Mixed-Order Phase Transition in a One-Dimensional Model

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We introduce and analyze an exactly soluble one-dimensional Ising model with long range interactions that exhibits a mixed-order transition, namely a phase transition in which the order parameter is discontinuous as in first order transitions while the correlation length diverges as in second order transitions. Such transitions are known to appear in a diverse classes of models that are seemingly unrelated. The model we present serves as a link between two classes of models that exhibit a mixed-order transition in one dimension, namely, spin models with a coupling constant that decays as the inverse distance squared and models of depinning transitions, thus making a step towards a unifying framework.

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The usual classification of phase transitions distinguishes between first order transitions, which are characterized by a discontinuity of the order parameter, and second order transitions in which the order parameter is continuous but the correlation length and the susceptibility diverge. However there are quite a number of cases for which this dichotomy between first order and second order transitions fails. In particular, some models exhibit phase transitions of mixed nature, which on the one hand have a diverging characteristic length, as typical of second order transitions, and on the other hand display a discontinuous order parameter as in first order transitions. Examples include models of wetting [1], DNA denaturation [2–4], glass and jamming transitions [5–8], rewiring networks [9], and some one-dimensional models with long range interactions [10–13]. A scaling approach for such transitions was introduced in Ref. [14]. Formulating exactly soluble models of this kind and probing their properties would be of great interest.

Two distinct classes of models that exhibit mixed transitions have been extensively studied: (a) one-dimensional spin models with interactions that decay as $1/r^2$ at large distances r, and (b) models of DNA denaturation and depinning transitions in $d = 1$ dimension. While in both classes the appropriate order parameter is discontinuous at the transition, the correlation length diverges exponentially in the first class and algebraically in the second. Placing the two rather distinct classes of models in a unified framework would provide a very interesting insight into the mechanism that generates these unusual transitions. This is the aim of the present work.

An extensively studied representative of class (a) is the one-dimensional Ising model with a ferromagnetic coupling that decays as $1/r^\alpha$ with $\alpha = 2$, which we shall call hereafter the inverse distance squared Ising (IDSI) model. While the model is not exactly soluble, many of its thermodynamic features have been accounted for. It was shown by Dyson that for $1 < \alpha < 2$ the model exhibits a phase transition to a magnetically ordered phase [15]. It was then suggested by Thouless, and later proved rigorously by Aizenman *et al.* [12], that in the limiting case $\alpha = 2$, the model exhibits a phase transition in which the magnetization is discontinuous [10]. This has been termed the Thouless effect. Using scaling arguments [16–18] and renormalization group analysis [19], which is closely related to the Kosterlitz-Thouless analysis, it was found that the correlation length diverges with an essential singularity as $\xi \sim e^{1/\sqrt{T-T_c}}$ for $T \to T_c$.

A paradigmatic example of models of class (b) is the Poland-Scheraga (PS) model of DNA denaturation [2–4] whereby the two strands of the molecule separate from each other at a melting, or denaturation, temperature. In this approach the DNA molecule is modeled as an alternating sequence of segments of bound pairs and open loops. While bound segments are energetically favored, with an energy gain $-\epsilon l$ for a segment of length l, an open loop of length l carries an entropy $sl - c \ln l$. Here $\epsilon, s > 0$ are model dependent parameters and c is a constant depending only on dimension and other universal features. For $c > 2$ the model has been shown to exhibit a phase transition of mixed nature, with a discontinuity of the average loop length that serves as an order parameter of the transition, and a correlation length that diverges as $(T_c - T)^{-1}$ at the melting temperature T_c.

In this Letter we introduce and study an exactly soluble variant of the IDSI model in which the the $1/r^2$ interaction applies only to spins that lie in the same domain of either up or down spins. This model can be conveniently represented within the framework of the Poland-Scheraga model, thus providing a link between these broadly studied classes of models. We find that on one hand the model exhibits an extreme Thouless effect whereby the magnetization m jumps from 0 to ± 1 at T_c, and on the other hand it exhibits an algebraically diverging correlation length $\xi \sim (T - T_c)^{-\nu}$, and consequently a diverging susceptibility. The power ν is model dependent and it varies with the model parameters. We also identify an additional order parameter, the average number of domains per unit length

n, which vanishes either continuously or discontinuously at the transition, depending on the interaction parameters of the model. In addition we find a similar type of transition (discontinuous with diverging correlation length) at nonzero magnetic field. This is in contrast to the IDSI model, which exhibits no transition for nonvanishing magnetic field [14]. Below we demonstrate these results by an exact calculation. We also present a renormalization group (RG) analysis that provides a common framework for studying both the IDSI and our model, elucidating the relation between the two.

The model is defined on a one-dimensional lattice with L sites where in site i, $1 \le i \le L$, the spin variable σ_i can be either 1 or -1. The Hamiltonian of the model is composed of two terms: a nearest neighbor (NN) ferromagnetic term $-J_{NN}\sigma_i\sigma_{i+1}$ and a long range (LR) term that couples spins lying within the same domain of either up or down consecutive spins. This intradomain interaction is of the form $-J(i-j)\sigma_i\sigma_j$ where $J(r)$ decays as $J_{LR}r^{-2}$ for large r. This is a truncated version of the IDSI model. Note, though, that the long range interaction is in fact a multispin interaction since it couples only spins that lie in the same domain. For domains of length $l \gg 1$ the energy due to the intradomain interactions is

$$E_d(l) \approx -J_{NN}(l-1) - J_{LR}\sum_{k=1}^{l}\frac{l-k}{k^2} = -bl + \tilde{c}\log l + \tilde{\Delta} + O(l^{-1}), \quad (1)$$

where b, $\tilde{c}$, and $\tilde{\Delta}$ are constants set by J_{NN} and J_{LR}. Without loss of generality one may set $b = 0$ since it contributes a constant to the total energy. Nearest neighbor domains interact only through the nearest neighbor interaction. The interaction $J_{NN} > 0$ can be made large enough so that $\Delta \equiv J_{NN} + \tilde{\Delta} > 0$ and, hence, domain walls are disfavored and the model is ferromagnetic. A configuration of the model is composed of a sequence of N domains of alternating signs whose lengths $\{l_i\}_{i=1}^{N}$ satisfy $\sum l_i = L$. The corresponding energy is

$$H(\{l_i\}, N) = \tilde{c}\sum_{i=1}^{N}\log(l_i) + N\Delta + O(1). \quad (2)$$

This representation of the model is reminiscent of the PS model, where $E_d(l)$ originates from the entropy of a denatured loop rather than its energy [2]. We also generalize Eq. (2) to include a magnetic field h, which couples to the magnetization $\sum_i(-1)^i l_i$.

This model is exactly solvable. The phase diagram of the model at zero magnetic field is presented in Fig. 1. The model exhibits a phase transition from a disordered phase ($m \equiv \sum_i^L \sigma_i/L = 0$) at $T > T_c$ to a fully ordered phase ($m = \pm 1$) at $T < T_c$, where T_c is the critical temperature. While m is discontinuous at the transition, the correlation length diverges and, hence, the transition is of mixed order.

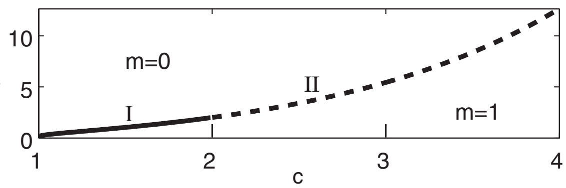

FIG. 1. The (T, c) phase diagram of the model (2) for zero magnetic field $h = 0$ and $\Delta = 1$. The transition line is marked as a continuous and dashed line in regions I ($1 < c \le 2$) and II ($c > 2$), respectively.

In addition to the magnetization, the transition may be characterized by another order parameter, the density of domains $n \equiv N/L$. In the disordered phase there is a macroscopic number of domains and, hence, $n > 0$, while in the ordered phase there is essentially a single macroscopic domain—a condensate—and, hence, $n = 0$. The behavior of n near the transition depends on the nonuniversal parameter $c \equiv \beta_c\tilde{c}$ where $\beta_c = (k_B T_c)^{-1}$ is the inverse transition temperature, which depends on the interaction parameters: for $1 < c \le 2$ (region I in Fig. 1) the density of domains decreases continuously to 0 as $T \to T_c$ from above, while for $c > 2$ (region II), n attains a finite value $n \to n_c$ as $T \to T_c$ from above, and it drops discontinuously to 0 at the transition.

The model also exhibits a condensation transition at finite magnetic field as presented in Fig. 2(a). The transition

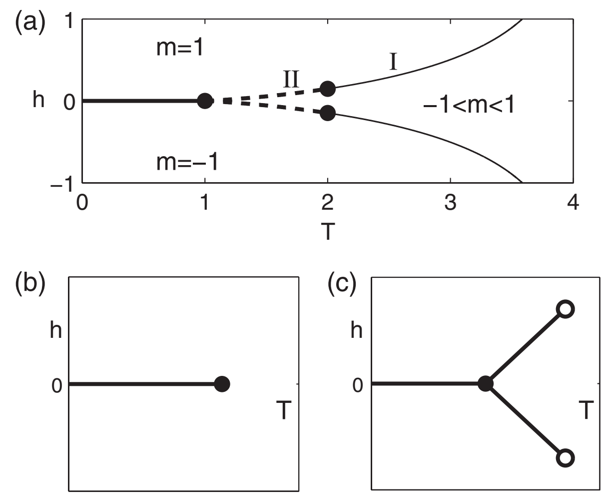

FIG. 2. (a) The (T, h) phase diagram of the model (2) compared with the phase diagram of (b) the IDSI model and (c) a schematic phase diagram of a typical first order transition. The parameters in (a) are $\tilde{c} = 4$ and $\Delta = \log(U(0))$ so that $T_c(h = 0) = 1$. Here the thick solid line is first order transition, the dashed lines represent mixed order transition, and the thin solid lines a second order transition. Tricritical points separating mixed order from second order transitions are indicated. In (b) and (c) the lines are first order. The terminal point in (b) is a mixed-order point. In (c) the solid point is a triple point while the empty circles are ordinary critical transitions.

at nonzero field does not involve symmetry breaking. It can be either second order, where both m and n change continuously to their ordered values $m = \pm 1$ and $n = 0$, or of mixed order, where both m and n change discontinuously at the transition. This depends on whether $c(h) \equiv \beta_c(h)\tilde{c}$ is greater or smaller than 2, where $\beta_c(h)$ is the magnetic-field dependent critical temperature. Qualitatively the phase diagram at a given magnetic field $h \neq 0$ is identical to that of the PS model, with $c(h)$ playing the role of c. On the other hand, the resulting phase diagram [Fig. 2(a)] is different from that of the IDSI model, presented in Fig. 2(b), for which no transition takes place at a nonvanishing magnetic field [14]. It is also different from the phase diagram of an ordinary first order transition such as the mean-field Ising spin 1 model, which is presented in Fig. 2(c), for which each of the finite h transition lines terminates at a critical point at some finite value of h. By contrast, the finite h transition lines in Fig. 2(a) extend to $h \to \infty$.

We shall now outline the derivation of the phase diagram (see Supplemental Material [20]). The Hamiltonian (2) represents a gas of noninteracting domains with a fugacity Δ. Correlation between domains is introduced, though, by the constraint that the sum of l_i is L, the chain length. The system is thus most conveniently studied within the grand canonical ensemble. The grand canonical partition function is given by

$$Q(p) = \sum_L Z(L) e^{\beta p L} \simeq \sum_L e^{-\beta L(F(\beta)-p)}, \quad (3)$$

where $Z(L)$ is the canonical partition function, $F(\beta)$ is the free energy per site, and p is effectively the pressure. Working with the symmetric boundary conditions $\sigma_1 = 1$ and $\sigma_L = -1$, a configuration is defined by a sequence of an even number of alternating + and − domains of variable sizes. Denoting by $U(p)$ the grand partition sum of a single domain and by $y \equiv e^{-\beta\Delta}$ the fugacity of domains, the explicit form of the grand partition sum is then

$$Q(p) \sim y^2 U(p)^2 + y^4 U(p)^4 + \cdots = \frac{y^2 U(p)^2}{1 - y^2 U(p)^2}, \quad (4)$$

$$U(p) = \sum_{l=1}^{\infty} \frac{e^{\beta p l}}{l^{\beta\tilde{c}}} = \Phi_{\beta\tilde{c}}(e^{\beta p}), \quad (5)$$

where $\Phi_\gamma(r)$ is the polylogarithm function [21]. Using the properties of the polylogarithm, or just inspecting the sum in Eq. (5), we see that for $p \leq 0$, $U(p)$ is an increasing function of p and a decreasing function of β. It also has a branch point at $p = 0$. In the thermodynamic limit $L \to \infty$, the most negative singularity of $Q(p)$ is given by $p^* = F(\beta)$ as this sets the radius of convergence of the sum in Eq. (3). The singularity can stem either from setting the denominator of Eq. (4) to zero, or from the branch point of $U(p)$, i.e.,

$$\text{(a) } U(p^*) = e^{\beta\Delta} \quad \text{or} \quad \text{(b) } p^* = 0 \quad (6)$$

The solution of (a) corresponds to the state with zero magnetization (no condensate) while (b) corresponds to the magnetic state. At high enough temperatures for which $\beta\tilde{c} < 1$ the sum $U(0) = \sum l^{-\beta\tilde{c}}$ diverges and a solution of type (a), with $p^* < 0$, exists. The solution p^* increases with increasing β and at the critical point β_c, for which $c = \beta_c\tilde{c} > 1$ and, hence, $U(0) < \infty$, p^* vanishes. It stays zero at all temperatures below T_c. Thus β_c is a singular point of the free energy $F(\beta) = p^*$. The freezing of the thermodynamic pressure p^* below T_c is mathematically similar to the freezing of the fugacity in Bose-Einstein condensation for free bosons [22].

We next proceed to show that there is a diverging length scale. Above the transition the probability to have a domain of size l is given by

$$P(l) \simeq \frac{Z(L-l) y l^{-\beta\tilde{c}}}{Z(L)} \simeq y \frac{e^{-l/\xi}}{l^{\beta\tilde{c}}}, \quad (7)$$

where we have used the fact that $Z(L) \simeq e^{-\beta p^* L}$, and defined $\xi = -(\beta p^*)^{-1}$. The length scale ξ can be regarded as a correlation length, and it diverges at the transition (for any c) as $p^* \to 0$. Expanding Eq. (6) (a) near the transition, it can be shown that $(-p^*)^{\min(c-1,1)} \sim (T - T_c)$. Hence we deduce that $\xi \sim (T - T_c)^{-\nu}$ with $\nu = \max[(1/(c-1)), 1]$, demonstrating the algebraic divergence of the correlation length for all $c > 1$.

The average density of domains is given by the usual relation $\langle n \rangle = -(\partial p^*/\partial\Delta)$. From this it is easy to see that at the low temperature phase $\langle n \rangle = 0$ since $p^* = 0$ regardless of Δ. As $\langle n \rangle \times \langle l \rangle = 1$ this implies that $\langle l \rangle = \infty$ for $T < T_c$. At the transition, where the correlation length ξ diverges, the average domain length is given by $\langle l \rangle = \sum_l l P(l) = \sum l^{-c+1}$ and, hence, it is finite if $c > 2$ and infinite if $1 < c \leq 2$. This implies that $\langle n \rangle$ drops continuously to 0 if $1 < c \leq 2$ and discontinuously if $c > 2$.

Finally we wish to show that the magnetization jumps at T_c from 0 to ± 1 for all $c > 1$. At zero magnetic field the system has spin reversal symmetry and, hence, as long as the symmetry is not spontaneously broken (i.e., at the high temperature phase) the magnetization is 0. The low temperature phase is characterized by a condensate, as was argued by the similarity to Bose-Einstein condensation and also as $\langle n \rangle = 0$; i.e., there is essentially a single macroscopic domain (plus maybe a subextensive number of microscopic domains). As the condensate is either of type +1 or −1, we find $\langle m \rangle = \pm 1$. This demonstrates the features of the phase diagram shown in Fig. 1.

We now consider the finite magnetic field case. The analysis of the transition in this case follows essentially the same steps as for the zero magnetic field case, with Eq. (6) replaced by

$$\text{(a) } U(p^* + h) U(p^* - h) = e^{2\beta\Delta} \quad \text{or} \quad \text{(b) } p^* = -|h|. \quad (8)$$

At finite h, the magnetization $m = -(\partial p^*/\partial h)$ is nonzero even in the high temperature phase. For $1 < c \leq 2$ it is continuous at T_c and the transition is an ordinary second order transition. For $c > 2$, $\langle m \rangle$ is discontinuous at T_c and the transition is of mixed nature as depicted in Fig. 2(a).

It is instructive to consider the RG flow of the model and compare it with that of the IDSI model. This provides a common analytical framework for both models and helps elucidating the mechanism behind their distinct features. The RG flow of the IDSI model was studied first by Anderson *et al.* [16–18] using scaling arguments and then more systematically by Cardy [19] and was shown to be of the Kosterlitz-Thouless type [23]. In particular the transition is characterized by a length that diverges as $\exp[(T - T_c)^{-1/2}]$. We show below that in our model the RG equations are of different form, yielding a correlation length that diverges with a power law. To proceed we consider a continuous version of the model, which captures the long wavelength behavior of the original model: we represent the domain boundaries (the kinks) as particles with impenetrable core of size a, placed on a circle at positions $\{r_i\}_{i=1}^N$, whereby, following Eq. (1), every pair of nearest neighbor particles i and $i+1$ attract each other logarithmically through a two body potential $\tilde{c}\log(r_{i+1} - r_i)$. The number of particles is not conserved, as the number of kinks in the spin representation fluctuates, and it is controlled by a fugacity y (equivalent to $e^{-\beta\Delta}$ above). The partition function is thus

$$Z = \sum_{N=0}^{\infty} y^N \int \prod_{i=1}^{N} \frac{dr_i}{a} \left(\frac{r_{i+1} - r_i}{a}\right)^{-\beta\tilde{c}} \Theta(r_{i+1} - r_i - a), \tag{9}$$

where Θ is the Heaviside step function. Assuming a small density of particles ($y \ll 1$), the renormalization procedure proceeds by rescaling the core size of the particle $a \to ae^{\kappa}$, as in Ref. [19]. The resulting flow equations in terms of the fugacity y and the scaled interaction strength $x = 1 - \beta\tilde{c}$ read

$$\frac{dy}{d\kappa} = xy + y^2; \qquad \frac{dx}{d\kappa} = 0. \tag{10}$$

The xy term in Eq. (10) compensates for the change in the $a^{-(N - N\beta\tilde{c})}$ factor in Eq. (9), and is the same as in the analysis of the IDSI model [19]. The second term (y^2) is the result of expanding the Θ function as $\Theta(r_{i+1} - r_i - ae^{\kappa}) \approx \Theta(r_{i+1} - r_i - a) - a\kappa\delta(r_{i+1} - r_i - a)$. Physically the second term of this expansion corresponds to the merging of two kinks due to the rescaling procedure, and, hence, it results in the y^2 term. As these are the only effects of the scale transformation, x remains invariant under it. The resulting flow diagram is presented in Fig. 3(a). In this flow there is a line of unstable fixed points for $y = -x$ each corresponding to a different value of c. A similar flow diagram has previously

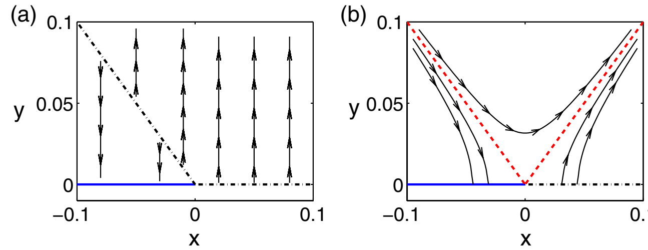

FIG. 3 (color online). RG flow for (a) the truncated model [Eq. (10)], and (b) the IDSI model (or XY model) [Eq. (11)]. Solid lines indicate attractive fixed points, unstable fixed points are marked by dashed-dotted lines, and the dashed line in (b) is a separatrix.

been found for the one-dimensional discrete Gaussian model with $1/r^2$ coupling [24,25].

Equation (10) can be compared with the RG equations for the IDSI model, which are the same as those of the XY model (under proper rescaling of parameters) [19,23]

$$\frac{dy}{d\kappa} = xy; \qquad \frac{dx}{d\kappa} = y^2. \tag{11}$$

Notice that in this case the merging of two kinks produces a dipole interaction, and, hence, the y^2 term renormalizes the interaction strength x. The renormalization flow of this model is presented in Fig. 3(b). It has only a single unstable fixed point for $x = y = 0$ in the relevant $x \leq 0$ regime.

One can calculate the temperature dependence of the correlation length of the truncated model by linearizing Eq. (10) near the fixed points. The result is $\xi \sim [(T - T_c)/|x|]^{1/x}$, which is the same as that found above for $c \leq 2$.

In conclusion, we have presented and analyzed a novel one-dimensional Ising model that displays a spontaneous symmetry breaking transition with diverging correlation length and an extreme Thouless effect, i.e., a discontinuous jump in magnetization (from 0 to ± 1). The model conveniently connects two widely studied classes of models, the Poland-Scheraga model and the IDSI. In addition to the magnetization we have identified another order parameter, the density of domains n, and have shown that it is either continuous or discontinuous at T_c depending on whether $c \leq 2$ or $c > 2$, respectively. This order parameter has not been discussed in the context of the IDSI model, and it would be interesting to explore its behavior in that case. We also showed that the model exhibits mixed transitions for nonzero magnetic field, unlike the IDSI model, and, hence, it does not fall into the classification of first order transition points appearing in Ref. [14]. We have also used a RG picture to explain the power law divergence of the correlation length in this model, in contrast to the essential singularity behavior of the correlation length in the IDSI model. It would be interesting to extend the present study to Potts type models and to consider the effect of disorder on the nature of the transition.

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