Constructing the GGE in integrable models: A Hilbert space Monte Carlo approach

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I. INTRODUCTION

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

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

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

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

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

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 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

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

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

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

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

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

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

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

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

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

Here $\vartheta(x)\equiv2\arctan(x)$. Similar to the Bethe quantum numbers 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

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

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

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

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

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

B. The Hilbert space Monte Carlo approach

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. Thus the probability of an eigenstate of the XXX chain with M particles is given as $(C_M^L - C_{M-1}^L)/C_{L/2}^L$.

Given a fixed particle number M the total number of eigenstates $D(\{\alpha_n\})$ corresponding to a string configuration $\{\alpha_n\}$ is given as

$$D(\{\alpha_n\}) = \prod_{i=1}^{M} C_{\alpha_i}^{L-\sum_{j=1}^{M} t_{ij}\alpha_j}. \tag{11}$$

Given the fixed particle number M and the string configuration $\{\alpha_j\}$, the GGE probability P_{GGE} of a generic eigenstate μ corresponding to a given choice of quantum numbers satisfying (10) is given as

$$P_{GGE}(\mu) = \frac{1}{Z}(L - 2M + 1)e^{-\sum_i \lambda_j \mathcal{I}_j}. \tag{12}$$

Here the factor $L - 2M + 1$ corresponds to the $SU(2)$ degeneracy. Notice that this assumes that all the conserved charges $\mathcal{I}_j$ are $SU(2)$ scalars.

Given two eigenstates μ and ν corresponding to eigenvalues of the conserved charges $\{M, \mathcal{I}_2, \mathcal{I}_3, \ldots, \mathcal{I}_N\}$ and $\{M', \mathcal{I}'_2, \mathcal{I}'_3, \ldots, \mathcal{I}'_N\}$ the transition probability is given as

$$\frac{P_{GGE}(\nu)}{P_{GGE}(\mu)} = \frac{L - 2M' + 1}{L - 2M + 1} e^{-\sum_j \lambda_j (\mathcal{I}'_j - \mathcal{I}_j)}. \tag{13}$$

This gives the Metropolis rule to be used in the Monte Carlo update as

$$T(\mu \to \nu) = \begin{cases} \frac{L-2M'+1}{L-2M+1} e^{-\sum_j \lambda_j (\mathcal{I}'_j - \mathcal{I}_j)}. & \text{if } \frac{P(\nu)}{P(\nu)} < 1 \\ 1 & \text{otherwise.} \end{cases}$$

III. THE CONSERVED CHARGES AND THEIR FLUCTUATIONS

IV. THE STRING ROOT DENSITIES

For infinite temperature the densities ρ_n are given as

$$\rho_n(x) = \sqrt{\frac{2}{\pi}} \frac{a_n}{n^2(n+2)^2 + (2(n+1)^2 + 2)x^2 + x^4} \tag{14}$$

where the sequence a_n is given as

$$a_n = \frac{2(n+1)^2}{(n+1)^2 + 1} \tag{15}$$

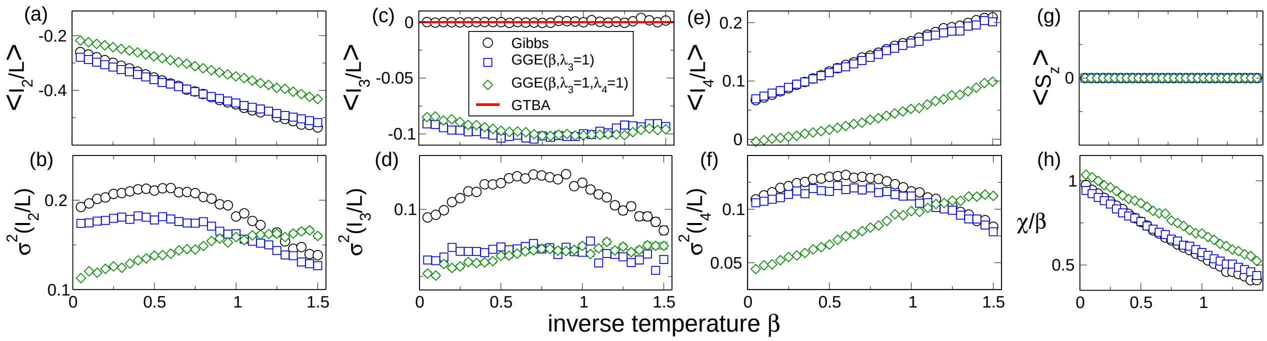

FIG. 1. The Generalized Gibbs Ensemble (GGE) for the Heisenberg spin chain with $L = 16$ sites. The GGE is constructed using the Monte Carlo method described in the paper. Only the first three conserved charges $\mathcal{I}_n$ ($n = 1, 2, 3$), with associated Lagrange multipliers λ_n, are included in the GGE. Here $\mathcal{I}_2$ is the Hamiltonian and $\lambda_2 \equiv \beta$ the inverse temperature. In all the panels different symbols correspond to GGEs with different values of λ_3, λ_4. The circles correspond to the Gibbs ensemble, i.e., $\lambda_3 = \lambda_4 = 0$. (a) The GGE average $\langle \mathcal{I}_2/L\rangle$ plotted as a function of β. (b) Variance of the GGE fluctuations $\sigma^2(\mathcal{I}_2/L) \equiv \langle(\mathcal{I}_2/L)^2\rangle - \langle\mathcal{I}_2/L\rangle^2$ as a function of β. (c)(d) and (e)(f): Same as in (a)(b) for $\mathcal{I}_3$ and $\mathcal{I}_4$, respectively. In all panels the dash-dotted lines are the analytical results obtained using the Generalized Thermodynamic Bethe Ansatz (GTBA). (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 conserved charges. (h) The GGE average $\langle\chi/\beta\rangle$ with χ the spin susceptibility.

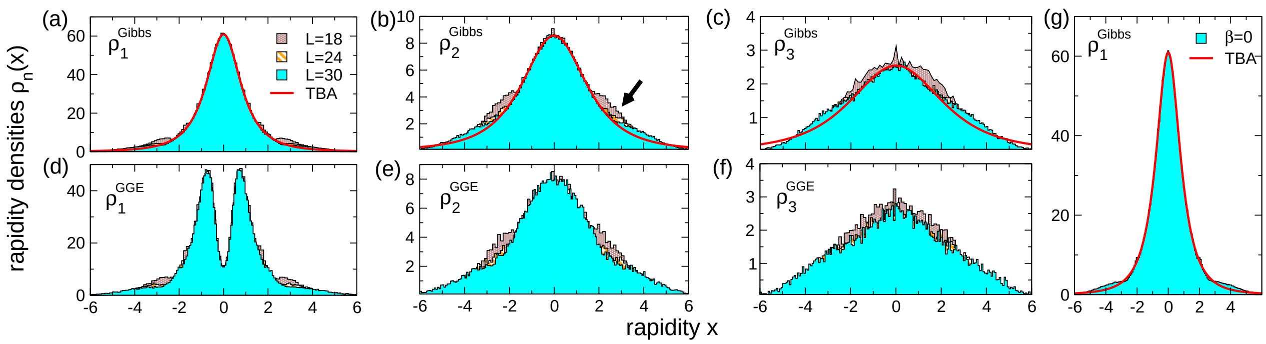

FIG. 2. The first three rapidity densities $\rho_n(\lambda)$ ($n = 1, 2, 3$) for the Gibbs (panels (a)(b)(c)) and the GGE equilibrium state (panels (d)(e)(f)). Here we consider the infinite temperature Gibbs ensemble. The GGE is constructed using only the two conserved charges $\mathcal{I}_2$ and $\mathcal{I}_4$. 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.

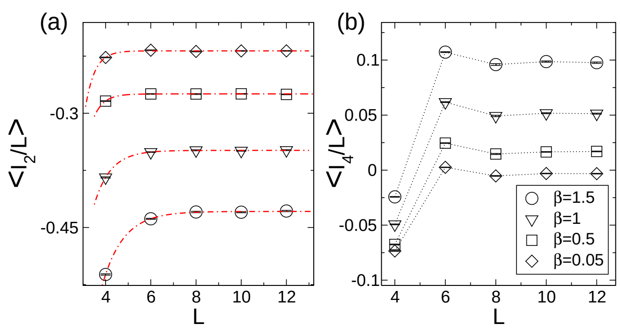

FIG. 3. Finite-size scaling of the GGE averages in the Heisenberg chain. Here the GGE is constructed using the conserved charges I_2, I_3, I_4, with associated Lagrange multipliers $\lambda_2, \lambda_3, \lambda_4$. I_2 is the Hamiltonian and $\lambda_2 \equiv \beta$ the inverse temperature. Here we 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.