

Constructing the GGE for the Heisenberg spin chain: A Hilbert space Monte Carlo approach

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I. INTRODUCTION

$$\rho^{GGE} = \frac{1}{Z} \exp \left(- \sum_j \lambda_j \mathcal{I}_j \right) \quad (1)$$

II. THE MODEL AND THE METHOD

A. The Heisenberg spin chain

The isotropic spin- $\frac{1}{2}$ Heisenberg (XXX) chain is defined by the Hamiltonian

$$\mathcal{H} \equiv J \sum_{i=1}^L \left[\frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + S_i^z S_{i+1}^z \right], \quad (2)$$

where $S_i^\pm \equiv (\sigma_i^x \pm i\sigma_i^y)/2$ are spin operators acting on the site i of the chain, $S_i^z \equiv \sigma_i^z/2$, and $\sigma_i^{x,y,z}$ the Pauli matrices. We fix $J = 1$ and use periodic boundary conditions identifying sites $L + 1$ and 1. Both the total spin $S_T^2 \equiv (\sum_i \vec{S}_i)^2$ and the total magnetization $S_T^z \equiv \sum_i S_i^z = L/2 - M$, with M being the number of down spins, commute with (2). Thus, the eigenstates of (2) can be labelled by M . Following the Bethe ansatz literature here we refer to the down spins as particles.

Each eigenstate of (2) is univocally identified by a set of M complex parameters (the so-called rapidities) $\{x_\alpha\}$ with $\alpha = 1, \dots, M$. These are solutions of a set of non linear algebraic equations, the Bethe equations

$$\arctan(x_\alpha) = \frac{\pi}{L} J_\alpha + \frac{1}{L} \sum_{\beta \neq \alpha} \arctan \left(\frac{x_\alpha - x_\beta}{2} \right). \quad (3)$$

Here $J_\alpha \in \frac{1}{2}\mathbb{Z}$ are the Bethe quantum numbers. Any choice

of $-L/2 \leq J_\alpha \leq L/2$ identifies a solution of the Bethe equations and an eigenstate of the XXX chain.

Besides the total magnetization and the momentum, the XXX chain has non-trivial conservation laws, due to the integrability. These extra conserved quantities \mathcal{I}_j are obtained as

$$\mathcal{I}_j \equiv \frac{i}{(j-1)!} \frac{d^j}{dx^j} \log(\Lambda) \Big|_{x=i}. \quad (4)$$

Here Λ in the Algebraic Bethe Ansatz approach is the eigenvalue of the transfer matrix of the XXX chain. This depends on a parameter x and on the set of rapidities $\{x_\alpha\}$ and it is given as

$$\Lambda(x, \{x_\alpha\}) \equiv \left(\frac{x+i}{2} \right)^L \prod_{\alpha} \frac{x - x_\alpha - 2i}{x - x_\alpha} + \left(\frac{x-i}{2} \right)^L \prod_{\alpha} \frac{x - x_\alpha + 2i}{x - x_\alpha}. \quad (5)$$

An important feature of the XXX chain is that in the thermodynamic limit $L \rightarrow \infty$, the solutions of (3) form “string” pattern in the complex plane (string hypothesis). Specifically, the rapidities forming a string of length $1 \leq n \leq M$ (n -string) are parametrized as

$$x_\gamma^{(n,j)} = x_\gamma^{(n)} - i(n-1-2j), \quad j = 0, 1, \dots, n-1. \quad (6)$$

Here $x_\gamma^{(n)} \mathbb{R}$ is the real part of the string (string center), and γ labels strings of the same length but with different centers.

Substituting the string hypothesis in (3) one obtains a set of the discrete Bethe-Takahashi equations for the string centers as

$$2L \arctan(x_\gamma^{(n)}/n) = 2\pi I_\gamma^{(n)} + \sum_{(m,\beta) \neq (n,\gamma)} \Theta_{m,n}(x_\gamma^{(n)} - x_\beta^{(m)}). \quad (7)$$

Here the scattering phases $\Theta_{m,n}$ are defined as

$$\Theta_{m,n}(x) \equiv \begin{cases} \vartheta\left(\frac{x}{|n-m|}\right) + \sum_{r=1}^{(n+m-|n-m|-1)/2} 2\vartheta\left(\frac{x}{|n-m|+2r}\right) + \vartheta\left(\frac{x}{n+m}\right) & \text{if } n \neq m \\ \sum_{r=1}^{n-1} 2\vartheta\left(\frac{x}{2r}\right) + \vartheta\left(\frac{x}{2n}\right) & \text{if } n = m \end{cases}$$

Here $\vartheta(x) \equiv 2 \arctan(x)$. Similar to the Bethe quantum num-

bers the Bethe-Takahashi quantum numbers $I_\gamma^{(n)}$ identify the

solutions of the Bethe-Takahashi equations. We denote as α_n the number of strings of length n in the rapidities identifying an eigenstate.

Clearly, for a generic eigenstate one has that $\sum_{n=1}^M \alpha_n = M$.

It can be shown that $I_\gamma^{(n)}$ are integers (half integers) if $L - \alpha_n$ is odd (even).

The energy and the total momentum associated to a given solution of the Bethe-Takahashi equations are given as

$$E(\{x_\gamma^{(n)}\}) = -L/4 + \sum_{n,\gamma} \frac{2n}{(x_\gamma^{(n)})^2 + n^2} \quad (8)$$

$$P(\{x_\gamma^{(n)}\}) = \sum_{n,\gamma} \frac{2\pi I_\gamma^{(n)}}{L} \quad (9)$$

One can show that the Bethe-Takahashi quantum numbers $I_\gamma^{(n)}$ obey the constraint

$$|I_\gamma^{(n)}| \leq \frac{1}{2}(L - 1 - \sum_{m=1}^M t_{mn}\alpha_m), \quad (10)$$

where $t_{mn} \equiv 2\min(m, n) - \delta_{mn}$.

B. The Hilbert space Monte Carlo approach

Given a set of conserved quantities \mathcal{I}_j

For a given number of particles M the total number of eigenstates with that number of particles is clearly given as $C_M^L - C_{M-1}^L$, with $C_y^x \equiv x!/(y!(x-y)!)$ the binomial coefficient.

III. THE CONSERVED CHARGES AND THEIR FLUCTUATIONS

IV. THE STRING ROOT DENSITIES

For infinite temperature the densities ρ_n are given as

$$\rho_n(x) = \sqrt{\frac{2}{\pi}} \frac{a_n}{n^2(n+2)^2 + (2(n+1)^2 + 2)x^2 + x^4} \quad (11)$$

where the sequence a_n is given as

$$a_n = \frac{2(n+1)^2}{(n+1)^2 + 1} \quad (12)$$

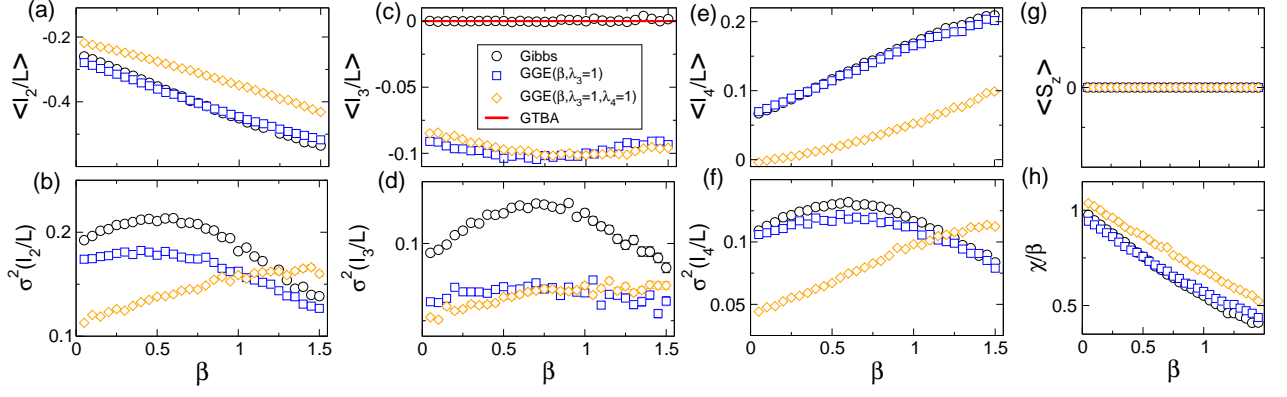


FIG. 1. The Generalized Gibbs Ensemble (GGE) for the finite-size Heisenberg spin chain with $L = 16$ sites. The GGE is constructed including the conserved charges I_2, I_3, I_4 . The corresponding Lagrange multipliers are denoted as $\lambda_2, \lambda_3, \lambda_4$. Here I_2 is the Hamiltonian and $\lambda_2 \equiv \beta$ the inverse temperature. (a) The GGE average $\langle I_2/L \rangle$ of I_2/L plotted as a function of β . The data are obtained using the Hilbert space Monte Carlo approach described in the manuscript. The different symbols correspond to GGEs with different fixed values of λ_3 and λ_4 . The circles correspond to the Gibbs ensemble. (b) The fluctuations $\sigma^2(I_2/L) \equiv \langle (I_2/L)^2 \rangle - \langle I_2/L \rangle^2$ as function of $0 \leq \beta \leq 1.5$. (c)(d) and (e)(f): Same as in (a)(b) for I_3 and I_4 , respectively. In all panels the dash-dotted lines are the analytical results obtained using the Generalized Thermodynamic Bethe Ansatz (GTBA) approach. (g) The GGE expectation value of the total magnetization $\langle S_z \rangle$. Notice that this is exactly zero due to the $SU(2)$ invariance of the Hamiltonian and the conserved charges. (h) The GGE average of the spin susceptibility χ : χ/β plotted versus β .

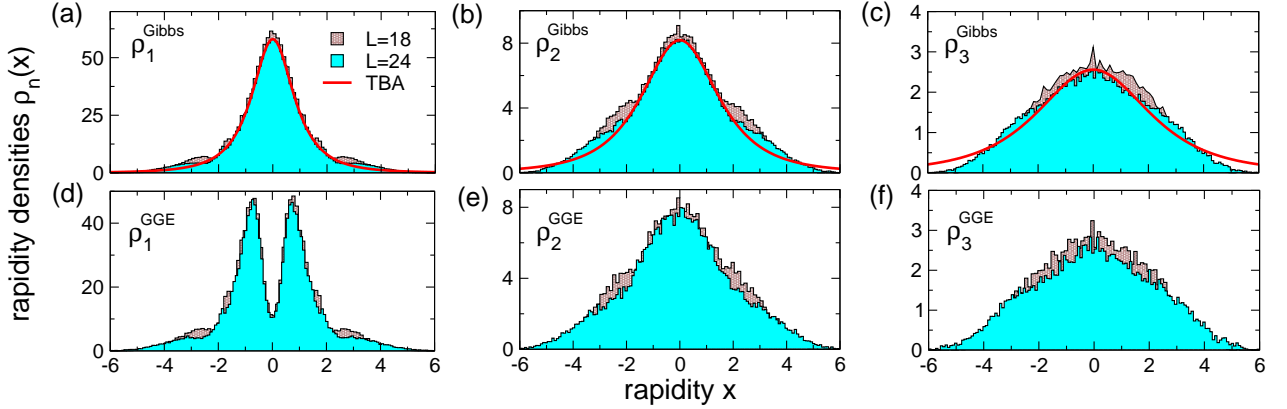


FIG. 2. The first three rapidity densities $\rho_n(\lambda)$ ($n = 1, 2, 3$) for the Gibbs (panels (a)(b)(c)) and the GGE equilibrium state (panels (d)(e)(f)). Here we consider the infinite temperature Gibbs ensemble. The GGE is constructed using only the two conserved charges I_2 and I_4 . The associated Lagrange multipliers are $\lambda_2 = 0$ and $\lambda_4 = 1$. The panels show the histograms of the rapidities x corresponding the n -strings for chains of three sizes $L = 18, 24, 30$ (corresponding to point, dashed, and full symbols). Here we restrict ourselves to the interval $-6 \leq x \leq 6$. For $L = 18$ all the histograms contain 100 bins, whereas for $L = 24$ they contain 140. In all the panels on the y -axes are divided by 10^3 for convenience. In panels (a)-(c) the lines are the Thermodynamic Bethe Ansatz (TBA) results.

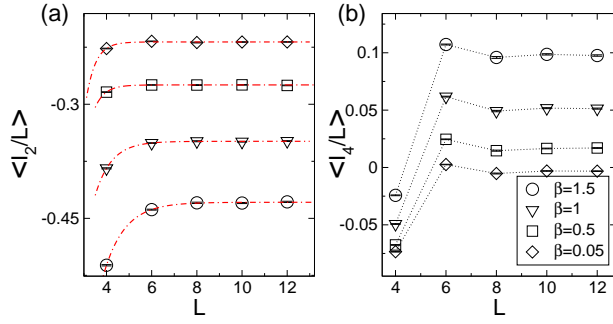


FIG. 3. Finite-size scaling of the GGE averages in the Heisenberg chain. Here the GGE is constructed using the conserved charges I_2, I_3, I_4 , with associated Lagrange multipliers $\lambda_2, \lambda_3, \lambda_4$. I_2 is the Hamiltonian and $\lambda_2 \equiv \beta$ the inverse temperature. Here we fix $\lambda_3 = \lambda_4 = 1$. (a) The GGE average $\langle I_2/L \rangle$ (Monte Carlo data) plotted versus the chain size L . Different symbols correspond to different values of β . The dash-dotted lines are fits to an exponential behavior. (b) Same as in (a) for I_4 .