Revista Brasileira de Flsica, Vol. 11, n.º 3, 1981

A Simple Derivation of the Thermodynamical Properties of the One-Dimensional Ising Model+

F. C. SÁ BARRETO

Departamento de Flsica, Universidade Federal de Mines Gerais and Departamento de Física, Universidade Federal de Pernambuco

and

I. P. FITIPALDI

Departamento de Física, Universidade Federal de Pernambuco

Recebido em 22 de Dezembro de 1980

The one-dimensional (or linear chain) Ising model is studied by means of a differential operator applied to an exact spin correlation function identity obtained by Callen. We derive the exact results for the zero-field magnetization, correlation function susceptibility, interna1 energy and specific heat. The general features and complexity of the present formalism For treating more realistic and complicated Ising problems are also briefly discussed. Owing to their simplicity, the method can easily be followed by first year graduate stuaents.

O modelo de Ising unidimensional (ou de cadeia linear) é estudado por meio de um operador diferencial aplicado a uma identidade exata para a função de correlação de spins obtida por Callen. Obtemos resultados exatos para a magnetização de campo zero, energia interna e calor especifico. Os traços gerais e a complexidade do presente formalismo para o tratamento de problemas de Ising mais realísticos e complicados são também discutidos brevemente. Devido à sua simplicidade, o método pode ser facilmente seguido por estudantes de primeiro ano de pós-graduação.

+ Work partially supported by CNPq and FINEP (Brazilian Agencies).

1. INTRODUCTION

The Ising model is certainly one of the most extensively studied many body systems[1]. The reason for this is due to the fact that it can describe fairly well numerous physical systems, as for example, magnetic spin system (ferro-and antiferromagnets), binary alloys (brass Zn-Cu), lattice gas, and so on.

The simplest form of the Ising model appears in one-dimension lattice (linear chain) for spin 1/2, with nearest-neighbor interactions and in the absence of an external field. It was in this form that W. Lenz[2] proposed it to his student Ising, in the early 1920, in order to study a magnetic phase transition[3]. Ising did not find a long-range order at any finite temperature. Indeed, one says that the Ising chain undergoes a "phase transition" at zero temperature..

However the two-dimensional (square lattice) Ising model in the absence of an external field does shows a phase transition at a finite temperature. It has been solved exactly by Onsager[4], in 1944, and it is now considered the turning point in the study of phase transition and critica1 phenomena. It is one of the few exactly solvable statistical mechanical models that exhibits a second order phase transition.

In this paper we present a simple derivation of the thermodynamical properties of the Ising linear chain, based on a method that can easily be followed by first year post graduate students. The method is achieved by introducing a differential operator into an exact spin correlation function equation obtained by Callen[5] in 1963 (here called by Callen's identity) as recently suggested by Kaneyoshi and co-workers[6,10]. Very recently severa1 useful theoretical technoques to deal with two- and three-dimensional Ising problems (not yet solved exactly) have been proposed based on these rigorous spin correlation relations[11,18].

The main purpose of this didactical work is, in çpite of its simplicity, to present an application of the differential operator technique to a solvable model in order to clarify the mathematical structure of the novel method. The ability of the formalism to deal with more realistic and complicated problems will be briefly discussed later on.

In section 2 we introduce the model and derive Callen's identity for the site magnetization. In section 3 the exponential differential operator, the basis of the present method, is introduced. In the following sections we study the magnetization (section 4), the correlation function and the susceptibility (section 5) and the internal energy and the specific neat (section 6). The last section is devoted to analyíis and comments on the extension and application of the present fornialism for higher dimensional lattices (square lattice) and for higher spin systems.

2. THE HAMILTONIAN MODEL AND CALLEN'S IDENTITY

The Hamiltonian for the Ising model in one dimension, in an external field h, is given by

$$H = -\frac{J}{2} \sum_{i,\delta} \sigma_i \sigma_{i+} - h \sum_i \sigma_i \,, \tag{1}$$

where the sum on i runs from 1 to N, with $\sigma_i = a_{i+N}$, and $\delta = \pm 1$. σ_i is the dynamical variable which can take two values, ± 1, and J in the coupling constant between neighboring sites.

If we interpret this hamiltonian as describing a rnagnetic system, then σ_i is the z-component of a spin operator ($\vec{S} = \frac{1}{2}\vec{\sigma}$) associated with the ion localized at site i which can have spin up ($\sigma_i = +1$) or down ($a_i = -1$) and J is the exchange interaction. The spin system is ordered when all spins are up (or down). The magnetic field is added in order to break the symmetry and to favour the ordered phase to be up or down. The parameter that measures the ordering of the system (called the long-range order parameter) is given by $m = \langle \sigma_i \rangle$. In the ordered phase $m \neq 0$, while in the disordered phase $m = 0$.

The expectation (average) value of the spin variable at the lattice site i is given by

$$\langle \sigma_i \rangle = \frac{\mathrm{Tr}\, \sigma_i e^{-\beta H}}{Z} \,, \tag{2}$$

where $Z = \mathrm{Tr}\, e^{-\beta H}$ and Tr(=trace) means the sum over all alowed states of the system. Here $\beta = 1/k_B T$, where k_B is the Boltzmann constant, and T is the absolute temperature.

Now, our objective is to obtain from (2) an identity which is more suitable foi calculation. This relation is known as Callen's identity[5] and it is valid for any dimensionality of the lattice with spin one-half although in this paper it will be only applied for the one-dimensional lattice.

Let us separate the hamiltonian (1) into two parts: one (denoted by H_i) which includes all contributions associated with the lattice site i, and the other (denoted by H') which does not depend on the site i. Then one has

$$H = H_i + H' , \tag{3}$$

where

$$H_i = -J\sigma_i \sum_{\delta} \sigma_{i+\delta} - h\sigma_i = -\sigma_i E_i , \tag{4}$$

and $E_i = J \sum_{\delta} \sigma_{i+\delta} + h$ is the local field on site i. (Note that E_i is a function of the spin variables of the neighbors of a_i, and therefore it does not depend on the site i).

We know that for every lattice site i and j the spin variables commute, i.e., $[\sigma_i, \sigma_j] = 0$, and therefore

$$[H_i, H'] = [H_i, H - H_i] = [H_i, H] = 0 . \tag{5}$$

This corninutativity, as a result of the algebra of the operators, plays a fundamental role ir! the derivation of Callen's identity. We will comment in section 6 about the sitcation when H_i and H' do not commute.

Let us write the trace in the following form,

$$\mathrm{Tr} = \prod_{k=1}^{N} \mathrm{tr}_{(k)} = \Big(\prod_{k \neq i = 1}^{N} \mathrm{tr}_{(k)} \Big) \mathrm{tr}_{(i)} = \mathrm{Tr}' \mathrm{tr}_{(i)} . \tag{6}$$

Here $\mathrm{tr}_{(k)} = \sum_{\sigma_k=-1}^{+1}$ stands for the trace associated with the variable at site k, and $\mathrm{Tr}' = \left(\prod_{k\neq i=1}^{N} \mathrm{tr}_{(k)} \right)$.

We can write expression (2) using (3), (5) and (6) as

$$\langle \sigma_i \rangle = \frac{1}{Z} \{ \mathrm{Tr}' \mathrm{tr}_{(i)} \sigma_i \; e^{-\beta (H_i + H')} \} = \frac{1}{Z} \{ \mathrm{Tr}' \; e^{-\beta H'} (\mathrm{tr}_{(i)} \sigma_i \; e^{-\beta H_i}) \} .$$

Inserting in the bracket $(\mathrm{tr}_{(i)} \; e^{-\beta H_i}) / (\mathrm{tr}_{(i)} \; e^{-\beta H_i}) = 1$, we get

$$\langle \sigma_i \rangle = \frac{1}{Z} \left\{ \mathrm{Tr}' \; e^{-\beta H'} \; \mathrm{tr}_{(i)} \; e^{-\beta H_i} \left(\frac{\mathrm{tr}_{(i)} \sigma_i e^{-\beta H_i}}{\mathrm{tr}_{(i)} e^{-\beta H_i}} \right) \right\}$$

$$- \frac{1}{Z} \left\{ \mathrm{Tr}' \mathrm{tr}_{(i)} e^{-\beta (H_i + H')} \left(\frac{\mathrm{tr}_{(i)} \sigma_i e^{-\beta H_i}}{\mathrm{tr}_{(i)} e^{-\beta H_i}} \right) \right\} ,$$

or,

$$\langle \sigma_i \rangle = \frac{1}{Z} \left\{ \mathrm{Tr} \; e^{-\beta H} \left(\frac{\mathrm{tr}_i \; \sigma_i \; e^{-\beta H_i}}{\mathrm{tr}_{(i)} e^{-\beta H_i}} \right) \right\} . \qquad (7)$$

Now, using equation (4) we can calculate explicitly the expression in the parentheses

$$\mathrm{tr}_{(i)} \; e^{-\beta H_i} = \mathrm{tr}_{(i)} \; e^{\beta \sigma_i E_i} = e^{\beta E_i} + e^{-\beta E_i}$$

$$\mathrm{tr}_{(i)} \sigma_i e^{-\beta H_i} = \mathrm{tr}_{(i)} \sigma_i \; e^{\beta \sigma_i E_i} = e^{\beta E_i} - e^{-\beta E_i} .$$

Substituting these results in (7) we ohtain

$$\langle \sigma_i \rangle = \frac{\mathrm{Tr} (e^{-\beta H} \tanh \beta E_i)}{Z} ,$$

or,

$$\langle \sigma_i \rangle = \langle \tanh \beta E_i \rangle \quad , \tag{8}$$

which is the single-site Callen's identity.

3. EXPONENTIAL DIFFERENTIAL OPERATOR

Let D be a differential operator $\frac{\partial}{\partial x}$ and let $e^{\alpha D}$ be an operator defined as (a is a parameter),

$$e^{\alpha D} = 1 + \alpha D + \frac{\alpha^2}{2!} D^2 + \frac{\alpha^3}{3!} D^3 + \ldots$$

Applying $e^{\alpha D}$ to a arbitrary function $f(x)$ it is easy to see that

$$e^{\alpha D} f(x) = f(x + \alpha) \quad . \tag{9}$$

Let us apply relation (9) into equation (8)

$$\langle \sigma_i \rangle = e^{(\beta E_i) D} \tanh x \Big|_{x=0} > = \langle e^{(\beta E_i) D} \rangle \tanh x \Big|_{x=0} \tag{10}$$

We take tanh x out of the average because it is a number, i.e., it does not contain any spin operator (the value of X should be taken equal to zero after all the operations have been perforrned).

Using the expression for the local field E_i [see eq. (4)], we get.

$$\langle \sigma_i \rangle = \langle e^{(\beta J \sum_{0} \sigma_{i+\delta} + \beta h) D} > \tanh x \Big|_{x=0}$$

$$= \langle e^{\beta J D \sum_{\delta} \sigma_{i+\delta}} e^{\beta h D} > \tanh x \Big|_{x=0}$$

$$= \langle e^{\beta J D \sum_{\delta} a_{i+\delta}} \rangle \tanh(x + \beta h) \Big|_{x=0}$$

In the last step we have applied the property (9) to the field dependent part. Now we can rewrite the above equation as

$$\langle \sigma_i \rangle = \langle \prod_{\delta} e^{(\beta J \sigma_{i+\delta}) D} \rangle \tanh(x+\beta h) \Big|_{x=0} , \qquad (11)$$

If we note that the spin operators σ_i have the property: $\sigma_i^2 = \sigma_i^4 = \ldots = 1$ and $\sigma_i = \sigma_i^3 = \sigma_i^5 = \ldots$ we can write, for any A,

$$e^{\lambda \sigma_i} = 1 + \lambda \sigma_i + \frac{\lambda^2}{2!} \sigma_i^2 + \frac{\lambda^3}{3!} \sigma_i^3 + \frac{\lambda^4}{4!} \sigma_i^4 + \ldots$$

$$= (1 + \frac{\lambda^2}{2!} + \frac{\lambda^4}{4!} + \ldots) + \sigma_i (\lambda + \frac{\lambda^3}{3!} + \frac{\lambda^5}{5!} + \ldots) .$$

Or,

$$e^{\lambda \sigma_i} = \cosh A + \sigma_i \sinh A . \qquad (12)$$

Using this result in (11), we obtain

$$\langle \sigma_i \rangle = \langle \prod_{\delta} [\cosh(\beta J D) + \sigma_{i+\delta} \sinh(\beta J D)] \rangle \tanh(x + \beta h) \Big|_{x=0} \qquad (13)$$

This result is exact and is valid for any lattice structure of a spin one-half Ising model with nearest-neighbor interactions. We will now use equation (13) to derive the thermodynamical properties of the Ising linear chain.

4. MAGNETIZATION

For the linear chain, δ can have only two values, ± 1. Therefore equation (13) yields

$$\langle\sigma_i\rangle = \langle\left[\cosh(\beta JD) + \sigma_{i+1}\sinh(\beta JD)\right]\left[\cosh(\beta JD) + \right.$$

$$\left. + \sigma_{i-1}\sinh(\beta JD)\right]\rangle \tanh(x + \beta h)\Big|_{x=0}$$

$$= \langle\left[\cosh^2(\beta JD) + (\sigma_{i+1}\sigma_{i-1})\cosh(\beta JD)\sinh(\beta JD) + \right.$$

$$\left. + \sigma_{i+1}\sigma_{i-1}\sinh^2(\beta JD)\right]\rangle \tanh(x + \beta h)\Big|_{x=0} \tag{14}$$

Using the definitions of $\cosh(\beta JD)$ and $\sinh(\beta JD)$ we get

$$\cosh^2(\beta JD) = \frac{1}{4}\left[e^{2\beta JD} + e^{-2\beta JD} + 2\right]$$

$$\sinh^2(\beta JD) = \frac{1}{4}\left[e^{2\beta JD} + e^{-2\beta JD} - 2\right]$$

$$\sinh(\beta JD)\cosh(\beta JD) = \frac{1}{4}\left[e^{2\beta JD} - e^{-2\beta JD}\right] . \tag{15}$$

Substituting these results in (14) and applying the exponential operator expression (9) in the function $\tanh(x+\beta h)$ and at the end taking $x=0$, we obtain after a simple algebra

$$\langle\sigma_i\rangle = a + b(\langle\sigma_{i+1}\rangle + \langle\sigma_{i-1}\rangle) + c\langle\sigma_{i+1}\sigma_{i-1}\rangle , \tag{16}$$

where

$$a = \frac{1}{2\left[1 - f^2(2\beta J)f^2(\beta h)\right]}\left\{2f(\beta h) - f^2(2\beta J)f(\beta h)\left(1 + f^2(\beta h)\right)\right\}$$

$$b = \frac{1}{2\left[1-f^2(2\beta J)f^2(\beta h)\right]}\left\{f(2\beta J)(1-f^2(\beta h))\right\} \qquad (17)$$

$$c = \frac{1}{2\left[1-f^2(2\beta J)f^2(\beta h)\right]}\left\{f^2(2\beta J)f(\beta h)(f^2(\beta h)-2)\right\} .$$

Here the function $f(y)$ is defined as $f(y) = \tanh y$.

The zero-field inagnetization can he easily ohtained' from (16), putting h=O into equation (16) to give $a = c = 0$ and $b = \frac{1}{2} f(2\beta J)$. Calling $m(T,h=0) = \langle\sigma_i\rangle$, which due to translational invariance is site independent, we get

$$m(T,h=0) = m(T,h=0)\tanh(2\beta J) . \qquad (18)$$

This shows that the zero-field magnetizãtion (order parameter) can be different from zero only when $\tanh(2\beta J)=1$, which occurs as $\beta \to \infty$. In other words, an ordered phase can only be attained at $T = 0$ [19].

5. CORRELATION FUMCTION AND SUSCEPTIBILITY AT ZERO FIELD

In order to obtain the magnetization in the presence of the field and the zero-field susceptibility, which is defined by

$$\chi_T(T,h=0) = \frac{\partial m(T,h)}{\partial h}\bigg|_{h=0} , \qquad (19)$$

we have to calculate the spin correlation function $\langle\sigma_{i+1}a_{i-1}\rangle$ which appears in (16).

One can prove, following the same procedure used to deduce the first Callen's identity [given by rnpression (8)], the two-site Callen's identity given by

$$\langle\sigma_k\sigma_i\rangle = \langle\sigma_k \tanh(\beta E_i)\rangle , \quad k \neq i . \qquad (20)$$

Again, going through the same steps from (10) to (16) we get,

$$\langle\sigma_k\sigma_i\rangle = a\langle\sigma_k\rangle + b(\langle\sigma_k\sigma_{i+1}\rangle + \langle\sigma_k\sigma_{i-1}\rangle) + c\langle\sigma_k\sigma_{i+1}\sigma_{i-1}\rangle \qquad (21)$$

with a, b and c given by (17).

Therefore, at zero field, we obtain from (21)

$$\langle\sigma_k\sigma_i\rangle = (\langle\sigma_k\sigma_{i+1}\rangle + \langle\sigma_k\sigma_{i-1}\rangle)\ \frac{1}{2}\ \tanh(2\beta J)\ .$$

Due to translational invariance, the correlation function depends only upon the distance between i and &, i.e.;

$$\langle\sigma_k\sigma_i\rangle \equiv \langle\sigma_0\sigma_{i-k}\rangle = \langle\sigma_0\sigma_r\rangle \equiv g(r)\ ,$$

where $r = i-k$ is a measure of the distance between spins, in units of a lattice constant. Therefore,

$$g(r) = [g(r+1) + g(r-1)]\ \frac{1}{2}\ \tanh(2\beta J)\ .$$

This equation can be rewritten as follows

$$2\ \mathrm{cotgh}(2\beta J) = \left[\frac{g(r+1)}{g(r)}\right] + \left[\frac{g(r)}{g(r-1)}\right]^{-1}\ ,$$

which implies that the right-hand site must be independent of r. Hence we can assume $g(r+1)/g(r) = \gamma$ and as a consequence (doing $r \to r-1$) we obtain $g(r)/g(r-1) = \gamma$ which implies the recursion relation $g(r+n) = \gamma^n g(r)$. Note that this only occurs because both ratios involve functions separated by one unit of distance sites. Thus, we get

$$2\ \mathrm{cotgh}(2\beta J) = \gamma + \gamma^{-1}\ ,$$

or

$$1 = (\gamma + \frac{1}{\gamma})\ \frac{1}{2}\ \tanh(2\beta J).$$

Solving this quadratic equation for γ, we obtain two solutions: $\gamma_1 = \tanh(\beta J)$ and $\gamma_2 = [\tanh(\beta J)]^{-1}$. In the high ternperature limit $(\beta = 0)$ we should expect that no correlation exist between the sites, as a consequence of the highly thermal disorder. Therefore, the only physically

acceptable solution is $\gamma = \tanh(\beta J)$. It is also a physical imposition that the correlation function should get smaller with increasing distances. In particular, for the Ising chain we shall take $g(r) = \gamma^r$. Note that this behaviour is also predicted by the recursion relation $g(r' + r) = \gamma^r \; g(r')$ when we assume an origen $r'=0$, with $g(0) = 1$. Therefore

$$g(r) = g_{i-k} = \left[\tanh(\beta J)\right]^r \quad . \tag{22}$$

In Fig.1 we show a plot of $g(r)$ as a function of r.

We can now calculate the zero-field susceptibility, starting from the equation (16) for the magnetization, rewritten as[21],

$$m(T,h) = \frac{\left[1-f^2(2\beta J)\,(1+2\langle\sigma_{i+1}\sigma_{i-1}\rangle\right] f(\beta h) \; - \; \frac{1}{2}\left[f^2(2\beta J)\,(1-2\langle\sigma_{i+1}\sigma_{i-1}\rangle)\right]}{\left[\,1 \; - \; f(2\beta J) \; + \; f(2\beta J)\,(1 \; - \; f(2\beta J))\,f^2(\beta h)\right]} \; f^3(\beta h), \tag{23}$$

where $\langle\sigma_{i+1}\sigma_{i-1}\rangle$ is given by (22), for $r=2$, when h is taken equal to zero.

After a simple algebra we obtain for $\chi_T(T,h=0) = \left.\frac{\partial m(T\,h)}{\partial h}\right|_{h=0}$, the exact result

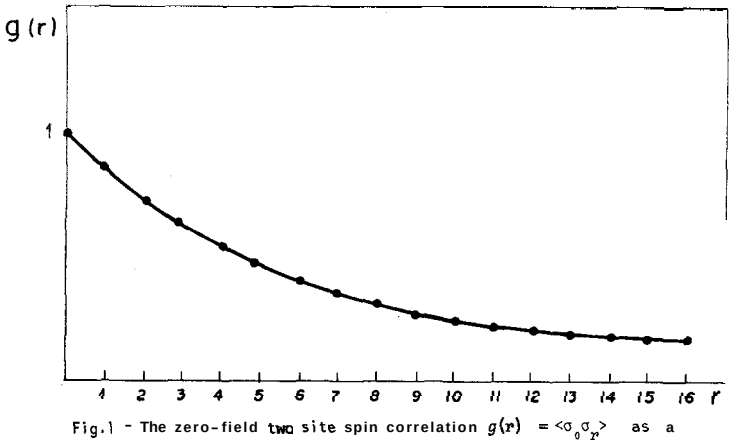

Fig.1 - The zero-field two site spin correlation $g(r) = \langle\sigma_0\sigma_r\rangle$ as a function of site separation r (in units of a lattice constant).

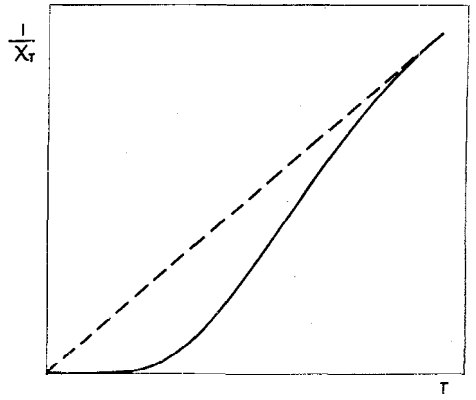

Fig.2 - The inverse zero-field susceptibiliry as a function of the temperature. Note that $\chi_T(T,h=0)$ diverges a $T=0$. The non-iriteracting limit case (dashed-line) is also plotted for the sake of comparison.

$$\chi_T(T,h=0) = \frac{1}{k_B T} e^{2J/k_B T} \quad , \tag{24}$$

which is shown as a function of temperature in Fig.2. As we see, inthe neighborhood of the critica1 temperature $T_c=0$ the zero-field susceptibility has an essential singularity, i.e. $\chi_T \sim \exp(1/T)$ as $T\to 0$. Notice also that the particular case of a non-interacting (perfect paramagnet) !inear chain Ising model is easily obtained from (24) allowing the exchange paraaeter J to approach zero.

6. INTERNAL ENERGY AND SPECIFIC HEAT

The internal energy of the system is given by

$$U = -J \sum_{i,\delta} \langle \sigma_i \sigma_{i+\delta} \rangle \quad , \tag{25}$$

which can be directly obtained using the spin correlation function, given by expression (22). So,

$$U = -J \sum_i \{\langle \sigma_i \sigma_{i+1} \rangle + \langle \sigma_i \sigma_{i-1} \rangle\} = -2JN \tanh(\beta J). \tag{26}$$

We will now present another way to calculate the internal

energy, which is useful when one deals with two- or three- dimensional lattices. In those situations the two spin correlation function is not known exactly (except for the square lattice[4]), and approximatiuns have to be made. We will comment about these approximations later in the paper.

Using relation (20), we can rewrite (25) as

$$U = - \sum_{\vec{i},\delta} J\langle\sigma_{i+\delta} \tanh(\beta E_i)\rangle = - \sum_{i} \langle E_i \tanh(\beta E_i)\rangle \ , \quad (27)$$

where $E_i = \sum_{\delta} J\sigma_{i+\delta}$. Introducing thedifferential operator $D=\partial/\partial x$, we have

$$U = - \sum_{i} \langle E_i \, e^{\beta E_i D} \rangle \tanh x \Big|_{x=0} \ . \quad (28)$$

Let us now define a new function $G_i(y,D)$ as

$$G_i(y,D) = \langle e^{\beta E_i D y} \rangle \ , \quad (29)$$

whose derivative with respect to the parameter y is

$$\frac{\partial}{\partial y} G_i(y,D) = \langle \beta E_i D \ e^{\beta E_i D y} \rangle \quad (30)$$

By comparing equations (28) and (30), we can immediatly see that

$$U = - \sum_{i} \left[\left\{ \frac{\partial}{\partial y} G_i(y,D) \ \frac{1}{D\beta} \right] \tanh x \right|_{x=0, \ y=1} \ , \quad (31)$$

which is completely general, with no approximation made.

For the Ising linear chain we obtain for $G_i(y,D)$ defined in equation (29), the result

$$G_i(y,D) = \langle [\cosh^2(\beta JDy) + (\sigma_{i+1} + \sigma_{i-1}) \sinh(\beta JDy) \cosh(\beta JDy) +$$

$$+ (\sigma_{i+1} \ \sigma_{i-1}) \sinh^2(\beta JDy)] \rangle \ , \quad (32)$$

and for its derivative we get

$$\frac{\partial G_i(y,D)}{\partial y} = \langle [(\beta JD)2\cosh(\beta JDy)\ \sinh(\beta JDy) +$$

$$+ (\beta JD)(\sigma_{i+1} + \sigma_{i-1})(\cosh^2(\beta JDy) + \sinh^2(\beta JDy))$$

$$+ (\beta JD)(\sigma_{i+1} - \sigma_{i-1})2\cosh(\beta JDy)\sinh(\beta JDy)] \rangle \quad . \tag{33}$$

Substituting this result in (31) and using relations (15) we obtain,

$$U = -\sum_i [Jf(2\beta J) + \langle \sigma_{i+1}\sigma_{i-1} \rangle Jf(2\beta J)] = -JNf(2\beta J)\ 1+f^2(\beta J) \quad , \tag{34}$$

which can be rewritten as

$$U = -2JN \quad \tanh(\beta J) \tag{35}$$

which is the same result obtained before as given by equation (26).

Now the zero-field specific heat, defined as $C_T(T,\ h=0) = \frac{dU}{dT}$, may be easily evaluated using equation (35)

$$C_T(T,h=0) = \frac{2J^2N}{k_B T^2}\ \mathrm{sech}^2\ (\frac{J}{k_B T}) \quad , \tag{36}$$

which goes to zero at $T=0$, in agreement with the rhird'law of thermodynamics. In Fig.3 we show $C(T,h=0)$ as a function of the temperature.

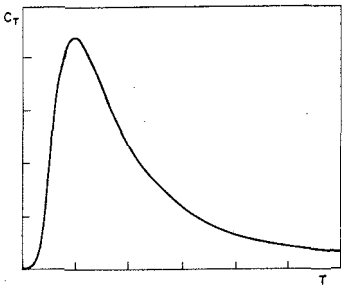

Fig.3 - The zero-field specific heat as a function of the temperature. Note that in agreement with the third law of thermodynamics $C_T(T,h=0)$ goes to zero at $T=0$.

7. CONCLUSION AND COMMENTS

In this paper we have presented a simple derivation of some thermodynamical properties of the spin 1/2 Ising linear chain by means of a novel differential operator scheme. The results obtained are all exact.

This was possible because we started from exact relations [see equations (8) and (20)] and for the linear chain two spin correlation functions do not enter in the calculation of the zero field magnetization [see equations (16-18)] and three spin correlations do not enter in the calculation of $g(r)$ [see equations (21-22)] and of $\chi_T(T,h=0)$ [see equations (23-24)].

For Ising systems Callen's identities are exact because H_i and H' commute [see equation (5)]. However for other models, as for example the transverse Ising model, the X-Y model and the Heisenberg model, H_i and H' do not commute. For those models it is not possible to obtain a simple exact relation. This impossibility resides in fact that

$$e^{-\beta(H_i+H')} \neq e^{-\beta H_i}\, e^{-\beta H'}\, e^{\frac{1}{2}[H_i,H']}, \qquad (37)$$

because the commutator $[H_i,H']$ is not a c-number, i.e., it does not commutes with both H_i and H'. However, it is possible to obtain a general relation for those models which can be used as a starting point for some approximation[22].

Even if we treated Ising models, for which the starting relations are exact, certain approximations have to be done if we deal with higher dimensional lattices[6-10] (where the number of neighbors is $z>2$).

One can easily check that for a square lattice the equation for the zero-field lattice rnagnetization obtained from equation (13), is given by

$$m(T,h=0) = 4a'm(T,h=0) + b'[\langle\sigma_1\sigma_2\sigma_3\rangle+\langle\sigma_1\sigma_2\sigma_4\rangle+\langle\sigma_2\sigma_3\sigma_4\rangle+\langle\sigma_1\sigma_3\sigma_4\rangle], \qquad (38)$$

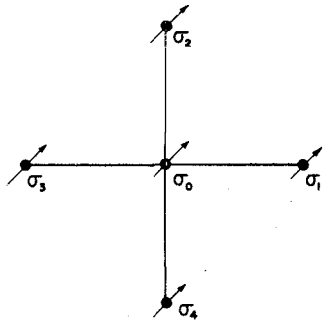

Fig.4 - The site notation for a square lattice.

where $m(T,h=0) = \langle\sigma_0\rangle$ [see Fig.4 for site lattice notation]. Here a' and b' are some functions of temperature.

Thus, we see from the above equation that in order to calculate $m(T,h=0)$ we must know the three spin correlation functions. If we generate the equations for these three spin correlation functions we will find its dependence on higher order functions, and a complicated set of coupled equations is obtained.

However we can approximate (13) neglecting the correlation between sites, as follows[6-10]

$$\langle\sigma_i\rangle \simeq \{\prod_{\delta} [\cosh(\beta JD) + \langle\sigma_{i+\delta}\rangle \sinh(\beta JD)]\} \tanh x\Big|_{x=0} \qquad (39)$$

Considering z neighbors (δ runs from 1 to z) and the translation invariance of the lattice, we have

$$m(T,h=0) = [\cosh(\beta JD) + m(T,h=0)\sinh(\beta JD)]^z \tanh x\Big|_{x=0} . \qquad (40)$$

This approximation is the simplest one that can be done and provides results that are better than the traditional mean field approximation[6-10].

As a final remark we must point out that the procedure presented in this paper has been applied by T.Kaneyoshi and collaborators to study a number of problems of interest. Other problems under study by the authors and colla'borators are: Susceptibility of planar lattice;

Thermodynamics of a pure and diluted transverse Ising model; Ising models with competing interactions; Dynamics of the Ising model near the critical point; Thermodynamical properties of a binary Ising alloy $A_p B_{1-p}$; Thermodynamical properties of a layered Ising ferromagnet. The extension and application of the present formaiism for higher spins systems has been already successfully achieved in order to study several problems of interest, such as [note that now the identity (12) is not valid any more]: Statistical mechanics of an one-dimensional Ising ferromagnet with single-site anisotropy; Phase transition of the Blume-Capel model; Effect of crystal-field anisotropy on magnetically ordered Ising systems; Dipolar and quadrupolar ordering in s = 3/2 Ising systems; Thermodynamical properties of the generalized Ising model.

Finally, several attempts to extend the present method in order to inçlude correlation effects are now under investigation and all these problems will be reported in near future.

The authors are indebted to Professors Mauricio D. Coutinho Filho, J.R.L. de Almeida and Silvio R. Salinas for the many enlightening and useful discussions which stimulated this publication. We are also, indebted to Professor T. Kaneyoshi for numerous valuable discussions associated with the differential operator method.

REFERENCES AND NOTES

1. For further discussion about the Ising model, the interested reader is referred to the following text books: H.E.Stanley, "Introduction to Phase Transition and Critical Fhenomena", Oxford University Press (1971); K.Huang, "Statistical Mechanics", Wiley, New York (1963), G.H. Wannier, "Statistical Physics", Wiley, New York (1966); McCoy and Wu, "The Two-Dimensional Ising Model", Harvard University Press, Cambridge (1973).
2. S.G.Brush, Rev.Mod.Phys. 39, 883 (1967).
3. E.Ising, Z.Phys. 31, 253 (1925).

4. L.Onsager, Phys.Rev. 65, 117 (1944); see also B.Kaufmann, Phys.Rev. 76, i232 (1949).

5. H.B.Callen, Phys. Lett. 4, 161 (1963) [see also, M.Suzuki, Phys. Lett. 19, 267 (1965)].

6. R.Honmura and T.Kaneyoshi, J.Phys. C 12, 3979 (1979); *11*, L973 (1978); Prog. Theor. Phys. 60, 635 (1978).

7. T.Kaneyoshi, I.P.Fittipaldi and H.Beyer, Phys. Stat. Sol. (b) *101*, (1980) (in press).

8. T.Kaneyoshi, I.P.Fittipaldi and H.Beyer (to be published).

9. T.Kaneyoshi and H.Beyer, J.Phys. Soc. of Japan, 49, 1306 (1980).

10. T.Kaneyoshi, J.Mag.Mag.Mat., *15/18*, 119 (1980); Phys. Lett. 76, 67 (1980).

11. F.B.Anderson, Phys. Rev. B*3*, 3950 (1971).

12. N.Matsudaira, J.Phys.Soc. of Japan, *35*, 1593 (1973).

13. B.Frank and O.Mitran, J.Phys. C 10, 2641 (1977); Solid St. Commun. 24, 343 (1977); J.Phy. C 11, 2087 (1978).

14. S.M.Girvin, J.Phys. C *11*, L427 (1978).

15. O.Mitran, J.Phys. C 12, 4871 (1979).

16. D.C.Mattis, Phys. Rev. B 19, 4937 (1979).

17. H.I.Zhang and D.Kim, Phys. Rev. B 21, 4173 (1980).

18. Y.Tanaka and N. Uryû, Phys.Rev. B 21, 1994 (1980).

19. For a discussion on the absence of long range order in a linear Ising chain for $T \neq 0$, see Wannier (Ref.1).

20. It is worth mentioning that a generalized Callen's identity can also be obtained by the same procedure described in the text, which reads.

$$\langle \{f\}\sigma_i \rangle = \langle \{f\} \tanh(\beta E_i) \rangle ,$$

where $\{f\}$ denotes an arbitrary spin function not including the i-th spin. We refer to Ref.5 for a better understanding of this point and to more explicit calculation.

21. An instructive check on the result (23) is to permit the field h to approach zero to get $m(T,h=0) = 0$. On the other hand, to reproduce the result (17) from equation (23) we should first multiply both sides by the denominator and only after performed the operations the value of h should be taken equal to zero.

22. This will be the aim of a future publication on thetransverse Ising model, by the authors and B.Žekš.