NOTE ON THE DIFFERENCE BETWEEN THE $a$-CYCLIC AND $c$-CYCLIC VERSION OF THE $XY$ MODEL

H.W. CAPEL
Instituut-Lorentz, Rijksuniversiteit te Leiden,
Leiden, The Netherlands

and

TH. J. SISKENS*
Department of Physics, Technological University of Twente,
Enschede, The Netherlands

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The transverse susceptibility of the c-cyclic version of the one-dimensional $XY$ model with respect to an infinitesimal magnetic field in the $x$-direction is investigated in more detail. Special attention is paid to the c-cyclic version of the one-dimensional Ising model. The c-cyclic susceptibility $\chi_{xx}$ is evaluated explicitly. The autocorrelation function of the magnetization $M_x$ turns out to be time dependent in the c-cyclic Ising model.

1. Introduction

The one-dimensional $XY$ model has been introduced by Lieb, Schultz and Mattis). Katsura$^2$) evaluated the free energy and the non-equilibrium properties were treated by Niemeyer$^3$). Since then the $XY$ model has been investigated extensively. Most treatments use the so-called c-cyclic version, which can be diagonalized exactly in terms of fermion operators. In many cases such as in the calculation of time-dependent correlations between $z$-components of spins, the c-cyclic model can be shown to produce exact results in the thermodynamic limit$^{4-6}$).

A more complicated quantity is the transverse susceptibility with respect to an infinitesimal magnetic field $B_x$ in the $x$ direction, $i.e.$

$$
\chi = \lim_{N \to \infty} \lim_{B_x \to 0} (\beta N)^{-1} \frac{\partial^2}{\partial B_x^2} \ln \langle e^{-\beta (H - B_x M_x)} \rangle 
$$

(1a)

$$
= \lim_{N \to \infty} N^{-1} \sum_{k,j=1}^{N} \int_0^\beta d\tau \langle \psi e^{i\mathbf{S}_j \cdot \mathbf{S}_k} e^{i \mathbf{S}_j \cdot \mathbf{S}_k} \rangle. 
$$

(1b)

* Present address: Instituut voor Theoretische Fysica, Universiteit van Amsterdam, The Netherlands.
where $\rho = e^{-\beta \mathcal{H}} \langle e^{-\beta \mathcal{H}} \rangle^{-1}$ is the density operator corresponding to the Hamiltonian $\mathcal{H}$ in the absence of $B_z$, $M_x = \sum_{j=1}^{N} S_j^x$ is the $x$-component of the magnetization and $\langle 0 \rangle \equiv \text{Tr} \, 0$ for an arbitrary operator $0$.

In ref. 7 we have given a high-temperature expansion up to order $\beta^6$ for the transverse susceptibility $\chi_a$ of the one-dimensional a-cyclic $XY$ model described by the Hamiltonian $\mathcal{H} = \mathcal{H}_a$, where

$$\mathcal{H}_a = \sum_{j=1}^{N} \{(1 + \gamma) S_j^x S_{j+1}^x + (1 - \gamma) S_j^y S_{j+1}^y - B_z S_j^z\} \quad (S_{N+1}^+ \equiv S_1). \quad (2)$$

Here $\gamma$ is the anisotropy parameter and $B_z$ is a magnetic field in the $z$-direction.

Using the Jordan-Wigner transformation

$$\alpha_j = \left( \prod_{k=1}^{j-1} P_k \right) S_j^x \sqrt{2}, \quad \beta_j = -\left( \prod_{k=1}^{j-1} P_k \right) S_j^y \sqrt{2}, \quad (3)$$

where

$$P_k = (2i) \alpha_k \beta_k = -2 S_k^z, \quad (4)$$

and where the $\alpha$'s and $\beta$'s are Hermitean operators satisfying the anticommutation relations

$$\{\alpha_i, \alpha_j\} = \{\beta_i, \beta_j\} = \delta_{ij}, \quad \{\alpha_i, \beta_j\} = 0; \quad (5)$$

the Hamiltonian $\mathcal{H}_a$ can be written\(^5\)

$$\mathcal{H}_a = \mathcal{H}_c + \frac{1}{2} h (P + 1). \quad (6)$$

Here $\mathcal{H}_c$ is the c-cyclic Hamiltonian given by

$$\mathcal{H}_c = \sum_{j=1}^{N} \left\{ \frac{1}{2} (1 + \gamma) \alpha_j \beta_{j+1} + \frac{1}{2} (1 - \gamma) \alpha_j \beta_{j+1} + i B_z \alpha_j \beta_j \right\},$$

$$\quad \left(\alpha_{N+1} \equiv \alpha_1, \beta_{N+1} \equiv \beta_1\right). \quad (7)$$

The operator $P$ is the product of all Jordan-Wigner factors $P = \prod_{j=1}^{N} P_j$ and the operator $h$ contains the operators (3) relative to site 1 and $N$, i.e.,

$$h = -i (1 + \gamma) \alpha_1 \beta_N - i (1 - \gamma) \alpha_N \beta_1$$

$$= \{2 (1 + \gamma) S_1^z S_N^x + 2 (1 - \gamma) S_1^y S_N^y\} P. \quad (8)$$

Using (6), (8) and the trivial relation $P^2 = 1$, $\mathcal{H}_c$ can be expressed by

$$\mathcal{H}_c = \mathcal{H}_a - \left\{ (1 + \gamma) S_1^x S_N^x + (1 - \gamma) S_1^y S_N^y \right\} (1 + P). \quad (9)$$
In ref. 7, the averages in eq. (16) with respect to the hamiltonian $\mathcal{H}_a$ were expressed in terms of averages with respect to the c-cyclic hamiltonian $\mathcal{H}_c$ (and also its c-anticyclic counter part) using a projection operator technique as in ref. 5. A difficulty was the occurrence of an operator containing the c-cyclic as well as the c-anticyclic hamiltonian $\mathcal{H}_{ac} \equiv \mathcal{H}_c + \mathcal{H}_a$. The c-cyclic averages were evaluated using the thermodynamic Wick theorem due to Bloch and de Dominicis.

We also investigated the spin correlation functions in eq. (1b) with respect to the c-cyclic hamiltonian $\mathcal{H}_c$. As a result of a high-temperature expansion we obtained the relation, cf. eq. (7.19) of ref. 7,

$$\langle \varrho_c e^{i \mathcal{H}_c} S_j^x e^{-i \mathcal{H}_c} S_{j+p}^x \rangle = \langle \varrho_a e^{i \mathcal{H}_a} S_j^x e^{-i \mathcal{H}_a} S_{j+p}^x \rangle \cdot \langle \varrho_c e^{i \mathcal{H}_c} e^{-i (\mathcal{H}_c + \mathcal{H}_a)} \rangle.$$ (10)

where $\varrho_c$ and $\varrho_a$ are the density operators corresponding to $\mathcal{H}_c$ and $\mathcal{H}_a$ respectively. Eq. (10) is valid, up to an arbitrary order in $\beta$, for sufficiently large values of $j$ and $N - j - p$.

From (10) one can expect the inequality

$$\chi_c \neq \chi_a,$$ (11)

where $\chi_c$ and $\chi_a$ are the c-cyclic and a-cyclic susceptibilities, which can be obtained from eq. (1b) by substituting $\mathcal{H} = \mathcal{H}_c$ and $\mathcal{H} = \mathcal{H}_a$ respectively. (In fact, $\chi_c$ was evaluated up to order $\beta^4$, cf. eq. (7.23) of ref. 7.)

The inequality (11) is only valid, if one first takes the limit $B_x \to 0$ and the thermodynamic limit $N \to \infty$ afterwards. If one defines “thermodynamic” susceptibilities $\tilde{\chi}_c$ and $\tilde{\chi}_a$ by interchanging the two limits in eq. (1a), then both susceptibilities should be equal. This is obvious from the relation

$$f(\mathcal{H}_c - B_x M_x) = f(\mathcal{H}_a - B_x M_x)$$ (12)

for the free energy per particle $f(\mathcal{H}) = \lim N^{-1} F(\mathcal{H})$, $F(\mathcal{H}) = -\beta^{-1} \ln \langle e^{-\beta \mathcal{H}} \rangle$, corresponding to the hamiltonians $\mathcal{H} = \mathcal{H}_c - B_x M_x$ and $\mathcal{H} = \mathcal{H}_a - B_x M_x$.

Eq. (12) is an immediate consequence of a special case of the Bogoliubov inequality

$$F(\mathcal{H}_0) - \| \mathcal{H}_1 \| \leq F(\mathcal{H}_0 + \mathcal{H}_1) \leq F(\mathcal{H}_0) + \| \mathcal{H}_1 \|,$$ (13)

where $\| \mathcal{H} \| = \sup \{ |(x, 0x)(x, x)^{-1} \}$ is the operator norm. Eq. (12) is obvious from (9) and (13), since the norm $\| (\mathcal{H}_c - \mathcal{H}_a) \|$ is finite.

Since there is no reason to doubt the validity of the relation $\tilde{\chi}_a = \tilde{\chi}_c$ for the a-cyclic model, eq. (11) implies that $\chi_c \neq \tilde{\chi}_c$; i.e. in the calculation of the susceptibility $\chi_{xx}$ for the c-cyclic chain the two limits $B_x \to 0$ and $N \to \infty$ cannot be interchanged. Note that for a direct evaluation of $\tilde{\chi}_a = \tilde{\chi}_c$ one should know the free energy of an $XY$ chain in the presence of $B_x$. In ref. 7 we calculated $\chi_{xx}$ for a finite chain in the limiting case $B_x \to 0$, taking the thermodynamic limit afterwards. The inequality (11) shows that the difference between the transverse sus-
ceptibilities per particle in the absence of a field \( B_\perp \) for finite a-cyclic and c-cyclic chains tends to a non-vanishing value in the thermodynamic limit.

As another consequence of (10) one can expect a difference between the c-cyclic and a-cyclic autocorrelation functions of the \( x \) component of the magnetization, i.e.,

\[
R_c(t) \neq R_a(t),
\]

where

\[
R_\varepsilon(t) \equiv \lim_{N \to \infty} N^{-1} \{ \langle \phi_\varepsilon M_x e^{i \mathcal{H}_\varepsilon t} M_x e^{-i \mathcal{H}_\varepsilon t} \rangle - \langle \phi_\varepsilon M_x \rangle^2 \} \quad (\varepsilon = c, a). \quad (15)
\]

In section 2 both inequalities (11) and (14) will be made more explicit for the simple case of an Ising model, where the c-cyclic quantities \( \chi_\varepsilon \) and \( R_\varepsilon(t) \) can be evaluated exactly without using high-temperature expansions or expansions in powers of \( t \). (Of course for this particular case the free energy per spin of the a-cyclic model in the presence of a magnetic field \( B_\perp \) is well known. Our purpose, however, is to show that the use of the c-cyclic version leads to an expression for \( \chi_\varepsilon \) different from \( \chi_a = \tilde{\chi}_a = \tilde{\chi}_c \).

2. Ising model

In this section we shall evaluate the c-cyclic correlation functions

\[
C_{jk}(\tau) \equiv \langle \phi_\varepsilon e^{i \mathcal{H}_\varepsilon \tau} S_j^x e^{-i \mathcal{H}_\varepsilon \tau} S_k^x \rangle \quad (\varepsilon = c, a), \quad (16)
\]

in the special case \( \gamma = 1, B_\perp = 0 \). The a-cyclic hamiltonian is then given by

\[
\mathcal{H}_a = 2 \sum_{j=1}^{N} S_j^x S_{j+1}^x \quad \text{ and } \quad S_{N+1}^x \equiv S_1^x. \quad (17)
\]

Since the spin components \( S_j^x \) commute with \( \mathcal{H}_a \), the a-cyclic time \( xx \) spin correlation functions and consequently the correlation function of \( M_x \) do not depend on time.

For the a-cyclic model we have

\[
\langle \phi_a S_j^x S_k^x \rangle = \frac{1}{4} \{ (-\tanh \frac{1}{2} \beta)^{j-k} + (-\tanh \frac{1}{2} \beta)^{N-1-k+j} \} \times \{ 1 + (-\tanh \frac{1}{2} \beta)^N \}^{-1},
\]

\[
\chi_a = \lim_{N \to \infty} \sum_{p=0}^{N-1} \beta \langle \phi_a S_1^x S_{1+p}^x \rangle = \frac{1}{4} \beta e^{-\beta} = \tilde{\chi}_a = \tilde{\chi}_c, \quad (19)
\]

\[
R_\varepsilon(t) = \frac{1}{4} e^{-\beta}. \quad (20)
\]
The equality \( \tilde{\alpha} = \frac{1}{2} \beta e^{-\beta} \) is well known; the equality \( \tilde{\alpha} = \tilde{\alpha}_c \) has been justified in section 1.

The Hamiltonian of the c-cyclic version of the Ising model reads

\[
H_c = H_a - 2S_1^x S_N^x (1 + P).
\]  

In the evaluation of the r.h.s. of (16) use will be made of the (anti)commutation relations

\[
\{P, S_k^x\} = 0, \quad [H_a, S_k^x] = 0, \quad [S_1^x S_N^x (1 \pm P), H_c] = 0
\]

and eq. (8) for the special case \( \gamma = 1, B = 0 \). Then

\[
C_{jk}(\tau) = \langle q_c e^{-2\pi S_1^x S_N^x (1 + P)} e^{iH_a^c S_j^x} e^{-\gamma H_c} S_k^x e^{2\pi S_1^x S_N^x (1 - P)} \rangle
\]

\[
= \langle q_c e^{-4\pi S_1^x S_N^x P} S_j^x S_k^x \rangle = \langle q_c e^{-\gamma} S_j^x S_k^x \rangle
\]

\[
= C_{kj}(\tau).
\]  

The operator \( e^{-\gamma} \), for \( \gamma = 1, B = 0 \), can be written

\[
e^{-\gamma} = \cosh \tau - 4S_1^x S_N^x P \sinh \tau = \cosh \tau + 2i \alpha \beta \sinh \tau.
\]  

Using the Jordan–Wigner transformation (3), the anti-commutation relations (5) and eq. (24) we obtain, \( p \geq 0 \),

\[
C_{jj+p} = \frac{1}{4} \langle q_c (\cosh \tau + 2i \alpha \beta \sinh \tau) (2i)^p \prod_{k=j}^{j+p-1} (\beta_k x_{k+1}) \rangle.
\]  

The r.h.s. of (25) can be evaluated using the thermodynamic Wick theorem and the relations, cf. eqs. (2.25), (2.29), (3.17)–(3.19) of ref. 7,

\[
\langle q_c x_{j+1} \rangle = \langle q_c \beta_j \beta_k \rangle = \frac{1}{2} \delta_{jk},
\]

\[
\langle q_c x_j \beta_k \rangle = \frac{1}{2} i (\tanh \frac{1}{2} \beta) \delta_{k-j-1}.
\]

As a result we obtain

\[
C_{jj+p}(\tau) = \frac{1}{4} (\tanh \frac{1}{2} \beta)^p (\cosh \tau - \sinh \tau \tanh \frac{1}{2} \beta).
\]  

The second factor in eq. (27), which is equal to \( \langle q_c e^{-\gamma} \rangle \) can also be obtained from the second factor on the r.h.s. of eq. (10) in the special case that \( \gamma = 1, B = 0 \), so that \([H_c, h] = 0\). Note that eq. (27) is also valid for a finite chain and
that the correlation function is independent of $j$. This is not true in the general case of the $XY$ model.

From eq. (27) we obtain immediately the c-cyclic susceptibility in the thermodynamic limit

$$
\chi_c = \int_0^\beta dx \left\{ C_{jj}(x) + \sum_{p=1}^\infty C_{jj+p}(x) \right\} 
= 2 \left( \tanh \frac{1}{2} \beta \right) \left\{ \frac{1}{4} + \frac{1}{2} \sum_{p=1}^\infty (-\tanh \frac{1}{2} \beta)^p \right\} = \chi_d 2 \beta^{-1} \tanh \frac{1}{2} \beta, \quad (28)
$$

which is clearly different from $\chi_a = \chi_a = \chi_c$. Substituting $\tau = -it$ in eq. (27), we find

$$
\langle q_c S_j^x e^{i t \hbar} e^{t \hbar} S_{j+p}^x e^{-i t \hbar} \rangle = \frac{1}{4} (-\tanh \frac{1}{2} \beta)^{k-j} (\cos t + i \sin t \tanh \frac{1}{2} \beta). \quad (29)
$$

The validity for $k < j$ can be seen by taking the hermitean conjugate of both members of the corresponding equation for $k > j$. As a result the auto-correlation function of the $x$ component of the magnetization is given by

$$
R_c(t) = \frac{1}{4} e^{-\beta} (\cos t + i \sin t \tanh \frac{1}{2} \beta). \quad (30)
$$

As a result of using the c-cyclic version the time auto-correlation function of $M_x$ is no longer a constant but depends on time. The time average of $R_c(t)$ vanishes (also in the case of the finite c-cyclic Ising model). Hence, the magnetization $M_x$ is an ergodic operator in the c-cyclic Ising model. (Both for finite $N$ and in the limit $N \to \infty$.) In the finite and infinite a-cyclic Ising chain $M_x$ is not an ergodic operator, since in the absence of $B_x$ the microcanonical and canonical averages of $M_x$ vanish, whereas the time average of $R_a(t)$ is given by (20).

### 3. Remark

So far we have restricted ourselves to the c-cyclic version of the Ising model. For the c-anticyclic version, which is defined by the hamiltonian

$$
\mathcal{H}_{ac} \equiv \mathcal{H}_c + h = \mathcal{H}_a - 2S^x_1 S^x_N (1 - P), \quad (31)
$$

the correlation functions $C'_{jj+p}$ are also given by the r.h.s. of (27), i.e.,

$$
C'_{jj+p}(x) \equiv \langle q_{ac} e^{i \hbar x} S_j^x e^{-i \hbar x} S_{j+p}^x \rangle = C_{jj+p}(x). \quad (32)
$$
This can be seen by the replacement $P \rightarrow -P$ in eq. (23), which leads to the \( c \)-anticyclic analogue of (25), \( i.e., \)

\[
C'_{j+p}(\tau) = \frac{1}{4} \left\langle \varrho_{ac} \left( \cosh \tau - 2i \alpha_{1} \beta_{N} \sinh \tau \right) \left( 2/i \right)^{p} \prod_{k=j}^{j+p-1} (\hat{\beta}_{k} \hat{\alpha}_{k+1}) \right\rangle. \quad (33)
\]

Now (32) is obvious from (33) noting that

\[
\left\langle \varrho_{ac} \alpha_{1} \beta_{N} \right\rangle = -\left\langle \varrho_{c} \alpha_{1} \beta_{N} \right\rangle, \quad (34)
\]

\[
\left\langle \varrho_{ac} \alpha_{j} \beta_{j-1} \right\rangle = \left\langle \varrho_{c} \alpha_{j} \beta_{j-1} \right\rangle \quad (j = 2, \ldots, N). \quad (35)
\]

From (32) we have the relations

\[
\chi_{ac} = \chi_{c}, \quad R_{ac}(t) = R_{c}(t). \quad (35)
\]

The susceptibility and the autocorrelation function of \( M_{c} \) in the \( c \)-cyclic and \( \hat{c} \)-anticyclic version are equal. Note that this is true even for the finite chain. In general, the properties of the \( c \)-cyclic and \( \hat{c} \)-anticyclic \( XY \) model are equal only in the thermodynamic limit.

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References