Recovering the equivalence of ensembles II: An Ising chain with competing short and long-range interactions

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Abstract
In a pioneer work, John Nagle has shown that an Ising chain with competing short and long-range interactions displays second and first-order phase transitions separated by a tricritical point. More recently, it has been claimed that Nagle’s model provides an example of the inequivalence between canonical and microcanonical calculations. We then revisit Nagle’s original solution, as well as the usual formulation of the problem in a canonical ensemble, which lead to the same results. Also, in contrast to recent claims, we show that an alternative formulation in the microcanonical ensemble, with the adequate choice of the fixed thermodynamic extensive variables, leads to equivalent thermodynamic results.

1 Introduction
In the beginning of the seventies, John Nagle [1][2] analyzed an Ising chain with antiferromagnetic interactions between nearest-neighbor sites, and the addition of equivalent-neighbor (mean-field) ferromagnetic interactions between all pairs of sites. Depending on the strength of the competition, this
system was shown to display second and first-order phase transitions separated by a “special critical point”, which was later named a tricritical point [3]. A few years ago, this problem has been revisited by some authors as one on the “paradigmatic examples” of the inequivalence of ensembles, in which the very localization of the tricritical point was supposed to depend on the ensemble (canonical or microcanonical) that was used to carry out the statistical calculations [4][5]. We have recently disproved similar claims of inequivalence of ensembles for a long-range version of a spin-1 Ising model [6]. In the present article we give arguments to show the equivalence of solutions in Nagle’s model.

The Hamiltonian of Nagle’s model in zero external field may be written as

\[ H = -J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - \frac{1}{2N} J_{LR} \left( \sum_{i=1}^{N} \sigma_i \right)^2, \]  

where \( \sigma_i = \pm 1 \) for \( i = 1, 2, ..., N \), the long-range interactions are ferromagnetic, \( J_{LR} > 0 \), and the presence of a tricritical point requires antiferromagnetic short-range interactions (\( J_{SR} < 0 \)). In his original work, Nagle obtained exact thermodynamic solutions by two elegant and complementary techniques, which already refer to different thermodynamic representations. Later, this model was solved by easier manipulations, in the usual canonical ensemble [7][8][9]. Due to its instructive features, and to a number of misconceptions in the literature, we begin by reviewing Nagle’s solution. We then resort to a Gaussian identity to establish the (same) solutions in the usual canonical ensemble. Finally, we use the corresponding Ising chain, with the exclusion of the long-range terms, to write an entropy function in the microcanonical ensemble. With the appropriate choice of the extensive variables, and properly accounting for the long-range interactions, we show that there are no discrepancies between canonical and microcanonical results.

2 Original solutions of Nagle

In the more detailed solution of the problem, Nagle considers the Hamiltonian of an Ising chain with the exclusion of the long-range interactions (\( J_{LR} = 0 \)) and in the presence of a field \( H \),

\[ H_I = -J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - H \sum_{i=1}^{N} \sigma_i. \]
Given the temperature \( k_B T = 1/\beta \) and the field \( H \), we write the usual form of the canonical partition function,

\[
Z_I = Z_I (T, H, N) = \sum_{\{\sigma_i\}} \exp \left[ \beta J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} + \beta H \sum_{i=1}^{N} \sigma_i \right],
\]

which can be analytically obtained by the transfer matrix technique. In the thermodynamic limit, the associated free energy per site, as a function of \( T \) and \( H \), is given by

\[
g_I = g_I (T, H) \sim -\frac{1}{\beta N} \ln Z_I,
\]

from which we obtain the magnetization per site,

\[
m = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sigma_i \right\rangle = -\left( \frac{\partial g_I}{\partial H} \right)_T.
\]

We then use a Legendre transformation to write another free energy, \( f_I = f_I (T, m) \), which is expressed as a function of temperature \( T \) and magnetization \( m \),

\[
f_I (T, m) = g_I (T, H) + mH.
\]

In this one dimensional system, there are no problems of convexity, and the field \( H \) can be eliminated by using equation (5).

Nagle then remarks that the energy per site of an additional term, of mean-field nature, may be written in terms of the magnetization, so that we have

\[
\frac{1}{N} \left\langle -\frac{1}{2N} J_{LR} \left( \sum_{i=1}^{N} \sigma_i \right)^2 \right\rangle = -\frac{1}{2} J_{LR} m^2.
\]

Taking into account that this term depends only on \( m \), the free energy \( f = f (T, m) \), associated with Nagle’s model, defined by the Hamiltonian of equation (1), is given by

\[
f = f (T, m) = f_I (T, m) - \frac{1}{2} J_{LR} m^2.
\]

This is the central equation of Nagle’s treatment. In analogy with a Landau expansion, the free energy \( f (T, m) \) may be written as a power series in terms of the magnetization,

\[
f (T, m) = a_0 (T) + a_2 (T) m^2 + a_4 (T) m^4 + a_6 (T) m^6 + \ldots,
\]
from which we obtain the critical line \( a_2 = 0; a_4 > 0 \) and the location of the tricritical point \( a_2 = a_4 = 0; a_6 > 0 \). It should be noted that this Landau expansion is written in terms of a density (the order parameter \( m \)) and that the coefficients of this expansion depend on the thermodynamic fields (in this case, the parameters \( \beta J_{SR} \) and \( \beta J_{LR} \)).

In the Appendix of his article, Nagle mentions an alternative calculation, in which the canonical partition function, in zero field, is written as

\[
Z(T, H = 0, N) = \sum_{M=-N}^{N} \exp \left[ \beta J_{LR} \frac{M^2}{2N} \right] \sum_{S=0}^{R} f_N(R, S) \exp \left[ -\beta J_{SR} (N - 4S) \right],
\]

where \( R = \min \{(N \pm M)/2\} \), \( S \) is the number of \((+, -)\) pairs, and

\[
f_N(R, S) = \frac{N}{S} \binom{R - 1}{S - 1} \binom{N - R - 1}{S - 1}.
\]

Although referring to a future publication, Nagle and Yeo never published the combinatorial derivation of \( f_N(R, S) \), which corresponds to the number of microstates of the system with fixed values of \( N, M \) and \( S \) (in other words, with fixed magnetization \( m \) and internal energy \( u \) associated with the short-range terms). This expression of \( f_N(R, S) \) is directly related to the entropy in the microcanonical ensemble in terms of the appropriate densities. In the thermodynamic limit, the partition function \( Z(T, H = 0, N) \) is given by the maximum term of the sum over \( M \) and \( S \). According to Nagle, all the results in zero field have been checked in this alternative formulation, in particular the location of the tricritical point.

The choice of independent variables and the alternative solutions of Nagle are already a firm indication of the equivalence of ensembles. The asymptotic form of the expression of \( f_N(R, S) \), which is directly related to the entropy in the microcanonical ensemble, has been independently written by several authors \[10\], even in recent work with claims of inequivalence of ensembles \[4\]. The most remarkable deduction has been published by Ernst Ising \[11\] in his famous article of 1925.
3 Solution in the canonical ensemble

The usual canonical partition function associated with Hamiltonian (1) is given by

\[ Z = Z(\beta J_{SR}, \beta J_{LR}) = \sum_{\{\sigma_i\}} \exp \left[ \beta J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} + \frac{\beta J_{LR}}{2N} \left( \sum_{i=1}^{N} \sigma_i \right)^2 \right]. \]  

(12)

Using the Gaussian identity

\[ \int_{-\infty}^{+\infty} dx \exp \left[ -x^2 + 2ax \right] = \sqrt{\pi} \exp (a^2), \]  

(13)

we have

\[ Z = \left( \frac{\beta J_{LR}N}{2\pi} \right)^{1/2} \int_{-\infty}^{+\infty} dy \exp [-\beta N f(y)], \]  

(14)

where

\[ f(y) = \frac{1}{2} J_{LR} y^2 - \frac{1}{\beta N} \ln Z_I, \]  

(15)

and \( Z_I \) is the canonical partition function of an Ising chain,

\[ Z_I = Z_I(\beta J_{SR}, \beta J_{LR}y) = \sum_{\{\sigma_i\}} \exp \left[ \beta J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} + \beta J_{LR}y \sum_{i=1}^{N} \sigma_i \right]. \]  

(16)

Also, we remark that these results can be obtained from an application of a well-known Bogoliubov identity [8].

In the thermodynamic limit we write

\[ f(y) \sim \frac{1}{2} J_{LR} y^2 - \frac{1}{\beta} \ln \lambda(y), \]  

(17)

where \( \lambda(y) \) is the largest eigenvalue of a transfer matrix,

\[ \lambda = \exp(\beta J_{SR}) \cosh(\beta J_{LR}y) + \left[ \exp(2\beta J_{SR}) \cosh^2(\beta J_{LR}y) - 2 \sinh(2\beta J_{SR}) \right]^{1/2}. \]  

(18)

We can analyze the critical behavior from an expansion of the asymptotic form of \( f(y) \) as a power series in \( y \),

\[ f(y) = A_0 + A_2 y^2 + A_4 y^4 + A_6 y^6 + ..., \]  

(19)
which is equivalent to Nagle’s expansion of the free energy $f(T,m)$, given by equation (9). The critical line comes from $A_2 = 0$, with $A_4 > 0$, and the tricritical point is located at $A_2 = A_4 = 0$, with $A_6 > 0$.

If we use Laplace’s method to calculate the asymptotic form of the integral (14), the saddle-point equation is given by

$$
\tilde{y} = \frac{\sinh (\beta J_{LR}\tilde{y}) \left[1 + D^{-1/2} \cosh (\beta J_{LR}\tilde{y})\right]}{\cosh (\beta J_{LR}\tilde{y}) + D^{1/2}},
$$

(20)

where

$$
D = \sinh^2 (\beta J_{LR}\tilde{y}) + \exp (-4\beta J_{SR}),
$$

(21)

so we have the corresponding free energy per spin,

$$
g = g(T) = -\frac{1}{2} J_{LR}\tilde{y}^2 - \frac{1}{\beta} \ln \lambda(\tilde{y}).
$$

(22)

In the next Section we derive again the equation of state (20) in the context of the microcanonical formulation. As in a typical mean-field calculation, there is always a paramagnetic solution, $\tilde{y} = 0$, but this solution becomes physically unacceptable in the ordered region of the phase diagram. If there are several solutions, we have to choose the absolute minima, which corresponds to using a Maxwell construction (and to recovering the convexity of the free energy).

From the equation of state (20), it is possible to check the location of the tricritical point, given by

$$
\beta J_{LR} = \exp (-2\beta J_{SR}),
$$

(23)

which corresponds to $A_2 = 0$, and

$$
\beta J_{LR} \left[\frac{1}{3} + \frac{4}{3} \exp (2\beta J_{SR}) - \exp (6\beta J_{SR})\right] = 1 + \exp (2\beta J_{SR}),
$$

(24)

which corresponds to $A_4 = 0$, in agreement with Nagle’s findings.

4 Solution in the microcanonical ensemble

According to the work of Nagle, it is convenient to begin by considering the Hamiltonian of an Ising chain, without the addition of mean-field terms and in the presence of an external field $H$, which can be written as

$$
\mathcal{H}_I = -J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - H \sum_{i=1}^{N} \sigma_i = U - HM,
$$

(25)
where the energy $U$ refers to the short-range interactions,

$$U = -J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1}; \quad M = \sum_{i=1}^{N} \sigma_i.$$  \hspace{1cm} (26)

Given $U$, $M$, and $N$, the number of microscopic states associated with this system may be formally written as a sum over spin configurations of a product of two delta functions,

$$\Omega_I = \Omega_I(U, M, N) = \sum_{\{\sigma_i\}} \delta \left( U + J_{SR} \sum_{i=1}^{N} \sigma_i \sigma_{i+1} \right) \delta \left( M - \sum_{i=1}^{N} \sigma_i \right). \hspace{1cm} (27)$$

We now introduce integral representations of these delta functions, and use the transfer matrix technique to carry out the sums. In the thermodynamic limit, it is straightforward to write

$$\Omega_I(U, M, N) \sim \int \int dk_1 dk_2 \exp \left[ N f(k_1, k_2) \right], \hspace{1cm} (28)$$

where

$$f(k_1, k_2) = k_1 u - k_2 m + \ln \lambda(k_1, k_2), \hspace{1cm} (29)$$

and

$$\lambda(k_1, k_2) = \exp (k_1 J_{SR}) \left\{ \cosh k_2 + \left[ \sinh^2 k_2 + \exp (-4k_1 J_{SR}) \right] \right\}, \hspace{1cm} (30)$$

with $u = U/N$ and $m = M/N$.

The entropy per particle as a function of $u$ and $m$ is given by

$$s_I = s_I(u, m) \sim \frac{k_B}{N} \ln \Omega_I \sim k_B f\left(\tilde{k}_1, \tilde{k}_2\right), \hspace{1cm} (31)$$

where $\tilde{k}_1$ and $\tilde{k}_2$ come from the saddle-point equations, $(\partial f/\partial k_1)_{k_2} = 0$ and $(\partial f/\partial k_2)_{k_1} = 0$,

$$u + J_{SR} = 2J_{SR} \frac{\exp (-4\tilde{k}_1) D^{-1/2}}{\cosh \tilde{k}_2 + D^{1/2}} \hspace{1cm} (32)$$

and

$$m = \frac{\sinh k_2 \left[ 1 + D^{-1/2} \cosh k_2 \right]}{\cosh k_2 + D^{1/2}}, \hspace{1cm} (33)$$
with
\[ D = \sinh^2 k_2 + \exp (-4k_1 J_{SR}) . \]  
(34)

In the entropy representation, we write the differential form
\[ ds_I = \frac{1}{T} du - \frac{H}{T} dm, \]  
(35)
from which we have the equations of state,
\[ \frac{1}{T} = \left( \frac{\partial s_I}{\partial u} \right)_m ; \quad -\frac{H}{T} = \left( \frac{\partial s_I}{\partial m} \right)_u . \]  
(36)

It is straightforward to use these equations, together with the saddle point equations (32) and (33), in order to show that
\[ \tilde{k}_2 = \beta H; \quad \tilde{k}_1 = \beta, \]  
(37)
which is an evidence of the equivalence of ensembles (in the absence of the mean-field interactions).

We now turn to Nagle’s model, with the addition of the long-range terms. In the presence of the equivalent-neighbor interactions, the internal energy is given by the sum of two terms,
\[ u = u_{SR} + u_{LR} = u_{SR} - \frac{1}{2} J_{LR} m^2 , \]  
(38)
so that both the energy associated with the short-range interactions, \( u_{SR} \), and the magnetization \( m \) should be fixed in the microcanonical formulation. Therefore, the entropy of Nagle’s model is still given by the expression \( s_I \), as in equation (31), but with the energy given by equation (38), which leads to a new differential form,
\[ ds = \frac{1}{T} du_{SR} - \frac{J_{LR} m^2}{T} dm - \frac{H}{T} dm . \]  
(39)

From this expression we have
\[ \frac{1}{T} = \left( \frac{\partial s}{\partial u_{SR}} \right)_m ; \quad -\frac{J_{LR} m^2}{T} = \left( \frac{\partial s}{\partial m} \right)_{u_{SR}} . \]  
(40)
where \( H_{ef} = H + J_{LR} m \) is an effective field, including the external field \( H \) and the effects of the long-range terms. Thus, in zero external field, we use
equations (37) to write $\tilde{k}_2 = \beta J_{LR} m$ and $\tilde{k}_1 = \beta$. Inserting these expressions into equations (33) and (34), we obtain

$$m = \frac{\sinh (\beta J_{LR} m) \left[ 1 + D^{-1/2} \cosh (\beta J_{LR} m) k_2 \right]}{\cosh (\beta J_{LR} m) + D^{1/2}},$$

(41)

where

$$D = \sinh^2 (\beta J_{LR} m) + \exp (-4 \beta J_{SR}),$$

(42)

which is identical to the equation of state (20) in the canonical ensemble, with the identification of $m$ with $\tilde{y}$ (and which already leads to the location of the tricritical point). In contrast to previous calculations, we do not find any disagreements in the thermodynamic behavior obtained from calculations in different ensembles.

5 Conclusions

We revisited the statistical analysis of a spin-1/2 Ising chain with antiferromagnetic interactions between nearest-neighbor sites, and the addition of equivalent-neighbor ferromagnetic interactions between all pairs of sites. This system, which is known to display second and first-order phase transitions separated by a tricritical point, has been used as one of the paradigmatic examples of inequivalence of canonical and microcanonical formulations. In contrast to these claims, we give arguments to show the equivalence of thermodynamic solutions in different ensembles.

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