

Wick's Theorem for Matrix Product States

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Matrix product states and their continuous analogues are variational classes of states that capture quantum many-body systems or quantum fields with low entanglement; they are at the basis of the density-matrix renormalization group method and continuous variants thereof. In this work we show that, generically, N -point functions of arbitrary operators in discrete and continuous translation invariant matrix product states are completely characterized by the corresponding two- and three-point functions. Aside from having important consequences for the structure of correlations in quantum states with low entanglement, this result provides a new way of reconstructing unknown states from correlation measurements, e.g., for one-dimensional continuous systems of cold atoms. We argue that such a relation of correlation functions may help in devising perturbative approaches to interacting theories.

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Quantum states of many-body systems or fields are characterized by their N -point correlation functions. Unsurprisingly, given their central status in the respective theories, there are many ways in which such correlation functions can be book-kept in terms of as simple as possible mathematical objects. For instance, prominent perturbative methods for the description of interacting field theories make extensive use of the relation between high-order and two-point correlators [1,2]. These methods, supported by Isserlis's or Wick's theorem [2], give rise to a practical way of identifying the propagators as the basic objects for the description of the situation at hand, as well as an interpretation in terms of virtual processes.

In this work we show that, remarkably, generic translation invariant matrix product states (MPS) [3–6] and their continuous analogues, cMPS or holographic states [7,8], are completely characterized by their two- and three-point functions. These states comprise a variational state class that approximates states with limited spatial entanglement well—an ubiquitous property for good reasons [5,6]—and are at the basis of the seminal density-matrix renormalization group method [6] and continuous versions thereof [7]. What is more, in our approach states and corresponding operators can be constructed such that their N -point correlation functions are completely characterized by their correlators of up to arbitrary odd order. We do so by proposing an explicit construction procedure of how to reconstruct higher-order correlation functions from lower-order ones. This insight has a number of interesting consequences.

To start with, a fruitful research program has emerged in recent years of revisiting questions in many-body theory within the variational set of matrix product states, now seen as a “theoretical laboratory.” This approach has the appealing feature that some links and statements that are in all generality too hard to capture analytically can be

formulated in a completely rigorous fashion. In this mindset, complete classifications of quantum phases have been given, new instances of Lieb-Schultz-Mattis theorems proven, or phase transitions of arbitrary order identified [9]. Our statement provides a new tool to grasp the structure of matrix product states and their analogues for quantum fields.

Our result also identifies matrix product states as a variational class that is similar to, but yet beyond, quasifree approaches. This observation may be even more interesting in light of the fact that it is not straightforward to construct natural classes generalizing Gaussian states: For example, it is known that any unitary evolution generated by quadratic polynomials in the canonical coordinates maps Gaussian states to Gaussian states. If one looks at the closure of the unitaries generated by the quadratic polynomials and a single further term, say, of third order, one does not arrive at a meaningful new variational class, but in fact generates a set dense in all unitaries [10].

More practically speaking, our result clearly opens up novel ways to think of reconstruction methods for quantum states. We show how one-dimensional lattice states and states of continuous systems such as cold atoms on top of atom chips [11] can be reconstructed or approximated using low-order correlation data only.

Finally, the most important implications may come from a fundamental insight into the inherent structural properties of correlations as such. Our result shows that many physically relevant states of limited entanglement correspond one to one to families of meromorphic functions with interdependent poles.

Matrix product states.—The main theorem of this Letter applies to *generic* translation invariant (continuous) matrix product states in the thermodynamic limit. Let us define what this means and fix some basic notation. A discrete

matrix product state vector of an ν -partite spin system with periodic boundary conditions is given by

$$|\psi_{\text{MPS}}\rangle = \sum_{s_\nu, \dots, s_1} \text{Tr}[A^{(\nu)}[s_\nu] \dots A^{(1)}[s_1]] |s_\nu, \dots, s_1\rangle, \quad (1)$$

where $A^{(i)}[s_i] \in \mathbb{C}^{d \times d}$ for all i . In this work we will focus on the thermodynamic limit, i.e., $\nu \rightarrow \infty$, and the translation invariant case, i.e., $A^{(i)}[s] = A^{(j)}[s]$ for all i, j . The finite bond dimension d will be arbitrary but fixed. In this setting, correlation functions of a set of operators $\{O_j\}$ labeled by an index j and with support on (different) sites i_k with $0 = i_1 < \dots < i_N$ take the form

$$\begin{aligned} & \langle O_{j_N}^{(i_N)} O_{j_{N-1}}^{(i_{N-1})} \dots O_{j_1}^{(i_1)} \rangle \\ &= \text{Tr}[M^{[j_N]} E^{i_N - i_{N-1} - 1} M^{[j_{N-1}]} \dots M^{[j_1]} E^\infty] =: C_{\mathbf{j}}^{(N)}(\mathbf{n}), \end{aligned} \quad (2)$$

with $M^{[j]} = \sum_{m,n} A^*[m] \otimes A[n] \langle m | O_j | n \rangle$, the transfer matrix $E = \sum_s A^*[s] \otimes A[s]$, and $E^\infty := \lim_{n \rightarrow \infty} E^n$, which exists when the state is normalized. The star indicates complex conjugation of the matrix elements. We have written the distances in a compact form as $\mathbf{n} = (i_2 - i_1 - 1, \dots, i_N - i_{N-1} - 1) \in \mathbb{Z}^{N-1}$ and summarized likewise $\mathbf{j} = (j_1, \dots, j_N)$. It is possible to consider finite-dimensional and infinite-dimensional local systems; in the latter case, the matrices $A[s]$ have to be chosen such that the infinite sums converge.

The expectation values are invariant under simultaneous conjugation of all $M^{[j]}$ and E with some invertible matrix, making it possible to consider an equivalent formulation where E is in its Jordan normal form (JNF), i.e., $E \mapsto J(E)$. We call the MPS *generic* if $J(E)$ has nondegenerate diagonal entries μ_1, \dots, μ_{d^2} and, moreover, if the largest absolute value occurs only once. We order the diagonal elements by their absolute value, in descending order. Note that in the thermodynamic limit normalization implies $|\mu_i| \leq 1$, where the one with the largest magnitude equals unity, i.e., $\mu_1 = 1$. In the future, we will simply say eigenvectors when we mean the *right* eigenvectors, i.e., $E|i\rangle = \mu_i|i\rangle$. The number of Schmidt coefficients, and hence the entanglement belonging to any contiguous bipartition of regions, is limited by $2d$.

Continuous MPS.—A one-dimensional nonrelativistic bosonic quantum field can be described in terms of field operators $\Psi(x)$ and $\Psi^\dagger(x)$, with $[\Psi(x), \Psi(x')^\dagger] = \delta(x - x')$ and $\Psi(x)|0\rangle = 0$, where $|0\rangle$ is the vacuum. A particular class of one-dimensional quantum fields is that of cMPS or holographic states [7] with state vectors

$$|\psi_{\text{cMPS}}\rangle = \text{Tr}_{\text{aux}} \left[\mathcal{P} e^{\int_0^L dx Q(x) \otimes \mathbb{1} + R(x) \otimes \Psi^\dagger(x)} \right] |\Omega\rangle, \quad (3)$$

where $Q(x)$ and $R(x)$ are x -dependent finite-dimensional complex matrices acting in a d -dimensional auxiliary space. Similar to the case of MPS, we focus on translation invariant cMPS, having constant Q and R , in the

thermodynamic limit $L \rightarrow \infty$. It is useful to introduce the Liouvillian matrix

$$T = Q^* \otimes \mathbb{1} + \mathbb{1} \otimes Q + R^* \otimes R. \quad (4)$$

A state of such a quantum field is completely characterized by all the possible normal ordered correlation functions of the operators $\Psi(x)$ and $\Psi^\dagger(x)$, e.g.,

$$\langle \Psi^\dagger(x_2) \Psi^\dagger(x_5) \dots \Psi(x_4) \Psi(x_3) \Psi(0) \rangle, \quad (5)$$

where the order of position labels is such that they increase in size from left to right within the Ψ^\dagger , decrease within the Ψ , and $0 = x_1 < \dots < x_N$. Correlation functions of cMPS are given by expressions involving only the auxiliary space. Let e^{T^∞} be a short notation for $\lim_{L \rightarrow \infty} e^{TL}$; this limit makes sense when the state is normalized.

For translation invariant cMPS, we consider the differences between points, $\tau_i = x_{i+1} - x_i$, and summarize them in a vector notation $\boldsymbol{\tau} = (\tau_1, \tau_2, \dots, \tau_{N-1}) \in \mathbb{R}^{N-1}$. Let the matrices $M^{[j]}$ be equal to $R^* \otimes \mathbb{1}$, $\mathbb{1} \otimes R$, or $R^* \otimes R$, etc. With this notation we represent all N th-order correlation functions in a compact and straightforward way. For example,

$$\begin{aligned} & \langle \Psi^\dagger(x_2) \Psi^\dagger(x_3) \Psi(x_2) \Psi(0) \rangle \\ &= \text{Tr}[M^{[1]} e^{T\tau_2} M^{[3]} e^{T\tau_1} M^{[2]} e^{T^\infty}] =: C_{\mathbf{j}}^{(3)}(\boldsymbol{\tau}), \end{aligned} \quad (6)$$

with $\boldsymbol{\tau} = (x_2, x_3 - x_2)$, $\mathbf{j} = (1, 3, 2)$, and $M^{[1]} = R^* \otimes \mathbb{1}$, $M^{[2]} = \mathbb{1} \otimes R$, and $M^{[3]} = R^* \otimes R$. Note that also in this case a gauge transformation is possible, corresponding to a simultaneous conjugation of T and the matrices $M^{[j]}$ by an invertible matrix, so that we can always go to a picture where T is in its JNF. The relationship between cMPS and channels directly implies [12] that the diagonal elements $\lambda_1, \lambda_2, \dots, \lambda_{d^2}$ of $J(T)$ are closed under conjugation. We call the cMPS *generic* if $J(T)$ has a nondegenerate diagonal and, moreover, the largest real part occurs only once. We order the eigenvalues in descending order by their real parts; the normalization of cMPS implies that it is non-positive and the largest one is zero, i.e., $\lambda_1 = 0$.

Main result.—In general, to characterize the full state of a quantum system one needs to specify all the correlation functions. One may ask the following question: “Is it possible to completely characterize a (continuous) matrix product state from low order correlation functions?” With the only initial assumption of a bond dimension d , we will show how to (i) certify that the given (c)MPS is generic and (ii) reconstruct the full state of a (c)MPS from low order correlation functions once (i) has been verified. Both aspects will be studied in detail in the following.

Data structure and transformations.—We will use both the Z and Laplace transform of correlation functions in their multidimensional form. For discrete MPS, the Z transform

$$Z_{\mathbf{j}}^{(N)}(\mathbf{s}) = \sum_{n_1, \dots, n_N} s_1^{n_1} \dots s_N^{n_N} C_{\mathbf{j}}^{(N)}(\mathbf{n}), \quad s_1, \dots, s_N \in \mathbb{C} \quad (7)$$

is applicable. Similarly, we have a Laplace transformation of the cMPS correlation functions

$$\mathcal{L}_{\mathbf{j}}^{(N)}(\mathbf{s}) = \int_0^\infty d^{N-1} \tau e^{-\mathbf{s} \cdot \boldsymbol{\tau}} C_{\mathbf{j}}^{(N)}(\boldsymbol{\tau}), \quad s_1, \dots, s_N \in \mathbb{C}. \quad (8)$$

Depending on the correlation data, these transformations will not converge everywhere. The key observation is that under the assumption of a nondegenerate diagonal of $J(E)$, we have

$$C_{\mathbf{j}}^{(N)}(\mathbf{n}) = \sum_{k_1, \dots, k_{N-1}=1}^{d^2} c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) (\mu_{k_{N-1}})^{n_{N-1}} \dots (\mu_{k_1})^{n_1}, \quad (9)$$

where

$$\begin{aligned} c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) \\ = \langle 1 | M^{[j_N]} | k_{N-1} \rangle \langle k_{N-1} | M^{[j_{N-1}]} \dots | k_1 \rangle \langle k_1 | M^{[j_1]} | 1 \rangle, \end{aligned} \quad (10)$$

and $\{|k\rangle\}$ denotes the basis where E obtains JNF. Note that $E^\infty = |1\rangle\langle 1|$. Considering $|\mu_i| \leq 1$ with $\mu_1 = 1$, we deduce that the Z transform—as a function in the complex variables $\{s_1, \dots, s_{N-1}\}$ —converges within the product of unit disks around the origin. It is possible, starting from this region, to reconstruct the whole meromorphic function (its poles and the residues) by analytic continuation. Another way of dealing with, e.g., experimental data, would be to fit functions of the given form using only the unit disk as support. Summarizing, we have access to

$$Z_{\mathbf{j}}^{(N)}(\mathbf{s}) = \sum_{k_1, \dots, k_{N-1}}^{d^2} \frac{c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})}{(1 - \mu_{k_1} s_1) \dots (1 - \mu_{k_{N-1}} s_{N-1})}. \quad (11)$$

Similar considerations apply to cMPS correlations, which, under the assumption of nondegenerate $J(T)$, turn into

$$C_{\mathbf{j}}^{(N)}(\boldsymbol{\tau}) = \sum_{k_1, \dots, k_{N-1}=1}^{d^2} c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) e^{\lambda_{k_1} \tau_1} \dots e^{\lambda_{k_{N-1}} \tau_{N-1}}, \quad (12)$$

with the same symbols $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$ as defined in Eq. (10). The integral in Eq. (8) yields meromorphic functions in higher dimensions of the form

$$\mathcal{L}_{\mathbf{j}}^{(N)}(\mathbf{s}) = \sum_{k_1, \dots, k_{N-1}}^{d^2} \frac{c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})}{(\lambda_{k_1} - s_1) \dots (\lambda_{k_{N-1}} - s_{N-1})}. \quad (13)$$

Since $\text{Re} \lambda_i \leq 0$, the region of convergence of the integral in Eq. (8) is the product of complex half-planes with positive

real part. Being a meromorphic function, it can be reconstructed using this data. Note that now $e^{T^\infty} = |1\rangle\langle 1|$. The fact that the diagonal of $J(E)$ and $J(T)$ is nondegenerate and has only finitely many elements played a crucial role in the derivation of the form of Eqs. (9) and (12).

Reconstruction theorem.—The form of the equations (11) and (13) implies that all poles are elements of $\{\lambda_i\}$ and $\{\mu_i^{-1}\}$, respectively. Depending on whether the corresponding residues $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$ are zero or not, the transforms of the correlation data may or may not reveal poles at these points. This makes it useful to give the following definition.

Definition 1 (p number): Given a (c)MPS with bond dimension d , we define the p number as the minimum order p such that d^2 distinct poles appear in the Z or Laplace transforms, respectively, in at least one correlation function of order less than or equal to p . If the minimum does not exist, we say that the p number is infinite.

Note that in this definition we only need *one* correlation function of *any* subset of operators of interest to show all poles in one of its arguments, in order to derive the p number. This provides a solution to the first task: If the p number of a (c)MPS is finite, we can directly claim that E or T has a nondegenerate Jordan diagonal. Now we are going to study in more detail not only the poles, but the full structure of correlation functions of (c)MPS. We work in the basis where E or T is in JNF. If a function $Z_{\mathbf{j}}^{(N)}$ or $\mathcal{L}_{\mathbf{j}}^{(N)}$ is given, each coefficient $c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1})$ can be extracted by finding the residue of the corresponding multipole. We can finally state the main theorem as follows.

Theorem 1 (Computing higher from lower correlation functions): A generic, translation invariant (c)MPS in the thermodynamic limit with p number p is completely characterized by the correlation functions of order $\ell \leq 2p - 1$. *Proof:* We merely need to consider the case in which p is finite. From the definition of the p number we know that $J(E)$, respectively $J(T)$, have a nondegenerate diagonal in the JNF, whose entries can be recovered from (the pole structure of the transforms of) the correlation functions of order $N \leq p$. This reduces the reconstruction of correlation functions to the reconstruction of the coefficients in Eq. (10). The problem now is to express every coefficient

$$c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) = M_{1, k_{N-1}}^{[j_N]} M_{k_{N-1}, k_{N-2}}^{[j_{N-1}]} \dots M_{k_1, 1}^{[j_1]}, \quad (14)$$

each associated with a unique set of poles, in terms of low-order coefficients $c^{(\ell)}$ with $\ell \leq 2p - 1$. From the definition of the p number we know that for each index k there is at least one nonzero coefficient $c_{\mathbf{j}(k)}^{(p(k))}(\dots, k, \dots) \neq 0$, with $p(k) \leq p$ and fixed $\mathbf{j}(k)$, having k as one of its indices. This allows us to write d^2 different versions of the identity (this is a scalar)

$$1^{(k)} = \frac{M_{1,\star}^{[j^{(k)}_{p(k)}]} \cdots M_{\star,k}^{[j^{(k)}_{\ell'}]} M_{k,\star}^{[j^{(k)}_{\ell'-1}]} \cdots M_{\star,1}^{[j^{(k)}_1]}}{c_{\mathbf{j}^{(k)}}^{(p(k))}(\dots, k, \dots)}, \quad (15)$$

where $k = 1, 2, \dots, d^2$, and the symbol \star stands for other indices which are irrelevant. Now we reorder the matrix elements in the numerator by shifting all matrix elements on the right-hand side of the index k simultaneously to the left-hand side, leaving the order of the other indices untouched, i.e., in the following way:

$$1^{(k)} = \frac{M_{k,\star}^{[j^{(k)}_{\ell'-1}]} \cdots M_{\star,1}^{[j^{(k)}_1]} M_{1,\star}^{[j^{(k)}_{p(k)}]} \cdots M_{\star,k}^{[j^{(k)}_{\ell'}]}}{c_{\mathbf{j}^{(k)}}^{(p(k))}(\dots, k, \dots)}. \quad (16)$$

We can finally put all these resolutions of the identity between the matrix elements in Eq. (14):

$$\begin{aligned} c_{\mathbf{j}}^{(N)}(k_1, \dots, k_{N-1}) \\ = M_{1,k_{N-1}}^{[j_N]} 1^{(k_{N-1})} M_{k_{N-1},k_{N-2}}^{[j_{N-1}]} 1^{(k_{N-2})} \cdots 1^{(k_1)} M_{k_1,1}^{[j_1]}. \end{aligned} \quad (17)$$

We recognize, in the numerator, several new strings of matrix elements resulting from the insertion. They have the same structure as in Eq. (14) but a lower order $\ell \leq 2p - 1$. This means that, for every N , all the coefficients $c^{(N)}$ can be written in terms of $c^{(\ell)}$ with $\ell \leq 2p - 1$. In other words, correlation functions of order less than or equal to $2p - 1$ are enough to reconstruct all the others. This proves the validity of the theorem.

Example.—It is instructive to consider the following case. Given a MPS or a cMPS with finite d , let the operators O_j and the state be such that the corresponding matrices $\tilde{M}^{[j]} = XM^{[j]}X^{-1}$ have only *nonzero* elements. Here, $J(\cdot) = X \cdot X^{-1}$ is the conjugation that takes E, T to their JNF. Note that the probability to have this situation in an experiment, or using a randomized (c)MPS and operators O_j , is 1. Under this condition, all two-point function transforms show all the poles; hence, $p = 1$. Computationally, all residues of all the poles of all N -point functions with $N \leq 3$ can be obtained. Hence we can, using the construction above, give explicit formulas that express all N -point functions in terms of the two- and three-point functions.

Applications in tomography.—The framework established here opens up novel ways to reconstruct unknown low-entanglement states from correlation data alone. Our approach gives rise to a complementary picture to the method of Ref. [13], where the reconstruction is based on a tomographic estimation of certain reduced states. We moreover address quantum field states and continuous systems, for which no method is known altogether. Consider the application to correlation data of atom counting experiments, or of split and recombined Bose condensates [11,14]. See the Supplemental Material [16] for detailed instructions.

Location of poles and decay behavior.—The decay behavior of contributions to the correlations follows

directly from the position of the poles on the complex plane; note the relation between poles and diagonal elements: $s_i = \mu_i^{-1}$ and $s_i = \lambda_i$, respectively. The MPS poles describing slow decay are sitting close to the unit circle, and the cMPS poles of this kind are close to the imaginary axis. An inclusion of matrix dimensions in a reconstruction of only a subspace of the auxiliary space can be guided by the relevance of the poles for the desired range of correlations.

Outlook.—A stimulating insight is given by the mathematical structure of the correlations, which are, as shown, related to meromorphic functions with interdependent residues. The structure of correlations is, moreover, linked to the quantitative limitation of entanglement between spatial regions on a fundamental level.

One might speculate that, based on the findings above—in particular, the relations of higher-order correlations to two- and three-point functions—some new insight into diagrammatic perturbative methods could be obtained. One future direction of investigation is virtual processes. In well-known perturbative methods for interacting field theories, the states of the interacting theory are described in terms of states of the noninteracting counterpart. This leads to a description in terms of quasifree states, determined by their two-point correlators, and puts the focus on propagators and an interpretation of the theory in terms of virtual processes. While this approach allows us to predict experimental data with very high precision [1], it gives rise to conceptual problems [17]. Hence, transfer of the structures discussed here to a relativistic setting might be interesting.

Of course, the relations underlying our approach are already summarized in a computationally efficient formal framework: the family of states known under the name of MPS, cMPS, and instances of projected entangled pair states. This means, given experimental data with the relations above, an optimal bookkeeping device would be, e.g., a MPS. However, say, series expansions in a perturbation approach starting from MPS and potentially leaving this class of states due to closing gaps etc. give rise to different sets of terms with different structure, and the MPS scheme is only one possible way to interpret it. A different summation order might yield a different optimal bookkeeping device in this context.

In a related line of thinking, there is the possibility that the meromorphic structure of the correlations, together with the interdependencies of the poles, enables a different mathematical understanding of the underlying renormalization procedure. Such an understanding might help to find variations of the renormalization procedure, including possibly meaningful and computationally efficient extensions of MPS and cMPS to higher dimensions.

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