (B-D) to plot a measurement of f from Eq. 29. We find that β from 0.5 to 0.7 result in similar graphs for all NLC orders. Therefore, we estimate that T goes to a power between 1.9 and 2.6 with temperature at the QCP. The precision of this calculation can be improved by taking higher orders of NLC to estimate β more accurately.

For χ_{xx}, we obtain different qualitative functional forms for orders of NLC as high as 11 as seen in Fig. 8. Further investigation of χ_{xx} would require more computational time to perform higher order NLC calculations.

VII. CONCLUSION

In this paper, we used the numerical linked-cluster (NLC) expansion to calculate the divergence of χ_{zz} at the QCP. We have also shown that NLC accurately calculates χ_{xx} in the paramagnetic phase at the thermodynamic limit. Future works could determine χ_{xx} in the ferromagnetic phase using other methods.

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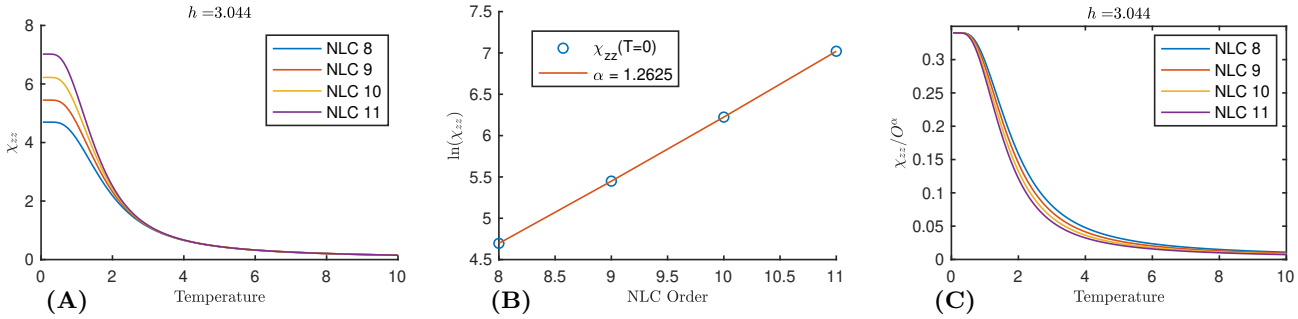

FIG. 6. Determining α for χ_{zz}. Panel (A) shows the χ_{zz} at the critical field strength for several orders of NLC against temperature. The χ_{zz} reaches a constant for small temperatures. We use the χ_{zz} at $T = 0.05$ in (B) to determine α by fitting the the log of χ_{zz} against the NLC order and the slope of this fit is α. The normalized χ_{zz} is shown in (C) where the y-axis is divided by $\mathcal{O}^{\alpha}$ where $\mathcal{O}$ is the order of the NLC.

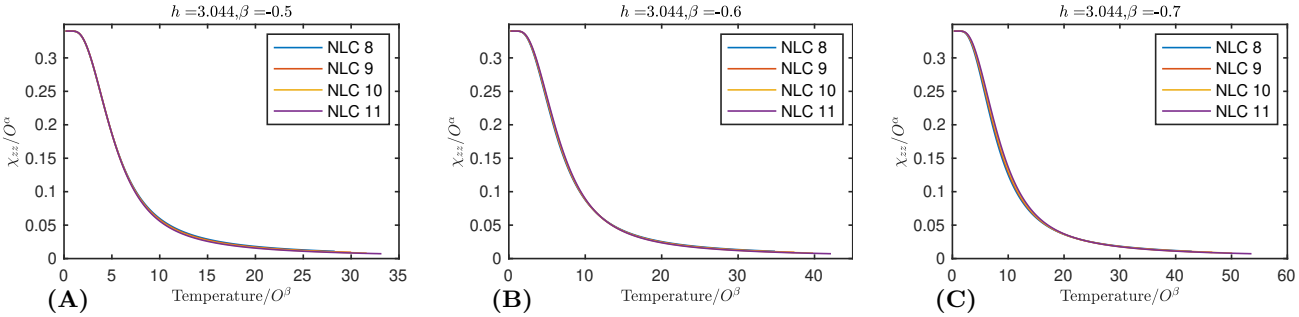

FIG. 7. Determining β for χ_{zz}. The χ_{zz} is graphed at the critical field strength for several orders against the temperature. The y-axis is normalized by dividing by $\mathcal{O}^{\alpha}$ where $\mathcal{O}$ is the NLC order and $\alpha = 1.2625$. The x-axis is normalized by dividing by $\mathcal{O}^{\beta}$ where beta is -0.5 in (A), -0.6 in (B), and -0.7 in (C). Hence, the graph shown is our measurement of f from Eq. 29. Since the graphs of f match for all orders, we know that the values of α and β are accurate.

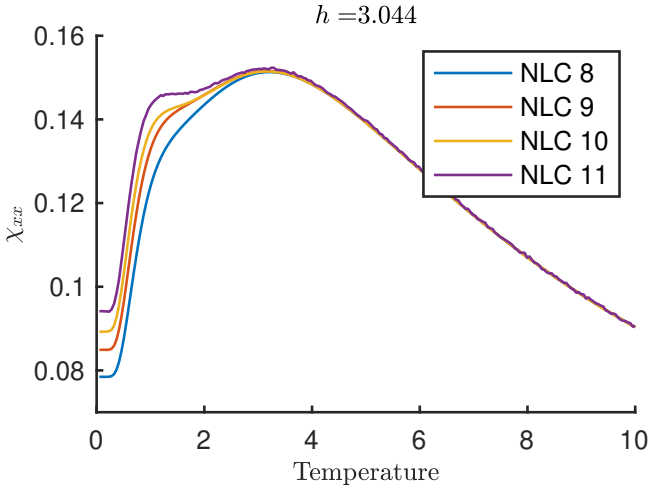

FIG. 8. NLC Calculation of χ_{xx} for Multiple Orders. Since the shape of the function changes up to 11th order, with a flat section at a temperature below 2 in 11th order, we cannot match χ_{xx} to the scaling behavior in Eq. 29. Higher order NLC calculations are needed.