Effective Field Theory of the Zero-Temperature
Triangular-Lattice Antiferromagnet: A Monte Carlo Study

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Abstract

Using a Monte Carlo coarse-graining technique introduced by Binder et al., we have explicitly constructed the continuum field theory for the zero-temperature triangular Ising antiferromagnet. We verify the conjecture that this is a gaussian theory of the height variable in the interface representation of the spin model. We also measure the height-height correlation function and deduce the stiffness constant. In addition, we investigate the nature of defect-defect interactions at finite temperatures, and find that the two-dimensional Coulomb gas scenario applies at low temperatures.

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I. INTRODUCTION

In recent years, there has been considerable interest in the study of classical spin systems with critical ground states. One of the best studied of these is the triangular-lattice Ising antiferromagnet (TIAFM) [1]. The critical behavior of these models can be understood based on an interface representation and an “effective” field theory which is gaussian in the height variable [2,3]. In this paper, we present an explicit construction of the effective field theory based on the study of Monte Carlo cell distribution functions [4] of the TIAFM. To accomplish this, a height mapping [5] is applied to the system and this variable is then coarse grained to obtain a continuum field theory. Our interest in this model was stimulated by the observation of anomalously slow dynamics in the compressible TIAFM [6]. In that model, the supercooled state exhibits an ergodicity-breaking transition which is reminiscent of the structural-glass transition. This glassy behavior is believed to arise from the interaction between strings and vortices [7]: the topological defects present in these models at finite temperature. In the pure TIAFM model, the gaussian theory implies that the vortices interact as charges of a 2-D Coulomb gas [8]. We have analyzed the defect-defect correlation function at finite temperatures to investigate the nature of the defect interactions. The 2-D simulations are consistent with the Coulomb gas picture at low densities of defects.

The motivation behind this numerical study was (1) to test the Monte Carlo cell distribution function technique in a model where the effective field theory is well established and (2) to establish a framework for the construction of effective field theories and effective defect-defect interactions in models such as the compressible TIAFM where no adequate field theory description exists.

The paper is organized as follows. In section II we describe the cell distribution function technique. In section III we present results from the coarse grained free-energy functional and compare our results to the gaussian theory. In section IV we verify the gaussian theory from a study of the height-height correlation function and in section V we describe the study of the defect-defect correlation functions. Section VI presents our conclusions and directions
for future work.

II. CELL DISTRIBUTION FUNCTIONS AND COARSE GRAINED FREE-ENERGY FUNCTIONALS

Binder and coworkers [9,10] have studied cell distribution functions of the three-dimensional Ising model on a cubic lattice and constructed coarse-grained Ginzburg-Landau Hamiltonians. In this section, we review this technique and present the results of its application to the triangular Ising ferromagnet as an example. We will describe the application of this technique to the zero-temperature TIAFM in the next section.

Given a microscopic Hamiltonian such as the Ising model, Monte Carlo (MC) methods can be used to sample the distribution functions \( P_L(\{s_i\}) \) of the coarse grained variables

\[
s_i = \frac{1}{L^2} \sum_{l \in \text{cell}} S_l,
\]

where \( S_l \) are the original microscopic spin variables, such as the Ising spins on the original lattice, and \( L \) is the cell size. The distributions \( P_L(\{s_i\}) \) are assumed to be of the form \( e^{-\beta F} \) with \( F \) having the Ginzburg Landau (GL) form in terms of the coarse-grained variables \( \{s_i\} \). This assumption is expected to be valid when \( L >> a \) (lattice spacing) but much smaller than the correlation length, such that the coarse grained variables do not fluctuate rapidly from cell to cell. If one could sample the total distribution function in MC simulations, then this connection could be exploited for the explicit construction of the GL Hamiltonian by simulating the microscopic model. Sampling the total distribution function is essentially an impossible task and therefore, we have followed Binder [10] in studying the two simplest reduced distribution functions, the single cell and the joint, nearest-neighbor, two-cell distribution functions which are then parameterized by the GL form. To illustrate how the cell distribution function method works, we briefly describe its application to the triangular Ising ferromagnet in zero magnetic field, where we choose the model system size to be 80x80 with periodic boundary conditions and the cell sizes \( L \) to be 4, 8, 10, 16, 20 and 40.
The microscopic Hamiltonian is:

\[ \mathcal{H}_{\text{sing}} = -J \sum_{\langle l \neq l' \rangle} S_l S_{l'} \]

The total distribution function \( P_L(\{s_i\}) \) is assumed to be:

\[ P_L(\{s_i\}) = \frac{1}{Z} e^{-\mathcal{F}_{GL}(\{s_i\})} \tag{1} \]

where \( Z \) is the partition function and the GL Hamiltonian has the form

\[ \mathcal{F}_{GL}(\{s_i\}) = \sum_i (\bar{r}_L s_i^2 + \bar{u}_L s_i^4) + \sum_{\langle ij \rangle} \bar{c}_L (s_i - s_j)^2. \tag{2} \]

The two reduced distribution functions, which are amenable to numerical calculations, are the two-cell joint distribution function \( P_L(s_i, s_j) \) and the single-cell distribution function \( P_L(s_i) \):

\[ P_L(s_i, s_j) = \int \prod_{\substack{l \neq i \atop <ij>}} ds_l P_L(\{s_l\}) \tag{3} \]

\[ P_L(s_i) = \int P_L(s_i, s_j) ds_j \tag{4} \]

The parameterization of the effective Hamiltonian is accomplished by sampling \( P_L(s_i, s_j) \) and \( P_L(s_i) \)

\[ P_L(s_i, s_j) = \frac{1}{Z'} \exp\{-(c_L(s_i - s_j)^2 + V_L(s_i) + V_L(s_j))\} \tag{5} \]

\[ P_L(s_i) = \frac{1}{Z''} e^{-V_L(s_i)} \tag{6} \]

where \( Z' \) and \( Z'' \) are normalization factors, and

\[ V_L(s_i) = -r_L s_i^2 + u_L s_i^4 \]

The \( r_L \) and \( u_L \) obtained from \( P_L(s_i, s_j) \) and \( P_L(s_i) \) respectively, can be different since the effect of the gradient term has been integrated over in the single-cell distribution function. Similar considerations imply that these coefficients can be different from \( \bar{r}_L, \bar{u}_L \) and
\( \bar{c}_L \) in Eq. 4. For small values of \( \bar{c}_L \), the coupling between different sites is small and all of these coefficients are expected to be approximately equal [10]. The coefficients \( r_L, u_L \), and \( c_L \), as functions of temperature (T) and cell size (L), can be estimated by fitting the measured distribution function \( P_L(s_i, s_j) \) to the model form (Eq. 5). It is well known that a temperature-driven second order transition exists for this Ising model and the exact result for \( T_c(\infty) = 3.6 \) [11]. Fig. 1 shows \( \frac{r_L(T)}{u_L(T)} \) as a function of temperature for different cell sizes. There is clear evidence for a temperature-driven second order transition at \( T_c(L) \) where the sign of the ratio changes. The L dependence of \( T_c(L) \) agrees with finite size scaling predictions [4]. The variation of \( \frac{c_L(T)}{u_L(T)} \) with cell size L (Fig. 2) shows temperature-dependent behavior as the size of the cells approach infinity. For temperatures above \( T_c(\infty) \), the ratio approaches a non-zero fixed point as \( L \) approaches infinity. For all other temperatures, this ratio approaches zero. The sampling of the single-cell distribution function \( P_L(s_i) \) (Eq. 6) leads to similar results for \( r_L \) and \( u_L \), which is consistent with the small value obtained for \( c_L \). These results support the assumptions that went into the construction of \( \mathcal{F}_{GL}\{s_i\} \).

The results of this section will be contrasted with the frustrated antiferromagnetic case in the next section. The application of the distribution-function technique to the TIAFM is based on the mapping to an interface model and height variables. The coarse graining of these height variables and the GL parameterization are described in the next section.

### III. RESULTS OF COARSE GRAINING AND COMPARISON WITH THE GAUSSIAN THEORY

#### A. Height Variables and coarse graining at T=0

One interesting property of the TIAFM is that the ground state ensemble has a one-to-one mapping onto an interface model [2][3][3]. This provides a simple way of studying the properties of zero-temperature TIAFM.

The discrete variables in the interface model are height variables \( \{z_l\} \), which are defined
on each site of the triangular lattice. The mapping from the TIAFM to an interface model is realized by the mapping from spin variables \( \{ S_i \} \) to height variables \( \{ z_i \} \). Specifying the height variable to be zero at a chosen site, the following rules (Fig. 3), provide a unique mapping from \( \{ S_i \} \) to \( \{ z_i \} \):

(1) Along d1 direction, \( \Delta z = -1 \) for opposite spins and \( \Delta z = +2 \) for same spins.

(2) Along d2 direction, \( \Delta z = -1 \) for opposite spins and \( \Delta z = +2 \) for same spins.

(3) Along d3 direction, \( \Delta z = +1 \) for opposite spins and \( \Delta z = -2 \) for same spins.

These height assignments are unique up to the choice of origin as long as we restrict ourselves to Ising configurations in the ground state ensemble, which is the set of states that do not have any completely frustrated plaquettes (all spins same). The microscopic Hamiltonian in terms of these height variables \( \{ z_i \} \) can be written directly from the mapping as

\[
\mathcal{H}\{z_i\} = -J \sum_{<ij>} (3 - 2|z_i - z_j|)
\]

The symmetries of the original Hamiltonian are reflected in \( \mathcal{H}\{z_i\} \). These include Ising up-down symmetry, and sub-lattice symmetry. In addition, \( \mathcal{H}\{z_i\} \) has a symmetry with respect to global, discrete shifts of the height variable. A detailed discussion of these symmetries can be found in Blöte et al. [3]. An interesting property of this mapping is that for any ground state the height variable modulo 3 is the same for all spins on the same sub-lattice.

Starting from \( \{ z_i \} \), we can define a new set of height variables \( \{ H_\mu \} \) which are situated on the dual lattice, by averaging the three neighboring \( z_i \) on each triangular plaquette:

\[
H_\mu = \frac{1}{3}(z_1 + z_2 + z_3) \quad \text{where} \quad z_1, z_2, \text{and} \quad z_3 \text{are on the three vertices of the } \mu^{th} \text{ plaquette} \]

as shown in Fig. 3. Since the sum of \( z_1, z_2, \) and \( z_3 \) are multiples of 3, the \( \{ H_\mu \} \) is a set of integers.

We apply the coarse graining technique to the height variables \( \{ H_\mu \} \). The coarse-graining cell is chosen to be a rhombus with the linear size \( L \) and the coarse-grained height variables
\{h_i\} are defined as the average of all the $H_\mu$ within the cell.

$$h_i = \frac{1}{N} \sum_{\mu \in \text{ith}} H_\mu$$

where $N$ is the total number of $H_\mu$ variables within the $i^{th}$ cell. The coarse-graining cell is depicted schematically in Fig. 3. As $L$ approaches infinity, the $\{h_i\}$ become continuous variables. The effective field theory is based on these continuous variables $\{h_i\}$, which describe the roughness of the interface. In the rough phase of the interface model, the average tilt of the interface, which is defined as the difference between $< h_m >$ and $< h_n >$ with $m^{th}$ cell and $n^{th}$ cell separated by the system size, is zero. For an arbitrary spin configuration, a tilt can be frozen in [5]. We will avoid such configurations in our simulations. Also $\{< h_i >\}$ may be non-zero for a general choice of height origin and the Hamiltonian should only depend on the fluctuation $h_i - < h_i >$ [5].

We performed Monte Carlo simulations on a system of size 600x600 shaped as a rhombus and looked at cell sizes 10, 15, 20, 30, 40, 50, 60, 75, 100. We set the initial configuration to be one of the flat states [12], where $\{H_\mu\}$ is uniform in space. The dynamics we use in the simulation is single spin-flip Metropolis algorithm at zero temperature, where the energy is not allowed to increase and thus not all spins are flippable. The first 20,000 configurations are discarded to ensure that measurements are taken in equilibrium. The sampling is done every ten MC steps and for a total of 6,000 configurations. Since we use single spin-flip MC dynamics, the average tilt is unchanged from its initial value of zero during the MC runs [13]. In the following sections, we will use $h_i$ to represent $h_i - < h_i >$.

B. Results and comparison with the gaussian theory

It has been conjectured [2,3] that in terms of the height variables, the continuum theory for the zero temperature TIAFM is gaussian:

$$\mathcal{F}(h(\vec{r})) = \int d\vec{r} \frac{\hat{c}}{2} (\nabla h(\vec{r}))^2$$

(7)
with a value of $\bar{c} = \pi/9$. This stiffness constant was identified by Bl"{o}te et al through the correspondence between the exact calculation of the spin-spin correlation function in the spin model [14] and the discrete height-height correlation function in real space in the interface model [5]. The stiffness constant was also obtained numerically by Zeng and Henley from measurements of the discrete height correlation function in Fourier space [12]. In this section, we deduce the stiffness constant by an explicit construction of the coarse-grained free energy.

Assuming a Ginzburg-Landau form for the Hamiltonian in terms of the continuous height variables,

$$F(h(\vec{r})) = \int d\vec{r} \left\{ \frac{\bar{a}}{2} h(\vec{r})^2 + \frac{\bar{c}}{2} (\nabla h(\vec{r}))^2 \right\}$$

we proceed to obtain $\bar{a}$ and $\bar{c}$ from our simulations by parameterizing the joint distribution function of the coarse-grained height variables $P_L(h_i, h_j)$.

As in the triangular ferromagnet, we study the nearest-neighbor joint distribution function of heights,

$$P_L(h_i, h_j) = \int \prod_{\langle i \neq j \rangle} dh_i P_L(\{h_i\})$$

where $P_L(\{h_i\})$ is the total cell distribution function. We parameterize the joint distribution function as

$$P_L(h_i, h_j) = \frac{1}{Z'} \exp\{-c_L(h_i - h_j)^2 + a_L(h_i^2 + h_j^2)\}$$

where $Z'$ is a normalization factor.

Anticipating a critical point at $T=0$, where $a_L \to 0$, we have neglected the quartic term in Eq. [10]. This will be justified a posteriori from our numerical study. From the joint distribution function, we can extract $a_L$ and $c_L$ as in the ferromagnetic Ising model.

We examine a typical $P_L(h, h^*)$ for cell size $L=50$. One-dimensional cuts of $P_L(h_i, h_j)$ at different fixed values $h_j = h^*$ are shown in Fig. [4]. The peak and shape of the cuts can
be deduced from the distribution function (Eq. 10) which is a product of two Gaussians, \( \exp(-a_L h^2) \) and \( \exp(-c_L (h - h^*)^2) \). When \( h^* \) differs from 0 by a large amount, the plots in Fig. 4 show that the actual peak of the cut is much closer to \( h^* \) than to 0, which implies that the \( \exp(-c_L (h - h^*)^2) \) is the dominant term in the product of Gaussians and the \( \exp(-a_L h^2) \) term acts more as a pre-factor modulating the amplitude of the peak. The width of the cut is also seen to be determined mainly by \( c_L \). Fig. 4 indicates that \( a_L \) is small compared with \( c_L \). We also analyze the importance of higher order gradient terms by measuring the non-gaussian parameter \( \langle g_L \rangle \) in the distribution of \( v \equiv \frac{1}{2}(h_i - h_j) \):

\[
g_L \equiv 1 - \frac{3 < v^2 >_L}{2 < v^4 >_L^2} \tag{11}
\]

We find \( g_L \) to be much smaller than 1, which is consistent with the assumed form of the gradient term in the joint distribution function. Extracting quantitative information about the coefficients \( a_L \) and \( c_L \) from fits to the distribution functions, turns out to be difficult because of the essential two-dimensional nature of the distribution function \( P_L(h_i, h_j) \) (\( c_L \) is large). Instead, we resort to measurement of moments for extracting quantitative information.

The parameters \( a_L \) and \( c_L \) can be related to the moments of \( \{h_i\} \). We have calculated various moments of these coarse-grained variables directly from the MC simulations. In general, the parameterization of the joint distribution function (such as Eq. 10) provides a connection between these moments and the coefficients of the GL Hamiltonian. For the model of Eq. 10, the relation between \( a_L \) and \( c_L \) and the moments can be shown to be:

\[
a_L = \frac{1}{2(<h^2> + <h_1h_2>)} \tag{12}
\]

\[
c_L = \frac{<h_1h_2>}{2(<h^2> + <h_1h_2>)(<h^2> - <h_1h_2>)} \tag{13}
\]

implying that

\[
\frac{c_L}{a_L} = \frac{<h_1h_2>}{(<h^2> - <h_1h_2>)} \tag{14}
\]
Here $h_1$ and $h_2$ refer to coarse-grained height variables on nearest-neighbor cells separated by the coarse-graining cell size $L$. These relations, between the parameters $a_L$ and $c_L$ and the moments, also provide the connection between $a_L$ and $c_L$ and the corresponding parameters $\bar{a}$ and $\bar{c}$ in continuum field theories such as in Eq. 8. Using the known expressions for the correlations functions in the continuum model in two dimensions [13], these relations are:

$$\bar{a} = 4 a_L L^{-2}$$

and

$$\bar{c} = 2 w_0 \frac{\ln(\pi)}{\pi} c_L$$

The factor $w_0 = \sqrt{3}/2$ arises from the volume per unit cell in the triangular lattice. The prediction from the gaussian theory is $\bar{a} = 0$ and $\bar{c} = \pi/9$. We expect that, if the gaussian theory is correct, then $\bar{a}$ should approach zero and $\bar{c}$ should remain constant as $L \to \infty$. Because of the connection to the continuum theory (Eq. 15), it is natural to fit $a_L/L^2$, to a second-order polynomial in $1/L$. The results of the fitting are shown in Fig. 5. The value of $\bar{a}$ can be deduced from the constant term extracted from the fitting and is found to be $6.183 \times 10^{-6}$ implying that the quadratic term in the Ginzburg-Landau Hamiltonian becomes negligible as $L \to \infty$. It is difficult to extract the value of $\bar{c}$ from the measured values of $c_L$ because of the fact that the errors increase with $L$ [16]. If, instead, we analyze $c_L/L^2$, the error bars actually decrease with $1/L$ as seen from Fig. 5, and this provides a more precise way of determining the value of $\bar{c}$. As shown in Fig. 5 the data for $c_L/L^2$ can be fit very well to a second-order polynomial in $1/L$ with vanishingly small coefficients of the constant and linear term in $1/L$. The value of $c_L$ obtained from this fit is 0.622. The standard deviations, calculated from the appropriate higher moments of $h_i$ and $h_j$ based on Eq. 12 and Eq. 13, are plotted as error bars.

These results for the parameters obtained from our analysis of the moments are completely consistent with the qualitative behavior deduced from the joint distribution functions, $P_L(h_i, h_j)$, shown in Fig. 5.
The results shown in Fig. 5 and Fig. 6 verify the gaussian nature of the continuum theory. The numerical value of $\bar{c}$ extracted by applying Eq. [16] to the fitted value of $c_L$ is 0.392, which is in very good agreement with the conjectured stiffness constant of $\pi/9 = 0.349$ [2].

**IV. HEIGHT-HEIGHT CORRELATION FUNCTION**

In this section we will briefly present our calculation of the correlation function of height variables in Fourier space, *i.e.*, the power spectrum of the height variable, which can be used to deduce the stiffness constant as in the investigation of Zeng and Henley [12]. In the next section we further extend this technique to study the defect-defect interactions at finite temperatures by measuring the defect density correlation function.

As implied by Eq. [4], the stiffness constant $\bar{c}$ of the interface model can be directly related to the correlation function of height variables $\{h_i\}$ in Fourier space.

$$\mathcal{F}\{h(\vec{r})\} = \int d\vec{r} \frac{\bar{c}}{2} (\nabla h(\vec{r}))^2 = \sum_{\vec{q}} \frac{\bar{c}}{2} |\vec{q}|^2 |h(\vec{q})|^2$$  \hspace{1cm} (17)

Thus, the correlation function $< |h(\vec{q})|^2 >$ is:

$$< |h(\vec{q})|^2 > = \frac{1}{\bar{c} |\vec{q}|^2}$$  \hspace{1cm} (18)

The stiffness constant $\bar{c}$ can be extracted from a knowledge of $< |h(\vec{q})|^2 >$. Numerical measurements of $< |h(\vec{q})|^2 >$ are, however, arduous, and instead, we study the correlation function of the discrete height variables, $< |H(\vec{q})|^2 >$, which should resemble $< |h(\vec{q})|^2 >$ for small $q$ except for a factor of $\sqrt{3}/2$ coming from the volume per lattice site. Therefore, the $< |H(\vec{q})|^2 >$ for small $q$ can be written as:

$$< |H(\vec{q})|^2 > = \frac{1}{c |\vec{q}|^2}$$  \hspace{1cm} (19)

where

$$c = \frac{2}{\sqrt{3}} \bar{c}$$  \hspace{1cm} (20)
We simulate a system of size 240x240. We start with the same flat states as the ones used in the coarse-graining simulations. After discarding the first 20,000 configurations, the simulations are sampled at every 10 MC steps for a total of 8,000 configurations. For each sampled configuration we calculate $|H(\vec{q})|$, the two-dimensional Fourier transform of the discrete height variables $\{H_\mu\}$ (cf section IIIA) and average $|H(\vec{q})|^2$ over the sampled MC configurations.

For simplicity, one-dimensional cuts of $< |H(\vec{q})|^2 >^{-1}$ along different directions in q-space are shown in Fig. 7. As seen from Fig. 7, different cuts collapse on top of one another only for small values of $q^2$. This is due to the fact that the correlation function is isotropic for small values of q because of the six-fold rotational symmetry of the triangular lattice. As seen from the insert, the anisotropy starts to be significant when $q^2 > 1.6$. We have fitted $< |H(\vec{q})|^2 >^{-1}$ to a second-order polynomial in $q^2$, restricting the fitting region to $q^2 < 0.2$. A value of $c = 0.414 \pm 0.016$ was extracted from the linear term of the fit. The non-linear terms were small, and an estimate of the error on $c$ was obtained from the standard deviation of the linear term extracted from fits to different segments of the curves ($q^2 < 0.2$). From Eq. 20, the stiffness constant can be deduced to be $\bar{c} = 0.360$, compared with 0.392 from our previous real space coarse-graining approach and $\pi/9 = 0.349$ from Blöte et al [5].

The similarity of the results obtained from the real-space analysis and the power-spectrum analysis is quite remarkable and underlines the strength of these numerical techniques. A comparison of the two different analysis techniques, however, makes it clear that the power-spectrum analysis is simpler to implement and is the more desirable technique. The question of how well either of these techniques will fare when applied to a model with general non-linear interactions, where very little is known analytically, is still open.

V. DEFECT INTERACTIONS

At finite temperatures, there are completely frustrated plaquettes which can be viewed as vortex excitations in the height variable $\bar{q}$. There are two types of vortices correspond-
ing to the two different orientations of the frustrated triangular plaquettes. These vortex 
excitations interact like charges via a two-dimensional Coulomb potential \[3,8\].

An alternative to the gaussian description is, therefore, a Coulomb gas description 
involving electric and magnetic charges corresponding to spin waves and vortices, respectively \[3,8\]. This connection suggests that extracting effective defect-defect interactions could be 
an alternative to constructing coarse-grained free energies. In complicated models and especially in analyzing dynamics, this might be the more viable alternative. We therefore wanted 
to numerically extract the effective vortex-vortex interaction in the TIAFM and verify the 
Coulomb gas scenario.

In the regime of low defect-density, where mean field theory is expected to hold, the effec-
tive interactions can be related to the density-density correlation function \[17\]. The appro-
priate mean-field theory for our system with positive and negative charges is Debye-Hückle 
theory \[17\] which predicts that the charge-density correlation function has the following 
form:

\[
< |\rho(q)|^2 > = \frac{\kappa^2}{4\pi} \frac{q^2}{q^2 + \kappa^2}
\]

where

\[
\kappa^2 = 4\pi ( < n_+ > + < n_- > )
\]

is the square of an inverse Debye-Hückle screening length. \(< n_\pm >\) are the average den-
sities of positive and negative charges and \(\rho(q) = n_+(q) + n_-(q)\), where \(n_\pm(q)\) are the Fourier 
transform of the real space charge density functions.

If the vortices in our model behave as a Coulomb gas, then we expect to find this behavior 
of the charge-density correlation function at low temperatures where the vortex density is 
low.

We studied the charge density correlation function in a manner similar to that em-
ployed in the previous section for studying the height-height correlation function. The MC 
simulations were performed on a 120x120 system and after discarding the first 10000 config-
The correlation function, $< |\rho(q)|^2 >$, was measured at several temperatures.

The simulation results are shown in Fig. 8 along with the fits to the Debye-Hücke form (Eq. 21). The figure shows a one-dimensional cut of $< |\rho(q)|^2 >$ along a particular direction. In contrast to the height power spectrum, the defect density power spectrum was found to be isotropic within the range of $q$ studied. The Debye-Hücke theory models the data well for all temperatures except the lowest temperature, $T = 0.6$, which is shown in the insert. The lowest temperature data is suspect because the defect density is low and statistics are difficult to obtain. The isotropy of the $< |\rho(q)|^2 >$ data imply that the screening length and, therefore, the interactions between the defects on the triangular lattice is isotropic down to length scales of the order of the lattice spacing.

From the fits to the Debye-Hücke theory the inverse square of the screening length, $\kappa^2$ can be extracted and compared to the analytic form given in Eq. (22) which uses as an input the measured defect density. In Fig. 9, the fitted values, $\kappa_f^2$ and the analytic values, $\kappa_a^2$ are plotted versus temperature. Except at the highest temperature, $T=2.0$, the agreement between the two different estimates is very good. Interestingly, the temperature at which the two $\kappa$’s differ significantly from each other is also where the defect density differs from a simple Arrhenius prediction corresponding to an activation energy of $4J$, the single-defect creation energy. The observation of the large defect density at $T=2.0$, $< n_+ > + < n_- > = 0.110$, indicates that the defects are covering the whole lattice at this temperature and the single-defect picture becomes inappropriate.

These numerical studies show that it is possible to extract effective defect-defect interactions from measurements of the defect-density power spectrum and verifies that the interaction, in the TIAFM, is Coulombic. A numerical measurement of the force between defects has been made via a study of the dynamics of the defects in TIAFM [15]. This study could not confirm the existence of a Coulomb force from the behavior of the defect density at long times, however, it was argued that the force could not be falling of more slowly than $1/r$. 


VI. CONCLUSION

Based on a mapping to an interface model, we have constructed a coarse-grained Hamiltonian for the zero-temperature TIAFM by studying the joint distribution function of the coarse-grained height variables. Our numerical work confirms that the effective field theory is gaussian in terms of the coarse-grained height variables and we obtain a numerical estimate of the stiffness constant which is in a good agreement with the analytical prediction. The connection between the parameters in joint distribution function and the moments of height variables eliminates the arduous work of directly relating the parameters of joint distribution function to those of the total distribution function. We also directly measured the power spectrum of the height and obtained a value of the stiffness constant, which is very close to the analytic prediction and the estimate from the real-space coarse-graining. This suggests that measurement of power-spectrum might provide a simple route towards the construction of effective field theories. We also demonstrated that effective defect-defect interactions can be extracted from numerical studies of the defect-density power spectrum.

The compressible TIAFM [19,20] is currently being studied using these techniques. The effective field theory and defect-defect interactions in this model are of interest for the study of alloys with the elastic interactions, and for the study of glassy dynamics [6].

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Larger cell size $L$ implies less cells for a given system size, thus less coarse grained height variables $\{h_i\}$ to average over for each sampled MC configuration.

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FIG. 1. The ratio $\frac{r_L(T)}{u_L(T)}$, calculated from the joint distribution function for different cell sizes. $T_c(L)$ is identified as the point where $\frac{r_L}{u_L} = 0$. The exact result for $T_c(\infty)$ is 3.6 [11].
FIG. 2. The ratio $\frac{c_L(T)}{u_L(T)}$, calculated from the joint distribution function for different temperatures, plotted as a function of $L^{-1}$. The curves can be divided into two groups. For those with temperatures higher than $T_c(\infty)=3.6$ (identified in the figure), the curves converge to a finite value. For those with temperatures lower than $T_c(\infty)$, the curves converge to zero.
FIG. 3. (a) The three nearest-neighbor directions d1, d2, d3, and the 6 nearest neighbors (black dots) of discrete height variables $z_i$ (open circle) mapped onto the rhombus-shaped lattice used in the simulation. (b) The coarse graining cell of size $L = 2$. The vertices (black dots) of lattice are \{z_i\} and the centers of the triangular plaquettes (open square) are \{H_\mu\}, each of which is defined as the average of the three surrounding $z_i$ variables. The coarse-grained height variable $h_l$ is defined as the average of all the $H_\mu$ variables within this cell.
FIG. 4. The cuts of $P_L(h, h^*)$ for cell size $L=50$ and different values of $h^*$, demonstrating the dominance of the gradient term (cf. text).
FIG. 5. Plots of $\bar{a}_L = a_L/L^2$ for different cell sizes. The open circles are the data points and the solid line is the second degree polynomial fit. The error bars are obtained from the standard deviations calculated from appropriate higher moments of $h_i$ and $h_j$. The fitting of $a_L/L^2$ leads to a constant term with a value of 6.183E-6, which implies that the quadratic term in the field theory $\bar{a}$ (cf. Eq. 15) becomes vanishingly small as $L \to \infty$. 
FIG. 6. Plots of $c_L/L^2$ for different cell sizes. The open circles are the data points and the solid line is the second degree polynomial fit. The error bars are the standard deviations calculated from appropriate higher moments of $h_i$ and $h_j$. The fitting of $c_L/L^2$ leads to a quadratic term with a coefficient 0.622, and vanishingly small constant and linear terms, which implies that the gradient term of the continuous theory (cf. Eq. 16), $\bar{c}$ approaches 0.392 as $L \to \infty$. 


FIG. 7. Plots of $<|H(\mathbf{q})|^2>^{-1}$ vs. $|\mathbf{q}|^2$. Different data sets are from the cuts of two-dimensional data along different directions in $q$-space. The correlation function shows significant anisotropy for $q^2 \geq 1.6$. The value of $c = 0.414 \pm 0.016$ is obtained from the fitting of curves in the region $q^2 < 0.2$ to a second-degree polynomial in $q^2$. The stiffness constant, $\bar{c}$, deduced from this fit is 0.360.
FIG. 8. Plots of the defect density correlation function at $T=1.0$, $1.2$, $1.5$, $2.0$. The data points are taken from cuts of two-dimensional data along one chosen direction since we did not observe any anisotropy (cf text), and the solid lines are from the fittings to a Debye-Hückle form (Eq. 21). The fittings lead to $\kappa_f^2$ at different temperatures. The $\kappa_f^2$ and the analytical values of $\kappa_a^2$ extracted from the total defect density for the same temperature (cf. Eq. 22) are shown in Fig. 9. The total defect density is 0.030, 0.051, 0.085, 0.110, respectively, for $T=1.0$, $1.2$, $1.5$, $2.0$. The inset shows the fitting at the lowest temperature, $T=0.6$ where the defect density is 0.003 and the results suffer from a lack of statistics.
FIG. 9. Plots of $\kappa_f^2$, the inverse screening length obtained from fitting compared to $\kappa_a^2$, the value obtained from Eq. 22. The two curves deviate significantly only at the highest temperature where the defect picture itself starts to break down (cf text).