

# Exact Overlaps for All Integrable Matrix Product States of Rational Spin Chains

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The overlaps between integrable matrix product states (MPSs) and Bethe states are important in both the nonequilibrium statistical physics and the AdS/CFT duality. We present the general MPS overlap formula. The result is a product of a ratio of Gaudin determinants and a prefactor. The Gaudin determinants depend on the spin chain but not on the MPS. The MPS dependent prefactor is given for all integrable MPSs of the  $\mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , and  $\mathfrak{sp}_N$  symmetric spin chains with arbitrary representations.

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**Introduction**—Over the past ten years, intensive research has been carried out on the topic of integrable boundary states. The overlaps between boundary and Bethe states have important applications in two areas of theoretical physics: nonequilibrium dynamics in statistical physics and the AdS/CFT duality.

A major breakthrough in the last decade has been the laboratory simulation of integrable statistical physics models [1–3]. A common feature of these studies is the experimental investigation of so-called quantum quenches, where certain initial states (the ground state of the pre-quenched system) are prepared and the resulting finite-time dynamics are monitored. This has launched an intensive theoretical investigation of the nonequilibrium dynamics of integrable models [4,5]. These studies are based on the so-called “quench action” method, which allows for the calculation of the long-term equilibrium state and the possibility of studying the time evolution of specific initial states [6–8]. The quench action method is based on explicit knowledge of the overlaps between the initial state and the Bethe eigenstates. This method has been successfully applied to a number of different models [9–12], but the investigated initial states were the so-called two-site product states, which have essentially minimal entanglement.

In parallel, the investigation of the AdS/CFT duality with defects by integrability methods has begun. The single-trace operators of the planar  $\mathcal{N} = 4$  super Yang-Mills theory ( $\mathcal{N} = 4$  SYM) can be mapped to Bethe states of an integrable spin chain at weak coupling [13]. It was found that the one-point functions of these single-trace operators

can be traced back to overlaps of matrix product states (MPS) and Bethe states for the so-called D3-D5 type domain wall defect of  $\mathcal{N} = 4$  SYM [14,15]. These overlap formulas, which give the one-point functions, have been determined in various limits [16–19]. This domain wall setup was also generalized to the Aharony-Bergman-Jafferis-Maldacena theory [20,21]. Similar boundary states have been found for other defects. In the presence of a giant graviton, some correlation functions are also given by boundary state overlaps in the  $\mathcal{N} = 4$  SYM [22] and in the Aharony-Bergman-Jafferis-Maldacena theory [23]. Boundary state overlaps also appear in the one-point functions in the presence of Wilson and ’t Hooft lines [24,25]. Most recently, integrable boundary states and their overlaps have emerged in the investigation of the Coulomb branch of  $\mathcal{N} = 4$  SYM [26]. The integrable conformal defects in  $\mathcal{N} = 4$  SYM have also been classified [27]. The physical significance of these defects is that they violate conformal [26] or supersymmetry [28] in certain configurations, which can lead to more realistic theories. Since for each of these examples the important physical quantities can be described by overlaps between boundary states and Bethe states, the investigation of the overlap formulas is important.

Because of the above applications in statistical physics and AdS/CFT duality, research on the overlaps of integrable boundary and Bethe states has been initiated. The definition of integrable boundary states first appeared in the context of 2D quantum field theories [29] and was later generalized to spin chains [30,31]. The first important observation regarding the overlaps was that they are proportional to the ratio of Gaudin determinants [32]. The Gaudin determinants are universal, i.e., they do not depend on the boundary state. The boundary state dependent part of the overlap function is the prefactor preceding the ratio. Later, this observation was used to conjecture overlap formulas [16,33,34]. There have been only a few

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proofs [32,35,36], mainly focused on spin 1/2 XXX or XXZ spin chains. It was not clear how these methods could be generalized to general spins or higher rank symmetries. Later, a method based on the algebraic Bethe ansatz was developed to determine and prove the overlap formulas of  $\mathfrak{gl}_N$  symmetric spin chains for any representations and any two-site product states [37–39]. Although these results are extremely general, they do not say anything about MPS overlaps. In terms of applications, the MPS overlaps are particularly important. For quantum quenches, the ground state of the prequench system can be approximated better with an MPS than with a two-site product state. Even in the AdS/CFT duality, the most interesting defects correspond to MPS boundary states [15,20,28].

In this Letter, we present the general overlap formula (19) for integrable MPSs of rational spin chains. Every integrable MPS corresponds to a  $K$  matrix that is a representation of a reflection algebra. One can define a series of commuting matrices ( $F$  operators) from the components of the  $K$  matrix. The spectrum of the  $F$  operators completely defines the MPS overlap formula. The definition of the  $F$  operators depends only on the reflection algebra. In the Supplemental Material (SM) [40], we give the definitions of the  $F$  operators for every reflection algebra of the  $\mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , or  $\mathfrak{sp}_N$  symmetric spin chains. These results give the overlaps for all integrable MPSs of the  $\mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , or  $\mathfrak{sp}_N$  symmetric spin chains with arbitrary representations.

The derivation of the overlaps can be found in a separate, more detailed paper [41]. For a broad class of MPSs in  $\mathfrak{gl}_N$  spin chains, the proofs are fully rigorous, while in the remaining cases the calculations involve some conjectures; for details, see the End Matter.

#### Integrable spin chains and matrix product states—

**Definitions for integrable spin chains:** In this Letter, we do not focus on a particular model, but instead work with a wide class of integrable spin chains. A spin chain is given by a Hamiltonian  $H$ , which acts on a Hilbert space  $\mathcal{H}$  with a tensor product structure:  $\mathcal{H} = (\mathbb{C}^d)^J$ , where  $d$  is the dimension of the one-site Hilbert space and  $J$  is the length of the spin chain. The model is integrable if there exists a generating function  $\mathcal{T}(u)$  of the commuting charges that commutes with the Hamiltonian

$$[H, \mathcal{T}(u)] = 0. \quad (1)$$

This generating function  $\mathcal{T}(u)$  is called the “transfer matrix.”

Let us introduce an auxiliary space  $\mathbb{C}^N$ . For integrable spin chains with periodic boundary conditions, the transfer matrix is

$$\mathcal{T}(u) = \sum_{j=1}^N T_{j,j}(u), \quad (2)$$

where  $T_{i,j}(u)$  are the entries of the monodromy matrix for  $i, j = 1, \dots, N$ . We also introduce the matrix notation in

the auxiliary space:  $T(u) = \sum_{i,j} e_{i,j} \otimes T_{i,j}(u) \in \text{End}(\mathbb{C}^N \otimes \mathcal{H})$ , where  $e_{i,j}$  are the unit matrices of  $\mathbb{C}^N$  with components  $(e_{i,j})_{a,b} = \delta_{i,a} \delta_{j,b}$ . The monodromy matrix satisfies the famous  $RTT$  relation

$$R_{1,2}(u-v)T_1(u)T_2(v) = T_2(v)T_1(u)R_{1,2}(u-v), \quad (3)$$

where  $R(u) \in \text{End}(\mathbb{C}^N \otimes \mathbb{C}^N)$  is the  $R$  matrix and the subscripts 1 and 2 label two copies of the auxiliary space. The  $RTT$  relation has two consequences: the  $R$  matrix must satisfy the Yang-Baxter equation

$$R_{1,2}(u-v)R_{1,3}(u)R_{2,3}(v) = R_{2,3}(v)R_{1,3}(u)R_{1,2}(u-v), \quad (4)$$

and the transfer matrix generates commuting operators

$$[\mathcal{T}(u), \mathcal{T}(v)] = 0. \quad (5)$$

In this Letter we investigate rational spin chains with Lie-algebra symmetries  $\mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , or  $\mathfrak{sp}_N$ . The  $\mathfrak{gl}(N)$  symmetric  $R$  matrix is

$$R(u) = \mathbf{1} + \frac{1}{u} \mathbf{P}, \quad \mathbf{P} = \sum_{i,j=1}^N e_{i,j} \otimes e_{j,i}. \quad (6)$$

The  $\mathfrak{o}_N$  and  $\mathfrak{sp}_N$  symmetric  $R$  matrices can be written as

$$R(u) = \mathbf{1} + \frac{1}{u} \mathbf{P} - \frac{1}{u + \kappa_N} \mathbf{Q}, \quad \mathbf{Q} = \sum_{i,j=1}^N \theta_i \theta_j e_{i,j} \otimes e_{\bar{i},\bar{j}}, \quad (7)$$

where  $\bar{i} = N + 1 - i$  and  $\kappa_N = (N \mp 2/2)$ . The minus or plus signs correspond to the  $\mathfrak{o}_N$  or  $\mathfrak{sp}_N$  algebras, respectively. For  $\mathfrak{o}_N$ ,  $\theta_i = +1$  and for  $\mathfrak{sp}_N$ ,  $\theta_i = \text{sgn}[i - (N + 1/2)]$ . The monodromy matrices are representations of the Yangian algebras  $Y(\mathfrak{g})$  [42], where  $\mathfrak{g} = \mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , or  $\mathfrak{sp}_N$ .

Let  $\tau(u|\bar{u})$  and  $|\bar{u}\rangle$  be the eigenvalues and eigenvectors of the transfer matrix  $\mathcal{T}(u)$ , where the set  $\bar{u} \equiv \{\bar{u}^j\}_{j=1}^n$  consists of subsets  $\bar{u}^j = \{u_k^j\}_{k=1}^{r_j}$ , and each  $u_k^j$  denotes a Bethe root. The  $n$  is the rank of the symmetry algebra ( $n$  for  $\mathfrak{gl}_{n+1}$ ,  $\mathfrak{o}_{2n+1}$ ,  $\mathfrak{sp}_{2n}$ , and  $\mathfrak{o}_{2n}$ ). The Bethe root  $u_k^\mu$  corresponds to the rapidity of a type  $a$  quasiparticle, and it must satisfy the Bethe equation [43]

$$\alpha_\mu(u_k^\mu) \prod_{\nu=1}^n \prod_{l=1}^{r_\nu} \frac{u_k^\mu - u_l^\nu - \frac{i}{2} C_{\mu,\nu}}{u_k^\mu - u_l^\nu + \frac{i}{2} C_{\mu,\nu}} = -1. \quad (8)$$

The coefficients  $C_{\mu,\nu}$  are the inner products of the simple roots of the corresponding algebra [40]. The functions  $\alpha_\mu(u)$  depend on the representations of the Hilbert space (and the inhomogeneities for inhomogeneous chains). A set

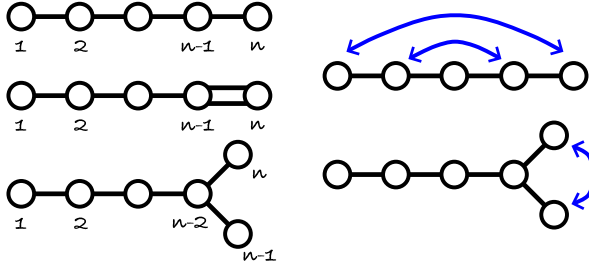


FIG. 1. Dynkin diagrams (first row  $\mathfrak{gl}_{n+1}$ , second row  $\mathfrak{o}_{2n+1}$  or  $\mathfrak{sp}_{2n}$ , third row  $\mathfrak{o}_{2n}$ ). On the right, the blue arrows show the nontrivial involutions  $\rho$  that correspond to achiral PS.

of the Bethe roots  $\bar{u}^\mu$  corresponds to a node  $\mu$  of the Dynkin diagram for  $\mu = 1, \dots, n$ ; see Fig. 1.

Integrable matrix product states: For even  $J$  let us define the following MPS:

$$\langle \text{MPS} | = \sum_{i_1, \dots, i_J} \text{Tr} \left[ \psi_{i_{J-1}, i_J}^{(J/2)} \dots \psi_{i_1, i_2}^{(1)} \right] \langle i_1, i_2, \dots, i_{J-1}, i_J |, \quad (9)$$

where  $\psi_{i,j}^{(k)} \in \text{End}(\mathbb{C}^{d_B})$  for  $i, j = 1, \dots, d$ ,  $k = 1, \dots, J/2$ , and  $d_B$  is the boundary (or bond) dimension. The matrices  $\psi_{i,j}^{(k)}$  can differ (i.e.,  $\psi_{i,j}^{(k)} \neq \psi_{i,j}^{(l)}$ ) for inhomogeneous chains, but they are given by the same functions as  $\psi_{i,j}^{(k)} \equiv \psi_{i,j}(\theta_k)$ , where  $\theta_k$ -s are the inhomogeneities. For homogenous chains it may happen that  $\psi_{i,j}^{(k)} = \omega_j \omega_i$ , in which case the MPS can also be defined for chains of even or odd length,

$$\langle \text{MPS} | = \sum_{i_1, \dots, i_J} \text{Tr}[\omega_{i_J} \dots \omega_{i_1}] \langle i_1, i_2, \dots, i_{J-1}, i_J |. \quad (10)$$

We also define states by “cutting the trace,”

$$\langle \Psi_{\alpha, \beta} | = \sum_{i_1, \dots, i_J} \left( \psi_{i_{J-1}, i_J}^{(J/2)} \dots \psi_{i_1, i_2}^{(1)} \right)_{\alpha, \beta} \langle i_1, i_2, \dots, i_{J-1}, i_J |, \quad (11)$$

where  $\alpha, \beta = 1, \dots, d_B$  are indices of the boundary space. The MPS is integrable if the states  $\langle \Psi_{\alpha, \beta} |$  satisfy the  $KT$  relation [38,44]

$$\sum_{k, \gamma} K_{i,k}^{\alpha, \gamma}(u) \langle \Psi_{\gamma, \beta} | T_{k,j}(u) = \sum_{k, \gamma} \langle \Psi_{\alpha, \gamma} | \hat{T}_{i,k}(-u) K_{k,j}^{\gamma, \beta}(u), \quad (12)$$

where the coefficients  $K_{i,j}^{\alpha, \beta}(u) \in \mathbb{C}$  define the  $K$  matrix  $\mathbf{K}_{i,j}(u) = \sum_{\alpha, \beta} K_{i,j}^{\alpha, \beta}(u) e_{\alpha, \beta}^B \in \text{End}(\mathbb{C}^{d_B})$ ,  $\mathbf{K}(u) = \sum_{i,j} e_{i,j} \otimes \mathbf{K}_{i,j}(u) \in \text{End}(\mathbb{C}^N \otimes \mathbb{C}^{d_B})$ . Here,  $(e_{\alpha, \beta}^B)_{a,b} = \delta_{\alpha,a} \delta_{\beta,b}$  are the elementary matrices of the boundary space  $\mathbb{C}^{d_B}$ . We also define the notation  $\langle \Psi | \in \mathcal{H}^* \otimes \text{End}(\mathbb{C}^{d_B})$ , which is a covector in the Hilbert space and a matrix in the boundary space:  $\langle \Psi | = \sum_{\alpha, \beta} \langle \Psi_{\alpha, \beta} | \otimes e_{\alpha, \beta}^B$ . Using this matrix notation

in the boundary space, the  $KT$  relation takes the compact form

$$\mathbf{K}(u) \langle \Psi | T(u) = \langle \Psi | \hat{T}(-u) \mathbf{K}(u). \quad (13)$$

Here, the tensors  $\mathbf{K}(u)$ ,  $\langle \Psi |$ , or  $T(u)$  act trivially on the Hilbert, auxiliary, or the boundary spaces, respectively.

There are two types of  $KT$  relation: the uncrossed  $KT$  relation, where  $\hat{T} = T$ , and the crossed  $KT$  relation [38,41], where

$$\sum_{k=1}^N \hat{T}_{k,i}(u) T_{k,j}(u) = \lambda_1(u) \lambda_1(-u) \delta_{i,j} \mathbf{1}. \quad (14)$$

Here, we used the pseudovacuum eigenvalue  $T_{1,1}(u)|0\rangle = \lambda_1(u)|0\rangle$  [45]. Assuming the  $K$  matrix is invertible, the condition

$$\langle \text{MPS} | \mathcal{T}(u) = \langle \text{MPS} | \hat{\mathcal{T}}(-u) \quad (15)$$

follows from the  $KT$  relation.

Another consequence of the  $KT$  relation is that the  $K$  matrix satisfies the reflection equation [38,41]

$$\begin{aligned} R_{1,2}(u-v) \mathbf{K}_1(-u) \bar{R}_{1,2}(u+v) \mathbf{K}_2(-v) \\ = \mathbf{K}_2(-v) \bar{R}_{1,2}(u+v) \mathbf{K}_1(-u) R_{1,2}(u-v), \end{aligned} \quad (16)$$

where

$$\bar{R}_{1,2}(u) = \begin{cases} R_{1,2}(u), & \text{for the uncrossed } KT, \\ R_{1,2}'(-u), & \text{for the crossed } KT. \end{cases} \quad (17)$$

The reflection equation defines reflection algebra with generators  $\mathbf{K}(u)$ . Let us consider its series expansion,

$$\mathbf{K}(u) = \mathcal{U} \otimes \mathbf{1} + u^{-1} \sum_{i,j=1}^N e_{i,j} \otimes \mathbf{k}_{i,j}^{(1)} + \mathcal{O}(u^{-2}), \quad (18)$$

where  $\mathcal{U} \in \text{Aut}(\mathbb{C}^N)$  and  $\mathbf{k}_{i,j}^{(1)} \in \text{End}(\mathbb{C}^{d_B})$ . The matrices  $\mathbf{k}_{i,j}^{(1)}$  generate a Lie-subalgebra  $\mathfrak{h}$  [46], and the  $K$  matrix is a representation of the twisted Yangian  $Y(\mathfrak{g}, \mathfrak{h})$  [47–50]. The reflection equation and the explicit form of  $\mathcal{U}$  define the twisted Yangian [41]. The classification of twisted Yangians is shown in Table I. This Lie-subalgebra  $\mathfrak{h}$  is also the symmetry algebra of both the  $K$  matrix and the MPS.

*Exact overlaps of integrable MPS—*

Pair structures: We now continue with the discussion of overlaps between the integrable MPSs and on-shell Bethe states. The integrability condition (15) is equivalent to nontrivial selection rules for the on-shell overlaps: the overlap is nonvanishing only when the Bethe roots exhibit

TABLE I. The reflections algebras  $Y(\mathfrak{g}, \mathfrak{h})$  and the corresponding PS. For  $Y(\mathfrak{o}_{2n}, \mathfrak{gl}_n)$ , the PS is chiral or achiral when  $n$  is even or odd. For  $Y(\mathfrak{o}_{2n}, \mathfrak{o}_M \oplus \mathfrak{o}_{2n-M})$ , the PS is chiral or achiral when  $n - M$  is even or odd. For chiral or achiral  $\mathfrak{o}_{2n}$  PS, the value of  $n_+$  is  $n$  or  $n - 1$ , respectively.

| $\mathfrak{g}$        | $\mathfrak{h}$                                    | $KT$ relation | PS                | $n_+$                   |
|-----------------------|---------------------------------------------------|---------------|-------------------|-------------------------|
| $\mathfrak{gl}_N$     | $\mathfrak{o}_N$ or $\mathfrak{sp}_N$             | Crossed       | Chiral            | $N - 1$                 |
|                       | $\mathfrak{gl}_M \oplus \mathfrak{gl}_{N-M}$      | Uncrossed     | Achiral           | $\lfloor (N/2) \rfloor$ |
| $\mathfrak{o}_{2n+1}$ | $\mathfrak{o}_M \oplus \mathfrak{o}_{2n+1-M}$     | Uncrossed     | Chiral            | $n$                     |
| $\mathfrak{sp}_{2n}$  | $\mathfrak{sp}_{2m} \oplus \mathfrak{sp}_{2n-2m}$ | Uncrossed     | Chiral            | $n$                     |
|                       | $\mathfrak{gl}_n$                                 | Uncrossed     | Chiral            | $n$                     |
| $\mathfrak{o}_{2n}$   | $\mathfrak{o}_M \oplus \mathfrak{o}_{2n-M}$       | Uncrossed     | Chiral or achiral | $n$ or $(n - 1)$        |
|                       | $\mathfrak{gl}_n$                                 | Uncrossed     | Chiral or achiral | $n$ or $(n - 1)$        |

pair structures (PSs), i.e.,  $\bar{u}^j = -\bar{u}^{\rho(j)}$  for  $j = 1, \dots, n$ . The  $\rho$  is an involution of the Dynkin diagram. If  $\rho$  is trivial (i.e.,  $\rho(j) = j$  for all  $j$ ), the PS is called “chiral.” If  $\rho$  is nontrivial, the PS is “achiral” [18]. There are two cases for nontrivial  $\rho$ : for  $\mathfrak{gl}_N$ ,  $\rho(j) = N - j$ ; for  $\mathfrak{o}_{2n}$ ,  $\rho(n - 1) = n$ ,  $\rho(n) = n - 1$ , and  $\rho(j) = j$  for  $j < n - 1$  (see Fig. 1). For  $\mathfrak{o}_{2n+1}$  and  $\mathfrak{sp}_{2n}$ , there is no nontrivial involution, so only a chiral PS is possible.

A set of Bethe roots  $\bar{u}^j$  is chiral if  $\rho(j) = j$ . The achiral PS can include chiral subsets. For an achiral  $\mathfrak{gl}_{2n}$  PS, node  $n$  is chiral, and for an achiral  $\mathfrak{o}_{2n}$  PS, nodes  $1, \dots, n - 2$  are chiral. For simplicity, we focus on the states where every chiral set contains an even number of elements. For the odd cases, see SM [40].

The PS halves the degrees of freedom: half of the Bethe roots can be expressed in terms of the other half. More precisely, the full set decomposes as  $\bar{u} = \bar{u}^+ \cup \bar{u}^-$ , with  $\bar{u}^+ \cap \bar{u}^- = \emptyset$  and  $\bar{u}^- = -\bar{u}^+$ . Let  $n_+$  be the number of sets in  $\bar{u}^+$ .

The physical interpretation of the overlaps is the annihilation of quasiparticles at the temporal boundary. The PS implies that the quasiparticles annihilate in pairs. The chiral PS indicates that the boundary preserves parity symmetry ( $P$ ), while an achiral PS implies that a quasiparticle annihilates with its antiparticle of opposite rapidity, meaning the MPS preserves  $CP$  symmetry. The residual symmetry  $\mathfrak{h}$  determines the PS (see Table I), and its derivation can be found in Appendix B of [18].

Overlap formula: The on-shell overlaps are given by

$$\frac{\langle \text{MPS} | \bar{u} \rangle}{\sqrt{\langle \bar{u} | \bar{u} \rangle}} = \underbrace{\left[ \sum_{k=1}^{d_B} \beta_k \prod_{j=1}^{n_+} \tilde{\mathcal{F}}_k^{(j)}(\bar{u}^{+,j}) \right]}_{\text{MPS dep.}} \times \underbrace{\sqrt{\frac{\det G^+}{\det G^-}}}_{\text{Bethe state dep.}}. \quad (19)$$

The overlap formula consists of two parts. The ratio of Gaudin determinants ( $G^\pm$ ) is independent of the MPS. It depends only on the Bethe roots. The Gaudin determinants are defined in SM [40] and have also appeared in several previous works [32,38,39].

The prefactor is the MPS dependent part. We introduced the shorthand notation  $\tilde{\mathcal{F}}_k^{(j)}(\bar{v}) = \prod_{v_l \in \bar{v}} \tilde{\mathcal{F}}_k^{(j)}(v_l)$ , where

$\tilde{\mathcal{F}}_k^{(j)}(u)$  are functions defined for  $j = 1, \dots, n_+$  and  $k = 1, \dots, d_B$ . These functions depend only on the  $K$  matrix and not on the specific representation of the Hilbert space. For each twisted Yangian  $Y(\mathfrak{g}, \mathfrak{h})$ , there exists a commuting subalgebra generated by operators  $\mathbf{F}^{(j)}(u)$  for  $j = 1, \dots, n_+$ . These  $F$  operators can be expressed in terms of the components of the  $K$  matrix. Since they commute, they can be simultaneously diagonalized, and their eigenvalues yield the functions  $\tilde{\mathcal{F}}_k^{(j)}(u)$ .

The prefactor also includes coefficients  $\beta_k \in \mathbb{C}$  for  $k = 1, \dots, d_B$ , which are the eigenvalues of the pseudovacuum overlap operator  $\mathbf{B} = \langle \Psi | 0 \rangle$ , which commutes with the  $F$  operators.

Physical interpretation: The prefactor represents the amplitude of the quasiparticles, while the Gaudin determinants account for the finite-size corrections. If  $d_B = 1$ , the prefactor reduces to a product of two-particle amplitudes  $\tilde{\mathcal{F}}^{(j)}(u)$ . If  $d_B > 1$ , the MPS corresponds to a superposition of  $d_B$  different boundaries. For the  $k$ th boundary, the two-particle amplitudes are  $\tilde{\mathcal{F}}_k^{(j)}(u)$ , and the total amplitude is a weighted sum over boundaries. This can also be interpreted as a thermal sum if  $\beta_k \rightarrow e^{-\beta \epsilon_k}$ . For each  $\epsilon_k$  is the energy of a state in the prequench system. From each such state, quasiparticles are emitted with amplitude  $\prod_j \tilde{\mathcal{F}}_k^{(j)}(\bar{u}^{+,j})$ . Thus, the MPS can be interpreted as a thermal state of the prequench system.

Example  $Y(\mathfrak{gl}_N, \mathfrak{o}_N)$ : We now provide the explicit form of the functions  $\tilde{\mathcal{F}}_k^{(j)}(u)$  for the reflection algebra  $Y(\mathfrak{gl}_N, \mathfrak{o}_N)$ . The nonvanishing overlaps require a chiral PS, in which case  $n_+ = N - 1$ , and thus we have  $N - 1$   $F$  operators.

We begin by defining a series of nested  $K$  matrices,

$$\mathbf{K}_{a,b}^{(k+1)}(u) = \mathbf{K}_{a,b}^{(k)}(u) - \mathbf{K}_{a,k}^{(k)}(u) \left[ \mathbf{K}_{k,k}^{(k)}(u) \right]^{-1} \mathbf{K}_{k,b}^{(k)}(u), \quad (20)$$

starting from the initial condition  $\mathbf{K}^{(1)} \equiv \mathbf{K}$ . The  $F$  operators are then constructed as

$$\mathbf{F}^{(k)}(u) = \left[ \mathbf{K}_{k,k}^{(k)}(u) \right]^{-1} \mathbf{K}_{k+1,k+1}^{(k+1)}(u), \quad (21)$$

for  $k = 1, \dots, N-1$ . These operators generate a commuting subalgebra and also commute with the operator  $\mathbf{B} = \langle \Psi | 0 \rangle$ , i.e.,

$$[\mathbf{F}^{(k)}(u), \mathbf{F}^{(l)}(v)] = [\mathbf{F}^{(k)}(u), \mathbf{B}] = 0, \quad (22)$$

for all  $k, l = 1, \dots, N-1$ . As a result, they can be simultaneously diagonalized

$$\begin{aligned} \mathbf{F}^{(k)}(u) &= \mathbf{A} \text{diag}[\mathcal{F}_1^{(k)}(u), \dots, \mathcal{F}_{d_B}^{(k)}(u)] \mathbf{A}^{-1}, \\ \mathbf{B} &= \mathbf{A} \text{diag}(\beta_1, \dots, \beta_{d_B}) \mathbf{A}^{-1}, \end{aligned} \quad (23)$$

where  $\mathbf{A}$  is an invertible matrix in the boundary space. Finally, the  $\tilde{\mathcal{F}}_k^{(j)}(u)$  functions of the overlap formula (19) are

$$\tilde{\mathcal{F}}_j^{(k)}(u) = \mathcal{F}_j^{(k)}(iu - k/2) \sqrt{\frac{u^2}{u^2 + 1/4}}. \quad (24)$$

This result provides the overlap formulas for any representation of the reflection algebra  $Y(\mathfrak{gl}_N, \mathfrak{o}_N)$ . The definitions for the other reflection algebras (listed in Table I) are structurally similar but technically more involved. The technical details of these definitions do not directly contribute to the understanding of the main results of the Letter, so we present them in SM [40].

*How to apply the formula*—Although the final result is quite general, its application is nontrivial. In this section, we outline the steps required to apply the overlap formula (19). A typical scenario involves an integrable spin chain with a given MPS, and the goal is to determine whether the MPS is integrable. If integrability is confirmed, the next step is to construct the corresponding overlap formula.

We assume that the monodromy matrix is known, satisfies the *RTT* relation (3), and commutes with the Hamiltonian of the model (1). For  $\mathfrak{gl}_N$  symmetric models, the inverse monodromy matrix (14) may also be required.

*Deciding on integrability*: To check whether the MPS is integrable, we use the condition (15), typically for small spin chain lengths [51]. Note that the spectral parameter of the monodromy matrix can be shifted, i.e.,  $T(u-a)$  also satisfies (3) and (1). Therefore, it may happen that only a shifted version of the integrability condition

$$\langle \text{MPS} | \mathcal{T}(u) = \langle \text{MPS} | \hat{\mathcal{T}}(-u+b) \quad (25)$$

is satisfied in the initial convention. In such cases, we simply redefine the monodromy matrix as  $T(u) \rightarrow T(u+b/2)$  to recover (15). In the  $\mathfrak{gl}_N$  case, we must also determine whether the uncrossed or crossed equation is satisfied.

*Finding the  $K$  matrix*: Once integrability is confirmed, the next step is to solve the *KT* relation (15) to find the  $K$

matrix. This can be done using the shortest possible spin chain ( $J=1$  or  $2$ ). Solving the *KT* relation is straightforward, as it is linear in  $\mathbf{K}(u)$ .

*Identifying the reflection algebra*: Next, identify the twisted Yangian  $Y(\mathfrak{g}, \mathfrak{h})$  associated with the  $K$  matrix. This can be done by identifying the symmetry algebra of either the MPS or the  $K$  matrix.

*Rotating the  $K$  matrix*: In some cases, the MPS may be in the “wrong direction” for applying the overlap formula. Specifically, the formulas for the  $F$  operators (20) and (21) assume that certain components of the  $K$  matrix are invertible. If this is not the case, we can apply a group transformation  $g \in G = \exp(\mathfrak{g})$  to rotate the  $K$  matrix,

$$\begin{aligned} \langle \Psi_{\alpha,\beta}^g | &= \langle \Psi_{\alpha,\beta} | \Delta(g), \\ \mathbf{K}^g(u) &= (\hat{g}^{-1} \otimes \mathbf{1}) \mathbf{K}(u) (g \otimes \mathbf{1}), \end{aligned} \quad (26)$$

where  $\hat{g} = g$  except in the crossed  $\mathfrak{gl}_N$  case, where  $\hat{g} = (g')^{-1}$ . The group action on the Hilbert space is given by the coproduct  $\Delta(g)$ . This transformation preserves the *KT* relation. Our goal is to find a group element of the form  $g(\varphi) = \exp(\varphi x)$  with  $x \in \mathfrak{g}$  and  $\varphi \in \mathbb{C}$  such that the  $F$  operators are well defined. The remaining steps are then performed using the rotated  $K$  matrix  $\mathbf{K}^{g(\varphi)}$  (if the rotation is necessary), and the limit  $\varphi \rightarrow 0$  is taken at the end.

*Calculating of the  $F$  operators*: With the  $K$  matrix and the associated reflection algebra  $Y(\mathfrak{g}, \mathfrak{h})$  identified, we compute the  $F$  operators and the corresponding functions  $\tilde{\mathcal{F}}_k^{(j)}(u)$  using the definitions provided in SM [40] for each case of  $Y(\mathfrak{g}, \mathfrak{h})$ .

*Conclusions and outlook*—In this Letter, we presented the exact overlap formula (19) for all integrable MPSs in  $\mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , and  $\mathfrak{sp}_N$  symmetric spin chains with arbitrary representations. For each MPS, there is a corresponding  $K$  matrix, which is a representation of a reflection algebra. The  $K$  matrix defines a series of commuting matrices—the  $F$  operators—whose spectrum determines the MPS overlap formula. In SM [40], we introduced the  $F$  operators for the reflections algebras associated with  $\mathfrak{gl}_N$ ,  $\mathfrak{o}_N$ , and  $\mathfrak{sp}_N$  symmetric spin chains.

The formula has been rigorously proven for the twisted Yangians  $Y(\mathfrak{gl}_N, \mathfrak{o}_N)$  and  $Y(\mathfrak{gl}_N, \mathfrak{gl}_{\lfloor N/2 \rfloor} \oplus \mathfrak{gl}_{\lceil N/2 \rceil})$ . The proof is detailed in [41], where strong evidence is also provided for the validity of the formula in other cases. In the End Matter, we briefly summarize the proof strategy and the additional checks performed.

A promising direction for future research is the extension of these results to graded spin chains, such as those with  $\mathfrak{gl}(M|N)$  or  $\mathfrak{osp}(M|2n)$  symmetry, or the Hubbard model. It is also likely that the formulas can be generalized to the trigonometric cases.

An alternative approach to computing MPS overlaps is based on dressing formulas [44]. While dressing formulas have the advantage of being applicable under general

twists, they must be computed separately for each representation of the reflection algebra. In contrast, the formulas presented in this letter are universal—they hold for all representations.

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## End Matter

The main result (19) has been proven for MPSs associated with the reflection algebras  $Y(\mathfrak{gl}_N, \mathfrak{o}_N)$  and  $Y(\mathfrak{gl}_N, \mathfrak{gl}_{\lfloor N/2 \rfloor} \oplus \mathfrak{gl}_{\lceil N/2 \rceil})$  [41]. In the remaining cases, strong arguments and numerical checks support the validity of the formula. In the End Matter, we briefly outline the proof and present additional verifications.

The proof described in [41] is essentially a generalization of the proof for the case  $d_B = 1$  presented earlier in [38]. For simplicity, let us start with  $\mathfrak{gl}_2$  spin chains. In this case, the monodromy matrix is  $2 \times 2$  in the auxiliary space, and during the use of the algebraic Bethe ansatz, the components are usually denoted as follows:

$$T(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}. \quad (\text{A1})$$

The pseudovacuum is the highest-spin state, which is annihilated by the  $C$  operator, i.e.,  $C(u)|0\rangle = 0$ . Bethe states can be generated from the pseudovacuum by applying  $B$  operators,

$$|\bar{u}\rangle = B(u_1) \dots B(u_r)|0\rangle. \quad (\text{A2})$$

Using the  $RTT$  relation (3), one can compute how the operators  $A$ ,  $B$ ,  $C$ , and  $D$  act on off-shell Bethe states, and the results can be expressed as linear combinations of new off-shell Bethe states. The key point is that the  $B$  operator increases, the  $C$  operator decreases, and the  $A$  and  $D$  operators do not change the number of Bethe roots. The main advantage of the  $KT$  relation (13) is that it allows us to obtain a recursion relation for the off-shell overlaps  $\langle \Psi | \bar{u} \rangle$ . This works as follows. The  $KT$  relation is a  $2 \times 2$  matrix in the auxiliary space, and we can take its (2,2) component,

$$\begin{aligned} & \mathbf{K}_{2,1}(z) \langle \Psi | B(z) + \mathbf{K}_{2,2}(z) \langle \Psi | D(z) \\ &= \langle \Psi | D(-z) \mathbf{K}_{2,2}(z) + \langle \Psi | C(-z) \mathbf{K}_{1,2}(z). \end{aligned} \quad (\text{A3})$$

Assuming that the matrix  $\mathbf{K}_{2,1}(z)$  is invertible, the action of the  $B$  operator on  $\langle \Psi |$  can be expressed in terms of the actions of the  $D$  and  $C$  operators. This means that in the overlap  $\langle \Psi | \bar{u} \rangle$  one of the  $B$  operators can be replaced by  $D$  and  $C$  operators. Since the action of  $D$  and  $C$  operators on a Bethe state can be expressed in terms of Bethe states with the same or fewer Bethe roots, the off-shell overlaps  $\langle \Psi | \bar{u} \rangle$  can ultimately be expressed in terms of overlaps with fewer Bethe roots, i.e., we obtain a recursion relation. This

recursion relation is very similar to the one obtained for the scalar product of Bethe states. Just as in the case of the scalar product [52,53], a sum formula can be derived for the off-shell overlaps, using the so-called coproduct property of the Bethe states and the boundary state  $\langle \Psi |$ . Following Korepin's argument [52,54], the on-shell overlap formula can then be derived from the sum formula.

The derivation can also be generalized to nested spin chains. For this, three prerequisites about Bethe vectors are needed: (1) a *recursion rule* that expresses a Bethe vector in terms of Bethe vectors that contain fewer roots of a certain type; (2) an *action formula* that expresses the action of the monodromy matrix elements on Bethe vectors in terms of Bethe vectors; and (3) a *coproduct formula*.

For  $\mathfrak{gl}_N$  spin chains, these were derived earlier in [53], so the proof for overlaps applies [41]. Since the calculations are based on the algebraic Bethe ansatz, the proof is valid for any representation in the quantum space. Furthermore, the calculation does not use the explicit form of the MPS; it only assumes that  $\langle \Psi |$  satisfies the  $KT$  relation. The  $KT$  relation is used to replace the “creation” operators of the Bethe vectors with “annihilation” operators, which requires inverting certain elements of the  $K$  matrix [see Eq. (A3) where  $\mathbf{K}_{2,1}$  must be inverted]. Based on this, the proof is valid for any MPS whose associated  $K$  matrix has certain invertible components. It turns out that this condition is satisfied for the  $K$  matrices corresponding to the algebras  $Y(\mathfrak{gl}_N, \mathfrak{o}_N)$  and  $Y(\mathfrak{gl}_N, \mathfrak{gl}_{\lfloor N/2 \rfloor} \oplus \mathfrak{gl}_{\lceil N/2 \rceil})$ , meaning that the overlap formula is proven for integrable MPSs with  $\mathfrak{o}_N$  and  $\mathfrak{gl}_{\lfloor N/2 \rfloor} \oplus \mathfrak{gl}_{\lceil N/2 \rceil}$  symmetry [41]. In the remaining cases  $[Y(\mathfrak{gl}_N, \mathfrak{sp}_N)$  and  $Y(\mathfrak{gl}_N, \mathfrak{gl}_M \oplus \mathfrak{gl}_{N-M})$  for  $M < N/2$ ], the method previously developed for simple tensor product states ( $d_B = 1$ ) [39] can be generalized to compute MPS overlaps [41]. This is not a rigorous proof, as the calculation involves some unproven assumptions. In these cases, additional checks were performed to validate the overlap formula; see below.

For orthogonal and symplectic spin chains, the overlap formula (19) has not yet been rigorously proven. In the calculations of [41], it was only assumed that the usual overlap formula (19) exists. However, this is a very well-founded assumption, as it has been verified in numerous previous cases [10,16,32–34,39,55–57] and no counterexamples are known. If we accept the existence of the overlap formula, then the unknown functions  $\tilde{\mathcal{F}}_k^{(j)}(u)$  appearing in the formula can be derived! Using the

embeddings  $\mathfrak{sl}_n \subset \mathfrak{o}_{2n+1}$ ,  $\mathfrak{sl}_n \subset \mathfrak{o}_{2n}$ , and  $\mathfrak{sl}_n \subset \mathfrak{sp}_{2n}$  the functions  $\tilde{\mathcal{F}}_k^{(j)}(u)$  for  $j = 1, 2, \dots, n-1$  can be obtained from the overlap formulas of  $\mathfrak{gl}_n$  spin chains. The remaining functions  $\tilde{\mathcal{F}}_k^{(n)}(u)$  can be determined using the algebra isomorphisms  $\mathfrak{sl}_2 \cong \mathfrak{sp}_2 \cong \mathfrak{o}_3$  and  $\mathfrak{sl}_2 \oplus \mathfrak{sl}_2 \cong \mathfrak{o}_4$ . For details, see Sec. 6 of [41].

A rigorous proof of the overlap functions for orthogonal and symplectic spin chains requires knowledge of the three prerequisites mentioned above (recursion, action, and coproduct formulas). In the case of  $\mathfrak{o}_{2n+1}$  these formulas are known [58], so the proof method based on the  $KT$  relation described above can likely be applied without further difficulties. For the cases of  $\mathfrak{o}_{2n}$  and  $\mathfrak{sp}_{2n}$ , the three prerequisites for Bethe vectors are currently not available.

The formulas that have not been rigorously proven underwent further validation. Each reflection algebra in Table I has one-dimensional representations corresponding to scalar-valued  $K$  matrices  $K(z)$ , where  $d_B = 1$ . The associated MPSs simplify to tensor product states, which are the  $\langle \delta |$  states. For tensor product states in  $\mathfrak{gl}_N$  spin chains, the overlap formulas were previously proven [38,39], and these results are compatible with the formulas in the Letter. For  $\mathfrak{o}_N$  and  $\mathfrak{sp}_{2n}$  spin chains, we numerically verified the  $\langle \delta |$  state overlap formulas in cases where the quantum space is constructed from the defining representations of the symmetry algebra  $N = 3, 4, 5, 6, 8$  and  $n = 1, 2, 4$ .

For every reflection algebra there exists a special MPS, which is the action of the transfer matrix on the  $\langle \delta |$  state, i.e.,

$$\langle \text{MPS}_\xi | = \langle \delta | T(\xi), \quad (\text{A4})$$

where  $\xi$  is an arbitrary parameter. The  $K$  matrix corresponding to this special MPS is

$$\mathbf{K}_{0,B}(z) = \bar{R}_{0,B}(-z - \xi) K_0(z) R_{0,B}(-z + \xi), \quad (\text{A5})$$

where  $B$  indicates the boundary space of the  $K$  matrix. From the defining Eq. (A4), it follows that the ratio of overlaps can be expressed in terms of the transfer matrix eigenvalue  $\tau(\xi|\bar{u})$ , on the other hand, the same ratio can be expressed using our overlap formula (19), i.e.,

$$\frac{\langle \text{MPS}_\xi | \bar{u} \rangle}{\langle \delta | \bar{u} \rangle} = \tau(\xi|\bar{u}) = \sum_{k=1}^{d_B} \beta_k \prod_{j=1}^{n_+} \frac{\tilde{\mathcal{F}}_k^{(j)}(\bar{u}^{+,j})}{\tilde{\mathcal{F}}_\delta^{(j)}(\bar{u}^{+,j})}, \quad (\text{A6})$$

where  $\tilde{\mathcal{F}}_\delta^{(j)}(u)$  are the one-particle overlaps corresponding to the  $\delta$  state. We have verified the correctness of this formula for every reflection algebra listed in Table I up to rank 4.

In the case of  $Y(\mathfrak{gl}_4, \mathfrak{sp}_4)$  it was possible to compare the (19) formula with previously numerically validated results. The paper [55] contains a class of MPSs built from the  $[s, 0]$  Dynkin-index representations of  $\mathfrak{sp}_4$  for all  $s \in \mathbb{Z}_+$ -ra. The case  $s = 1$  is given in SM Sec. VII B 2 [40]. We also performed numerical calculations for  $s = 2, 3, 4, 5$ , and the results agree. For higher-rank cases, one can use a special class of  $K$  matrices for  $Y(\mathfrak{gl}_{2n}, \mathfrak{sp}_{2n})$  [59],

$$\mathbf{K}_{i,j}(u) = g_{i,j} + \frac{1}{u - 1/2} F_{i,j}, \quad (\text{A7})$$

where  $g_{i,j} = -g_{j,i}$  is an arbitrary antisymmetric matrix and  $F_{i,j}$  is a representation of the  $\mathfrak{sp}_{2n}$  algebra, i.e.,  $F_{i,j} = F_{j,i}$  and

$$[F_{i,j}, F_{k,l}] = g_{k,j} F_{i,l} - g_{i,l} F_{k,j} - g_{i,k} F_{j,l} + g_{l,j} F_{k,i}. \quad (\text{A8})$$

It turns out that the MPSs from [55] belong to this class of  $K$  matrices when  $F_{i,j}$  are the  $[s, 0]$  Dynkin-index representations of  $\mathfrak{sp}_4$ . We have numerically verified the correctness of the formula for the  $[0, 1]$ ,  $[1, 1]$  and  $[0, 2]$  representations as well. Since the overlaps for the  $\delta$  states (representation with Dynkin index  $[0, 0]$ ) were derived earlier [39], in the numerical calculations we explicitly computed the ratio of overlaps between the MPS and the  $\delta$  states and compared it with the ratio given by the overlap formula (19), which automatically cancels the Gaudin factor that does not explicitly depend on the MPS. Using this method, we also verified the correctness of the formula for  $K$  matrices of type (A7) for  $n = 3$  for the representations  $[1, 0, 0]$ ,  $[0, 1, 0]$ , and  $[0, 0, 1]$ .

For orthogonal spin chains, it is also possible to perform a separate check for the  $\mathfrak{o}_6$  case. Here, we can use the fact that  $\mathfrak{o}_6 \cong \mathfrak{sl}_4$ , meaning that  $\mathfrak{gl}_4$  and  $\mathfrak{o}_6$  spin chains are equivalent, with the only differences being in conventions. At the level of  $K$  matrices, the following correspondences hold: (i)  $Y(\mathfrak{o}_6, \mathfrak{o}_3 \oplus \mathfrak{o}_3) \cong Y(\mathfrak{gl}_4, \mathfrak{o}_4)$  and  $Y(\mathfrak{o}_6, \mathfrak{o}_5) \cong Y(\mathfrak{gl}_4, \mathfrak{sp}_4)$  (chiral pair structures), and (ii)  $Y(\mathfrak{o}_6, \mathfrak{o}_6) \cong Y(\mathfrak{gl}_4, \mathfrak{gl}_4)$ ,  $Y(\mathfrak{o}_6, \mathfrak{o}_2 \oplus \mathfrak{o}_4) \cong Y(\mathfrak{gl}_4, \mathfrak{gl}_2 \oplus \mathfrak{gl}_2)$  and  $Y(\mathfrak{o}_6, \mathfrak{gl}_3) \cong Y(\mathfrak{gl}_4, \mathfrak{gl}_1 \oplus \mathfrak{gl}_3)$  (achiral pair structures). In all cases, there is an exact match between the overlap formulas.