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 $S_T^z\equiv\sum_iS_i^z=L/2-M$, 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 $-L/2\le J_\alpha\le L/2$ 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 $1\le n\le M$ (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

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

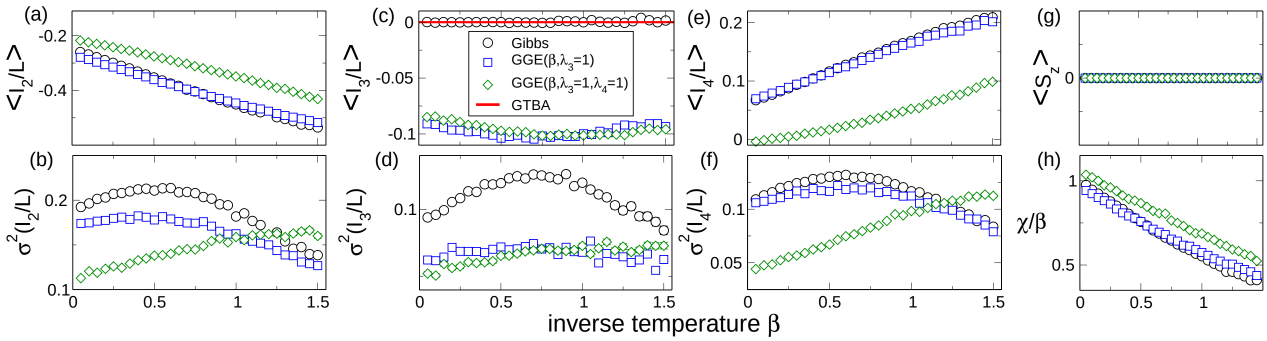

FIG. 1. The Generalized Gibbs Ensemble (GGE) for the Heisenberg spin chain with $L = 16$ sites: numerical results obtained using the Hilbert space Monte Carlo sampling. Only the first three conserved charges $\mathcal{I}_n$ ($n = 1, 2, 3$), with associated Lagrange multipliers λ_n, are included in the GGE. Here $\mathcal{I}_2$ is the Hamiltonian and $\lambda_2 \equiv \beta$ the inverse temperature. In all the panels different symbols correspond to 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 $\langle S_z \rangle = 0$ due to the $SU(2)$ invariance of the conserved charges. (h) χ/β plotted versus β, with χ being the magnetic susceptibility per site.

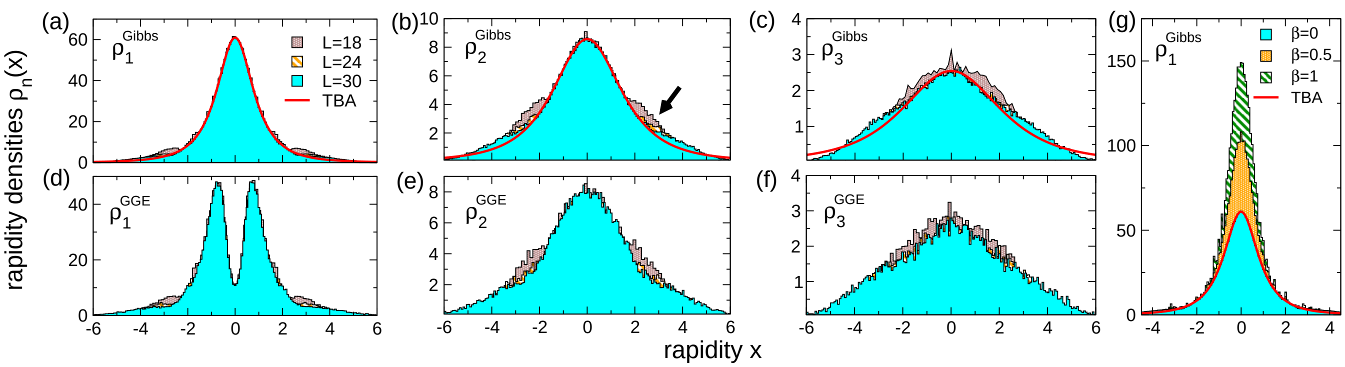

FIG. 2. The rapidity densities $\rho_n(x)$ (for $n = 1, 2, 3$) for the infinite temperature Gibbs (panels (a)-(c)) and the GGE equilibrium states (panels (d)-(f)): Numerical results for the Heisenberg spin chain obtained using the Hilbert space Monte Carlo sampling. Here the GGE is constructed including only $\mathcal{I}_2$ and $\mathcal{I}_4$ with fixed Lagrange multipliers $\lambda_2 = 0$ and $\lambda_4 = 1$. In all the panels the data are the histograms of the n-strings rapidities sampled in the Monte Carlo. The width of the histogram bins is $\Delta x = 2/L$. In each panel different histograms correspond to different chain sizes L. All the histograms are divided by 10^3 for convenience. In (b) the arrow is to highlight the finite-size effects. In panels (a)-(c) the lines are the Thermodynamic Bethe Ansatz (TBA) results. (g) Finite-temperature effects: Monte Carlo data for ρ_1^{Gibbs} for different values of the inverse temperature β.

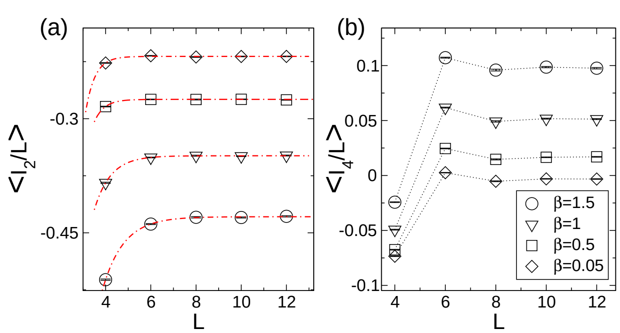

FIG. 3. Finite-size scaling of the GGE averages in the Heisenberg chain: Numerical results obtained from the Hilbert space Monte Carlo sampling. Here the GGE is constructed including $\mathcal{I}_2, \mathcal{I}_3, \mathcal{I}_4$, with Lagrange multipliers $\lambda_2 = \beta, \lambda_3 = \lambda_4 = 1$. (a) $\langle \mathcal{I}_2/L \rangle$ plotted versus the chain size L for several values of β. The dash-dotted lines are exponential fits. (b) Same as in (a) for $\mathcal{I}_4$.