Thermodynamic curvature for a two-parameter spin model with frustration

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Microscopic models of realistic thermodynamic systems usually involve a number of parameters, not all of equal macroscopic relevance. We examine a decorated $(1+3)$ Ising spin chain containing two microscopic parameters: a stiff parameter K mediating the long-range interactions, and a sloppy J operating within local spin groups. We show that K dominates the macroscopic behavior, with varying J having only a weak effect, except in regions where J brings about transitions between phases through its conditioning of the local spin groups with which K interacts. We calculate the heat capacity C_H, the magnetic susceptibility χ_T, and the thermodynamic curvature R. For large $|J/K|$, we identify four magnetic phases: ferromagnetic, antiferromagnetic, and two ferrimagnetic, according to the signs of K and J. We argue that for characterizing these phases, the strongest picture is offered by the thermodynamic geometric invariant R, proportional to the correlation length ξ. This picture has correspondences to other cases, such as fluids.

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In microscopic models, the parameters setting the strength of the interactions among the model elements are not usually all equal in importance for determining the overall macroscopic character of the system. Some of these parameters have only a weak influence over the macroscopic properties. The sorting of parameters according to whether they are macroscopically important or unimportant, or stiff or sloppy, has recently seen systematic examination by Sethna *et al.* [1,2] in a number of contexts with methods based on the Fisher information matrix (FIM) corresponding to the microscopic parameters.

In this analysis [1,2], let us imagine that we have some data set $\mathcal{D}$ taken for a macroscopic system with an underlying microscopic model containing n adjustable constants θ^α ($\alpha \in \{1,2,\ldots,n\}$). Each set of values θ^α produces for $\mathcal{D}$ a value of χ^2, the sum of squares of residuals of the data fit. The FIM $\mathbf{g}$ is the Hessian of χ^2 with respect to the θ^α. The eigenvalues of $\mathbf{g}$ may be sorted in terms of size, and on decreasing correspond to progressively less significant linear combinations of the θ^α. Namely, θ^α associated with small eigenvalues may be varied with little effect on χ^2, and, hence, have little importance at the macroscopic level.

In this paper we propose an alternative expression of these ideas in the thermodynamic realm, and with a somewhat different FIM, one based on thermodynamic parameters rather than microscopic model constants. This FIM results from thermodynamic fluctuation theory [3,4]. However, our basic agenda of sorting microscopic model parameters according to their effect on the macroscopic behavior is the same in spirit as that of Sethna *et al.* [1,2]. Our analysis focuses in particular on the invariant thermodynamic Ricci curvature scalar R of the thermodynamic FIM. R reveals information about the character of mesoscopic fluctuating structures. Our viewpoint is that such structures play a significant role in mediating the transition from microscopic to macroscopic [3].

Thermodynamic curvature R is an element of thermodynamic metric geometry. A pioneering paper was authored by Weinhold [5] who introduced a thermodynamic energy inner product. This led to the work of Ruppeiner [6] who wrote a Riemannian thermodynamic entropy metric to represent thermodynamic fluctuation theory, and was the first to systematically calculate R. A parallel effort was authored by Andresen, Salamon, and Berry [7] who began the systematic application of the thermodynamic entropy metric to characterize finite-time thermodynamic processes. R has been worked out in a number of discrete systems [8–15]. Another recent evaluation of R was Ref. [16].

We illustrate our ideas with a decorated $(1+3)$ Ising spin chain containing two microscopic parameters: a stiff parameter K mediating the long-range interactions, and a sloppy parameter J operating within local spin groups. We show that K dominates the macroscopic behavior, except in cases where varying J brings about transitions between phases through its conditioning of the local spin groups with which K interacts. In addition to R, we calculate the heat capacity C_H, and the magnetic susceptibility χ_T. We show that C_H is not very effective at displaying the order characterizing the various magnetic phases. χ_T does a better job, but we argue that R offers the cleanest picture of the magnetic order resulting from K. This is the first evaluation of R in a spin model with two coupling parameters.

A significant property of R is that, at zero magnetic field, R is proportional to the correlation length ξ in both the ferromagnetic and the ferrimagnetic phases. Namely, near critical points of fluid and spin systems (including critical points at $T=0$),

$$\xi^d = -\tfrac{1}{2}R, \tag{1}$$

where d is the spatial dimensionality (here, $d=1$) [3,13]. As a convenience for $d=1$, we use the notation

$$-\tfrac{1}{2}R = \xi_R, \tag{2}$$

for purposes of comparing R and ξ.

Although the model employed here is too simple to fully bring out what Sethna *et al.* [1,2] have in mind (here the spin

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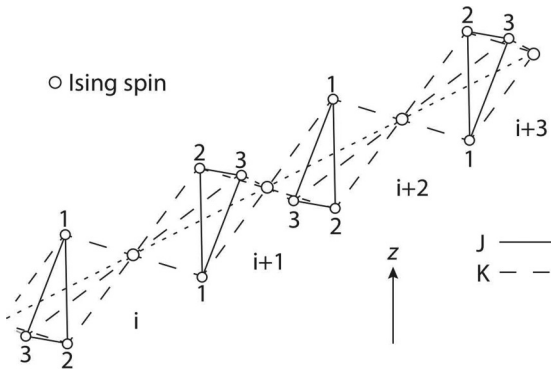

FIG. 1. The decorated (1 + 3) Ising chain. The N lattice basis elements, each consisting of a single Ising spin and a three Ising spin plaquette, are enumerated by an index $i \in \{1,\ldots,N\}$, with periodic boundary conditions $(N+1) \leftrightarrow 1$. The plaquette spins are enumerated by an index $\alpha \in \{1,2,3\}$. Spins within a plaquette interact with each other via a parameter J, and with the single neighboring Ising spins via a parameter K.

groups merely tend to lock into place with each other, instead of having the effects of their local fluctuations averaged out at the mesoscopic level), our use of the terminology stiff or sloppy seems nevertheless appropriate, and sets an agenda for future exploration.

In the theory of critical phenomena, the terms relevant and irrelevant are used for variables, which either affect or do not affect universal critical properties [17]. Our toy model has critical points (at $T = 0$), so we could certainly pitch our discussion in terms of critical phenomena. However, we present our ideas in a broader context, and we get strong results even well beyond what might be termed the critical point regime.

Figure 1 shows our spin model, which contains instances of ferromagnetism, antiferromagnetism, and ferrimagnetism. The model consists of N single Ising spins $\sigma_i = \pm 1$, alternating with N triangular Ising spin plaquettes $\sigma_{i\alpha} = \pm 1$. Two such interlaced sublattices offer the possibility of noncanceling magnetic moments, characteristic of ferrimagnetic states [18].

The Hamiltonian $\mathcal{H}$ is a sum over block Hamiltonians $\mathcal{H}_i$,

$$\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}_i, \tag{3}$$

where

$$\begin{aligned}\mathcal{H}_i = &-\tfrac{1}{2}H\sigma_i + J[\sigma_{i1}\sigma_{i2} + \sigma_{i1}\sigma_{i3} + \sigma_{i2}\sigma_{i3}] \\ &+ K(\sigma_i + \sigma_{i+1})(\sigma_{i1} + \sigma_{i2} + \sigma_{i3}) - H(\sigma_{i1} + \sigma_{i2} + \sigma_{i3}) \\ &- \tfrac{1}{2}H\sigma_{i+1},\end{aligned} \tag{4}$$

with coupling parameters (J,K), and magnetic field H parallel to the z axis, shown in Fig. 1. This block Hamiltonian is that of the solved quantum Ising-Heisenberg chain $(N \to \infty)$ with anisotropy Δ set to zero [19]. The solution yields the transfer matrix $\mathbf{T} = \{\{T_{11},T_{12}\},\{T_{21},T_{22}\}\}$ with:

$$\begin{aligned}T_{11} = &\, 2e^{-h-3\beta J}\cosh(h + 2\beta K) \\ &\times [2\cosh(2h + 4\beta K) + 3e^{4\beta J} - 1],\end{aligned} \tag{5}$$

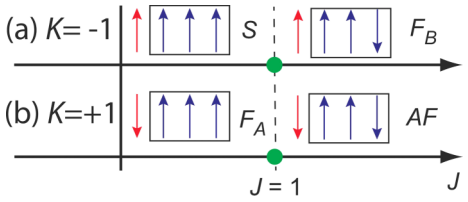

FIG. 2. (Color online) The ground-state spin configurations, as a function of J and for $H \downarrow 0$, for (a) $K = -1$ and (b) $K = +1$. S denotes the saturated phase, F_A and F_B the ferrimagnetic phases, and AF the antiferromagnetic phase. These spin configurations repeat over the entire lattice. $J = 1$ marks the phase boundary for $K = \pm 1$.

$$T_{12} = T_{21} = 6e^{\beta J}\cosh(h) + 2e^{-3\beta J}\cosh(3h), \tag{6}$$

and

$$\begin{aligned}T_{22} = &\, 2e^{h-3\beta J}\cosh(h - 2\beta K) \\ &\times [2\cosh(2h - 4\beta K) + 3e^{4\beta J} - 1].\end{aligned} \tag{7}$$

Here, $\{\beta,h\} = \{1/T,-H/T\}$, with T the temperature. Boltzmann's constant $k_B = 1$. $\mathbf{T}$ has two eigenvalues λ_+ and λ_-, ordered as $\lambda_+ > \lambda_-$. The thermodynamic potential per lattice constant (a lattice constant is the distance between spins σ_i and σ_{i+1}) is

$$\phi(\beta,h) = \ln \lambda_+. \tag{8}$$

ξ, in units of lattice constants, for a decorated Ising chain is [20]

$$\xi^{-1} = \ln\left(\frac{\lambda_+}{\lambda_-}\right). \tag{9}$$

ξ is nonthermodynamic since it may not be calculated from $\phi(\beta,h)$.

A simple reference model for our discussion consists of a chain of Ising spins alternating with single superspins $S_i = \pm p$, where p is a positive integer, in place of the triangular spin plaquettes. A large $|J|$ will lock the three spins in each plaquette into specific configurations with respect to each other, with all three spins in the same direction (J negative) or with one spin in the opposite direction from the other two (J positive), as shown in Fig. 2. These configurations correspond to p either 3 or 1 in the superspin model, which has block Hamiltonian

$$\mathcal{H}_{Si} = -\tfrac{1}{2}H\sigma_i + K_S(\sigma_i + \sigma_{i+1})S_i - HS_i - \tfrac{1}{2}H\sigma_{i+1}, \tag{10}$$

and one coupling parameter, the stiff parameter K_S. The transfer matrix method allows for an easy solution.[1]

Let us restrict attention in this paper to zero magnetic field $H = 0$. We consider only the values $K = -1,0,+1$, which cover the full model. This point is established by the identity $\phi(\beta,h,J,K) = \phi(\beta|K|,h,J/|K|,K/|K|)$, which follows from

[1]The idea of lumping triplets of spins into single spins was explored by Rojas and Alcaraz [21] in a more general setting than is considered here. These authors map with local gauge transformations, and do not assume that $|J|$ is necessarily large.

Eqs. (5)–(8). The ground-state spin configurations for $K = \pm 1$ are shown in Fig. 2. There is a saturated ferromagnetic state S, with all of the spins up, a ferrimagnetic state F_A, with all three plaquette spins up, and the single Ising spin down, a ferrimagnetic state F_B, with frustrated plaquette spins (two up and one down, with the down spin in any of the three positions), and the single Ising spin directed with the plaquette majority spins, and an antiferromagnetic state AF, with frustrated plaquette spins, and the single Ising spin directed with the plaquette minority spin. Appropriate wave function symmetrization was done when combining the three spins in every plaquette [19]. Details involve paired F_B and AF ground states. These show up in the transfer matrix elements Eqs. (5)–(7), but do not figure into the present discussion. The F_B and AF phases have zero magnetic field entropy per lattice constant $s = \ln 3$ as $T \to 0$, due to frustration.

If $|J/K|$ is large, then the spins in each plaquette lock into place with each other, according to the sign of J, as in Fig. 2. One expects the $(1+3)$ Ising chain to conform to the superspin chain in this limit, according to the sign of J, with positive J corresponding to the frustrated $p = 1$, and negative J corresponding to $p = 3$. Otherwise, only the value of $K(=K_S)$ is important, with variations in J causing little effect. For $K = 0$ we expect paramagnetic behavior, with only small organized fluctuating structure size.

The invariant R results directly from an information theoretic thermodynamic metric, with metric elements $g_{\alpha\beta} = \phi_{,\alpha\beta}$. The thermodynamic coordinates are $(x^1, x^2) = (\beta, h)$, and the comma notation denotes differentiation [3,22]. Generally [3],

$$R = \frac{1}{2}\begin{vmatrix} \phi_{,11} & \phi_{,12} & \phi_{,22} \\ \phi_{,111} & \phi_{,112} & \phi_{,122} \\ \phi_{,112} & \phi_{,122} & \phi_{,222} \end{vmatrix} \Bigg/ \begin{vmatrix} \phi_{,11} & \phi_{,12} \\ \phi_{,12} & \phi_{,22} \end{vmatrix}^2 . \qquad (11)$$

R is in units of lattice constants, and depends on derivatives of ϕ up to third-order. For fluid systems R was found to be negative when attractive intermolecular interactions dominate, such as near critical points, and positive in cases where repulsive interactions dominate, such as in solids [23–26]. $R = 0$ for the (noninteracting) paramagnet [8]. The sign of R has been less explored in spin systems, though recently it was shown that the kagome Ising model (2D) in a magnetic field has R diverging to $\pm\infty$ on opposite sides of the phase transition line ($R < 0$ on the ferromagnetic side, and $R > 0$ on the frustrated side) [15].

Let us define the heat capacity per lattice constant at constant H, $C_H = T(\partial s/\partial T)_H$, with entropy per lattice constant $s = \phi - \beta\phi_{,\beta} - h\phi_{,h}$. Also define the magnetic susceptibility $\chi_T = (\partial m/\partial H)_T$, with magnetization per lattice constant $m = -\phi_{,h}$. Figure 3 shows C_H, χ_T, and $\xi_R = -R/2$ as functions of J for several values of T, and for $K = -1, 0, +1$. In all cases with large $|J/K|$, these three functions reach asymptotic values independent of J, and equal to the corresponding values of the superspin chains with $K_S = K$.

As J increases from very negative values, and reaches the neighborhood of $J = 1$ ($J = 0$ for $K = 0$), all three thermodynamic functions go through transitional values as the corresponding superspin value p goes from 3 to 1. For $K = \pm 1$, the transition is between the phases shown in Fig. 2. In the transitional regime, the sloppy parameter J is clearly very relevant to the thermodynamic behavior, and we can expect no concordance with the superspin chain.

For the paramagnetic state $K = 0$, we have $|\xi_R| \leqslant 1$ lattice constants in all cases, as shown in Fig. 3(f). Such small values for $|\xi_R|$ are characteristic of situations with weak interactions among constituents. For $\{K, J, H\} = \{0,0,0\}$, $\xi_R = -1/16$ for all T, leading to the common crossing point shown in Fig. 3(f). For (K, J, H) all zero, the spins are randomly directed for all T, with $s = 4 \ln 2$, and $C_H = 0$, as shown in Fig. 3(d). χ_T shows a contrast between different K's, having diminished values for the paramagnet. Nevertheless, χ_T diverges ($\propto \beta$) for the paramagnet in the limit $\beta \to \infty$, in contrast to $|\xi_R|$, which continues to signal that nothing is going on at long lattice distances. For $K = 0$, the nonthermodynamic $\xi = 0$ for all J, so clearly the strictly local J by itself never produces fluctuations with large spatial extent.

For $K = \pm 1$, and for $|J|$ not too small, Fig. 3 shows strong divergences for χ_T and ξ_R as $\beta \to \infty$ in the S and F_A states. Weaker divergences are present in the F_B state. C_H is the same for $K = \pm 1$, since both cases have the same entropy function $s = s(T)$. In the transition regime, to the right of the peaks in Figs. 3(a) and 3(g), C_H shows a region of nearly temperature independent behavior. For decreasing J, values of ξ_R become the same for $K = \pm 1$, as seen in Figs. 3(c) and 3(i), reflecting a zero magnetic field symmetry for the S and F_A states. However, this symmetry is not displayed by χ_T.

For $K = +1$, χ_T in Fig. 3(h) has the curves crossing near $J = 5/4$, with the crossing depending weakly on β. ξ_R in Fig. 3(i) shows negative minima in the transition region on going from the F_A to the AF state. These minima grow deeper as the temperature decreases. Similar behavior was seen in the Takahashi gas, a one-dimensional system of hard rods with both attractive and repulsive interactions, during a pseudo-phase-transition from gaslike to liquidlike [27]. By the lattice gas analogy (discussed below), the correspondence between these negative ξ_R features is not unexpected. There is no corresponding feature in the transition from the S to the F_B state in Fig. 3(c).

The best way to characterize divergences as $\beta \to \infty$ consists of low temperature, zero magnetic field, series expansions in powers of the small parameter $w = e^{-2p|K|\beta}$. In the S, F_A, and F_B phases we find that, to leading order, $\xi_R = w^{-1}/4$, with the same divergence for ξ, in accord with Eq. (1). These series results (independent of J) are strong, holding (with $K \pm 1$) for all integer values of J except $J = 0,1$ in the transition region. The corresponding superspin chains have the same series. The absence of J in both w and the series coefficient $1/4$ further illustrate J's irrelevance out of the transition region. To leading order, $\chi_T = 2^p \beta w^{-1}$ for $K = -1$, and $\chi_T = 2\beta w^{-1}$ for $K = +1$, except for $J = 0,1$. These series for χ_T are not as clean as those for ξ_R, but they make the same point about J.

Let us supplement the series results for ξ_R and ξ with two examples spanning a range of β. Figure 4 shows excellent agreement between ξ_R and ξ in both the S and F_B phases, down to length scales less than about a lattice constant. The concordance with the corresponding superspin chain (not shown here) is likewise excellent. Outside the transition regime for J, the quality of these results is representative of that for other values of J, and clearly extends well beyond the critical region.

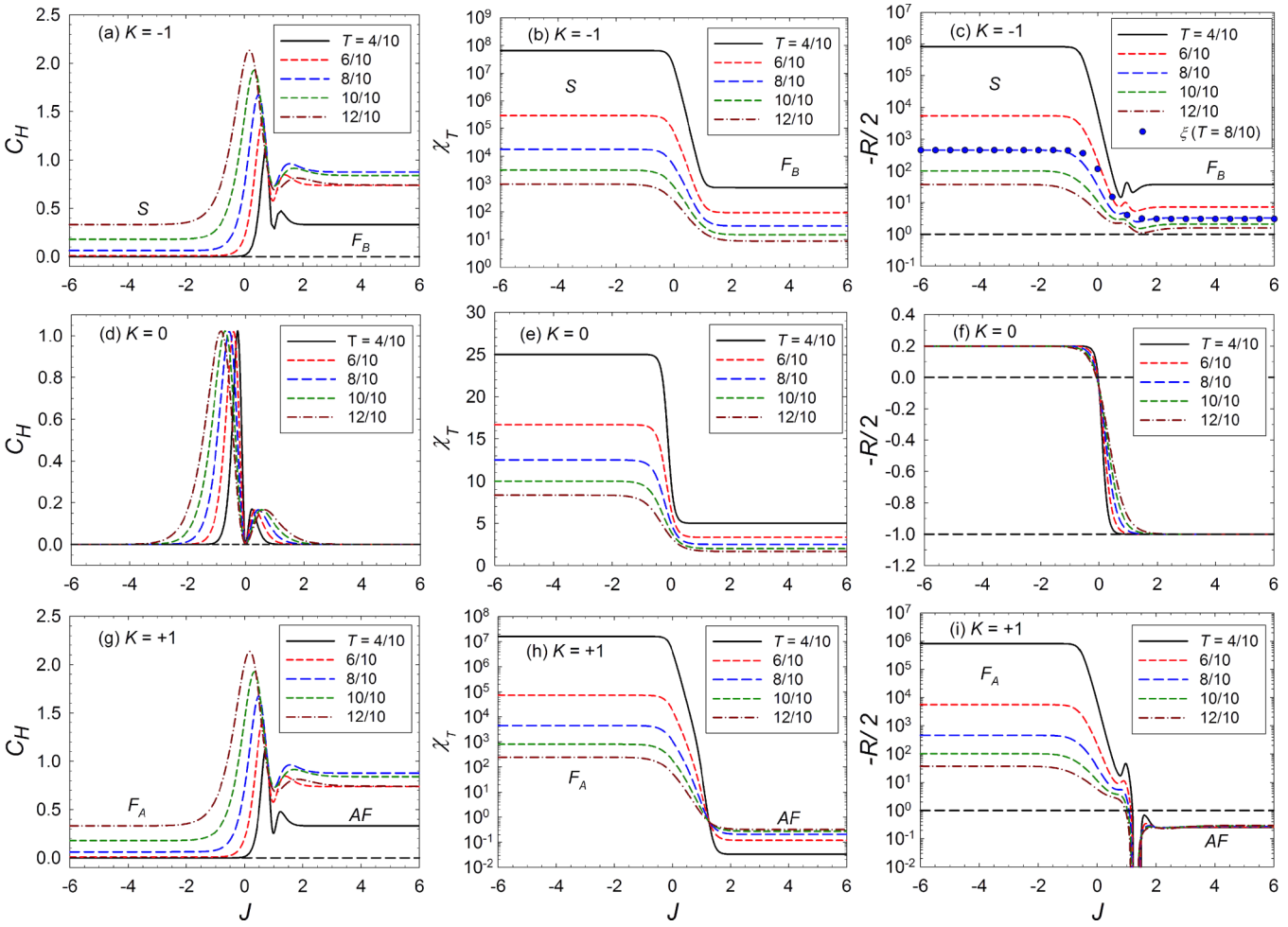

FIG. 3. (Color online) The heat capacity C_H, the magnetic susceptibility χ_T, and the thermodynamic curvature $\xi_R = -R/2$ as functions of J for several values of T, and for the three distinct cases $K = -1,0,+1$. Cases in the plateau regimes, with J not near 1, are commensurate with the appropriate superspin chains. The dots in (c) show ξ for $T = 8/10$, in good agreement outside the transition regime with the corresponding ξ_R. There are negative values of ξ_R in Fig. 3(i) near $J = 1$, which are omitted on the log scale.

Let us turn now to the antiferromagnetic AF state. Series expansions show that to leading order in w, $\xi_R = 1/4$, and $\chi_T \propto \beta w$, for $J \geqslant 2$ with $K = +1$, findings evident in Figs. 3(h) and 3(i), and in concordance with the corresponding superspin chains. To leading order, $\xi = w^{-1}/4$, also in concordance with the corresponding superspin chain.

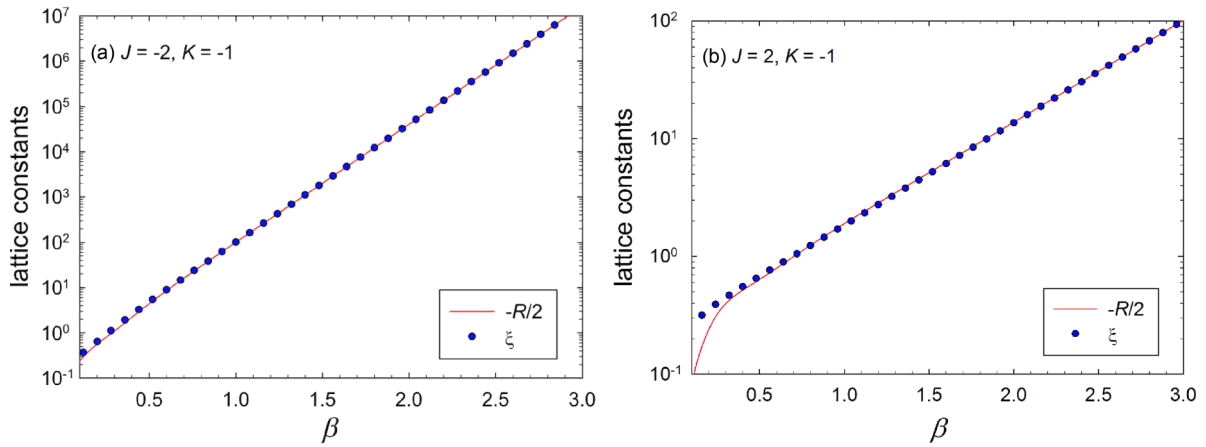

FIG. 4. (Color online) (a) $\xi_R = -R/2$ and ξ for the saturated phase S at zero magnetic field, with $\{J,K\} = \{-2,-1\}$. The agreement between ξ_R and ξ is excellent even to regimes with ξ_R less than about a lattice constant. (b) the corresponding quantities for the ferrimagnetic phase F_B with $\{J,K\} = \{+2,-1\}$. The agreement between ξ_R and ξ is likewise excellent, except when ξ_R has value a fraction of a lattice site.

Clearly, ξ_R is quite different from ξ for antiferromagnets, as ξ diverges in the same way as the ferromagnet, while $|\xi_R|$ has small value. This has long been known for the simple Ising chain [8].

Physically understanding ξ_R for the antiferromagnet benefits from a comparison with fluid systems. Ferromagnetic Ising spin models prefer to have aligned adjacent spins, and critical point properties analogous to those for fluid models. The lattice gas model offers a formal correspondence [28]. In the lattice gas model, spin up corresponds to a cell occupied by an atom, and spin down corresponds to an empty cell. Thus, the Ising ferromagnet corresponds to a fluid model with a preference for adjacent occupied cells. Near the critical point, a bunching of atoms, of characteristic size ξ, is brought about by the attractive interatomic interactions. The critical point models are characterized by uniformly negative R [23], and by the asymptotic equality Eq. (1). The S, F_A, and F_B states, where all or the majority of spins point in the same direction, and where there is a critical point at $T = 0$, corresponds to a fluid near its critical point. The behavior displayed here is certainly consistent with this expectation. We thus think of ferromagnetic spin interactions as attractive.

We might logically think of the antiferromagnetic interactions as repulsive, with positive R, but such thinking is in need of some refinement. Antiferromagnetism tends to have disaligned adjacent spins, corresponding to nearest-neighbor atoms avoiding each other in the lattice gas. Outside the transition region for J, calculation shows that $|R|$ in the AF phase tends to be uniformly small, of the order of a lattice constant. Although the sign of R for the antiferromagnet is generally negative here, there are cases for this model with the parameter $\Delta \neq 0$ where either sign occurs, though with $|R|$ always of the order of a lattice constant. As was shown by May *et al.* [25,26], solid models tend to have small positive R, and condensed liquid states tend to have small $|R|$, with R positive or negative depending on the density. By this measure, the antiferromagnetism here corresponds to the condensed liquid state. In any case, the results we have obtained here for the antiferromagnetic states are fully in accord with expectations from the fluid or solid context.

In conclusion, we have shown that in the zero magnetic field $(1 + 3)$ Ising chain here, the macroscopic order is connected with the stiff parameter K, whose repeated application connects all of the spins in the chain. The sloppy parameter J, operating only within local spin groups, affects the long-range behavior mostly through its conditioning of the local spin plaquettes for the interaction with K. Our analysis emphasized the role of the thermodynamic curvature R at characterizing the resulting magnetism. The ferromagnetic and the ferrimagnetic phases take on negative curvatures, diverging as the correlation length ξ as temperature $T \to 0$. The antiferromagnet may have positive or negative R, with $|R|$ of the order of a lattice constant. We suggest that at zero magnetic field such characteristics, which link directly to fluids or solids through the lattice gas analogy, may be general in spin models. Future research adds a magnetic field ($H \neq 0$), and a full Heisenberg interaction between the plaquette spins ($\Delta \neq 0$). Also, most interesting to work out would be a model where the effect of local spin interactions actually average out at the macroscopic level. This would relate our ideas of connecting R from the thermodynamic fluctuating FIM fully to those of Sethna *et al.* [1,2].

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