One-dimensional inhomogeneous Ising model with periodic boundary conditions

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In this paper, we focus on the essential difference between the inhomogeneous one-dimensional Ising model with open and periodic boundary conditions. We show that, although the profile equation in the periodic case becomes highly nonlocal, due to a topological collective mode, there exists a local free-energy functional in an extended space and one can solve the inhomogeneous problem exactly.

I. INTRODUCTION

Since the inhomogeneous one-dimensional (1D) Ising model was first solved[1] ten years ago by the inverse method (i.e., expressing the external field as a functional of the magnetization), there have been several similar approaches to the problem.[2-4] But all of the solvable cases are with an open boundary. Although, due to the short-range interactions, boundary conditions do not affect the thermodynamics, there is still a qualitative difference between the open and the periodic systems. For the latter, the profile equation becomes nonlocal, which precludes a simple solution even in the inverse approach. However, we will see that such a solution does exist on the expanded space of spins together with a collective mode, and we will examine the nature of the mode.

II. THE RECURSIVE EQUATION FOR THE SINGLE-SITE FUNCTIONS

The one-dimensional inhomogeneous Ising model with external field u_x, chemical potential μ, and coupling $-J$ is determined by the partition function (we set $\beta \equiv 1/kT$ to unity)

$$\Xi = \sum_{\{\sigma_x\}} \prod_{x=1}^{N} W_x(\sigma_x) e(\sigma_x, \sigma_{x+1}) , \tag{1}$$

where $h_x = \mu - u_x$, $W_x(\sigma_x) = \exp(h_x \sigma_x)$, $e(\sigma_x, \sigma y) = \exp(J\sigma_x \sigma_y)$, and $\sigma_{N+1} \equiv \sigma_1$.

To extend the previous technique[1] in a natural way, we define

$$\Xi_{x,x'}(\sigma,\sigma') = W_x(\sigma) \sum_{\{\sigma''\}} e(\sigma, \sigma''_{x-1}) W_{\sigma''_{x-1}} \cdots e(\sigma''_{x'+1}, \sigma') W_{x'}(\sigma') .$$

From this definition, we immediately get the following recursion relations:

$$\begin{aligned} \Xi_{x,x'}(\sigma,\sigma') &= W_x(\sigma) \sum_{\sigma''} e(\sigma,\sigma'') \Xi_{x-1,x'}(\sigma'',\sigma') , \\ \Xi_{x,x'}(\sigma,\sigma') &= W_{x'}(\sigma') \sum_{\sigma''} \Xi_{x,x'+1}(\sigma,\sigma'') e(\sigma'',\sigma') . \end{aligned} \tag{2}$$

On combining the two, we have

$$\begin{aligned} \frac{\Xi_{x+1,x'+1}(\sigma,\sigma')}{W_{x+1}(\sigma)} &= \sum_{\sigma'',\sigma'''} e(\sigma,\sigma'') \frac{\Xi_{x,x'}(\sigma'',\sigma''')}{W_{x'}(\sigma''')} e^{-1}(\sigma''',\sigma') , \\ \frac{\Xi_{x-1,x'-1}(\sigma,\sigma')}{W_{x'-1}(\sigma')} &= \sum_{\sigma'',\sigma'''} e^{-1}(\sigma,\sigma'') \frac{\Xi_{x,x'}(\sigma'',\sigma''')}{W_x(\sigma'')} e(\sigma''',\sigma') . \end{aligned} \tag{3}$$

Now if we define a new function $m_x(\sigma,\sigma') \equiv \Xi_{x,x}(\sigma,\sigma')\Xi^{-1}$, then the magnetization is clearly given by $m_x = \sum_{\sigma=\pm} \sigma m_x(\sigma,\sigma) W_x(\sigma)^{-1}$. By setting $x'=x$ in Eq. (3), we obtain recursion relations for the single-site functions, but these are not all independent. We know there can be only three independent equations, since their traces are equivalent. The three independent equations can be obtained by letting $\sigma'=\sigma$, multiplying by σ and summing over σ,

$$m_{x+1} = \sum_{\sigma,\sigma',\sigma''} \sigma e(\sigma,\sigma') m_x(\sigma',\sigma'') W_x(\sigma'')^{-1} e^{-1}(\sigma'',\sigma) ,$$

$$m_{x-1} = \sum_{\sigma,\sigma',\sigma''} \sigma e^{-1}(\sigma,\sigma') m_x(\sigma',\sigma'') W_x(\sigma')^{-1} e(\sigma'',\sigma) ,$$

then letting $\sigma'=-\sigma$, multiplying by σ and summing over σ,

$$\sum_{\sigma} m_{x+1}(\sigma,-\sigma) W_{x+1}(-\sigma)^{-1} = \sum_{\sigma''} m_x(\sigma'',-\sigma'') W_x(-\sigma'')^{-1} .$$

If we define $s=\sinh(2J)$, $c=\cosh(2J)$, $V_x = W_x(-1)^2$, $a_x = cm_x - sm_{x+1}$, and $b_x = cm_x - sm_{x-1}$, after eliminating $m(-1,1)$ and $m(1,-1)$, we obtain the basic recursion relation for V,

$$\frac{2a_{x+1}V_{x+1}+b_{x+1}(1+V_{x+1}^2)}{V_{x+1}^2-1}=\frac{2b_xV_x+a_x(1+V_x^2)}{V_x^2-1}\ . \quad (4)$$

III. SOLUTION OF THE NONLINEAR DIFFERENCE EQUATION

Equation (4) is much easier to solve than its appearance suggests. We first note the following identity:

$$\left[\frac{2aV+b(1+V^2)}{V^2-1}\right]^2=\left[\frac{2bV+a(1+V^2)}{V^2-1}\right]^2+b^2-a^2\ .$$

Hence, defining

$$q_x=[2b_xV_x+a_x(1+V_x^2)](V_x^2-1)^{-1}\ ,$$

(4) can be written as $q_{x+1}^2-q_x^2=a_{x+1}^2-b_{x+1}^2$. Because $b_{x+1}^2-a_x^2=m_{x+1}^2-m_x^2$, the general solution to (4) takes on the form

$$q_{x+1}^2-a_{x+1}^2+m_{x+1}^2=q_x^2-a_x^2+m_x^2=C(\mathbf{m})\ , \quad (5)$$

where C is a symmetric, and hence almost certainly nonlocal function of all of the m_x's which cannot be determined from the difference equation because of the periodicity.

From the definitions of q and V, we conclude that the "profile equation" for our system can be written as

$$h_x=\tfrac{1}{2}\ln\frac{a_x+(a_x^2-m_x^2+C)^{1/2}}{-b_x+(b_x^2-m_x^2+C)^{1/2}}\ . \quad (6)$$

The signs in front of the square roots are determined by $h_x\to\pm\infty$ as $m_x\to\pm1$. The foregoing also points to the fact that the nonlocal profile (6) becomes local if the magnetization at any site is fixed, e.g., if $|h_1|=\infty$, so that $|m_1|=1$, then $b_1=(b_1^2-m_1^2+C)^{1/2}$ or $a_1=-(a_1^2-m_1^2+C)^{1/2}$ tells us that $C=1$, and the model reduces to the usual open boundary case. Equation (6) will also become local if the external field at any site is fixed.

IV. THE NATURE OF THE COLLECTIVE VARIABLE

There remains the problem of determining the precise form of the global, nonlocal, collective variable C. For this let us recall that if $\Omega=-\ln\Xi$ is the grand potential, then $m_x=-\partial\Omega/\partial h_x$. It follows that $\partial m_x/\partial h_y=\partial m_y/\partial h_x$ as well as $\partial h_x/\partial m_y=\partial h_y/\partial m_x$, the "integrability conditions." These guarantee the existence of an $\Omega(\mathbf{h})$ and $F^B(\mathbf{m})$, where $h_x=\partial F^B/\partial m_x$. Since the equation of state (6) would be local if we could extend the space to also include C, we examine the derivative

$$\frac{\partial h_x}{\partial m_y}=\left.\frac{\partial h_x}{\partial m_y}\right|_C+\left.\frac{\partial h_x}{\partial C}\right|_m\frac{\partial C}{\partial m_y}\ . \quad (7)$$

If $|x-y|>1$, the first term on the right is absent, so that

$$\frac{\partial C}{\partial m_x}\Big/\left.\frac{\partial h_x}{\partial C}\right|_m=\frac{\partial C}{\partial m_y}\Big/\left.\frac{\partial h_y}{\partial C}\right|_m\ .$$

But any site can be reached by jumps $\Delta x\geq2$, and so we conclude that for any x,

$$\frac{\partial C}{\partial m_x}=K\frac{\partial h_x}{\partial C} \quad (8)$$

for suitable index-independent K, a differential relation that C has to satisfy. Furthermore, since (8) implies that the second term on the right in (7) is symmetric, so must be the first term:

$$\left.\frac{\partial h_x}{\partial m_y}\right|_C=\left.\frac{\partial h_y}{\partial m_x}\right|_C$$

for any x and y. We conclude that indeed there exists a free energy F on the combined $\{\mathbf{m},C\}$ space such that

$$h_x=\frac{\partial F(\mathbf{m},C)}{\partial m_x}\ . \quad (9)$$

$F(\mathbf{m},C)$ is only unique up to a function of C; we can make it unique by introducing $w(C)$ such that

$$F(\mathbf{m},C(\mathbf{m}))-w(C(\mathbf{m}))=F^B(\mathbf{m})\ . \quad (10)$$

Hence defining

$$\bar{F}(\mathbf{m},C)=F(\mathbf{m},C)-w(C)\ , \quad (11)$$

we see that

$$h_x=\frac{\partial}{\partial m_x}\bar{F}(\mathbf{m},C)\ , \quad (12)$$

$$0=\frac{\partial}{\partial C}\bar{F}(\mathbf{m},C)\ , \quad (13)$$

and $\bar{F}(\mathbf{m},C(\mathbf{m}))=F^B(\mathbf{m})$.

V. THE RELATION BETWEEN C AND Ω

To further explore the relation of C to more familiar thermodynamic quantities, one may guess first, on physical grounds, that C should only relate to the two extreme states (i.e. $\{\sigma^+\,|\,\sigma_x=1,\ \forall x\}$ or $\{\sigma^-\,|\,\sigma_x=-1,\ \forall x\}$, since C reflects the cyclic symmetry of the periodic lattice, which has nothing to do with the inhomogeneity, and this is exactly characteristic of the extreme states. This means C ought to be a function of the two probabilities $P(\sigma^+)$ and $P(\sigma^-)$. On the other hand, we know from the limiting behavior, $C\to1$ when $|h_x|\to\infty$, that C must take the form $1+\Phi(P(\sigma^+),P(\sigma^-))$. Further more, the function Φ can only depend on the product of the two probabilities, because Φ has to be invariant under the change $\sigma^+\leftrightarrow\sigma^-$ and go to zero symmetrically with respect to either state [in particular, to the lowest order, $\Phi\propto P(\sigma^+)P(\sigma^-)\to0$, when $|h_x|\to\infty$ for any x]. This suggests that C is a function of the grand partition function $\Xi=[P(\sigma^+)P(\sigma^-)]^{1/2}$, and therefore of the grand potential Ω. In the appendix, we give a theorem which proves the assertion by showing the proportionality of the two partial derivatives $\partial\Omega/\partial m_x$ and $\partial C/\partial m_x$ (with an index-independent coefficient), hence the functional relation between Ω and C. Once this relation is recognized, the explicit form can be obtained exactly by studying the homogeneous model itself.

For the homogeneous Ising model, where $h_x = h$, $\forall x$, the eigenvalues of the transfer matrix are[5]

$$\lambda_{1,2} = e^J \cosh h \pm (e^{2J} \sinh^2 h + e^{-2J})^{1/2} , \tag{14}$$

From the definitions of q and a, we have

$$C = q^2 + m^2 - a^2 = m^2 \left[1 + \frac{e^{-4J}}{\sinh^2 h} \right] , \tag{15}$$

so that

$$C = 1 - 4\frac{(\lambda_1\lambda_2)^N}{(\lambda_1^N + \lambda_2^N)^2} = 1 - 4\frac{(e^{2J} - e^{-2J})^N}{\Xi^2} . \tag{16}$$

Therefore, $\Phi = -4(1 - e^{-4J})^N P(\sigma^+) P(\sigma^-)$. From (16), we can see explicitly how C is related to the grand partition function Ξ. It is equal to unity when the field at any site goes to infinity in magnitude or when the temperature goes to infinity, or when $N \to \infty$. It is always no less than one for ferromagnetic Ising coupling (i.e., $J > 0$), but it is less or greater than 1 for antiferromagnetic coupling (i.e., $J < 0$) according to whether the size of the lattice, N, is even or odd.

Furthermore, the Ω-C relation allows us to determine the function $w(C)$ in (10) and consequently $\bar{F}$ of (11) by studying the homogeneous case. To do this, we choose a linear path in $\mathbf{m}$ space: $m_x^\lambda = \lambda m_x$ as λ goes from 0 to 1, and integrate (9),

$$\begin{aligned} F(\mathbf{m}, C) &= \sum m_x \int_0^1 d\lambda\, h_x(\lambda \mathbf{m}, C) \\ &= \sum m_x h_x + \frac{\sqrt{C}}{2} \sum \left[\ln \left[\frac{m_x^2 - a_x^2}{m_x^2 - b_x^2} \right]^{1/2} \frac{(C + a_x^2 - m_x^2)^{1/2} + a_x}{(C + b_x^2 - m_x^2)^{1/2} - b_x} \right. \\ &\qquad \left. \times \frac{m_x\sqrt{C} + b_x^2 - m_x^2 - b_x(C + b_x^2 - m_x^2)^{1/2}}{m_x\sqrt{C} + a_x^2 - m_x^2 + a_x(C + a_x^2 - m_x^2)^{1/2}} - \ln \left[\frac{(m_x - a_x)(m_x - b_x)}{(m_x + a_x)(m_x + b_x)} \right]^{1/2} \right] . \end{aligned} \tag{17}$$

In particular, for the homogeneous system, where $a = e^{-2J} m$, $C = m^2(1 + e^{-4J}/\sinh^2 h)$,

$$F(m, C) = Nmh + \frac{\sqrt{C}}{2} \left[\ln \frac{1 - \sqrt{C}}{1 + \sqrt{C}} - \ln \tanh J \right] . \tag{18}$$

On the other hand, since for the homogeneous system

$$F^B(m) = Nmh + \Omega = Nmh + \tfrac{1}{2}\ln(1 - C) + \text{const} , \tag{19}$$

we conclude that

$$\begin{aligned} w(C) &= F(m, C) - F^B(m) \\ &= -\tfrac{1}{2}[(1 + \sqrt{C})\ln(1 + \sqrt{C}) \\ &\qquad + (1 - \sqrt{C})\ln(1 - \sqrt{C}) + \sqrt{C} \ln \tanh J] , \end{aligned} \tag{20}$$

which combines with $F(\mathbf{m}, C)$ to yield the free energy $\bar{F}$ in the expanded space.

VI. CONCLUSION

The one-dimensional periodically bounded Ising lattice is certainly one of the simplest systems to exhibit a nontrivial collective mode. A question which has received no satisfactory general answer is how an efficient equilibrium description such as the free-energy density functional incorporates such a mode into what would otherwise be a local structure. We have found that, at least in this special case, the simplest resolution of the question lies in expanding configuration space to include mode amplitude together with local coordinates. The corresponding "internal" Helmholtz free energy $\bar{F}$ which can be chosen as numerically equal to the true free energy F^B, serves as generating function for the local chemical potential which is conjugate to the local spin density, and specifies the amplitude of the collective mode by the condition that its conjugate vanishes. It is not hard to see how this conceptual structure may extend to more complex systems, as well as to dynamics. We intend to report on these issues in the near future.

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APPENDIX

Theorem. If $h_x = \partial F^B(\mathbf{m})/\partial m_x = \partial \bar{F}(\mathbf{m}, C)/\partial m_x |_C$, and C is a homogeneous function of m for fixed $\mathbf{h}$, then C is a function of Ω.

Proof. Supposing C is a homogeneous function of degree n for fixed $\mathbf{h}$, then

$$\left[\sum m_y \frac{\partial}{\partial m_y} \bigg|_C + nC \frac{\partial}{\partial C} \right] h_x = 0 ;$$

therefore,

$$\begin{aligned} -\frac{\partial \Omega}{\partial m_x} &= \sum m_y \frac{\partial h_y}{\partial m_x} \bigg|_C + \left[\sum m_y \frac{\partial h_y}{\partial C} \right] \frac{\partial C}{\partial m_x} \\ &= \sum m_y \frac{\partial h_x}{\partial m_y} \bigg|_C + \left[\sum m_y \frac{\partial h_y}{\partial C} \right] K \frac{\partial h_x}{\partial C} \\ &= \left[-nC + \sum m_y \frac{\partial C}{\partial m_y} \right] \frac{\partial h_x}{\partial C} \\ &= \frac{1}{K} \left[\left[-n + \sum m_y \frac{\partial}{\partial m_y} \right] C \right] \frac{\partial C}{\partial m_x} , \end{aligned}$$

where use has been made of (8) which is valid under the condition of the theorem. For the inhomogeneous 1D Ising model, $n = 2$, as may be seen from (6).

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