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From interacting particles to equilibrium statistical ensembles

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We argue that a particle language provides a conceptually simple framework for the description of anomalous equilibration in isolated quantum systems. We address this paradigm in the context of integrable models, which are those where particles scatter completely elastically and are stable against decay. In particular, we demonstrate that a complete description of equilibrium ensembles for interacting integrable models requires a formulation built from the mode occupation numbers of the underlying particle content, mirroring the case of noninteracting particles. This yields an intuitive physical interpretation of generalized Gibbs ensembles, and reconciles them with the microcanonical ensemble. We explain how previous attempts to identify an appropriate ensemble overlooked an essential piece of information, and provide explicit examples in the context of quantum quenches.

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The last decade has seen experimental techniques in optical lattices establish themselves as a fruitful playground for testing paradigms of quantum statistical physics [1–4]. A hallmark achievement has been the observation of anomalous equilibration in ultracold bosonic condensates [5–9] where the nonergodic character of quantum dynamics is attributed to the fact that they lie in the vicinity of an integrable point [10–24]. It became clear that a new framework would be required to properly describe such anomalous relaxation processes. In this work, we advocate a shift from conventional interpretations by offering a simple conceptual framework centered around the notion of particles. We argue that the consideration of anomalous equilibration in isolated quantum many-body systems naturally leads to the study of integrable models since they possess stable particle excitations. The techniques of integrability in turn allow for a complete description of generalized equilibrium states.

Recent efforts on the subject have predominantly revolved around the notions of prethermalization and generalized Gibbs ensembles (GGE). By invoking locality and entropy extremization, the GGE was introduced as the canonical statistical ensemble in which the Hamiltonian is supplemented with an extensive amount of additional conservation laws stemming from integrability. Initial studies focused on noninteracting particles, for which the conserved operators forming the GGE are the single-particle mode numbers [25–34]. Formulating the GGE for genuinely interacting models turned out to be more elusive, however, due to the less obvious structure of the local conservation laws [35–45].

In this work, we address the problem from a different viewpoint, and exploit the fact that, in contrast to generic (ergodic) dynamical systems, integrable systems exhibit stable collective excitations which can be identified as particles. While in noninteracting systems particles do not experience mutual collisions, the distinguishing property of interacting integrable models is that particles undergo a completely elastic scattering without particle production or decay [46,47]. The scattering is thus nondiffractive, meaning that momenta of the outgoing particles are simply the rearranged initial momenta. Here, we convey how anomalous thermalization in integrable systems reflects the existence of particles and use this insight

to put forward a complete and universal description of local equilibrium states.

It turns out that our perspective demystifies and clarifies the physical picture of the unconventional equilibration seen in nonergodic interacting models, unifying its description with the case of noninteracting theories. Another advantage of adopting particle interpretation is that it eliminates the need of rather technical and subtle concepts introduced in the previous literature, e.g., recently advocated “weaker forms” of locality such as quasilocality [23,48] and semilocality [17], and makes the logic of the “truncated GGE” obsolete [33]. These auxiliary concepts, we argue, only undesirably obfuscate a clean physical picture. The very existence of an extensive hierarchy of higher (local and nonlocal) conservation laws is in fact a direct manifestation of the completely factorizable scattering of particles. It is the particles that are the inherently local objects of integrable theories [46].

In a closed quantum system, relaxation towards local equilibrium is typically formulated as an initial value problem, the so-called quantum quench, where a question of main interest is to characterize local equilibria which emerge as quasistationary states in the unitary relaxation process. This task can be naturally explained in the particle language, owing to the fact that integrability ensures that particles have infinite lifetimes and undergo completely elastic scattering. This observation implies that the information about the particle content at the initial time gets preserved for arbitrary long times. As we shall shortly discuss, this not only suffices to fully characterize the content of the stationary state, but it also proves necessary.

Prescribing an initial state can be viewed as exciting a macroscopic number of particles which subsequently participate in a scattering process. A local equilibrium state emerges dynamically after long times. However, the latter can only be meaningfully defined for a thermodynamically large system, which allows for a simplified description due to two mechanisms: *dephasing* and *eigenstate thermalization hypothesis* (ETH). Dephasing amounts to discarding the information contained in the dynamical phases from eigenstates at the same energy density [39,49], which averages out in the course of the relaxation process. ETH states that individual

microstates which are related by nonextensive modifications of quantum numbers are locally indistinguishable and give the same (generalized) free energy and expectation values of local observables [50]. No distinction between microcanonical and canonical ensembles is necessary as the former are understood as an unbiased collection of eigenstates which share the same set of distributions of quantum numbers, which for thermodynamically large systems exactly matches the canonical description, with the density operators of the particles providing a labeling of the microcanonical shells [50].

The task of finding and parametrizing the stationary state after a quench therefore amounts to detect the particle distributions from the initial state. There exist various strategies for performing this technical step. For instance, the one pursued in the seminal works on interacting quenches was to employ the quench action method [39,49] (see Appendix E) and compute the leading thermodynamic contribution of the overlap coefficients between the initial state and Bethe eigenstates [42–44]. While this has been successfully accomplished for certain special states [51], it seems to pose a formidable task for generic states. This can be overcome with the approach of Ref. [52] which derives exact operator representations for $\hat{\rho}_j$, allowing for efficient extraction of the particle densities from initial states which admit a (exact or approximate) representation in terms of matrix-product states [41,48].

The remaining discussion is devoted to rigorous justification of our claims. By carefully revisiting the previous formulations we shall demonstrate that our proposal not only unveils the true character of local conserved quantities, but it also captures a part of the manifold of equilibrium ensembles missed by previous proposals.

I. GENERALIZED GIBBS ENSEMBLES

The concept of a generalized Gibbs ensemble (GGE) has been proposed, conventionally given in the form [25–28]

$$\hat{\varrho} = \mathcal{Z}^{-1} \exp \left[- \sum_i \lambda_i \hat{Q}_i \right], \quad (1)$$

where \hat{Q}_i is some appropriately chosen set of conserved operators, λ_i the associated Lagrange multipliers, and $\mathcal{Z} = \text{Tr} \hat{\varrho}$. The GGE rests on the “principle of locality”, which states that the properties of local observables are completely characterized by including all local conserved charges \hat{Q}_i . This provides a greatly simplified description compared to the diagonal ensemble, which retains the entire information about the initial condition.

All proposals to date have attempted to define the GGE in terms of the Hamiltonian and other local charges obtained from the traditional algebraic Bethe ansatz procedure [53,54]. These suffer from two major drawbacks, however, (i) they shed no light on the physical interpretation of the charges \hat{Q}_i , and (ii) the question as to whether a given trial set of charges provides a complete and nonredundant characterization of local equilibria for a given model remained obscure. In fact, we shall show with explicit examples that the set of local charges from the previous proposals omits a crucial part of the local information necessary to characterize general equilibrium states. The shift

of perspective which we advocate in this work overcomes these difficulties.

As the entire spectrum of an integrable model is characterized in terms of stable particles, the number operators of these particles provide the most natural complete set for the local conserved \hat{Q}_i in Eq. (1). Specifically, expressing the ensemble in terms of particle density operators $\hat{\rho}_j(v)$, it takes the form

$$\hat{\varrho} = \mathcal{Z}^{-1} \exp \left[- \sum_j \int_{\mathbb{R}} dv \mu_j(v) \hat{\rho}_j(v) \right], \quad (2)$$

where the index j runs over distinct particle types, v is a rapidity variable which parametrizes their momenta $p_j(v)$, and $\mu_j(v)$ are rapidity-dependent chemical potentials. The eigenvalue densities ρ_j of the operators $\hat{\rho}_j$ completely determine the macrostates of the system [50]. Individual microstates drawn from the same macrostate differ only by rearrangements of the occupation of the $L\rho_j(v)dv$ quantum numbers in a rapidity window dv , and thus have a negligible effect on the local correlations in the thermodynamic limit. The entropy takes the universal form given explicitly below [cf. Eq. (12)]. This is understood as the integrable analog of ETH used to characterize the thermalization of eigenstates in ergodic interacting systems [55–58].

Heisenberg model. We focus on the prototypical integrable model, the Heisenberg spin- $\frac{1}{2}$ chain,

$$\hat{H} \simeq - \sum_i \vec{S}_i \cdot \vec{S}_{i+1}. \quad (3)$$

The particle content (cf. Appendix A), with respect to a fully polarized state, consists of magnons and j -particle bound states thereof, with momenta [59]

$$p_j(v) = -i \log \left[\frac{\left(v + j \frac{i}{2} \right)}{\left(v - j \frac{i}{2} \right)} \right]. \quad (4)$$

Recently, a set of local charges $\hat{X}_j(v)$ for the Heisenberg model has been identified [60], which allows macrostates to be uniquely determined from the values of charge densities X_j via string-charge duality [52]. This takes the form of a discrete wave equation

$$\rho_j = \square X_j, \quad (5)$$

where \square is a d’Alembertian on $X_j(v)$ defined for a set of functions $f_j(v)$ as

$$\square f_j = f_j^+ + f_j^- - f_{j-1} - f_{j+1}, \quad (6)$$

where $f_j^\pm(v) = f_j(v \pm \frac{i}{2} \mp i0^+)$ and 0^+ denotes an infinitesimal which acts as a regulator.

Although previous attempts at identifying a complete ensemble were built directly from a discrete basis of charges obtained from \hat{X}_j , the strategy they used was to incorporate the knowledge of charge densities to enforce constraints on the space of macrostates, thus tacitly bypassing the canonical form of Eq. (1) which is merely a formal series. Since it remains unclear how to unambiguously interpret it, we instead employ a continuous set of local charges $\hat{X}_j(v)$ and cast the most

recently proposed GGE [23,48] in the analytic form

$$\hat{\rho} = \mathcal{Z}^{-1} \exp \left[- \sum_j \int_{\mathbb{R}} dv \lambda_j(v) \hat{X}_j(v) - \lambda_z \hat{S}^z \right], \quad (7)$$

where functions $\lambda_j(v)$ are Lagrange multipliers and λ_z couples to the magnetization \hat{S}^z . While this appears reasonable, due to the correspondence between particle's distributions ρ_j and charge densities X_j in Eq. (5), it however fails to capture generic equilibrium states. In the following, we carefully examine the structure of equilibrium states, highlight the origin of this incompleteness, and provide explicit examples in the context of a quantum quench scenario. This leads us to the conclusion that the complete description of thermodynamic ensembles necessitates the particle-based formulation of Eq. (2).

II. TECHNICAL BACKGROUND

Integrability of the model provides a commuting family of operators \hat{T}_j , known as transfer matrices (defined in Appendix B). Following Refs. [48,52,60], a set of conserved charges is naturally identified:

$$\hat{X}_j(v) = \frac{1}{2\pi i} \partial_v \log \hat{T}_j \left(v + \frac{i}{2} \right). \quad (8)$$

These are Hermitian for $v \in \mathbb{R}$, and local for

$$v \in \mathcal{P} \equiv \left\{ v \in \mathbb{C} : |\text{Im}(v)| < \frac{1}{2} \right\}, \quad (9)$$

a domain in the complex plane known as the ‘‘physical strip’’.

The eigenvalue densities X_j of the charges \hat{X}_j are expressed in terms of the particle densities compactly as

$$X_j = G_{j,k} \star \rho_k, \quad G_{j,k} = \sum_{m=1}^j a_{|j-k|-1+2m}, \quad (10)$$

where the kernel $a_j(v) = -\frac{1}{2\pi} \partial_v p_j(v)$, $(f \star g)(v) \equiv \int_{\mathbb{R}} dt f(v-t)g(t)$ denotes convolution, and repeated indices are summed over. The matrix kernel G is the Green's function of the discrete d'Alembertian \square ,

$$(\square G_{j,k})(v) = \delta_{j,k} \delta(v). \quad (11)$$

This enables to invert the relationship between X_j and ρ_j , which yields Eq. (5). The thermodynamics of integrable models is conveniently treated in the language of thermodynamic Bethe ansatz (TBA) [50,59,61–63]. We shall proceed with minimal technicality, and refer the reader to Appendix C and references therein. The partition function is cast as a functional integration over the densities ρ_j ,

$$\mathcal{Z} = \int \mathcal{D}[\rho_j] \exp \left[-L \sum_j \int_{\mathbb{R}} dv (\mu_j(v) \rho_j(v) + \mathfrak{s}_j(v)) \right],$$

where the combinatorial weight is given by the Yang-Yang entropy density per mode [50],

$$\mathfrak{s}_j(v) = \rho_j \log \left(1 + \frac{\bar{\rho}_j}{\rho_j} \right) + \bar{\rho}_j \log \left(1 + \frac{\rho_j}{\bar{\rho}_j} \right). \quad (12)$$

The functions $\bar{\rho}_j$ represent the densities of unoccupied modes, which obey the Bethe-Yang equations [50,59]

$$\rho_j + \bar{\rho}_j = a_j - a_{j,k} \star \rho_k, \quad (13)$$

where the integral kernels $a_{j,k}$ are given by $a_{j,k} = G_{j,k-1} + G_{j,k+1}$. The dominant contribution to \mathcal{Z} in the thermodynamic limit is given by the saddle point, yielding a set of coupled nonlinear integral equations known as the TBA equations [64,65]

$$\log Y_j = \mu_j + a_{j,k} \star \log (1 + Y_k^{-1}), \quad (14)$$

written in terms of Y functions $Y_j = \bar{\rho}_j / \rho_j$. Together, Eqs. (13) and (14) completely determine the equilibrium state. They provide the direct relationship between the set of chemical potentials μ_j and the set of macrostates ρ_j , demonstrating the completeness of the ensemble given in Eq. (2).

For practical purposes, it is useful to switch to an alternative formulation of the TBA equations. The infinite sum in Eq. (14) can be eliminated with the use of kernel identities, yielding a local form

$$\log Y_j = d_j + s \star \log[(1 + Y_{j-1})(1 + Y_{j+1})], \quad (15)$$

where the source terms are

$$d_j = \mu_j - s \star (\mu_{j-1} + \mu_{j+1}), \quad (16)$$

and the convolution kernel

$$s(v) = [2 \cosh(\pi v)]^{-1}. \quad (17)$$

These are equivalent to Eq. (14) when supplemented with the large- v asymptotics of the Y functions. To proceed, care must be taken when inverting the convolution with s , as the *pseudoinverse* defined through

$$s^{-1} \star f = f^+ + f^- \quad (18)$$

has a nontrivial null space (see, e.g., [66,67]). In particular, while $s^{-1} \star (s \star f) = f$ for any function f , in general $s \star (s^{-1} \star f) \neq f$. We therefore decompose the source terms as

$$d_j = s \star \lambda_j + d_j^\theta, \quad (19)$$

where

$$\lambda_j = s^{-1} \star d_j, \quad (20)$$

and the ‘‘singular components’’ d_j^θ are annihilated by s^{-1} . Applying s^{-1} to Eq. (15) and exponentiating, yields the modified Y -system relations

$$Y_j^+ Y_j^- = e^{\lambda_j} (1 + Y_{j-1})(1 + Y_{j+1}). \quad (21)$$

In the process, the singular components are not lost, but are instead encoded in the analytic data of the Y functions: their poles and zeros in the physical strip \mathcal{P} . Equation (21) is reobtained by convolving the logarithm of Eq. (21) with s , after multiplying out the singularities ξ with the functions [67–69]

$$t(v; \xi) = \tanh \left[\frac{\pi}{2} (v - \xi) \right], \quad |\text{Im}(\xi)| < \frac{1}{2}, \quad (22)$$

which satisfy $t^+ t^- = 1$. As a result, the singular components are of the form

$$d_j^\theta(v) = \sum_a \log t(v; \xi_a^{j,z}) - \sum_b \log t(v; \xi_b^{j,p}), \quad (23)$$

where $\{\xi_a^{j,z}\}$ and $\{\xi_b^{j,p}\}$ are, respectively, the sets of zeros and poles of the Y function Y_j in \mathcal{P} .

We now address the question of the generality of the charge-based GGE of Eq. (7). Using Eq. (10), this ensemble takes the form of Eq. (2) with

$$\mu_j = G_{j,k} \star \lambda_k + \lambda_z j. \quad (24)$$

Naively, the two ensembles could then be assumed equivalent. The crucial point, however, is that the Lagrange multipliers λ_j are blind to the singular components d_j^θ . In fact, as $\square\mu_j = \lambda_j$, the Lagrange multipliers precisely match the functions λ_j introduced in the decomposition of Eq. (19).

Put another way, the d'Alembertian \square inherits a null space from s^{-1} , and $\square\mu_j = \lambda_j$ demonstrates that the Lagrange multipliers λ_j of Eq. (7) *cannot* encode the components of μ_j in this null space. In the following section, we provide evidence that singular component contributions are a generic feature of equilibrium states. To conclude, it is worthwhile to stress that the null space of \square does not cause a problem for the string-charge duality relations [Eqs. (5) and (10)] as the densities ρ_j on which \square acts already provide the full description of a macrostate.

III. EXAMPLES

We now explicitly demonstrate this limitation of the charge-based GGE of Eq. (7) with some examples in the context of a quantum quench. Starting from an initial state $|\Psi\rangle$, the equilibrium macrostate ρ_j reached in the long-time limit is determined from the expectation values of the particle density operators

$$\rho_j(v) = \lim_{L \rightarrow \infty} L^{-1} \langle \Psi | \hat{\rho}_j(v) | \Psi \rangle. \quad (25)$$

As described above, it is convenient to encode a macrostate in the Y functions, $Y_j = \bar{\rho}_j / \rho_j$. The condition that the charge-based GGE is a valid ensemble is the absence of poles and zeros of these functions in the physical strip \mathcal{P} .

The best studied quenches are those from the ‘‘dimer’’ state

$$|D\rangle = \frac{1}{2^{L/2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)^{\otimes L/2}, \quad (26)$$

and the Néel state

$$|N\rangle = |\uparrow\downarrow\rangle^{\otimes L/2}, \quad (27)$$

for which the Y functions are explicitly known [70,71]. For the dimer quench these are [52]

$$Y_j(v) = \frac{j(j+2)v^2}{[v + (j+1)\frac{i}{2}][v - (j+1)\frac{i}{2}]}. \quad (28)$$

The double zero at the origin immediately indicates that the Lagrange multipliers λ_j in the charge-based GGE are not sufficient to capture it. Indeed, the source terms

$$d_j(v) = \log \tanh\left(\frac{\pi}{2}v\right), \quad (29)$$

determined through Eq. (15), are in the null space of s^{-1} , from which it follows that $\lambda_j = 0!$ We stress that the state is by no means close to the infinite-temperature Gibbs state in terms of local correlation functions. Previous works mistakenly assigned nontrivial λ_j for this state [48,70,71], resulting in the

incorrect interpretation of the GGE. The important point is that due to the nontrivial null space of s^{-1} , it is *not* permissible to define λ_j via Fourier transform, namely, $\mathcal{F}[\lambda_j] \neq \mathcal{F}[d_j]/\mathcal{F}[s]$.

The Néel state is similar. Again, the source terms

$$d_j(v) = (-1)^{j+1} \log \tanh\left(\frac{\pi}{2}v\right)^2 \quad (30)$$

consist solely of singular components, indicating $\lambda_j = 0$ for this state also. Indeed, these two examples are members of a particular class of initial states, whose equilibrium states can be cast as the partition function of a vertex model for which the initial state provides an *integrable* boundary [72]. Generic initial states do not admit such a description.

We thus also consider more general product states. A complete analytic treatment is now out of scope, as the complexity of ρ_j , computed via Eq. (25), grows quickly with j . Nevertheless, the lowest Y functions are straightforwardly determined. A particular example is the state composed of alternating two-site domain walls $|\uparrow\downarrow\downarrow\uparrow\rangle^{\otimes L/4}$. Explicit expressions are unwieldy (see Appendix D). They indicate nontrivial λ_j , and that Y_1 has four zeros at $\pm(0.382 \pm 0.234i)$ and two poles at $\pm 0.155i$. These analytic data indicate that again the resulting equilibrium state is not captured by the GGE of Eq. (7).

IV. CONCLUSION

We have shown that a complete description of equilibrium states in interacting integrable models requires the ensemble to be constructed from the number operators of the model's particle content. Any attempt to reduce the description inevitably leads to a loss of information, rendering a part of the equilibrium manifold inaccessible. The proposal naturally extends the established framework for noninteracting particles to the interacting integrable regime. The effect of nontrivial scattering in the interacting case is that excitations about an equilibrium state get nontrivially dressed by the correlations of the state (see, e.g., [50,73]).

Our hope is that the particle-based perspective which we advocate here creates a platform for the study of equilibration as one leaves the integrable points. The resulting loss of factorized scattering induces time scales up to which the particle-based description of ensembles may be expected to accurately capture statistical properties of quasistationary states, the so-called prethermalized regime [74–77].

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APPENDIX A: STRING HYPOTHESIS AND BETHE-YANG EQUATIONS

Any eigenstate of the isotropic Heisenberg spin chain of finite length L is associated a unique set of M rapidities. These are obtained from solutions to Bethe quantization conditions

$$e^{ip(v)L} \prod_{k=1}^M S_{1,1}(v - v_k) = -1, \quad v = \{v_j\}_{j=1}^M, \quad (\text{A1})$$

where M/L is the magnetization density,

$$p(v) = -i \log \left(\frac{u + \frac{i}{2}}{u - \frac{i}{2}} \right), \quad (\text{A2})$$

and the scattering amplitude $S_{1,1}$ is a member of a complete set of scattering amplitudes

$$S_j(v) = \frac{v - j\frac{i}{2}}{v + j\frac{i}{2}}, \quad (\text{A3})$$

$$S_{j,k} = S_{|j-k|} S_{j+k} \prod_{m=1}^{\min(j,k)-1} S_{|j-k|+2m}^2. \quad (\text{A4})$$

In the *thermodynamic limit* ($L \rightarrow \infty$, $M \rightarrow \infty$, keeping M/L fixed), the solutions (rapidities) v_j , $j = 1, 2, \dots, M$ (referred to as the Bethe roots) in the complex plane organize in a special way and permit to partition the entire spectrum in terms of particles. A central feature of generic integrable models is the formation of *bound states*, representing stable particles which exhibit elastic scattering without particle production. In terms of solutions v_j ($j = 1, \dots, M$) to Eq. (A1), these comprise of rapidities with nonzero imaginary parts which share common real parts. According to the *string hypothesis* [59,61,62], the spectra of a thermodynamically large system can be partitioned in terms of complex-valued solutions, which physically represent multimagnonic excitations called the strings. A k -string solution ($k \in \mathbb{N}$) centered at $v_\alpha^k \in \mathbb{R}$ is parametrized as

$$\{v_\alpha^{k,l}\} = \left\{ v_\alpha^k + (k+1-2l)\frac{i}{2} : l = 1, 2, \dots, k \right\}, \quad (\text{A5})$$

suppressing exponentially small deviations in system size L .

In the $L \rightarrow \infty$, the string centers become dense on real axis and condense. This allows to introduce distributions of Bethe j strings ρ_j and their hole counterparts $\bar{\rho}_j$ (unoccupied solutions allowed by Bethe quantization condition). In the thermodynamic limit, the quantization condition (A1) gets replaced by linear integral equations which are customary called the Bethe-Yang equations [50,59,61]

$$\rho_j + \bar{\rho}_j = a_j - a_{j,k} \star \rho_k, \quad (\text{A6})$$

where here and below we assume summation convention over repeated indices, and introduce convolution operation $(f \star g)(v) = \int_{\mathbb{R}} dt f(v-t)g(t)$. The integral kernels a_j and $a_{j,k}$ represent the “kinematic data”, i.e., encode full scattering data

among all distinct types of strings. Specifically, they are the derivatives of scattering phase shifts

$$a_j(v) = \frac{1}{2\pi i} \partial_v \log S_j(v), \quad (\text{A7})$$

$$a_{j,k}(v) = \frac{1}{2\pi i} \partial_v \log S_{j,k}(v). \quad (\text{A8})$$

APPENDIX B: LOCAL CHARGES AND THERMODYNAMIC SPECTRA

In accordance with the standard practice in Yang-Baxter integrable models [53,54], we introduce an infinite set of quantum transfer operators

$$\hat{T}_j(v) = \text{Tr}_{\mathcal{V}_j} \hat{L}_j^{(1)}(v) \hat{L}_j^{(2)}(v) \dots \hat{L}_j^{(L)}(v), \quad (\text{B1})$$

defined as traces over L -fold spatially ordered products of Lax operators $\hat{L}_j^{(i)}(u)$ acting in the tensor product $\mathcal{H} \otimes \mathcal{V}_j$, where $\mathcal{H} \cong \mathcal{V}_1^{\otimes L}$ is the Hilbert space of the spin chain. Specifically, Lax operators take the form

$$\hat{L}_j^{(i)}(v) = \mathbb{1}_1^{\otimes(i-1)} \otimes \hat{L}_j(v) \otimes \mathbb{1}_1^{\otimes(L-i)}, \quad (\text{B2})$$

$$\hat{L}_j(v) = v \mathbb{1}_1 \otimes \mathbb{1}_j + i \sum_{\alpha=\{x,y,z\}} \hat{S}_1^\alpha \otimes \hat{S}_j^\alpha, \quad (\text{B3})$$

where \hat{S}_j^α denotes spin- $j/2$ operators acting in \mathcal{V}_j which enclose the algebraic relations $[\hat{S}_j^a, \hat{S}_j^b] = i \epsilon_{abc} \hat{S}_j^c$.

Conserved operators \hat{T}_j mutually commute,

$$[\hat{T}_j(v), \hat{T}_{j'}(v')] = 0, \quad (\text{B4})$$

for all values of $j, j' \in \mathbb{N}$ and $v' \in \mathbb{C}$, as implied by the Yang-Baxter relation. A set of local charges is then defined through their logarithmic derivatives [48,60]

$$\hat{X}_j(v) = \frac{1}{2\pi i} \partial_v \log \frac{\hat{T}_j^+(v)}{\phi^{[+j]}(v)}, \quad (\text{B5})$$

where $\phi = T_0^+$ and the spectral parameter v should be restricted to the *physical strip* \mathcal{P} , defined as the strip

$$\mathcal{P} = \left\{ v \in \mathbb{C} : |\text{Im}(v)| < \frac{1}{2} \right\}. \quad (\text{B6})$$

We note that the conserved operators $\hat{X}_j(v)$ are only defined on \mathcal{P} [23], and become singular as the boundary is approached. The Heisenberg spin-chain Hamiltonian H is proportional to the charge $\hat{X}_1(0)$. By convention, we adopt $\hat{H} \equiv \hat{X}_1(0)$.

The action of \hat{X}_j on Bethe eigenstates in the $L \rightarrow \infty$ limit has been obtained in Refs. [48,52]. Expressed in terms of Bethe root densities ρ_j they take the compact form

$$X_j = G_{j,k} \star \rho_k, \quad (\text{B7})$$

with

$$G_{j,k} = \sum_{m=1}^{\min(j,k)} a_{|j-k|-1+2m}. \quad (\text{B8})$$

Inverting relation (B7) amounts to find an operator \square such that $(\square G_{j,k})(v) = \delta_{j,k} \delta(v)$. To this end, we employ kernel identities [59]

$$a_j - I_{j,k} \star a_k = s \delta_{j,1}, \quad (\text{B9})$$

where the convolution kernel reads as

$$s(v) = \frac{1}{2 \cosh(\pi v)}, \quad (\text{B10})$$

and the incidence matrix $I_{j,k} \equiv \delta_{j,k-1} + \delta_{j,k+1}$ expresses how distinct types of particles interact with each other. As Eq. (B9), special attention has to be paid to the pole structure of a_1 . To properly account for the singularity at the boundary of \mathcal{P} we introduce a pseudoinverse

$$s^{-1} \star f = f^+ + f^-, \quad (\text{B11})$$

where

$$f^\pm(v) \equiv f(v \pm \frac{i}{2} \mp i0^+) \quad (\text{B12})$$

for some positive infinitesimal 0^+ . It has to be stressed that s^{-1} is only a left inverse of s ,

$$s^{-1} \star (s \star f) = f, \quad (\text{B13})$$

while in general there exist functions f for which

$$s \star (s^{-1} \star f) \neq f. \quad (\text{B14})$$

This means that s^{-1} has a nontrivial null space [66,67]. With aid of the pseudoinverse we define a discrete d'Alembertian \square , defined on a set of functions f_j as

$$\square f_j = s^{-1} \star f_j - I_{j,k} f_k \equiv f_j^+ + f_j^- - f_{j-1} - f_{j+1}. \quad (\text{B15})$$

The action of \square on the scattering kernels gives

$$\square a_j = \delta_{j,1} \delta, \quad \square a_{j,k} = I_{j,k} \delta. \quad (\text{B16})$$

It is now clear from definition (B8) that $G_{j,k}$ represents the Green's function of \square ,

$$\square G_{j,k} = \delta_{j,k} \delta. \quad (\text{B17})$$

Relation (B7) can now be readily inverted by applying \square on both sides, yielding

$$\rho_j = \square X_j. \quad (\text{B18})$$

The distributions of holes $\bar{\rho}_j$ can be obtained from Bethe-Yang equations (A6) and read as

$$\bar{\rho}_j = a_j - s^{-1} \star X_j. \quad (\text{B19})$$

Before proceeding, we wish to emphasize that the identification (B18) captures two vital ingredients for a proper formulation of complete set of equilibrium ensembles, that is, (i) the importance of the physical strip \mathcal{P} and (ii) the role of the regulator in the definition (B12).

APPENDIX C: CANONICAL AND LOCAL FORM OF TBA EQUATIONS

We now turn our attention to the statistical ensemble

$$\hat{\rho} = \mathcal{Z}^{-1} \exp \left[- \sum_j \int_{\mathbb{R}} dv \mu_j(v) \hat{\rho}_j(v) \right], \quad (\text{C1})$$

where the normalization $\mathcal{Z} = \text{Tr} \hat{\rho}$ represents the partition sum. A standard approach to perform thermodynamic considerations is to work under the string hypothesis and introduce

a discrete set of Y functions,

$$Y_j = \frac{\bar{\rho}_j}{\rho_j}, \quad (\text{C2})$$

given as ratios of hole and particle densities for each string species. In the thermodynamic limit (by accounting for the Yang-Yang entropy as described in the text), a functional representation for the partition sum yields an infinite set of coupled nonlinear integral equations

$$\log Y_j = \mu_j + a_{j,k} \star \log(1 + Y_k^{-1}). \quad (\text{C3})$$

Introducing the inverse of the matrix kernel ($a+1$), defined via

$$(a+1)_{j,k}^{-1} \star f_k = f_j - I_{j,k} s \star f_k, \quad (\text{C4})$$

enables to disentangle Eq. (C3) into a locally coupled form

$$\log Y_j = d_j + I_{j,k} s \star \log(1 + Y_k), \quad (\text{C5})$$

referred to as the local TBA equations. The source terms d_j are related to the chemical potentials

$$d_j = \mu_j - I_{j,k} s \star \mu_k. \quad (\text{C6})$$

A subtle point here is that any constant term in μ_j does not enter in d_j as $1 \star s = \frac{1}{2}$. Equation (C3) can be reobtained by casting Eq. (C5) as

$$\log \tilde{Y}_j - I_{j,k} s \star \log(\tilde{Y}_k) = I_{j,k} s \star \log(1 + Y_k^{-1}), \quad (\text{C7})$$

where $\tilde{Y}_j(v) = Y_j(v)/Y_j(\infty)$, and convolving with kernel ($a+1$).

Modified Y-system. Equation (C5) represents a set of coupled nonlinear integral equations defined on the real line. Equivalently, these can be analytically continued in the complex rapidity plane, resulting in an algebraic form a set of functional relations

$$Y_j^+ Y_j^- = e^{\lambda_j} (1 + Y_{j-1}) (1 + Y_{j+1}), \quad (\text{C8})$$

which we refer to as the *modified Y-system* [we stress that shifts on the left-hand side are defined with the prescription given by Eq. (B12)].

We now exhibit the equivalence between Eq. (C8) and TBA equations (C5). Since Y functions of generic equilibrium states are meromorphic functions inside the physical strip \mathcal{P} , a naive "integration" of the (modified) Y -system (C8) into TBA equations by virtue of Cauchy theorem is not possible. Singular parts of $\log Y_j$ can nevertheless be easily remedied. Let us suppose that Y functions Y_j possess a set of zeros and poles in \mathcal{P} , located at $\{\xi_{j,a}^z\}$ and $\{\xi_{j,b}^p\}$, respectively, with the large- v asymptotics $Y_j^{(\infty)}$. Using functions

$$t(v; \xi) = \tanh\left(\frac{\pi}{2}(v - \xi)\right), \quad \text{Im}(\xi) < \frac{1}{2}, \quad (\text{C9})$$

which satisfy the property $t^+ t^- = 1$, we introduce a set of renormalized Y functions $\tilde{Y}_j(v)$,

$$\tilde{Y}_j(v) = \frac{Y_j(v) \prod_b t(v; \xi_b^{j,p})}{Y_j^{(\infty)} \prod_a t(v; \xi_a^{j,z})}, \quad (\text{C10})$$

which still satisfy the same modified Y -system (C8) but are now analytic in \mathcal{P} and have asymptotic behavior

$\lim_{|v| \rightarrow \infty} \tilde{Y}_j(v) = 1$. Now convolving with s after taking the logarithm gives back the local TBA equations

$$\log Y_j = d_j^\theta + s \star \lambda_j + I_{j,k} s \star \log(1 + Y_k), \quad (\text{C11})$$

where we introduced the splitting of the source terms $d_j = s \star \lambda_j + d_j^\theta$, with the singular part

$$d_j^\theta = \sum_a \log t(v; \xi_a^{j,z}) - \sum_b \log t(v; \xi_b^{j,p}). \quad (\text{C12})$$

It is worthwhile remarking that the physical solutions correspond to real valued $Y_j(v)$ on the real axis, requiring the singularities ξ to always appear in complex-conjugated pairs.

Going in the opposite direction, i.e., transforming Eq. (C11) is straightforwardly obtained by applying s^{-1} to both sides and subsequently taking the exponent. In the process, the information from the singular part d_j^θ gets transferred into the analytic structure of Y functions, while λ_j enter the modified Y -system (C8) as the nonuniversal (i.e., node-dependent) part. Notice that setting $\lambda_j \equiv 0$ recovers the universal form which is common in the literature, governing states whose physical input (TBA source terms) consist solely from the null-space components.

Gibbs equilibrium. The cleanest example of a state which fulfils the modified set of functional relations (C8) is the canonical Gibbs equilibrium, corresponding to bare dispersions $\mu_j^{\text{Gibbs}} = \beta a_j$. Due to absence of zero modes, this is equivalent to have $\lambda_j^{\text{Gibbs}} = \mu_j^{\text{Gibbs}}$, with

$$\lambda_j(v) = \beta \delta_{j,1} \delta(v), \quad (\text{C13})$$

restoring the well-known TBA source term

$$d_j^{\text{Gibbs}} = s \star \lambda_j^{\text{Gibbs}} = \beta s. \quad (\text{C14})$$

APPENDIX D: EXACT SOLUTIONS OF QUANTUM QUENCHES

Below we explain how to detect zero modes given a macrostate ρ_j^Ψ . In the context of a quench protocol ρ_j^Ψ can be understood as equilibrium states of a quench with the initial condition $|\Psi\rangle$. We first consider two simple product states which have represented toy examples in previous studies of quantum quenches in the Heisenberg model [41,43,44,48,52,70–72].

Dimer state. We first consider the so-called dimer state

$$|\text{D}\rangle = \frac{1}{2^{L/2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)^{\otimes L/2}. \quad (\text{D1})$$

The associated macrostate ρ_j expressed in terms of Y functions reads as [52]

$$Y_j(v) = \frac{j(j+2)v^2}{[v + (j+1)\frac{i}{2}][v - (j+1)\frac{i}{2}]}. \quad (\text{D2})$$

These can be quickly verified to obey the standard form of Y -system relations [65,78,79]

$$Y_j^+ Y_j^- = (1 + Y_{j-1})(1 + Y_{j+1}), \quad (\text{D3})$$

representing a specialization of Eq. (C8) when $\lambda_j \equiv 0$. These relations have a purely group-theoretic origin and represent the kinematic input to the problem. The physical input of the solution is encoded in analytic properties of Y_j^D in the complex

plane. In the present case it consists of a double zero at the origin $v = 0$ and a pair of simple poles at $\pm(j+1)\frac{i}{2}$, while the large- v asymptotics matches that of the infinite-temperature Gibbs equilibrium, that is, $Y_j(v) \sim j(j+2)$ as $|v| \rightarrow \infty$. The only physically relevant input lies inside the strip \mathcal{P} , where we find for every function Y_j a double zero at the origin, yielding the local TBA source terms

$$d_j(v) = \log t(v; 0)^2. \quad (\text{D4})$$

The TBA source terms obey the fusion property

$$\square g_j = 0, \quad (\text{D5})$$

where

$$g_1(v) = \log \left(4v^2 \left(v + \frac{i}{2} \right) \left(v - \frac{i}{2} \right) \right). \quad (\text{D6})$$

Néel state. The antiferromagnetic (Néel) state

$$|\text{N}\rangle = |\uparrow\downarrow\rangle^{\otimes L/2} \quad (\text{D7})$$

represents another particularly simple example which can be treated exactly (see, e.g., [43,70]). The initial two Y functions read as explicitly [52]

$$Y_1(v) = \frac{4v^2(12v^2 + 19)}{\left(v + \frac{i}{2}\right)\left(v - \frac{i}{2}\right)(v+i)(v-i)}, \quad (\text{D8})$$

$$Y_2(v) = \frac{\left(v + \frac{i}{2}\right)\left(v - \frac{i}{2}\right)(2v^4 + 7v^2 + 2)}{v^2(v+i)(v-i)\left(v + \frac{3i}{2}\right)\left(v - \frac{3i}{2}\right)}, \quad (\text{D9})$$

whereas the higher ones can be computed from the Y -system relations (D3). Importantly, the analytic data of Y_j inside \mathcal{P} are now given by double zeros (poles) for index j being odd (even). This implies

$$\mu_1(v) = \log \left(\frac{16v^2}{\left(v + \frac{i}{2}\right)\left(v - \frac{i}{2}\right)} \right), \quad (\text{D10})$$

while the higher source terms follow from the fusion condition

$$\mu_j = \sum_{k=1}^j \mu_1^{[j+1-2k]}. \quad (\text{D11})$$

It is worth stressing that the two examples given here in fact represent atypical initial conditions. This is attributed to the fact that the TBA source have only components from d_j^θ , implying $\lambda_j \equiv 0$. General initial states $|\Psi\rangle$ on the other hand involve nonvanishing λ_j or, put differently, are given by functions μ_j which do violate the fusion condition (D11). A practical drawback of this is that a full specification of a macrostate ρ_j goes beyond the knowledge of only μ_1 .

Generic states. Here, we analyze a nontrivial periodic state of 2-spin ferromagnetic domain walls

$$|\Phi\rangle = |\uparrow\uparrow\downarrow\downarrow\rangle^{\otimes L/4}, \quad (\text{D12})$$

representing one of the simplest generic initial states. This state has already appeared in previous studies of quantum

quench applications as the initial condition in Refs. [41,80]. Expressions for the first few Y functions can be computed

$$Y_1(v) = \frac{(64v^6 + 112v^4 - 20v^2 + 5)(192v^6 + 784v^4 + 1124v^2 + 491)}{(4v^2 + 1)(4v^2 + 5)(256v^8 + 1024v^6 + 1696v^4 + 1248v^2 + 29)}, \quad (\text{D13})$$

with four zeros at $\pm(0.382 \pm 0.234i)$ and two poles at $\pm 0.155i$, in \mathcal{P} . It can furthermore be easily verified analytically that the universal form of the Y -system (D3) is now no longer satisfied (see also [80]). This specifically means that after subtracting the singular components d_j^θ from the TBA source terms d_j , we are left with nonvanishing components $s \star \lambda_j$ which in turn determine the node-dependent terms λ_j in the modified Y -system relations (C8).

APPENDIX E: QUENCH ACTION

The quench action approach [39,49] has been introduced as a functional integral approach towards time evolution of local observables in thermodynamically large integrable many-body systems. The steady-state limit of the evolution is entirely determined from the stationary part of the quench action functional

$$\mathcal{Z}_{\text{QA}} = \int \mathcal{D}[\rho_j] \exp(-L S_{\text{QA}}), \quad (\text{E1})$$

analytically, but are already rather formidable. The initial Y function for instance reads as

with

$$S_{\text{QA}} = \sum_j \int_{\mathbb{R}} dv \left(\mu_j(v) \rho_j(v) + \mathfrak{s}_j(v) \right). \quad (\text{E2})$$

The state-dependent terms μ_j represent the mode decomposition of the (density of the) logarithmic overlap between $|\Psi\rangle$ and a general macrostate, namely,

$$\sum_j \int_{\mathbb{R}} dv \mu_j(v) \rho_j(v) \equiv \lim_{L \rightarrow \infty} L^{-1} \log |\langle \Psi | \{v_j\} \rangle|^2. \quad (\text{E3})$$

Saddle-point evaluation of the functional \mathcal{Z}_{QA} yields a sought-for macrostate ρ_j . As the choice of notation already suggests, μ_j of Eq. (E3) are nothing but the chemical potentials corresponding to individual particle modes. This can be most easily seen by comparing Eq. (E3) with the form of Eq. (C1), implying that \mathcal{Z}_{QA} coincides with the partition sum \mathcal{Z} of the generalized Gibbs ensemble $\hat{\rho}$.

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