QUANTUM SPIN CHAINS AT FINITE TEMPERATURES

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This is a pedagogical review on recent progress in the exact evaluation of physical quantities in interacting quantum systems at finite temperatures. 1D quantum spin chains are discussed in detail as typical examples.

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1. Introduction

The evaluation of the thermal average of physical quantities is one of the main aims in statistical mechanics. The density matrix of a system is the most fundamental quantity to achieve this aim. Its diagonalization, however, becomes exponentially difficult with growing system size $L$. One inevitably has to give up this procedure in the thermodynamic limit. An alternative approach for quantum systems is to diagonalize the Hamiltonian, and to sum up the contributions from each eigenstate. This means to divide the problem into two parts: (1) diagonalize, and (2) sum up. Again, both procedures become exponentially difficult with the increase of $L$.

In this article we re-consider this problem for integrable quantum spin chains. We will show how the integrability helps bypassing the difficulties and yields exact estimates. The first problem, the diagonalization of the Hamiltonian, can, in principle, be solved by the celebrated Bethe ansatz. The second step, however, remains as a cliff wall. A first breakthrough, the string hypothesis approach, was achieved in the early 70’s.\textsuperscript{1,2} In this approach one introduces so-called root density functions of strings and holes of various lengths for the diagonalization. The free energy becomes a func-
tional of these density functions, which is claimed to be exact near its minimum. Therefore the variational estimate (w.r.t. density functions), with a fixed energy of the system, yields the exact free energy. The string hypothesis formulation can be regarded as a micro-canonical approach. It is supported by many consistency tests. We conclude that within the string hypothesis approach the diagonalization is achieved, but the summation is cleverly avoided.

In order to evaluate thermal expectation values of operators, it is better to deal with the canonical ensemble. We therefore consider an alternative approach based on the Quantum Transfer Matrix (QTM).\(^4,5\) It utilizes an exact mapping between a 1D quantum system at finite temperatures and a 2D classical system. At first sight the formulation may look tautological and may seem to be suffering from the need of “summation”. Yet, the main claim of the QTM formulation is that this is not the case. As in the the string hypothesis approach the “summation” can be avoided. Moreover, the QTM makes the evaluation of many quantities of physical relevance straightforward.

This article is organized as follows. In Sec. 2, we present a review on the QTM formulation. The results for the bulk quantities will be summarized in Sec. 2.3. In the rest of Sec. 2, we supplement arguments to justify the formula in Sec. 2.3. The non-linear integral equation (NLIE) will be explained in Sec. 3 together with an example for the explicit evaluation of bulk quantities. The evaluation of the reduced density matrix elements (DME) will be discussed in Sec. 4.

2. The QTM formulation

2.1. The problem

Let \( \mathcal{H} \) be the Hamiltonian of a 1D quantum system of size \( L \) and \( V \) its space of states. Our goal is to calculate the thermal expectation value of any physical quantity \( \mathcal{O} \) at temperature \( T(=1/\beta) \) in the limit \( L \to \infty \),

\[
\langle \mathcal{O} \rangle = \lim_{L \to \infty} \frac{\text{tr}_V \mathcal{O} e^{-\beta \mathcal{H}}}{Z_{1D}(\beta)} = \frac{Z_{1D}(\beta)}{\text{tr}_V e^{-\beta \mathcal{H}}} = \sum_j e^{-\beta E_j}.
\]

Here \( E_j \) stands for an eigenvalue of \( \mathcal{H} \).

The definition requires both diagonalization and summation. Below we shall show how we can avoid the latter within the framework of QTM.

\( ^a \)The Boltzmann constant \( k_B \) is set to be unity in this report.
2.2. The Baxter-Lüscher formula

To be concrete, we specify a Hamiltonian. As a prototypical integrable lattice system we choose the 1D spin \( \frac{1}{2} \) XXZ model,

\[
\mathcal{H} = J \sum_{j=1}^{L} \left( \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta (\sigma_j^z \sigma_{j+1}^z + 1) \right) = \sum_{j=1}^{L} \hat{h}_{j,j+1}
\]

where the \( \sigma^a \) (\( a = x, y, z \)) are the Pauli matrices. The periodic boundary conditions (PBCs) imply \( \sigma^a_{L+1} = \sigma^a_1 \). The anisotropy is parameterized as \( \Delta = \cos \gamma \). The Hamiltonian acts on “the physical space” \( V_{\text{phys}} \equiv \bigotimes_{j=1}^{L} V_j \) where \( V_j \) denotes the \( j \)th copy of a two-dimensional vector space \( c_1 e_+ + c_2 e_- \). The trace in (1) must be performed over \( V_{\text{phys}} \). By definition the “Hamiltonian density” \( \hat{h}_{j,j+1} \) is the \( j \)th summand in the first sum in (2). It acts non-trivially only on \( V_j \otimes V_{j+1} \).

The above Hamiltonian is integrable in the following sense. Let \( R(u,v) \) be the \( U_q(\hat{sl}_2) \) R matrix,

\[
R(u,v) = \begin{pmatrix}
1 + \frac{u-v}{2} & \frac{[u-v]}{2} & \frac{-q+u}{q-v} & \frac{-q}{q-1}
\end{pmatrix}
\]

depending on the spectral parameters (or rapidities) \( u, v \in \mathbb{C} \). We define \( E^\alpha_{\beta} \) s.t. \( (E^\alpha_{\beta})_{i,j} = \delta_{\alpha,i} \delta_{\beta,j} \). Then the matrix elements \( R^{\alpha \gamma}_{\beta \delta} \) can be read off from

\[
R(u,v) = \sum_{\alpha, \beta, \gamma, \delta = 1, 2} R^{\alpha \gamma}_{\beta \delta} (u,v) E^\alpha_{\beta} \otimes E^\gamma_{\delta}.
\]

The index 1(2) refers to \( e_+ (e_-) \). See fig. 1 for a graphic representation. We put arrows, to distinguish the \( R \) matrix from other \( R \) matrices appearing below. The reader should not confuse them with physical variables.
By $R_{j,j+1}(u,v)$ we mean the $R$ matrix acting non-trivially only on the tensor product $V_j(u) \otimes V_{j+1}(v)$ of $U_q(\hat{sl}_2)$ modules. We also introduce the intertwiner $R'_{j,j+1}(u,v) = P_{j,j+1}R_{j,j+1}(u,v)$, where $P : V_j(u) \otimes V_{j+1}(v) \to V_{j+1}(v) \otimes V_j(u)$. Then, with $q = e^{i\gamma}$, we have the expansion
\[
R'_{j,j+1}(u,0) = 1 + \frac{\gamma}{4J \sin\gamma} u (\hat{h}_{j,j+1} + \hat{h}'_{j,j+1}) + O(u^2),
\]
where $\hat{h}'_{j,j+1} := iJ \sin \gamma (\sigma^z_j - \sigma^z_{j+1})$. We introduce the row-to-row (RTR) transfer matrix $T_{\text{RTR}}(u) \in \text{End}(V_{\text{phys}})$,
\[
T_{\text{RTR}}(u) = \text{tr}_{a} R_{a,L}(u,0) R_{a,L-1}(u,0) \cdots R_{a,1}(u,0).
\]
With the lattice translation operator $e^{iP}$, shifting the state by one site, we obtain the Baxter-Lüscher formula
\[
T_{\text{RTR}}(u) = e^{iP} (1 + \frac{\gamma u}{4J \sin\gamma} \hat{H} + O(u^2)).
\]
Note that the $\hat{h}'_{j,j+1}$ terms cancel due to the PBCs. The huge symmetry $U_q(\hat{sl}_2)$ is at the bottom of the integrability of the Hamiltonian.

### 2.3. A summary of results for bulk quantities

We first present the formula for the free energy per site in the QTM formalism. A supplemental discussion will be given in subsequent sections.

We introduce the transposed $R$ matrix $R^t_{j,k}(u,v)^7$ by $(R^t)^{\alpha\gamma}_{\beta\delta}(u,v) = R^{\beta\alpha}_{\gamma\delta}(v,u)$. See fig. 2. The QTM does not act on $V_{\text{phys}}$ but on a fictitious space $V_{\text{Trotter}} = V_1(u) \otimes V_2(-u) \otimes \cdots V_{N-1}(u) \otimes V_N(-u)$. The fictitious system size $N$ is often referred to as the Trotter number. The parameter $u$ is fixed to be
\[
u = -\frac{4\beta J \sin\gamma}{\gamma N} = -\frac{4J \sin\gamma}{\gamma NT}.
\]
In its most sophisticated version, the QTM is explicitly defined by,
\[
T_{\text{QTM}}(x,u) = \text{tr}_{a} R_{a,N}(ix,-u) R^t_{a,N-1}(ix,u) \cdots R_{a,2}(ix,-u) R^t_{a1}(ix,u).
\]
The new parameter $x$ will later play the role of a spectral parameter. The factor $i$ is introduced for convenience.

We are now in a position to write down the formula for the free energy per site in the thermodynamic limit, $f = -\lim_{L \to \infty} \frac{T}{L} \ln Z_{1D}(\beta)$.

**Theorem 2.1.** Let $\Lambda_0$ be the largest eigenvalue of $TQT M(0,u)$. Then the free energy per site is solely given by $\Lambda_0$,

$$f = -\lim_{N \to \infty} T \ln \Lambda_0. \quad (6)$$

The limit $N \to \infty$ is referred to as the Trotter limit. As was announced earlier, eq. (6) expresses $f$ without recourse to any summation. We also note that $\ln \Lambda_0$ itself is already intensive, which may reflect the size dependent interaction of the system.

The quantitative analysis of (6) is most efficiently performed by means of the NLIE. Having in mind the examples, from now on we are considering only for $J = \frac{1}{4}$, $\gamma \to 0$ and $u = -\frac{2}{N}$, consequently. Let $a$ be the unique solution to the NLIE,

$$\ln a(x) = \beta \epsilon_0(x + i) - \int_C \frac{2}{(x - y)^2 + 4} \ln A(y) \frac{dy}{\pi} \quad (7)$$

$$\epsilon_0(x) = h + \frac{2}{(x - i)(x + i)} \quad A := 1 + a.$$

Here the contour $C$ is a closed narrow loop which encircles all “Bethe roots”. We added a Zeeman term $\frac{1}{4} \sum_j \sigma_j^z$ to the Hamiltonian so that $\text{diag}(\exp(-\beta h), \exp(\beta h))$ is inserted in the trace in (5). Then we have the following

**Theorem 2.2.** The free energy per site can be evaluated in terms of the solution to the NLIE,

$$\beta f = \frac{\beta}{2}(1 + h) - \int_C \frac{1}{x(x + 2i)} \ln A(x) \frac{dx}{\pi}. \quad (8)$$

Note that the NLIE (7) and the expression for $f$ in (8) are independent of $N$. The extension to arbitrary $J, \gamma$ is straightforward.

Below we shall comment on the derivation of the formula. By presenting supplementary arguments, we wish to convince the reader that the above formalism, seemingly complicated, is actually necessary and efficient for many purposes. Hereafter we set again $h = 0$ for simplicity.

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To be precise, there are, in general, several equivalent versions of NLIEs. We present one of these below.
2.4. The 1D quantum partition function as a 2D classical partition function

We define a rotated R matrix \( \tilde{R}(u, v) \) by \( \tilde{R}_{\alpha\gamma}^{\beta\delta}(u, v) = R_{\delta\gamma}^{\beta\alpha}(v, u) \) (fig. 3). Then we introduce a rotated transfer matrix \( \tilde{T}_{RTR}(u) \in \text{End}(V_{\text{phys}}) \) by

\[
\tilde{T}_{RTR}(u) = \text{tr}_{a} \tilde{R}_{a,L}(-u, 0) \tilde{R}_{a,L-1}(-u, 0) \cdots \tilde{R}_{a,1}(-u, 0).
\]

Analogous to (4) \( \tilde{T}_{RTR}(u) = e^{-iP(1 + uH + O(u^2))} \). We thus obtain an important identity,

\[
Z_{1D}(\beta) = \lim_{N \to \infty} \text{tr}_{V_{\text{phys}}} \left( T_{\text{double}}(u) \right)^{\frac{N}{2}} \bigg|_{u \to -\frac{\beta}{N}} \quad (9)
\]

where \( T_{\text{double}}(u) := T_{RTR}(u) \tilde{T}_{RTR}(u) \). The rhs of (9) can be interpreted as a partition function of a 2D classical system defined on \( N \times L \) sites (fig. 4),

\[
Z_{1D}(\beta) = \lim_{N \to \infty} Z_{\text{2D classical}}(N, L, u = -\frac{\beta}{N}).
\]

This equivalence lies in the heart of the QTM formalism. The expression (9) itself, however, is of no direct use for the actual evaluation of physical quantities for the following reason. Let the eigenvalue spectrum of \( T_{RTR}(u) \) be \( \lambda_0(x) > \lambda_1(x) \geq \lambda_2(x) \geq \cdots \). We introduced \( x = i^{-1}(u + 1) \) for technical reasons. It is easy to see that \( \tilde{T}_{RTR}(u) \) has the same spectrum. Thus,

\[
\text{tr}_{V_{\text{phys}}} \left( T_{\text{double}}(u) \right)^{\frac{N}{2}} = \left( \lambda_0(x) \right)^{N} \left( 1 + \left( \frac{\lambda_1(x)}{\lambda_0(x)} \right)^{N} + \left( \frac{\lambda_2(x)}{\lambda_0(x)} \right)^{N} + \cdots \right). \quad (10)
\]

The eigenvalue \( \lambda_{j}(x) \) is characterized by its zeros \( \pm \theta_{a} (a = 1, 2, \ldots) \) on the real axis (holes). We know numerically that for low excitations, \( \theta_{a} \sim \ln L \) and also that \( \lambda_{j}(x) \) is analytic and nonzero in the strip \( |\Re x| \leq 1 \) except at \( \pm \theta_{a} \). Let us introduce an analytic and nonzero function near the real axis, \( \lambda_{j}^{\Sigma}(x) = \prod_{a} \text{th} \left( \frac{x - \theta_{a}}{2} \right) \text{th} \left( \frac{x + \theta_{a}}{2} \right) \lambda_{j}^{\Sigma}(x) \). It approximately satisfies the inversion relation for \( L \gg 1 \),

\[
\lambda_{j}^{\Sigma}(x - i)\lambda_{j}^{\Sigma}(x + i) = \phi(x), \quad (11)
\]
where φ(x) is a known function common to any j. Thus, we simply have
\[ \left| \frac{\lambda_j(x)}{\lambda_0(x)} \right| = \left| \prod_a \text{th} \left( \frac{\pi}{4}(x - \theta_a) \text{th} \left( \frac{\pi}{4}(x + \theta_a) \right) \right) \right|. \]

For very low excitations, we take a single pair of holes, substitute \( \theta_a \sim \frac{2}{\pi} \ln \frac{2\pi L}{L_j} \) and take the large \( L \) limit. Then we arrive at the estimate (\( u \sim 0 \))
\[ \left| \frac{\lambda_j(x)}{\lambda_0(x)} \right| \sim e^{-|u|} \text{th} \left( \frac{\pi}{4} \right) \text{th} \left( \frac{\pi}{4} \right) \sim e^{-\Delta_j \frac{\pi}{4} |u|}. \]  

(12)

For a usual 2D classical system we can consider an infinitely long cylinder and take \( N L \gg 1 \). We thus have to take into account only the first term on the rhs in (10). By contrast, the spectral parameter depends on the fictitious system size \( u = -\frac{\beta}{N} \) in the present case. Therefore, as long as \( T \neq 0 \), we have
\[ \left| \frac{\lambda_j(x)}{\lambda_0(x)} \right| \sim e^{-\frac{\Delta_j \pi}{4} |u|} \sim e^{-\Delta_j \frac{\pi}{4} N L}, \]

(12)

Fig. 5 presents numerical evidence for the above argument. The left figure shows the histogram of the distribution of \( |\lambda_j/\lambda_0| \) for \( q = 1, L = 10, u = -0.01 \) in the sector with vanishing magnetization. One clearly sees that the maximum of the distribution lies near \( |\lambda_j/\lambda_0| \sim 1 \). The right figure magnifies the region near \( |\lambda_j/\lambda_0| \sim 1 \). The maximum is located around \( |\lambda_j/\lambda_0| \sim 0.96 \). We believe that, with increasing \( L \), the peak moves towards \( |\lambda_j/\lambda_0| \sim 1 \). These findings are consistent with (12). Hence, we conclude that infinitely many terms of the sum in the rhs of (10) contribute non-trivially, and eq. (9) is of no practical use.
Fig. 5. The distribution of eigenvalues. The horizontal axis is the absolute value of the eigenvalues normalized by the largest one. The left figures ranges over [0,1] in the horizontal direction, and the right one is zoomed into the range [0.93,1].

2.5. **Commuting QTM**

A crucial observation was made in reference.\(^4\) We start from the same two-dimensional classical model in fig. 4. We consider, however, the transfer matrix propagating in horizontal direction, that is, \(T'_{\text{QTM}}(u)\). Equivalently, one can rotate the system by 90°. Then we define a transfer matrix propagating in vertical direction, \(T_{\text{QTM}}(u)\) (see fig. 2.5). The latter is more convenient for our formulation.

The partition function is then given by,

\[
Z_{1D}(\beta) = \lim_{N \to \infty} \text{tr}_{\text{V Trotter}} (T_{\text{QTM}}(u))^L \bigg|_{u=-\frac{\beta}{N}}.
\]

Let the eigenvalue spectrum of \(T_{\text{QTM}}(u)\) be \(\Lambda_0(u) > \Lambda_1(u) \geq \Lambda_2(u) \geq \cdots\). Then we have an expansion similar to (10)

\[
\text{tr}_{\text{V Trotter}} (T_{\text{QTM}}(u))^L = \left(\Lambda_0(u)\right)^L + \left(\frac{\Lambda_1(u)}{\Lambda_0(u)}\right)^L + \left(\frac{\Lambda_2(u)}{\Lambda_0(u)}\right)^L + \cdots.
\]
Our physical interest is in the free energy per site \( f \) in the thermodynamic limit \( L \to \infty \).

\[
f = -\frac{1}{\beta} \lim_{L \to \infty} \lim_{N \to \infty} \left\{ \ln \Lambda_0(u) + \frac{1}{L} \ln \left( 1 + \left( \frac{\Lambda_1(u)}{\Lambda_0(u)} \right)^L + \left( \frac{\Lambda_2(u)}{\Lambda_0(u)} \right)^L + \cdots \right) \right\} \bigg|_{u=-\frac{\beta N}{N}}.
\]

(15)

**Proposition 2.1.** *The two limits in (15) are exchangeable.*

We supplement an argument which claims that the second term in the second line in (15) is negligible for \( L \to \infty \). The previous argument, using the inversion relation (11) cannot be applied directly as the spectral parameter \( u \) is already fixed as \( -\frac{\beta N}{N} \) in the present problem.

We introduce a slight generalization, a commuting QTM \( T_{\text{QTM}}(x, u) \), by assigning the parameter \( i x \) in “horizontal” direction. The substitution \( x = 0 \) recovers the previous results. The precise definition is shown in (5).

Hereafter we drop the \( u \) dependence as it is always \( -\frac{\beta N}{N} \). Let \( T_{\text{QTM}}(x) \) be the corresponding monodromy matrix. Then it is easy to see that monodromy matrices are intertwined by the same \( R \) matrix as in the RTR case,

\[
R(x, x') T_{\text{QTM}}(x) \otimes T_{\text{QTM}}(x') = T_{\text{QTM}}(x') \otimes T_{\text{QTM}}(x) R(x, x').
\]

(16)

This immediately proves the commutativity of \( T_{\text{QTM}}(x) \) with different \( x \)’s.

The most important consequence of introducing \( x \) is that we have the inversion relation in this new “coordinate”,

\[
\Lambda_j^x(x - i) \Lambda_j^x(x + i) = \psi(x, u)
\]

(17)

where we set again \( \Lambda_j(x) = \prod_a \text{th} \left( \frac{x}{2} - \theta_a \right) \text{th} \left( \frac{x}{2} + \theta_a \right) \Lambda_j^x(x) \). Note that \( \Lambda_j^x(x) \) also depends on the “old” spectral parameter \( u \), which is set to be \( -\frac{\beta N}{N} \) on both sides. The known function \( \psi \) is again independent of \( j \). The analysis of the Bethe ansatz equation associated to the QTM implies that \( \theta_a \sim \frac{\beta}{2} \ln \frac{4}{\pi} \) for large \( \beta \). Then, proceeding as before, we obtain,

\[
\left| \frac{\Lambda_j(x)}{\Lambda_0(x)} \right| \sim e^{-\frac{\Delta_j}{\beta} \text{ ch} \frac{\pi x}{2}} \quad \text{thus} \quad \left| \frac{\Lambda_j(x)}{\Lambda_0(x)} \right|^L \sim e^{-\frac{\Delta_j L}{\beta} \text{ ch} \frac{\pi x}{2}}.
\]

The diagonalization for fixed \( N \) clearly shows the gap between the eigenvalues, which is consistent with the above argument. Thus, at any finite temperature, the second term in (15) is negligible for \( L \to \infty \). We then conclude that the formula (6) is valid.

Although we made use of the integrability of the model in the above argument, the validity of the formula is actually independent of it. See the proof in reference.\(^4\)
3. Diagonalization and NLIE

3.1. Bethe roots

Thanks to (16), one can apply the machinery of the quantum inverse scattering method, devised originally for the diagonalization of $T_{RTR}$, to the diagonalization of $T_{QTM}$. We skip the derivation and present only results relevant for our subsequent discussion\(^c\). We fix $N$ for a while. Then the eigenvalue of $T_{QTM}$ is given by

\[
\Lambda^{(N)}(x) = a(x) \frac{Q(x - 2i)}{Q(x)} + d(x) \frac{Q(x + 2i)}{Q(x)}
\]

\[
a(x) := \phi_{+}(x + 2i)\phi_{-}(x) \quad d(x) := \phi_{-}(x - 2i)\phi_{+}(x)
\]

\[
Q(x) := \prod_{j=1}^{m} (x - x_j) \quad \phi_{\pm}(x) := \left(\frac{x \pm u}{\pm 2i}\right)^{N/2}.
\]

The different sets of Bethe roots $\{x_j\}$ correspond to the different eigenvalues. They satisfy the Bethe ansatz equation (BAE),

\[
\frac{a(x_j)}{d(x_j)} = -\frac{Q(x_j + 2i)}{Q(x_j - 2i)} \quad 1 \leq j \leq m.
\]

For the largest eigenvalue the number of roots $m$ equals $N/2$.

To evaluate $f$ via (6) we need the largest $\Lambda^{(N)}$ for $N \to \infty$. This means we must deal with infinitely many roots in the limit, which resembles the situation encountered in the evaluation of the free energy in the thermodynamic limit of a classical 2D model by means of the RTR transfer matrix. Still, we would like to comment on the qualitative difference in the root distribution between such “standard” case and the problem under discussion.

Fig. 7 shows the distribution of the positive half of BAE roots for the largest eigenvalue of $T_{RTR}$ (left) and $T_{QTM}$ (right) for various system sizes. The distribution of RTR roots behaves smoothly for large system size. The limiting shape of the distribution (the root density function) is a smooth function satisfying a linear integral equation. For $T_{QTM}$, on the other hand, a few large roots remain isolated at almost the same positions as $N$ increases, while close to the origin more and more Bethe roots cluster.

Let us describe this in detail. Using the NLIE technique, we can derive an approximate BAE equation (see the discussion after (25)),

\[
\frac{N}{2} \ln\left(\frac{\tanh \frac{\pi i}{4} (x_j - \frac{\delta}{2})}{\tanh \frac{\pi i}{4} (x_j + \frac{\delta}{2})}\right) \sim (2I_j + 1)\pi i.
\]

\(^c\)A technical remark: the vacuum is conveniently chosen $(+, -, +, -, \cdots)$. 

The hole $\theta_a$ corresponds to the branch cut integer $I_{\text{max}} = \frac{N}{2} - \frac{1}{2}$, and this implies $\theta_a \sim \frac{1}{\pi} \ln \beta$ for $\beta \gg 1$, which was used in the last subsection.

Near the origin, we set $x_j = \frac{2}{N} \hat{x}_j$, and obtain the approximate distribution of $\hat{x}_j$ as an algebraic function,

$$\rho(\hat{x}) = \lim_{N \to \infty} \frac{I_{j+1} - I_j}{N(\hat{x}_{j+1} - \hat{x}_j)} \sim \frac{1}{2\pi(\hat{x}^2 + 1)}.$$ 

This differs from the usual root density function which decays exponentially as $|x| \to \infty$. In the original variable, if we take the Trotter limit naively,

$$\rho(x) \sim \lim_{|u| \to 0} \frac{|u|}{2\pi(x^2 + u^2)} \sim \frac{1}{2} \delta(x).$$

Namely the distribution of the BAE roots for $T_{\text{QTM}}$ is singular in the Trotter limit. We thus conclude that the usual root density method may not be applicable, and we have to devise a different tool.

Let us stress again that the cancellation of of the order of $N$ many terms in $\ln \Lambda^{(N)}$ is a unique property of the QTM. In the RTR case $O(L)$ many terms can survive, and we obtain intensive quantities (e.g., the free energy per site) only after dividing by $L$. On the other hand, $\ln \Lambda^{(N)}$ is already an intensive quantity, as remarked after Theorem 2.1. The cancellation is thus vital. The $O(e^N)$ terms, $a(x), d(x)$ must be canceled by the denominator $Q(x)$, resulting in $O(1)$ quantities. According to this point of view, (18) is (again) not practical, as the ratios of $O(e^N)$ terms are still present. Thus, we understand (18) still as a starting point, not as the goal.

One must intrinsically deal with a finite size system with coupling constant $u$ depending on the Trotter size, and then take the Trotter limit. Such an attempt was executed first numerically by extrapolation in $N$. The analytic low temperature expansion was performed based on the Wiener-Hopf method. Below we shall present the most sophisticated approach which utilizes the commuting QTM in a most efficient manner.
3.2. Non-linear Integral Equation (NLIE)

The introduction of the new spectral parameter $x$ plays a fundamental role. Instead of dealing with the BAE roots directly, we make use of the analyticity of specially chosen auxiliary functions in the complex $x$ plane.

There are various approaches. One of them is to introduce the fusion hierarchy of the QTM, which contains the original $T_{\text{QTM}}$ as $T_1$. In place of the BAE one uses the functional relations among fusion transfer matrices,

$$T_m(x - i)T_m(x + i) = \psi_m(x) + T_{m-1}(x)T_{m+1}(x).$$

Here $\psi_1$ is nothing but $\psi$ in the inversion relation (17), where the small term $T_0T_2/\psi_1$ was neglected. As $\{T_m\}$ constitutes a commuting family, the same relation holds among the eigenvalues. We thus use the same symbol $T_m$ for the eigenvalue. After a change of variables, $y_m(x) = T_{m-1}(x)T_{m+1}(x)/\psi_m(x)$, one can transform the algebraic equations into integral equations under certain assumptions on the analyticity of $y_m$. The resultant equations coincide with the Thermodynamic Bethe Ansatz equations.\textsuperscript{10,11} The string hypothesis is thus replaced by an assumption on the analyticity of $y_m$. The coupled set of equations may fix the values of $T_1(x)$. Then $\Lambda_0 = T_1(0)$ yields the free energy per site $f$. A technical problem in this approach is that we must deal with an infinite number of $y_m$ functions, which requires a truncation of the equations in an approximate manner.

Below we shall discuss another approach originally devised in the context of the evaluation of finite size corrections.\textsuperscript{12} We define the auxiliary function $a_N(x)$ by the ratio of the two terms in $\Lambda^{(N)}(x)$ (18),

$$a_N(x) = \frac{d(x)Q(x + 2i)}{a(x)Q(x - 2i)} \quad \mathfrak{A}_N(x) = 1 + a_N(x).$$

The suffix $N$ is introduced to recall that we are fixing $N$ finite here. The BAE (19) is equivalent to the condition

$$a_N(x_j) = -1 \quad \text{or} \quad \ln a_N(x_j) = (2I_j + 1)\pi i.$$

We also note that $\lim_{|x|\to\infty} a_N(x) = 1$ by construction.

We then adopt the following assumptions for the analytic properties of $\mathfrak{A}_N(x)$ corresponding to the largest eigenvalue. They are supported by numerical calculations.

1. There are $\frac{N}{2}$ simple zeros of $\mathfrak{A}_N(x)$ on the real axis. They coincide with the BAE roots. There are additional zeros, sufficiently far away from the real axis, so that $\mathcal{C}$ does not include them inside.
The only pole of $\mathfrak{A}_N(x)$ in $\exists x \in [-1, 1]$ is located at $x = iu$ and is of order $N^2$.

Once these assumptions are granted, one immediately derives the following NLIE,

$$\ln a_N(x) = \ln \frac{\phi_-(x + 2i)\phi_+(x)}{\phi_+(x + 2i)\phi_-(x)} - \int_C \frac{2}{(x-y)^2 + 4} \ln A_N(y) \frac{dy}{\pi}. \quad (23)$$

The largest eigenvalue $\Lambda$ can be similarly represented by

$$\ln \Lambda(N)(x) = \ln (\phi_+(x + 2i)\phi_-(x - 2i)) + \int_C \frac{\ln A_N(y)}{(x-y)(x-y-2i)} \frac{dy}{\pi}. \quad (24)$$

Note that only the driving term in (23) depends on $N$. We can thus take the Trotter limit easily, with $a := \lim_{N \to \infty} a_N$, and obtain the NLIE in (7) (for $h = 0$). To evaluate the free energy one has to first set $x = 0$, then take the Trotter limit. Or otherwise one meets a spurious divergence. Then we obtain the expression for the free energy in Theorem 2.2.

One still needs to make an effort to achieve a high numerical accuracy, especially at very low temperatures. The introduction of another pair of auxiliary functions solves this problem. We define $\bar{a}_N, \bar{A}_N$ by

$$\bar{a}_N(x) = (a_N(x))^{-1}, \quad \bar{A}_N(x) = 1 + \bar{a}_N(x).$$

Numerically one finds that $|a_N| \ll 1$ for $\exists x \geq 0$. Thus, we use $a_N, \bar{A}_N$ in the upper half plane and $\bar{a}_N, \bar{A}_N$ in the lower half plane. It is straightforward to rewrite (23) in the coupled form,

$$\ln a_N(x) = D_+^{(N)}(x) + \int_{C_+} F(x-y) \ln A_N(y) \frac{dy}{2\pi} - \int_{C_-} F(x-y) \ln A_N(y) \frac{dy}{2\pi}, \quad (25)$$

$$\ln \bar{a}_N(x) = D_-^{(N)}(x) + \int_{C_-} F(x-y) \ln \bar{A}_N(y) \frac{dy}{2\pi} - \int_{C_+} F(x-y) \ln \bar{A}_N(y) \frac{dy}{2\pi}$$

$$D_{\pm}^{(N)} = \frac{N}{2} \ln \left( \frac{\text{th} \frac{\pi}{2}(x + iu)}{\text{th} \frac{\pi}{2}(x - iu)} \right), \quad F(x) = \int_{-\infty}^{\infty} \frac{e^{-ikx}}{1 + e^{2|k|}} \, dk,$$

where $C_+(C_-)$ is a straight contour slightly above (below) the real axis. In the first (second) equation we understand that $x \in C_+(C_-)$. Note that the convolution terms bring only minor contributions as they are defined on those contours where the auxiliary functions are small. Therefore the main contributions come from the known functions. This enables us to perform numerics with high accuracy. We can drop the convolution terms for the lowest order approximation. Thanks to eq. (22) this leads to eq. (20).
Similarly, for the largest eigenvalue we have
\[
\ln \Lambda^{(N)}(x) = \varepsilon^{(N)}(x) + \int_{C_+} K_+(x-x') \ln \ln \mathcal{A}_N(x') \frac{dx'}{2\pi} + \int_{C_-} K_-(x-x') \ln \ln \bar{\mathcal{A}}_N(x') \frac{dx'}{2\pi},
\]
\[
K_{\pm}(x) = K(x \pm i), \quad K(x) = \frac{\pi}{2 \text{ch} \frac{x}{2}},
\]
\[
\varepsilon^{(N)} = \ln \phi_+(x+2i) \phi_-(x-2i) + N^2 \int e^{-|k|-i\varepsilon} \frac{\text{dh}}{k \text{ch} k} dk.
\]
We obtain the NLIE and the eigenvalue in the Trotter limit by replacing \(a_N \to a\) etc. and
\[
D^{(N)}_{\pm} \to -\frac{\pi i \beta}{2 \text{sh} \frac{x}{2}}, \quad \varepsilon^{(N)} \to -\frac{\beta}{2} \int \frac{1}{1 + e^{2|k|}} dk.
\]
For the actual calculation, it is even better to deal with \(b(x) := a(x+i)\) and \(\bar{b}(x) := \bar{a}(x-i)\) so that the singularities of \(\ln(1+b), \ln(1+b)\) are away from the integration contours. We omit, however, the details.

As a concrete example for the evaluation of bulk quantities we plot the susceptibility, \(\chi = \partial^2 f\), in fig. 8 (left). Note that at low temperatures the physical result in the Trotter limit (solid line) deviates from its finite Trotter number approximation. The above approach has been successfully applied to many models of physical relevance.\(^{13–19}\)

The correlation length \(\xi\) characterizes the decay of correlation functions at large distance, e.g.,
\[
\langle \sigma^+_x \sigma^-_y \rangle \sim e^{-\frac{|x-y|}{\xi}} \quad |x-y| \gg 1.
\]
It is evaluated from the ratio of the largest and the second largest eigenvalues of the QTM. For the second largest eigenvalue state, our assumption (1) on $A$ is no longer valid: a pair of holes $\theta_a$ lies on the real axis, and they are zeros of $\mathfrak{A}$ other than Bethe roots. Nevertheless, a small modification leads to a set of equations that fixes the second largest eigenvalue. The resultant NLIE has a form similar to (25) containing, however, additional inhomogeneous terms. Fig. 8 (right) shows a plot of $\xi T$ against temperature for the XXZ model with $q = e^{i\pi p}$ for $p = 3, 4, 5$.

When $h \neq 0$, we have to replace $a(x), d(x)$ in (18) by $e^{-\beta h/2}a(x), e^{\beta h/2}d(x)$. Then we add $\beta h (-\frac{\beta h}{2})$ to the rhs of (23) ((24)). Also $D_{\pm}^{(N)}$ must be replaced by $D_{\pm}^{(N)} \pm \frac{\beta h}{2}$.

Before closing this section, we would like to mention another formulation of thermodynamics also based on the QTM. It is described by a NLIE for $\Lambda_j$ directly and allows one to efficiently calculate high temperature expansions. The good numerical accuracy in the low temperature region is, however, hard to achieve. Moreover, we point out that the equation is the same for any eigenvalue. Thus, one should know a priori good initial values in order to select the convergence to the desired eigenvalue.

4. DME (Density Matrix Elements) at finite temperatures

The deep understanding of a model requires ample knowledge of its correlation functions. We would therefore like to go beyond their asymptotic characterization by the correlation length $\xi$ (26).

The evaluation of correlation functions has been defying many challenges in the past. Considerable progress was made only recently for the $T = 0$ correlations, based on vertex operators, on the $qKZ$ equation and on QISM. The third approach is the most relevant for our purpose. For $T = 0$ it first requires the solution of the “inverse problem”, that is, one has to represent the spin operators in terms of the QISM operators $A(u), B(u), C(u), D(u)$. Then, by algebraic manipulations, one obtains the correlation functions as combinatorial sums of expectation values of QISM operators, which are finally converted into (multiple) integrals.

At first glance, the case $T > 0$ seems far more difficult, as one expects that a summation of the contributions from all excited states is necessary. We argue here that, as above, the QTM helps us to avoid this summation and that, moreover, one does not have to solve the “inverse problem” within the QTM framework. The combinatorics, on the other hand, can be done in parallel to $T = 0$, because the QISM algebra is the same in both cases.

Let us explain why we can bypass the inverse problem in the QTM
formalism. This can be most quickly done in a graphical manner. To be specific, we need to evaluate $D_{\beta_1 \ldots \beta_m}^{\alpha_1 \ldots \alpha_m} := \langle E_{\alpha_1}^{\beta_1} \ldots E_{\alpha_m}^{\beta_m} \rangle = \frac{\text{tr}_{\text{phys}} \exp(-\beta H) E_{\alpha_1}^{\beta_1} \ldots E_{\alpha_m}^{\beta_m}}{\text{tr}_{\text{phys}} \exp(-\beta H)}$.

Using the logic of section 2, we can represent $\exp(-\beta H)$ by a “2D partition function”. Therefore $D_{\beta_1 \ldots \beta_n}^{\alpha_1 \ldots \alpha_n}$ can be represented by a modified 2D partition function: Start from the $N \times L$ classical system (fig. 4) with periodic boundaries in both directions. Then cut $n$ successive vertical bonds at the bottom row, and fix the variables at both sides of the cut. As we are adopting PBCs in the vertical direction this is equivalent to fixing the configuration of $n$ successive bonds at the top and at the bottom. See fig. 9 (left).

As previously, we rotate the lattice by 90°. See fig. 9 (right). Obviously we can write $D_{\beta_1 \ldots \beta_n}^{\alpha_1 \ldots \alpha_n}$ in terms of elements of the monodromy matrix $T_{\text{QTM}}(x)$. By introducing independent spectral parameters $\xi_i$ we obtain

$$
(D)_{\beta_1 \ldots \beta_n}^{\alpha_1 \ldots \alpha_n}(\xi_1, \ldots, \xi_n) = \frac{\langle \Phi_0 | (T_{\text{QTM}})_{\beta_1}^{\alpha_1}(\xi_1) \ldots (T_{\text{QTM}})_{\beta_n}^{\alpha_n}(\xi_n) | \Phi_0 \rangle}{\langle \Phi_0 | T_{\text{QTM}}(\xi_1) \ldots T_{\text{QTM}}(\xi_n) | \Phi_0 \rangle}.
$$

Here $\Phi_0$ denotes the largest eigenvalue state of the QTM, which is given by acting with $B$ operators on the vacuum. As any $(T_{\text{QTM}})_{\beta_1}^{\alpha_1}(\xi_1)$ is represented by a QISM operator, we reach an expression for DME purely in terms of QISM operators without solving the inverse problem.

At the same time, the problem for $T > 0$ is not so simple in view of the analyticity. We consider $D_{++}^{++}$ as a concrete example. After employing the
similar to (27) is also possible for the integration contour is already fixed for the Trotter limit is thus unknown. The most significant difference is that we cannot resort to the root density function. The explicit form of \( w_{j,k} \) is characterized by a simple algebraic relation. Note that the above algebraic expression is formally identical for \( w \) in the thermodynamic limit. Then the algebraic relation for \( w_{j,k} \rightarrow g(x_j, \xi_k) \) is solved with the explicit result \( g(x, \xi) = \frac{1}{4 \operatorname{ch} \frac{1}{2}(x - \xi + i)} \)

\[
D_{++}^{\pm} (\xi_1, \xi_2) = \left( \int dx dx' \frac{(x' - \xi_2)(x - \xi_1 - 2i)}{\xi_{2,1}(x - x' - 2i)} \right) \left[ g(x, \xi_1) g(x', \xi_1) \right] \left[ g(x, \xi_2) g(x', \xi_2) \right] - \frac{\xi_{1,2} + 2i}{\xi_{1,2}} \int dx \frac{(x - \xi_1)}{(x - \xi_1 + 2i)} g(x, \xi_1) - \frac{\xi_{2,1} + 2i}{\xi_{2,1}} \int dx \frac{(x - \xi_2)}{(x - \xi_2 + 2i)} g(x, \xi_2) + 1 \right).
\]

Third, we can freely move the integration contours. Every time it passes the singularity of \( g(x) \), it brings extra contributions and they cancel the “tails” (the 2nd to the 4th terms above). We finally obtain

\[
D_{++}^{\pm} (\xi_1, \xi_2) = \int dx dx' \frac{(x' - \xi_2 + i)(x - \xi_1 - i)}{\xi_{2,1}(x - x' - 2i)} \left[ g(x + i, \xi_1) g(x' + i, \xi_1) \right] \left[ g(x + i, \xi_2) g(x' + i, \xi_2) \right]. \tag{27}
\]

Without such a compact expression, it is hard to proceed further.

On the other hand, \( \mathfrak{A} \) is quite non-trivial for \( T > 0 \). As noted previously, we can not resort to the root density function. The explicit form of \( w_{j,k} \) in the Trotter limit is thus unknown. The most significant difference is that the integration contour is already fixed for \( T > 0 \). Thus, we cannot apply the above trick to swallow tails into the ground state.

Nevertheless, with an appropriate choice of a further auxiliary function \( G(x, \xi) \), it was shown that a compact multiple integral representation, similar to (27) is also possible for \( T > 0 \).\(^{27,28}\)

\[
D_{++}^{\pm} (\xi_1, \xi_2) = \int \frac{dx}{\mathfrak{A}(x)} \int \frac{dx'}{\mathfrak{A}(x')} \frac{(x - \xi_1 - 2i)(x' - \xi_2)}{4\pi^2 \xi_{1,2}(x - x' - 2i)} \left[ G(x, \xi_1) G(x', \xi_1) \right] \left[ G(x, \xi_2) G(x', \xi_2) \right].
\]

The formula for any other DME is similarly known.

It is a big progress to obtain the multiple integral representation for DMEs. The representation is, however, not yet optimal. Although one can
use it for the numerical analysis at sufficiently high temperatures, it suffers from numerical inaccuracy at low temperatures.\textsuperscript{29,30} We thus would like to reduce it to (a sum of) products of single integrals.

The factorization of DME at $T = 0$ has been performed by brute force, with the extensive use of the shift of contour technique.\textsuperscript{31,32} Based on studies of the $q$KZ equation, a hidden Grassmannian structure behind DME has been found.\textsuperscript{33} It naturally explains the factorization of the multiple integral formula through the nilpotency of operators. The explicit form of DME consists of two pieces, the algebraic part, evaluated from a matrix element of $q$-oscillators, and the transcendental part, related to the spinon-$S$ matrix.

On the other hand, we still do not have a finite temperature analogue of the $q$KZ equation. We are nevertheless able to factorize the multiple integrals for small segments.\textsuperscript{34} The explicit results also consist of two parts. Surprisingly the algebraic part remains identical to the $T = 0$ case, while the transcendental part can be interpreted as a proper finite temperature analogue to the spinon-$S$ matrix. This finally enables us to perform an accurate numerical analysis of the correlation functions.\textsuperscript{35} We show plots of $\langle \sigma_z^1 \sigma_z^4 \rangle$ for $\Delta = \frac{1}{\sqrt{2}}$ with various magnetic fields in fig. 10. The results from a brute force calculation are also plotted, which supports the validity of our formula. Such high accuracy calculation can clarify the quantitative nature of interesting phenomena such as the quantum-classical crossover.\textsuperscript{36} Recently a proof of the existence of factorization of the DMEs for $T > 0$ was obtained, again by using the Grassmannian structure.\textsuperscript{37} See also the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure10.png}
\caption{The plots of $\langle \sigma^x_1 \sigma^x_4 \rangle$ (left) and $\langle \sigma^y_1 \sigma^y_4 \rangle$ (right) for $\Delta = \frac{1}{\sqrt{2}}$ with various magnetic fields by NLIEs (continuous line).}
\end{figure}
further development\cite{38} in this direction based on NLIEs.

5. Summary and discussion

We presented a brief review on the recent progress with the exact thermodynamics of 1D quantum systems. The QTM is found to be an efficient tool, and it offers a framework to evaluate quantities of physical interest, including DME. The NLIE combines into the framework nicely, yielding high accuracy numerical results.

The factorization of the multiple integral formula at $T > 0$ is yet to be further explored. It seems e.g. quite plausible that the qKZ equation could be extended to finite temperatures. This might be an important next step.

There are certainly many interesting questions left open. For example, can we have the QTM formulation starting from a continuum system? What is the generalization of the multiple integral formula to models with higher spin? The study of such questions is underway.

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