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XX Heisenberg Spin Chain and an Example of Path Integral with "Automorphic" Boundary Conditions

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Dedicated to the memory of A.G.Izergin

Abstract

New representation for the generating function of correlators of third components of spins in the XX Heisenberg spin chain is considered in the form given by the fermionic Gaussian path integrals. A part of the discrete anti-commuting integration variables is subjected to "automorphic" boundary conditions in respect of imaginary time. The situation when only a part of the integration variables is subjected to the unusual boundary conditions generalizes more conventional ones when "automorphic" boundary conditions appear for all sites in the lattice spin models. The results of the functional integration are expressed in the form of determinants of the matrix operators. The generating function, as well as the partition function of the model, are calculated by means of zeta-regularization. Certain correlation functions at nonzero temperature are obtained explicitly.

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1 Introduction

The correlation functions of the quantum models which can be solved by the Bethe ansatz method [1] can be represented as the Fredholm determinants of certain linear integral operators. One of such *determinant* representations has been obtained in [2] for a simplest equal-time correlator of one-dimensional model of "impenetrable" bosons, which are described by the quantum non-linear Schrödinger equation with infinite coupling. The result [2] has been generalized to the case of correlators with different time arguments [3], and also to the case of the Heisenberg XX spin chain [4]. The determinant representations of the correlation functions enable to deduce the integrable non-linear partial differential equations for the correlators [1, 5].

In its turn, path integration technique can be used to calculate the correlation functions in various quantum models [6, 7]. A path integration approach has been suggested in [8] to calculate the generating function of correlators of third components of spins in the XX and XY Heisenberg spin models on a cyclic chain. The path integrals obtained in [8] for the XX-case lead to the answers in the determinant form [9]. Further, the determinant representations have been deduced in [10] for the equal-time temperature correlators of all components of spins in the anisotropic XY-chain. Multiple integration over a set of the Grassmann coherent states (instead of the path integration) is used in [10]. Subsequent development of the approach [10] can be found in [11]. It should be noticed that XX model also still continues to attract attention [12], and determinant representations for the correlators in integrable models are also actively studied [13].

The idea to use path integration technique for obtaining certain determinant formulas for XX and XY Heisenberg models looks attractive. Therefore, another version of the path integration approach is developed in the given paper to represent both the partition function and the generating function of correlators of third components of spins in the Heisenberg XX-model. The approach proposed below is based on a technical note pointed out in Refs.[14] which are concerned with the index theory and supersymmetric quantum mechanics. Path integration is used in [14] to evaluate traces of the corresponding operators, and for some cases the functional integration is defined in [14] over trajectories subjected to non-conventional "automorphic" boundary conditions with respect of imaginary time.

Path integrals considered in the present paper are also over a set of variables a part of which is subjected to "automorphic" boundary condition (while another part – to usual requirements of a fermion/boson-type). It should be noticed that our path integral representations do not imply a straightforward implementation of the proposal [14]: a special restoration of invariance of the Lagrangian under shifts of imaginary time by a period is required. The method of zeta-regularization is used below to handle the determinants obtained. The generating function, as well as the partition function of the model, are calculated. Certain correlation functions at nonzero temperature are obtained explicitly. It is demonstrated that the path integration approach proposed admits a considerable simplification and enough transparency for the problem in question.

¿From a physical viewpoint, basic ideas of zeta-regularization (ζ-regularization) have been formulated in [15, 16]. In mathematical literature, usage of ζ-regularization is usually traced to [17]. ζ-Regularization turned out to be rather useful in physics to calculate, say, the instanton determinants [18, 19], the Casimir energy on manifolds [20], as well as the axial and conformal anomalies [21]. One should be referred to [15–17, 22] for exposition

of ζ-regularization.

The paper is organized as follows. Section 2 contains the basic notations and introductory remarks. The representation for the generating function of correlators of $\sigma_z^{(k)}$-operators (and also for the partition function) in the form given by the fermionic path integrals with "automorphic" boundary conditions is obtained in Section 3 ($\sigma_z^{(k)}$ implies σ_z at kth site). The most important formulas of ζ-regularization are given in Section 4. Moreover, the partition function of the model is calculated in Section 4 with the use of the generalized ζ-function in the series form. The generalized ζ-function in the form of a Mellin transform is defined in Section 5, and it is used to calculate the generating function of the correlators of spins. Differentiation of the integrals obtained with respect to a parameter is also considered in Section 5, and some specific correlators are calculated. Discussion in Section 6 concludes the paper.

2 Notations

Let us consider the Heisenberg XX-model (which is an isotropic limit of more general XY-model, [23]) on a chain of the length M (M is even). Let $Q(m)$ be the number of particles operator on the first m sites of the chain ($m \leq M$). We shall calculate $\exp(\alpha Q(m))$ averaged over the ground state of the model (our notations, though conventional, correspond to [4, 10]),

$$\langle e^{\alpha Q(m)} \rangle \equiv \langle \Phi_0 \mid e^{\alpha Q(m)} \mid \Phi_0 \rangle,$$

using the formula

$$\langle e^{\alpha Q(m)} \rangle = \frac{\mathrm{Tr}\left(e^{\alpha Q(m)} e^{-\beta H_{XX}}\right)}{\mathrm{Tr}\left(e^{-\beta H_{XX}}\right)}, \quad \alpha \in \mathbb{C}, \tag{1}$$

where H_{XX} is the Hamiltonian, β is inverse temperature, and Tr means trace of operator. The Hamiltonian of the model, H_{XX}, will be taken in the fermionic representation [23, 24]. In fact, H_{XX} considered by us appears after the Jordan–Wigner transformation from initial Pauli spin variables to the canonical fermionic variables subjected to the anti-commutation relations:

$$\{c_k, c_n\} = \{c_k^\dagger, c_n^\dagger\} = 0, \quad \{c_k, c_n^\dagger\} = \delta_{kn}.$$

In these notations, $Q(m) \equiv \sum_{k=1}^{m} c_k^\dagger c_k$.

It can be verified, that H_{XX} commutes with the total number of particles $\mathcal{N} \equiv Q(M)$, while the parity operator $(-1)^{\mathcal{N}}$ anti-commutes with the canonical variables,

$$\{(-1)^{\mathcal{N}}, c_n\} = \{(-1)^{\mathcal{N}}, c_n^\dagger\} = 0,$$

and it commutes with H_{XX} since the latter is bilinear in c_n, $c_n^\dagger$. Therefore, two projectors $P^\pm = \frac{1}{2}(1 \pm (-1)^{\mathcal{N}})$ can be defined in such way, that H_{XX} can be written in the form [24]:

$$H_{XX} = H^+ P^+ + H^- P^-,$$

$$H^\pm = -\frac{1}{2} \sum_{n=1}^{M} (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + h\mathcal{N} - \frac{hM}{2}, \tag{2}$$

where $h > 0$ is an external magnetic field. The superscript $^{\pm}$ in (2) implies the following boundary conditions at the ends of the chain:

$$\begin{aligned} c_{M+1} &= -c_1, \quad c^{\dagger}_{M+1} = -c^{\dagger}_1 \quad \text{for} \quad H^{+}, \\ c_{M+1} &= +c_1, \quad c^{\dagger}_{M+1} = +c^{\dagger}_1 \quad \text{for} \quad H^{-}. \end{aligned} \tag{3}$$

We shall calculate the required average (1), i.e.,

$$G(m) \equiv \frac{1}{Z}\,\mathrm{Tr}\left(e^{\alpha Q(m)} e^{-\beta H}\right)$$

(the index XX is omitted), using the formula [10]:

$$G(m) = \frac{1}{2Z}(G^{+}_F Z^{+}_F + G^{-}_F Z^{-}_F + G^{+}_B Z^{+}_B - G^{-}_B Z^{-}_B), \tag{4.1}$$

where

$$\begin{aligned} G^{\pm}_F Z^{\pm}_F &\equiv \mathrm{Tr}\left(e^{\alpha Q(m)} e^{-\beta H^{\pm}}\right), \\ G^{\pm}_B Z^{\pm}_B &\equiv \mathrm{Tr}\left(e^{\alpha Q(m)} (-1)^{\mathcal{N}} e^{-\beta H^{\pm}}\right), \end{aligned} \tag{4.2}$$

and $H^{\pm}$ are defined by (2), (3). By an analogy with (4), the partition function $Z \equiv \mathrm{Tr}\,(\exp(-\beta H))$ can also be written in the form

$$\begin{aligned} Z &= \frac{1}{2}(Z^{+}_F + Z^{-}_F + Z^{+}_B - Z^{-}_B), \\ Z^{\pm}_F = \mathrm{Tr}\,(e^{-\beta H^{\pm}}), &\quad Z^{\pm}_B = \mathrm{Tr}\,((-1)^{\mathcal{N}} e^{-\beta H^{\pm}}) \end{aligned} \tag{5}$$

((4) results in (5) at $\alpha \to 0$).

The representations for $G^{\pm}_F Z^{\pm}_F$ and $G^{\pm}_B Z^{\pm}_B$ are obtained in [8] as the path integrals over the Grassmann variables. As the result, the final answers in [8] take the form of determinants of finite-dimensional matrices. The anti-commuting functional variables in [8], $\xi_n(\tau)$, turn out to satisfy conventional (anti-)periodicity rules with respect of imaginary time $\tau : \xi_n(\tau) = \pm\xi_n(\tau + \beta)$ (at nth site).

The following observation can be found in Refs.[14], which are concerned with the index theory and supersymmetric quantum mechanics. Let a, $a^{\dagger}$ be some fermionic canonical operators. Let us consider a unitary operator $Q_{\vartheta} \equiv \exp(i\vartheta a^{\dagger} a)$ of $\mathcal{U}(1)$-transformation, which acts on $a, a^{\dagger}$ as follows:

$$Q_{\vartheta} a Q^{\dagger}_{\vartheta} = e^{-i\vartheta} a, \quad Q_{\vartheta} a^{\dagger} Q^{\dagger}_{\vartheta} = e^{i\vartheta} a^{\dagger}.$$

When calculating $\mathrm{Tr}\,(Q_{\vartheta} \exp(-\beta H))$, it turns out to be quite natural to come to a path integral over a variable subjected to "automorphic" boundary condition: $\xi(\tau) = -e^{i\vartheta}\xi(\tau + \beta)$. The latter implies that the integration variable is transformed accordingly to a nontrivial representation of $\mathcal{U}(1)$ when τ is shifted by the period β. Let us note that another example of "automorphic" boundary condition can be found in [25] where spin 1 and 1/2 chain models are studied by the method of functional integration.

It is not difficult to note that $\exp(\alpha Q(m))$ behaves analogously:

$$e^{\alpha Q(m)} c_n e^{-\alpha Q(m)} = \begin{cases} e^{-\alpha} c_n, & 1 \le n \le m \\ c_n, & m < n \le M, \end{cases} \tag{6}$$

and one can use the idea [14] when calculating $G_F^{\pm}Z_F^{\pm}$, $G_B^{\pm}Z_B^{\pm}$ (4.2). The "automorphic" condition arises for all sites in the models considered in [25]. It can be guessed that the peculiarity due to (6) will be concerned with $m \leq M$, and the "automorphic" condition should be expected to appear only for a part of sites.

To conclude, let us define the coherent states using the fermionic operators c_n, $c_n^{\dagger}$ which possess the Fock vacuum $\mid 0\rangle$:

$$c_n \mid 0\rangle = \langle 0 \mid c_n^{\dagger} = 0, \quad \forall n, \quad \langle 0 \mid 0\rangle = 1.$$

Namely,

$$\begin{aligned} \mid x(n)\rangle &= \exp\left\{\sum_{k=1}^{M} c_k^{\dagger} x_k(n)\right\} \mid 0\rangle \equiv \exp(c^{\dagger}x(n)) \mid 0\rangle, \\ \langle x^*(n) \mid &= \langle 0 \mid \exp\left\{\sum_{k=1}^{M} x_k^*(n) c_k\right\} \equiv \langle 0 \mid \exp(x^*(n)c), \end{aligned} \tag{7}$$

where n is the discrete index running from 1 to N, and the shorthand notations are used: $\sum_{k=1}^{M} c_k^{\dagger}x_k \equiv c^{\dagger}x$, $\prod_{k=1}^{M} dx_k \equiv dx$, etc. In fact, N independent coherent states are defined which are labeled by independent complex-valued Grassmann parameters $x_k^*(n)$, $x_k(n)$. The following relations hold for the states (7):

$$c_k \mid x(n)\rangle = x_k(n) \mid x(n)\rangle, \quad \langle x^*(n) \mid c_k^{\dagger} = \langle x^*(n) \mid x_k^*(n),$$

$$\langle x^*(n) \mid x(n)\rangle = \exp(x^*(n)x(n)).$$

3 The path integral

Let us turn to the problem of rewriting (4) and (5) in a path integral form. For definitness, let us consider

$$G_F^{\pm}Z_F^{\pm} = \int dz\, dz^* e^{z^*z} \langle z^* | e^{\alpha Q(m)} e^{-\beta H^{\pm}} | z\rangle, \tag{8}$$

where the trace of the operator is understood as the integral over the anti-commuting variables [26], and the coherent states $\langle z^*|, |z\rangle$ are defined as follows:

$$\langle z^*| = \langle 0| \exp(z^*c), \quad |z\rangle = \exp(c^{\dagger}z)|0\rangle.$$

In order to go over to the path integral, let us divide the interval $[0, \beta]$ into N parts of the length β/N, and let us represent $\exp(-\beta H^{\pm})$ as a product of N identical exponentials. Inserting N completeness relations between the exponentials, let us transform (8) into

$$\begin{aligned} G_F^{\pm}Z_F^{\pm} = \int dz\, dz^* \prod_{n=1}^{N} dx^*(n)dx(n) \exp\left(z^*z - \sum_{n=1}^{N} x^*(n)x(n)\right) \\ \times \langle z^*| e^{\alpha Q(m)} |x(1)\rangle \langle x^*(1)| e^{-\frac{\beta}{N}H^{\pm}} |x(2)\rangle \ldots \langle x^*(N)| e^{-\frac{\beta}{N}H^{\pm}} |z\rangle, \end{aligned} \tag{9}$$

where $\mid x(n)\rangle$ and $\langle x^*(n) \mid$ are defined in (7).

Using the properties of the coherent states we evaluate the following entries:

$$\langle z^*|e^{\alpha Q(m)}|x(1)\rangle = \exp\left(e^{\alpha}\sum_{k=1}^{m} z_k^* x_k(1) + \sum_{k=m+1}^{M} z_k^* x_k(1)\right),$$

$$\langle x^*(n)|e^{-\frac{\beta}{N}H^{\pm}}|x(n+1)\rangle_{N\gg 1}^{\simeq}$$

$$\simeq \exp\left(x^*(n)x(n+1) - \frac{\beta}{N}H^{\pm}(x^*(n), x(n+1))\right),$$

$$H^{\pm}(x^*(n), x(n+1)) \equiv -\frac{1}{2}\sum_{k=1}^{M}(x_k^*(n)x_{k+1}(n+1) + x_{k+1}^*(n)x_k(n+1))$$

$$+h\sum_{k=1}^{M} x_k^*(n)x_k(n+1) - \frac{hM}{2}.$$

Inserting them to (9), we obtain:

$$G_F^{\pm}Z_F^{\pm} = \int dz\, dz^* \prod_{n=1}^{N} dx^*(n)dx(n)\, \exp\left\{\sum_{k=1}^{m} z_k^*(z_k + e^{\alpha}x_k(1))\right.$$

$$+\sum_{k=m+1}^{M} z_k^*(z_k + x_k(1)) + x^*(1)(x(2) - x(1)) + \ldots + x^*(N)(z - x(N))$$

$$\left.-\frac{\beta}{N}(H^{\pm}(x^*(1), x(2)) + \ldots + H^{\pm}(x^*(N), z))\right\}. \tag{10}$$

Let us denote $x(N+1) \equiv z$, $x_k^*(0) \equiv e^{\alpha}z_k^*$ (for $1 \le k \le m$) or z_k^* (for $m < k \le M$), and impose the conditions

$$\begin{aligned} x_k(0) &= -e^{-\alpha}x_k(N+1), \quad 1 \le k \le m, \\ x_k(0) &= -x_k(N+1), \qquad m < k \le M, \end{aligned}$$

and perform $N \to \infty$. As the result, R.H.S. of (10) acquires the integral form:

$$\int \prod_{\tau\in[0,\beta]} dx^*(\tau)dx(\tau) \exp\left(\int_0^{\beta} \mathcal{L}(\tau)d\tau\right), \tag{11.1}$$

where $\mathcal{L}(\tau)$ denotes the Lagrangian:

$$\mathcal{L}(\tau) = x^*(\tau)\frac{dx}{d\tau} - H^{\pm}(x^*(\tau), x(\tau)), \tag{11.2}$$

and the functional variables $x(\tau)$, $x^*(\tau)$ are subjected to the conditions:

$$\begin{aligned} x_k(\tau) &= -e^{-\alpha}x_k(\tau+\beta), \quad 1 \le k \le m, \\ x_k(\tau) &= -x_k(\tau+\beta), \qquad m < k \le M. \end{aligned} \tag{11.3}$$

Generally speaking, the fields $x_k^*(\tau)$ are independent integration variables. It is convenient to subject $x_k^*(\tau)$ to a requirement analogous to (11.3) but with e^{α} instead of $e^{-\alpha}$.

The derivation of the representation (11) follows [14] strictly, and it does not take into account the peculiar character of our problem: the conditions (11.3) characterize two independent sets of sites. In their turn, the Hamiltonians $H^{\pm}$ with the nearest neighbour coupling are diagonal just in the momentum representation. Therefore, the following circumstance becomes essential (which is new in comparison with [14, 25]).

It can be assumed that a certain representation of the group of shifts of τ by the period β, i.e., $\tau \to \tau+\beta$, is defined by the traditional (anti-)periodicity rules $x_k(\tau) = \pm x_k(\tau+\beta)$, $k \in \{1, \ldots, M\}$, as well as by the conditions (11.3). The action $\int_0^\beta \mathcal{L}(\tau)d\tau$ in the exponent of (11.1) is a well-defined object provided $\mathcal{L}(\tau)$ is invariant under the shifts of τ. Such invariance takes place for a conventinal boundary condition provided $\mathcal{L}(\tau)$ is even in powers of the fields.

Let us use (11.3) to calculate the variation $\delta\mathcal{L}(\tau)$:

$$\delta\mathcal{L}(\tau) = \mathcal{L}(\tau+\beta) - \mathcal{L}(\tau) =$$

$$= \frac{1}{2}\Big[(e^{\alpha}-1)\Big(x^*_{m+1}(\tau)x_m(\tau) + x^*_M(\tau)x_{M+1}(\tau)\Big) +$$

$$+(e^{-\alpha}-1)\Big(x^*_m(\tau)x_{m+1}(\tau) + x^*_{M+1}(\tau)x_M(\tau)\Big)\Big].$$

The case of the origin of $\delta\mathcal{L}(\tau)$ is simple: the cyclic quadratic form

$$\sum_{k=1}^{M}(x^*_k x_{k+1} + x^*_{k+1}x_k)$$

is invariant under

$$x_k \to \pm e^{\alpha}x_k, \quad x^*_k \to \pm e^{-\alpha}x^*_k, \tag{12}$$

provided $k \in \{1, \ldots, M\}$ (the homogeneous "gauge" transformation), and it is not invariant provided (12) is valid only for a part of sites (the nonhomogeneous transformation). The rule (11.3) implies a nonhomogeneous representation of shifts $\tau \to \tau+\beta$, and, thus, the invariance turns out to be broken for $\mathcal{L}(\tau)$ (11.2). However, this symmetry can straightforwardly be restored as follows: one should replace $H^{\pm}(x^*(\tau), x(\tau))$ in the limiting formula (11.1) by another form of the following type:

$$\widetilde{H}^{\pm}(\tau) = -\frac{1}{2}{\sum_{k=1}^{M}}'(x^*_{k+1}(\tau)x_k(\tau) + x^*_k(\tau)x_{k+1}(\tau))$$

$$+h\sum_{k=1}^{M}x^*_k(\tau)x_k(\tau) - \frac{1}{2}\Big[x^*_{m+1}(\tau)x_m(\tau)e^{-\frac{\alpha}{\beta}\tau} + x^*_m(\tau)x_{m+1}(\tau)e^{\frac{\alpha}{\beta}\tau}$$

$$+x^*_{M+1}(\tau)x_M(\tau)e^{\frac{\alpha}{\beta}\tau} + x^*_M(\tau)x_{M+1}(\tau)e^{-\frac{\alpha}{\beta}\tau}\Big] - \frac{hM}{2},$$

where $\sum'$ means that the indices $k = m, M$ are omitted. The Lagrangian

$$\widetilde{\mathcal{L}}(\tau) = x^*(\tau)\frac{dx}{d\tau} - \widetilde{H}^{\pm}(\tau)$$

is invariant under $\tau \to \tau + \beta$, the integration measure in (11.1) is also invariant, and, finally, we obtain:

$$G_F^{\pm} Z_F^{\pm} = \int \prod_{\tau \in [0,\beta]} dx^*(\tau) dx(\tau) \exp\left(\int_0^{\beta} \widetilde{\mathcal{L}}(\tau) d\tau \right). \tag{13}$$

The main statement of the present paper reads that the representation (13) (together with the conditions (11.3)) is a well-defined relation which is alternative to the functional representation obtained in [8]. The actual calculation below is to argue this assertion. Equations (11.3) remind the definition of an automorphic function (automorphic form, [27]):

$$g^* f \equiv f(gu) = r(g) f(u)\,,$$

where $f(u)$ is an appropriate function (form), g is an elememt of a group of transformations acting on the argument u (thus generating an action of g^* on f), and $r(g)$ denotes a representation of g^*. It is why we can formally consider (11.3) as "authomorphic" boundary conditions to distinguish them from more conventional rules of fermionic/bosonic (at $\alpha = i\pi k, k \in \mathbb{Z}$) type.

Let us pass in (13) to the momentum representation:

$$\begin{aligned} x_k(\tau) = &\quad (\beta M)^{-1/2} \sum_p e^{i(\omega\tau - i\frac{\alpha}{\beta}\tau + qk)} x_p, \quad 1 \le k \le m, \\ x_k(\tau) = &\quad (\beta M)^{-1/2} \sum_p e^{i(\omega\tau + qk)} x_p, \qquad\quad m < k \le M, \end{aligned} \tag{14.1}$$

where $p = (\omega, q)$, and the summation goes over the Matsubara frequencies $\omega = \pi T(2n+1)$, $n \in \mathbb{Z}$, and over the quasi-momenta $q \in X^{\pm}$. Two sets $X^{\pm}$,

$$\begin{aligned} X^{+} = &\quad \{q = -\pi + \pi(2l-1)/M \mid l = 1, \ldots, M\}, \\ X^{-} = &\quad \{q = -\pi + 2\pi l/M \mid l = 1, \ldots, M\}, \end{aligned} \tag{14.2}$$

correspond to two boundary conditions (3). Let us substitute (14.1) into (13), rescale $x_p \exp(i(m+1)q/2) \to x_p$, and obtain:

$$\begin{aligned} G_F^{\pm} Z_F^{\pm} &= \int \prod_{\omega_F, q \in X^{\pm}} dx_p^* dx_p \exp(S^{\pm}(\alpha)), \\ S^{\pm}(\alpha) &= \sum_p (i\omega - \varepsilon_q) x_p^* x_p + \frac{\alpha}{\beta} \sum_{\omega_F, q, q'} Q^{(0)}_{qq'} x^*_{\omega q} x_{\omega q'} + \frac{Mh\beta}{2}, \end{aligned} \tag{15.1}$$

where $\varepsilon_q = h - \cos q$ is the band energy of the quasi-particles,

$$Q^{(0)}_{qq'} = \frac{1}{M} \frac{\sin\frac{m}{2}(q-q')}{\sin\frac{q-q'}{2}}, \tag{15.2}$$

ω_F denotes summation over the fermionic frequencies, and $q, q' \in X^{+}$ or X^{-}.

Let use the known formula for multiple Grassmann integrals [26],

$$\int dx^* dx \exp(-x^* \mathcal{M} x) = \det \mathcal{M},$$

to obtain the following formal answers:

$$G_F^{\pm} Z_F^{\pm} = e^{Mh\beta/2} \mathrm{Det} \left[(-i\omega_F + \varepsilon_q)\delta_{pp'} - \frac{\alpha}{\beta}\, \delta_{\omega\omega'} Q^{(0)}_{qq'} \right], \tag{16.1}$$

$$G_B^{\pm} Z_B^{\pm} = e^{Mh\beta/2} \mathrm{Det} \left[(-i\omega_B + \varepsilon_q)\delta_{pp'} - \frac{\alpha}{\beta}\, \delta_{\omega\omega'} Q^{(0)}_{qq'} \right], \tag{16.2}$$

and

$$Z_F^{\pm} = e^{Mh\beta/2} \mathrm{Det}\, [(i\omega_F - \varepsilon_q)\delta_{pp'}], \tag{17.1}$$

$$Z_B^{\pm} = e^{Mh\beta/2} \mathrm{Det}\, [(i\omega_B - \varepsilon_q)\delta_{pp'}], \tag{17.2}$$

where ω_F and ω_B are the fermionic and bosonic frequencies. The symbol Det denotes determinants of "infinite-dimensional" matrices, while 'det' is reserved for conventional matrices. The modification of all the calculations for (16.2) and (17.2) is straightforward. It is convenient to denote the matrix operators, which appear in (16) and (17), as $A(\alpha) \equiv A_\alpha$ and A, respectively.

4 Zeta-regularization.

We shall use ζ-regularization [15, 16, 22] in order to assign meaning to the determinants (16), (17). Notice that, in principle, the partition function of XY-model can be written with minor (in comparison with (17)) modifications [10]:

$$\begin{aligned} Z &= \frac{1}{2}(Z_F^+ + Z_F^- + Z_B^+ - Z_B^-), \\ Z_F^{\pm} &\equiv \mathrm{Tr}\,(e^{-\beta H^{\pm}_{XY}}) = e^{-\beta E_0^{\pm}} \mathrm{Det}\, [(i\omega_F - E_q)\delta_{pp'}], \\ Z_B^{\pm} &\equiv \mathrm{Tr}\,((-1)^{\mathcal{N}} e^{-\beta H^{\pm}_{XY}}) = e^{-\beta E_0^{\pm}} \mathrm{Det}\, [(i\omega_B - E_q)\delta_{pp'}], \end{aligned} \tag{18}$$

where

$$E_0^{\pm} \equiv -\frac{1}{2} \sum_{q \in X^{\pm}} E_q, \quad E_q = (\varepsilon_q^2 + \gamma^2 \sin^2 q)^{1/2}.$$

Thus, let us turn, for a generality, to regularization of (18) instead of (17).

We shall begin with the introductory notes. Usually, a generalized ζ-function is related to an elliptic operator. Precisely, let $\mathcal{A}$ be a non-negative elliptic operator of order $p > 0$ on a compact d-dimensional smooth manifold. Let its eigen-values λ_n being ennumerated by the multi-index n. The series

$$\zeta(s \mid \mathcal{A}) = \sum_{\lambda_n \neq 0} (\lambda_n)^{-s}, \tag{19}$$

which is convergent at $\Re s > d/p$, defines the generalized ζ-function of the operator $\mathcal{A}$. This series defines $\zeta(s \mid \mathcal{A})$ as the meromorphic function of the variable $s \in \mathbb{C}$, which can be analytically continued to $s = 0$. The formal relation

$$\lim_{s \to 0} \frac{d\zeta}{ds}(s \mid \mathcal{A}) = \lim_{s \to 0} \left[- \sum_{\lambda_n \neq 0} \frac{\log \lambda_n}{(\lambda_n)^s} \right] = -\log \left(\prod_{\lambda_n \neq 0} \lambda_n \right)$$

allows to define a regularized determinant of $\mathcal{A}$ as follows:

$$\log \mathrm{Det}\, \mathcal{A} = -\zeta'(0 \mid \mathcal{A}). \tag{20}$$

The Riemann ζ-function,

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s}, \quad \Re s > 1, \tag{21}$$

and the generalized ζ-function,

$$\zeta(s, \alpha) = \sum_{n=0}^{\infty} (n+\alpha)^{-s}, \quad \alpha \neq 0, -1, -2, \ldots, \tag{22}$$

which are meromorphic in s, have a simple pole at $s = 1$ with residue 1, and possess a continuation at $s = 0$ [28], can be formally considered as particular cases of $\zeta(s \mid \mathcal{A})$ (19). Notice that $\zeta\left(s, \frac{1}{2}\right)$ is the Gurvitz ζ-function, and $\zeta(s, 1) = \zeta(s)$.

Starting with (19), one can represent $\zeta(s \mid \mathcal{A})$ as a Mellin transform:

$$\zeta(s \mid \mathcal{A}) = \frac{1}{\Gamma(s)} \int_0^{\infty} t^{s-1} [\mathrm{Tr}\,(e^{-\mathcal{A}t}) - \dim(\ker \mathcal{A})] dt. \tag{23}$$

The integral (23) is defined at sufficiently large positive $\Re s$ (precisely, at $\Re s > d/p$); for other $\Re s$ its analytic continuation is required. The formula (23) can be related [21, 22] to the definition of $\mathrm{Det}\, \mathcal{A}$ by means of the proper time regularization [29]:

$$\log \frac{\mathrm{Det}\, \mathcal{A}}{\mathrm{Det}\, \mathcal{A}_0} = \mathrm{Tr}\, \left[\int_0^{\infty} (e^{-\mathcal{A}_0 t} - e^{-\mathcal{A}t}) \frac{dt}{t} \right]. \tag{24}$$

The definitions by means of (20), (23), and by means of (24) coincide up to an infinite additive constant.

Now one can pass to the calculation of (18). Let us define the following series, which can be expresed through $\zeta(s, \alpha)$ (22):

$$\begin{aligned} \zeta_F^{\pm}(s \mid A) &\equiv \sum_{\omega_F, q \in X^{\pm}} (i\omega_F - E_q)^{-s} \\ &= \left(\frac{\beta}{2\pi i}\right)^s \sum_{q \in X^{\pm}} \left[\zeta\left(s, \frac{1}{2} + i\frac{\beta E_q}{2\pi}\right) + (-1)^s \zeta\left(s, \frac{1}{2} - i\frac{\beta E_q}{2\pi}\right) \right], \end{aligned} \tag{25}$$

$$\begin{aligned} \zeta_B^{\pm}(s \mid A) &\equiv \sum_{\omega_B, q \in X^{\pm}} (i\omega_B - E_q)^{-s} \\ &= \left(\frac{\beta}{2\pi i}\right)^s \sum_{q \in X^{\pm}} \left[\zeta\left(s, i\frac{\beta E_q}{2\pi}\right) + (-1)^s \zeta\left(s, -i\frac{\beta E_q}{2\pi}\right) \right] - \sum_{q \in X^{\pm}} (-E_q)^{-s}. \end{aligned} \tag{26}$$

The analytic continuations for $\zeta(s, z)$ are known [28]:

$$\zeta(0, z) = \frac{1}{2} - z, \quad \zeta'(0, z) = \log \frac{\Gamma(z)}{(2\pi)^{1/2}}, \tag{27}$$

and they lead to the following answers:

$$
\begin{aligned}
-\lim_{s\to 0}\frac{d}{ds}\,\zeta_F^{\pm}(s\mid A) &= \sum_{q\in X^{\pm}}\log(1+e^{c\beta E_q}),\\
-\lim_{s\to 0}\frac{d}{ds}\,\zeta_B^{\pm}(s\mid A) &= \sum_{q\in X^{\pm}}\log(1-e^{c\beta E_q}),
\end{aligned}
\tag{28}
$$

where $c=\pm 1$ due to an arbitrariness when differentiating $(-1)^s=\exp(\pm i\pi s)$. The series $\zeta_F^{\pm}(s\mid A)$ and $\zeta_B^{\pm}(s\mid A)$ should be considered as the generalized ζ-functions of the diagonal operators A in the series form (19).

Choosing $c=-1$, and combining (28) with (20), one obtains the following relations of the XY-model [9, 10]:

$$
\begin{aligned}
Z_F^{\pm} &= e^{-\beta E_0^{\pm}}\prod_{q\in X^{\pm}}(1+e^{-\beta E_q}) = \prod_{q\in X^{\pm}} 2\cosh\frac{\beta E_q}{2},\\
Z_B^{\pm} &= e^{-\beta E_0^{\pm}}\prod_{q\in X^{\pm}}(1-e^{-\beta E_q}) = \prod_{q\in X^{\pm}} 2\sinh\frac{\beta E_q}{2}.
\end{aligned}
\tag{29}
$$

The total partition function should be calculated accordingly to (5), the free energy is $F=-(1/\beta M)\log Z$, while arbitrariness in the choice of c does not influence the magnetization $M_z=-\partial F/\partial h$ and the entropy $S=-\partial F/\partial T$. Specifically, one gets in the thermodynamic limit:

$$
F=-\frac{1}{2\pi\beta}\int_0^{\pi}\log(2(1+\cosh\beta E_q))dq. \tag{30}
$$

All the formulas obtained can be reduced at $\gamma\to 0$ to the XX-model.

5 Determinats of the operators $A(\alpha)$

5.1 The regularization

Thus, in the previous section we have defined ζ-functions of the diagonal operators A (17), (18) in the series form. Let us now use (23) to calculate the regularized determinants of the non-diagonal operators $A(\alpha)$ (16). For instance, let us calculate $G_F^{\pm}$ (16.1).

Let us begin with the formal integral

$$
\frac{1}{\Gamma(s)}\int_0^{\infty} t^{s-1}\mathrm{Tr}\,\left[e^{(i\omega_F-\widehat{\varepsilon}+\frac{\alpha}{\beta}\widehat{Q})t}\right]dt, \tag{31}
$$

where $\widehat{\varepsilon}$ and $\widehat{Q}$ imply the matrices in the momentum space, diag $\{\varepsilon_q\}$ and $Q_{pq}^{(0)}$ (15.2), accordingly, while the indices p, q run independently over X^+ or X^-. Convergence of the integral (31) at the upper bound is respected at $h>h_c=1$ (h_c is the critical magnetic field [4]). Regularization is necessary at the lower bound.

Let us use the asymptotical relation

$$
\mathrm{Tr}\,\left[e^{(i\omega_F-\widehat{\varepsilon}+\frac{\alpha}{\beta}\widehat{Q})t}\right]\underset{t\to 0}{\longrightarrow}\phi_0,
$$

where $\phi_0 \equiv \phi_0(A_\alpha)$ is an infinite constant equal to $\mathrm{Tr}\,(\delta_{pp'}) \equiv \sum_{\omega_F} \mathrm{tr}\,(\widehat{\delta})$ ($\widehat{\delta}$ is a unit $M \times M$ matix). Let us define the function $\rho(t)$:

$$\rho(t) \equiv \mathrm{Tr}\,\left[e^{(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta}\widehat{Q})t}\right] - \phi_0, \quad t \in [0,1[\,, \tag{32}$$

and divide the integral (31) into two parts. We rewrite (31) using (32) as follows:

$$\frac{1}{\Gamma(s)} \int_1^\infty t^{s-1} \mathrm{Tr}\,\left[e^{(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta}\widehat{Q})t}\right] dt + \frac{1}{\Gamma(s)} \int_0^1 t^{s-1} \rho(t) dt + \frac{\phi_0}{s\Gamma(s)}. \tag{33}$$

The function $\rho(t)$ is a formal series in powers of t^n, $n \geq 1$. Besides,

$$\frac{1}{s\Gamma(s)} \simeq 1 + \gamma s + o(s), \quad \gamma = -\psi(1), \tag{34}$$

where $\psi(z) = (d/dz)\log\Gamma(z)$. Therefore, (33), which is regular at $s \to 0$, defines an analytic continuation of (31) at any $\Re s \geq 0$. It just can be considered as the definition of $\zeta_F^{\pm}(s \mid A_\alpha)$ in the right half-plane of $\mathbb{C} \ni s$.

Let us now consider the constant ϕ_0 and the coefficients which define $\rho(t)$. These numbers turn out to be nonzero for differential operators on manifolds [22]. In our situation all these coefficients are infinite, but finite values can be assigned to them by means of (21), (22).

First of all, using $\zeta(0) = -\frac{1}{2}$ one obtains:

$$\phi_0 = M \sum_{\mathbb{Z}} 1 = M(2\zeta(0) + 1) = 0,$$

where $\sum_{\mathbb{Z}}$ can equivalently be replaced by $\sum_{\mathbb{Z}+\frac{1}{2}}$, and $2\zeta(0)+1$ – by $2\zeta\left(0, \frac{1}{2}\right)$ ("ζ-regularized measure" of the set $\mathbb{Z}$ is zero). Further, the divergence of the coefficients at the powers of t in $\rho(t)$ is given by the divergent sums

$$\sum_{n \in \mathbb{Z}+\frac{1}{2}} n^m.$$

It is reasonable to consider such sums as zeros at $m = 2k+1$, $k \in \mathbb{Z}^+$, since $\left(l + \frac{1}{2}\right)^m$ are odd. If $m = 2k$, $k \in \mathbb{Z}^+$, then

$$\sum_{n \in \mathbb{Z}+\frac{1}{2}} n^m = 2 \sum_{l=0}^{\infty} \left(l + \frac{1}{2}\right)^m = 2\zeta\left(-2k, \frac{1}{2}\right) = 2\left(\frac{1}{2^{2k}} - 1\right)\zeta(-2k).$$

But $\zeta(-2k) = 0$ at $k \geq 1$. It can be concluded that "ζ-regularized" coefficients are zero for $A(\alpha)$, and, thus, only the first term is relevant in (33).

Let use (34) to pass from (33) to the relation:

$$-\lim_{s \to 0} \frac{d}{ds} \zeta_F^{\pm}(s \mid A_\alpha) = -\int_1^\infty \mathrm{tr}\,\left[e^{(-\widehat{\varepsilon} + \frac{\alpha}{\beta}\widehat{Q})t}\right] \left(\sum_{\omega_F} e^{i\omega_F t}\right) \frac{dt}{t} - \int_0^1 \rho(t) \frac{dt}{t} - \gamma\phi_0, \tag{35}$$

where the Poisson formula enables to sum up over ω_F. Then, R.H.S. of (35) takes the form:

$$-\mathrm{tr}\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\left(e^{-\beta\widehat{\varepsilon}+\alpha\widehat{Q}}\right)^k-\int_0^1\rho(t)\frac{dt}{t}-\gamma\phi_0$$

$$=\log\det\left(1+e^{-\beta\widehat{\varepsilon}+\alpha\widehat{Q}}\right)-\int_0^1\rho(t)\frac{dt}{t}-\gamma\phi_0.$$

Let us also take into account that $\widehat{Q}^2=\widehat{Q}$, and so $e^{\alpha\widehat{Q}}-1=(e^{\alpha}-1)\widehat{Q}$. Therefore,

$$G_F^{\pm}=\frac{\mathrm{Det}\,\left[(i\omega_F-\varepsilon_q)\delta_{pp'}+\frac{\alpha}{\beta}\,\delta_{\omega\omega'}Q^{(0)}_{qq'}\right]}{\mathrm{Det}\,\left[(i\omega_F-\varepsilon_q)\delta_{pp'}\right]}=\det\left[1+(e^{\alpha}-1)\widehat{Q}(1+e^{\beta\widehat{\varepsilon}})^{-1}\right]. \qquad (36)$$

Additional renormalization of $\rho(t)$ and ϕ_0 (to zero, in fact) is irrelevant for $G_F^{\pm}$, i.e., for the ratio of the determinants. However, when $m=M$, the corresponding operator A_α becomes diagonal since $\widehat{Q}$ becomes the unit matrix $\widehat{\delta}$. In this case, we can consider ζ-function in the series form (19). Transparent adjusting of (25)–(28) at $m=M$ gives the same answer as (35) with $\rho(t)$ and ϕ_0 being zero.

In an analogous way we obtain:

$$G_B^{\pm}=\det\left[1+(e^{\alpha}-1)\widehat{Q}(1-e^{\beta\widehat{\varepsilon}})^{-1}\right].$$

It should be pointed out that, say, $G_F^{\pm}$ (36) (i.e., the ratio of two Det 's) can be regularized in a way looking more conventionally:

$$G_F^{\pm}=\mathrm{Det}\,\left[\delta_{pp'}+\frac{\alpha}{\beta}\,\frac{\delta_{\omega\omega'}Q^{(0)}_{qq'}}{i\omega_F-\varepsilon_q}\right]. \qquad (37)$$

Using the series formula

$$\log G_F^{\pm}(\alpha)=\mathrm{Tr}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k}\,\left[\frac{\alpha}{\beta}\,\frac{\delta_{\omega\omega'}Q^{(0)}_{qq'}}{i\omega_F-\varepsilon_q}\right]^k$$

to calculate (37) one can check that (36) and (37) have the same numerical coefficients at the powers of α.

5.2 Differentiation of the determinants

It is necessary to differentiate the generating function (1) over α at $\alpha=0$ when calculating the correlators of third components of spins (the operator of third component of spin, $\sigma_z^{(m)}$, is defined as σ_z at mth site) as follows [1, 4]:

$$\lim_{\alpha\to 0}\frac{d^n}{d\alpha^n}\,G(m).$$

In fact, with regard at (31), it is suffice to do only a first differentiation. The other ones would occur as usual differentiations of matrices [30].

The operator in question, $A(\alpha)$, is linear in α: $A(\alpha) \equiv A_1 + \alpha A_2$. Let us calculate the first derivative of Det $A(\alpha)$ using the formal integral (33):

$$\frac{(d/d\alpha)\mathrm{Det}\, A(\alpha)}{\mathrm{Det}\, A(\alpha)} = -\frac{d}{d\alpha}\left(\int_0^\infty \mathrm{Tr}\,(e^{A(\alpha)t})\frac{dt}{t}\right) \tag{38}$$

(the regularization at $t \searrow 0$ is irrelevant for the differentiation over the parameter). In the spirit of the Ray–Singer–Schwarz lemma [31], we shall use in (38) the following relation:

$$\frac{d}{d\alpha}\Big(\mathrm{Tr}\,(e^{A(\alpha)t})\Big) = t\frac{d}{dt}\,\mathrm{Tr}\,\Big(B(\alpha)e^{A(\alpha)t}\Big), \quad B(\alpha) \equiv A_2 A^{-1}(\alpha).$$

Then, the integral over t can be calculated, and one obtains:

$$\frac{(d/d\alpha)\mathrm{Det}\, A_\alpha}{\mathrm{Det}\, A_\alpha} = \mathrm{Tr}\, B(\alpha)$$

$$= \mathrm{Tr}\,\left(\frac{\widehat{Q}}{\beta}(i\omega_F - \widehat{\varepsilon} + \frac{\alpha}{\beta}\widehat{Q})^{-1}\right) = \mathrm{tr}\,\Big(\widehat{Q}(1+e^{\beta\widehat{\varepsilon}-\alpha\widehat{Q}})^{-1}\Big), \tag{39}$$

where the Cauchy formula for matrices [30] is used to sum up over the frequencies. Knowing (39), one can calculate all the differentiations required:

$$\lim_{\alpha\to 0}\frac{(d/d\alpha)\mathrm{Det}\, A_\alpha}{\mathrm{Det}\, A_\alpha} = \mathrm{tr}\,\Big(\widehat{Q}(1+e^{\beta\widehat{\varepsilon}})^{-1}\Big),$$

$$\lim_{\alpha\to 0}\frac{(d^2/d\alpha^2)\mathrm{Det}\, A_\alpha}{\mathrm{Det}\, A_\alpha} = \mathrm{tr}\,\Big(\widehat{Q}(1+e^{\beta\widehat{\varepsilon}})^{-1}\Big) + \tag{40}$$

$$+\mathrm{tr}^{\,2}\Big(\widehat{Q}(1+e^{\beta\widehat{\varepsilon}})^{-1}\Big) - \mathrm{tr}\,\Big(\widehat{Q}(1+e^{\beta\widehat{\varepsilon}})^{-1}\widehat{Q}(1+e^{\beta\widehat{\varepsilon}})^{-1}\Big),$$

etc.

To conclude the section, let us use the formulas obtained to calculate the correlators $\langle\sigma_z^{(m)}\rangle$ and $\langle\sigma_z^{(m+1)}\sigma_z^{(1)}\rangle$. To this end, let us rewrite (40):

$$\langle Q(m)\rangle = \frac{m}{M}\sum_q (1+e^{\beta\varepsilon_q})^{-1}, \tag{41}$$

$$\langle Q^2(m)\rangle = \frac{m}{M}\sum_q (1+e^{\beta\varepsilon_q})^{-1} + \frac{m^2}{M^2}\left[\sum_q (1+e^{\beta\varepsilon_q})^{-1}\right]^2 -$$

$$-\sum_{p,q}\Big(Q_{pq}^{(0)}\Big)^2 (1+e^{\beta\varepsilon_p})^{-1}(1+\varepsilon^{\beta\varepsilon_q})^{-1}. \tag{42}$$

One obtains from (41) in the thermodynamic limit:

$$\sigma_z \equiv \langle\sigma_z^{(m)}\rangle = 1 - \frac{1}{\pi}\int_{-\pi}^{\pi}\frac{dq}{1+e^{\beta\varepsilon_q}}, \tag{43}$$

where the definitions

$$\langle\sigma_z^{(m)}\rangle = 1 - 2\mathcal{D}_1\langle Q(m)\rangle$$

and $\mathcal{D}_1 f(m) = f(m) - f(m-1)$ are used. The result (43) agrees with the magnetization $\mathcal{M}_z = -\partial F/\partial h$, which is calculated by means of F (30). We obtain from (42) ($m > 0$):

$$\langle \sigma_z^{(m+1)} \sigma_z^{(1)} \rangle = \sigma_z^2 - \frac{1}{\pi^2} \left| \int_{-\pi}^{\pi} \frac{e^{imq}}{1 + e^{\beta \varepsilon_q}} \, dq \right|^2 ,$$

where the definitions

$$\langle \sigma_z^{(m+1)} \sigma_z^{(1)} \rangle = 2\mathcal{D}_2 \langle Q^2(m) \rangle + 2\sigma_z - 1$$

and $D_2 f(m) = f(m+1) - 2f(m) + f(m-1)$ are used. The answers obtained reproduce correctly the result of [4], and, thus, they witness in favour of the strategy chosen which stems from the functional definition (11.3), (13).

6 Discussion

The path integral representations for the partition function and for the generating function of static correlators of third components of spins in the XX Heisenberg chain are obtained in the present paper. The present paper is close to [14], where a path integration with "automorphic" boundary conditions has been used to calculate traces of some operators in the index theory, and to [25] where the partition functions of spin 1 and 1/2 chain models have been also obtained in the form of path integrals over variables subjected to "automorphic" boundary conditions. The distinction between [14, 25] and the present paper consists in the fact that the "automorphic" boundary conditions appear only for a part of sites (several first ones) of the chain model in question. It is interesting that the situation, when only a part of the lattice variables is subjected to the unusual boundary conditions in imaginary time, can successively be handled.

The path integrals in question are regularized by means of zeta-regularization. It is demonstrated that, from a practical viewpoint (i.e., if only differentiations over the parameter α are needed), the formula for the first derivative of the generating function can be obtained without regularization of the Mellin integral at the lower bound.

The paper provides further development of the technical finds discussed in [14] and [25], and it can be useful in practical calculations for other models where vacuum averages (traces) of operator exponentials similiar to our $\exp(\alpha Q(m))$ are of importance.

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