TOWARDS A BETTER UNDERSTANDING OF THE MATRIX PRODUCT
FUNCTION APPROXIMATION ALGORITHM IN APPLICATION TO QUANTUM
PHYSICS

MORITZ AUGUST\* AND THOMAS HUCKLE\†

Abstract. We recently introduced a method to approximate functions of Hermitian Matrix Product Operators
or Tensor Trains that are of the form \(\text{Tr} f(A)\). Functions of this type occur in several applications, most notably in
quantum physics. In this work we aim at extending the theoretical understanding of our method by showing several
properties of our algorithm that can be used to detect and correct errors in its results. Most importantly, we show that
there exists a more computationally efficient version of our algorithm for certain inputs. To illustrate the usefulness
of our finding, we prove that several classes of spin Hamiltonians in quantum physics fall into this input category.
We finally support our findings with numerical results obtained for an example from quantum physics.

Key words. tensor decompositions, matrix product states, tensor trains, numerical analysis, Lanczos method,
Gauss quadrature, quantum physics

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1. Introduction. Approximating functions of the form \(\text{Tr} f(A)\) where \(f : \mathbb{C}^{N \times N} \rightarrow \mathbb{C}^{N \times N}\) is analytic and smooth for large Hermitian matrices \(A \in \mathbb{C}^{N \times N}\) is a problem of interest in areas such as computational chemistry, graph theory or quantum physics. In quantum
physics, fundamental properties of states of many particle systems such as the entanglement
entropy, the trace norm, heat capacity or expectation values are defined as functions of this
form [43].

While computing \(\text{Tr} f(A)\) is not challenging for small to medium size matrices, it becomes significantly harder for larger matrices of size \(2^L\) with \(L \gg 20\) where numerical diagonalization becomes computationally infeasible. We have recently addressed this issue
by presenting an algorithm [2] that is able to approximate such functions even for matrices of
very high dimensionality via a combination of the global Krylov method with its connection
to Gauss-type quadrature and the matrix product state (or tensor train) tensor decomposition
scheme. Our method constructs a basis \([U_1, \ldots, U_K]\) of \(\text{span}\{A^0, A^1, \ldots, A^{K-1}\}\) where
\(U_i \in \mathbb{C}^{N \times N}\) and yields the projection \(T_K\) of \(A\) onto that space, which is used to approximate
the desired function.

We have shown that our algorithm converges to the exact result or an arbitrarily good
approximation thereof in the case of exact arithmetics and exact representation of the \(U_i\).
While this result is instructive to understand the theoretical capability of the method, in prac-
tice the tensor decomposition is used to approximate \(A\) and the \(U_i\) and hence introduces an
approximation error into the calculations. Unfortunately, it is very difficult to analyze the
propagation of such approximation errors over the course of a complete run of the algorithm
and their influence on the final function approximation. It is therefore important to gain a
deeper understanding of theoretical properties of partial results of the computation, namely
the \(U_i\) and \(T_i\), in order to be able to detect and possibly correct unwanted artifacts caused by
the approximation errors. In addition to that, we would of course like to avoid unnecessary
operations that might introduce approximation errors and waste runtime whenever possible.
Thus, in this work we present several results regarding analytical properties of the \(U_i\) and
\(T_i\) in the exact case and also show how these results can be used to obtain a more efficient
version of our algorithm for a certain case of input matrices \(A\).

\*Department of Informatics, Technical University of Munich, 85748 Garching, Germany (august@in.tum.de)
\†Department of Informatics, Technical University of Munich, 85748 Garching, Germany (huckle@in.tum.de)
Algorithm 1: Approximation Algorithm

\textbf{Input :} MPO $A[D_A] \in \mathbb{C}^{N \times N}$, Starting orthogonal MPO $U[D_{init}] \in \mathbb{C}^{N \times N}$, Number of Dimensions $K$, Maximal Bond-Dimension $D_{max}$, Stopping Criteria $S$

\begin{algorithmic}
\State $U_0 \leftarrow 0$;
\State $V_0 \leftarrow U$;
\State $D \leftarrow D_{init}$;
\For{$i \leftarrow 1; i \leq K$}
\State $\beta_i \leftarrow \sqrt{\text{innerProduct}(V_{i-1}, V_{i-1})}$;
\If{$\beta_i = 0$}
\State break;
\EndIf
\State $U_i \leftarrow \text{multiply}(1/\beta_i, V_{i-1})$;
\State $D \leftarrow \min(D_{max}, D \cdot D_A)$;
\State $V_i \leftarrow \text{multiply}(A, U_i, D)$;
\State $D \leftarrow \min(D_{max}, D + D_{U_{i-1}})$;
\State $V_i \leftarrow \text{sum}(V_i, -\beta_i U_{i-1}, D)$;
\State $\alpha_i \leftarrow \text{innerProduct}(U_i, V_i)$;
\State $D \leftarrow \min(D_{max}, D + D_{U_i})$;
\State $V_i \leftarrow \text{sum}(V_i, -\alpha_i U_i, D)$;
\State $V_T \Lambda_T V_T^\ast \leftarrow \text{spectralDecomposition}(T_i)$;
\State $G f \leftarrow \beta_i^2 e_1^T V_T f(\Lambda_T) V_T^\ast e_1$;
\If{$\text{checkStop}(G f, \Lambda_T, S)$}
\State break;
\EndIf
\EndFor
\textbf{Output:} Approximation $G f$ of $\text{Tr}_f(A)$
\end{algorithmic}

While our algorithm is of general nature, as was hinted at above an important field of application can be found in numerical quantum physics. Here, tensor networks have already been applied with great success for some time [16, 44, 50, 24, 48, 53, 52, 49, 38] but so far a method to approximate functions of the type considered here was lacking. Because of this, we will additionally present an analysis of possible use cases of our newly discovered algorithmic improvement for the application of spin Hamiltonians, an important problem in numerical quantum physics.

The rest of this work is structured as follows: in Section 2, we briefly introduce our method. Equipped with this knowledge, we present our analytical findings in Section 3. In Section 4, we then present our analysis of possible applications of the previously introduced results in quantum physics. Following this, we proceed to provide numerical evidence of the correctness of our claims regarding the existence of an improved version of our algorithm in Section 5. Finally, we conclude this work in Section 6.

2. The Algorithm. As we have stated above, our goal is to approximate functions of the form $\text{Tr}_f(A)$. For smaller to medium sized matrices, there already exists a well-established method to achieve this in performing a Gauss-type quadrature via the projection of $A$ onto a Krylov space starting with a carefully chosen initial vector [7, 5, 18, 46, 39].

For symmetric or Hermitian matrices, the global Lanczos method recently was introduced as a formulation of the classical Lanczos method in terms of basis matrices with the
Frobenius inner product defined as
\[ \langle U_i, U_j \rangle = \text{Tr}U_i^*U_j \]
and \( U_i, U_j \in \mathbb{C}^{N \times M} \) [7]. Note that this inner product acts on whole matrices, meaning that the global Lanczos method differs from other block Krylov methods in that it only orthogonalizes complete matrices. The algorithm iteratively builds up a basis \( U_i = [U_1, U_2, \ldots, U_i] \) of the Krylov space and yields the partial global Lanczos decomposition
\[ AU_i = U_i\hat{T}_i + \beta_{i+1}U_{i+1}E_i^T \]
where \( \hat{T}_i = T_i \otimes I_M \in \mathbb{R}^{iM \times iM} \) and \( E_i^T = [0, \ldots, 0, I_M] \in \mathbb{R}^{M \times iM} \). It was shown that the connection between Lanczos method and Gauss quadrature extends to the global Lanczos method and that hence for an initial matrix \( U \in \mathbb{C}^{N \times M} \) \( \text{Tr}U^*f(A)U \) yields a Gauss quadrature of \( \text{Tr}f(A) \). However, for the algorithm to remain computationally efficient, it is required that \( M \ll N \) and consequentially \( U \) can not be orthogonal/unitary. This implies that the method does in general not converge to the exact result and sampling over multiple starting matrices is required. Additionally, for very large matrices even the computation of the aforementioned inner product becomes infeasible.

To allow for approximations of larger matrices, we reformulated the global Lanczos algorithm in terms of matrix product operators (MPO) which support all basic linear algebra operations. A matrix product operator decomposes a matrix \( A \in \mathbb{C}^{N \times N} \) such that
\[ A_{ij} = A_{i_1 \ldots i_L j_1 \ldots j_L} = \text{Tr}C_1^{i_1 j_1}C_2^{i_2 j_2} \cdots C_L^{i_L j_L} \]
where the indices \( i, j \) are split up into \( i_1, \ldots, L \) and \( j_1, \ldots, j_L \) respectively and are called the physical indices. W.l.o.g. we here assume all physical indices to be of equal dimension \( d = 2 \). This corresponds to the assumption that \( N = d^L \). The \( C_k \in \mathbb{C}^{D \times D \times d \times d} \) are called the core tensors where \( D \) will in the following be referred to as the bond dimension or the auxiliary index. It follows that \( C_k^{i_k j_k} \) is a matrix of size \( D \times D \) and hence the right-hand side of the above equation yields a scalar. The matrix product operator representation of a matrix requires \( Ld^2D^2 \) parameters which for suitable choices of \( D \) either poses an approximation or suffices for an exact representation. Typically, \( D \) is chosen such that \( Ld^2D^2 \in \mathcal{O}(\text{poly}(L)) \) yields an efficient representation. Note that especially in numerical quantum physics, it is possible and common to formulate matrices of interest, such as Hamiltonians, directly as matrix product operators and perform computations on them so that an explicitly stored matrix is at no point required. While explaining the decomposition in more detail exceeds the scope of this section, we refer the interested reader to the overview articles [44, 37, 21].

Our algorithm can thus be perceived as the global Lanczos algorithm reformulated for matrix product operators. However the differences between the methods extend beyond the different possible sizes of the input matrices. In our algorithm, we are able to start our computation with an orthogonal/unitary matrix of the same dimensionality as \( A \). Hence, instead of the previous equation
\[ \text{Tr}U^*f(A)U \approx \text{Tr}f(A) \]
with \( U \in \mathbb{C}^{N \times M} \) and \( M \ll N \), in our method it holds
\[ \text{Tr}U^*f(A)U = \text{Tr}f(A) \]
and \( U \in \mathbb{C}^{N \times N} \) orthogonal/unitary. This implies that our algorithm converges to the exact result or an arbitrarily close approximation of it in the case of exact arithmetics and no approximations. Our general algorithm is shown in Algorithm 1. Note that the subfunctions
For the sake of clarity, we explicitly state the update rules for $U$ errors in the computed basis matrices. As we will make use of these equations in all following proofs of this section, it is worthwhile to explicitly state the update rules

$$U_{n+1} = (AU_n - \alpha_{n+1}U_n - \beta_nU_{n-1})/\beta_{n+1}$$

and

$$\alpha_{n+1} = \text{Tr}U_n^*U_{n+1}$$

as implied by Algorithm 1.

We begin by stating a result about the inheritance of tracelessness of the basis matrices from the input $A$.

**Theorem 1.** If $A \in \mathbb{C}^{N \times N}$ is traceless and $U_0 \in \mathbb{C}^{N \times N} = I_N/\beta_0$, all basis matrices $U_i \in \mathbb{C}^{N \times N}, i \in \{1, \cdots, K\}$ as constructed by the algorithm are traceless.

**Proof.** We prove the statement by induction over the iteration number $n$ of the algorithm. For $n = 1$, it is easy to see that $\text{Tr}U_1 = \text{Tr}A/(\beta_1\beta_0) = 0$ as $\alpha_1 = \text{Tr}A/\beta_0^2 = 0$. We now obtain for $n = 2$ that $\text{Tr}U_2 = (\beta_1\beta_0\text{Tr}U_1U_1 - \alpha_2/(\beta_1\beta_0)\text{Tr}A - \beta_1/\beta_0\text{Tr}I)/\beta_2 = 0$. This establishes the inductive basis.

In the inductive step for $n \geq 2$ we then have

$$\text{Tr}U_{n+1} = (\text{Tr}AU_n - \alpha_{n+1}\text{Tr}U_n - \beta_n\text{Tr}U_{n-1})/\beta_{n+1}$$

$$= (\text{Tr}AU_n - \alpha_{n+1}0 - \beta_n0)/\beta_{n+1}$$

$$= 0$$

Since it is possible to efficiently compute the trace of a given MPO, this property of the $U_i$ can be efficiently checked for and, if desired, enforced during a run of the algorithm.

Next, we present a result about the commutation relation of $A$ and the $U_i$ that will also become useful for proving subsequent statements.

**Theorem 2.** If $A \in \mathbb{C}^{N \times N}$ commutes with $U_0 \in \mathbb{C}^{N \times N}$, $A$ commutes with all basis matrices $U_i \in \mathbb{C}^{N \times N}, i \in \{1, \cdots, K\}$ as constructed by the algorithm.
Proof. We again prove the statement by induction over the iteration number $n$. To start, we note that $[U_1, A] = ((AAU_0 - \alpha_1 AU_0) - (AAU_0 - \alpha_1 AU_0))/\beta_1 = 0$.

In the inductive step for $n \geq 1$, it is now straightforward to see that

$$[U_{n+1}, A] = [(AU_n - \alpha_{n+1} U_n - \beta_n U_{n-1}) - (AAU_n - \alpha_{n+1} AU_n - \beta_n AU_{n-1})]/\beta_{n+1} = 0$$

\[ \square \]

Corollary 1. We note that any $A \in \mathbb{C}^{N \times N}$ commutes with $I_N$. Thus it follows that the above statement holds for Algorithm 1.

As for the previous result, this property can be efficiently checked for during an execution of the algorithm assuming MPO representation of the $U_i$ by computing the Frobenius norm, which is efficiently computable for MPOs, of the distance between $AU_i$ and $U_i A$.

The following finding addresses the symmetry properties of the basis matrices in relation to the input $A$ and the initial basis matrix $U_0$.

Theorem 3. If $A \in \mathbb{R}^{N \times N}$ is symmetric, persymmetric or centrosymmetric and $U_0 \in \mathbb{R}^{N \times N}$ is symmetric, persymmetric or centrosymmetric and commutes with $A$, all basis matrices $U_i \in \mathbb{R}^{N \times N}, i \in \{1, \cdots, K\}$ as constructed by the algorithm are symmetric, persymmetric or centrosymmetric.

Proof. As for the above statements, we prove this statement by induction over the iteration number $n$. To establish the inductive basis, we observe that for the case of symmetry $U_1^T = ((AU_0)^T - \alpha_1 U_0^T)/\beta_1 = (AU_0 - \alpha_1 U_0)/\beta_1 = U_1$. Likewise, we find that $U_1 J = (AU_0 - \alpha_1 U_0)/\beta_1 J = J((AU_0)^T - \alpha_1 U_0^T)/\beta_1 = J U_1^T$ for persymmetry and finally $J U_1 = J(AU_0 - \alpha_1 U_0)/\beta_1 = (AU_0 - \alpha_1 U_0)/\beta_1 J = U_1 J$ for centrosymmetry.

For $n \geq 1$, we can now make the inductive step by

$$U_{n+1}^T = ((AU_n)^T - \alpha_{n+1} U_n^T - \beta_n U_{n-1}^T)/\beta_{n+1}$$

$$=(U_n A - \alpha_{n+1} U_n - \beta_n U_{n-1})/\beta_{n+1}$$

$$=U_{n+1}$$

for symmetry,

$$U_{n+1} J = (AU_n - \alpha_{n+1} U_n - \beta_n U_{n-1})/\beta_{n+1} J$$

$$=(J A^T U_n^T - \alpha_{n+1} J U_n^T - \beta_n J U_{n-1}^T)/\beta_{n+1}$$

$$=J U_{n+1}^T$$

for persymmetry and

$$J U_{n+1} = J(AU_n - \alpha_{n+1} U_n - \beta_n U_{n-1})/\beta_{n+1}$$

$$=(AU_n J - \alpha_{n+1} U_n J - \beta_n U_{n-1} J)/\beta_{n+1}$$

$$=U_{n+1} J$$

for centrosymmetry. \[ \square \]

Corollary 2. As can be easily verified based on its proof, the above statement extends to the case of hermiticity, perhermiticity and centrohermiticity when $A, U_i \in \mathbb{C}^{N \times N}, i \in \{0, \cdots, K\}$.

Corollary 3. We note that the matrix $I_N$ is symmetric, persymmetric and centrosymmetric as well as hermitian, perhermitian and centrohermitian. Hence the above statements hold for Algorithm 1.
These symmetry properties can as well be tested efficiently in a manner similar to the way the commutation relation can be checked since \( J \), like \( I \), permits a formulation in MPO format with minimal bond dimension. Additionally, symmetries could be leveraged to obtain more efficient representations of the \( U_i \) by reflecting them in the structure of the MPOs and thus obtaining more efficient and stable expressions.

We now turn our attention to a description of the \( U_i \) in terms of polynomials as might seem natural given the underlying Lanczos algorithm. However, we restrict our analysis to the particular case where all \( \alpha_i = 0 \) to obtain a result that will become important in the proof of the subsequent statement.

**Theorem 4.** If for \( A \in \mathbb{C}^{N \times N} \) all \( \alpha_i = 0 \), \( i \in \{1, \ldots, K\} \) as computed by the algorithm and \( U_0 \in \mathbb{C}^{N \times N} = I_N / \beta_0 \), then all \( U_i \in \mathbb{C}^{N \times N} \), \( i \in \{1, \ldots, K\} \) are polynomials of the form \( \sum_{j \in 2N_0 \leq 1} c_j A^j \) if \( i \) is even and \( \sum_{j \in 2N-1 \leq 1} c_j A^j \) if \( i \) is odd.

**Proof.** We again prove the statement by induction over the iteration number \( n \). We establish the inductive basis by observing that \( U_0 = A^0 / \beta_0 \), \( U_1 = A / (\beta_1 \beta_0) \), \( U_2 = A^2 / (\beta_2 \beta_1 \beta_0) - \beta_1 / (\beta_2 \beta_0) A^0 \) and \( U_3 = A^3 / (\beta_3 \beta_2 \beta_1 \beta_0) - (\beta_2^2 + \beta_1^2) / (\beta_3 \beta_2 \beta_1 \beta_0) A \) are all polynomials of the types specified above.

In the inductive step, we then find for even \( n \) that

\[
U_{n+1} = (AU_n - \beta_n U_{n-1}) / \beta_{n+1}
\]

\[
= \left( A \sum_{j \in 2N_0 \leq n} c_j A^j - \beta_n \sum_{j \in 2N-1 \leq n-1} d_j A^j \right) / \beta_{n+1}
\]

\[
= \left( \sum_{j \in 2N-1 \leq n+1} c_j A^j - \beta_n \sum_{j \in 2N-1 \leq n-1} d_j A^j \right) / \beta_{n+1}
\]

\[
= \sum_{j \in 2N-1 \leq n+1} (c_j - \beta_n d_j) / \beta_{n+1} A^j
\]

and analogously for odd \( n \)

\[
U_{n+1} = (AU_n - \beta_n U_{n-1}) / \beta_{n+1}
\]

\[
= \left( A \sum_{j \in 2N-1 \leq n} c_j A^j - \beta_n \sum_{j \in 2N_0 \leq n-1} d_j A^j \right) / \beta_{n+1}
\]

\[
= \left( \sum_{j \in 2N_0 \leq n+1} c_j A^j - \beta_n \sum_{j \in 2N_0 \leq n-1} d_j A^j \right) / \beta_{n+1}
\]

\[
= \sum_{j \in 2N_0 \leq n+1} (c_j - \beta_n d_j) / \beta_{n+1} A^j
\]

where we defined \( d_{n+1} := 0 \). \( \square \)

We can now use this result to obtain a more profound insight.

**Theorem 5.** If \( A \in \mathbb{C}^{N \times N} \) has a spectrum that is point-wise symmetric around zero and \( U_0 \in \mathbb{C}^{N \times N} = I_N / \beta_0 \), all the \( \alpha_i \), \( i \in \{1, \ldots, K\} \) as computed by the algorithm are zero.

**Proof.** As done previously, we prove this statement by induction over the iteration number \( n \). We start by observing that by assumption \( \text{Tr} A = 0 \) and hence \( \alpha_1 = \text{Tr} A / \beta_0^2 = 0 \). Consequently, we have that \( \alpha_2 = \text{Tr}(AU_1)^*U_1 = 1/(\beta_1 \beta_0)^2 \text{Tr} A^3 = 0 \) which is our inductive basis.
Now for the inductive step, we begin by noting that it follows from the inductive hypothesis that all $U_i, i \in \{1, \cdots, n\}$ are polynomials of the form defined in the previous statement. Then for odd $n$, it follows that

$$\alpha_{n+1} = \text{Tr} U_n U_n^* A$$
$$= \text{Tr} \left( \sum_{j \in 2N-1 \leq n} c_j A^j \right) \left( \sum_{j \in 2N-1 \leq n} c_j A^{*j} \right) A$$
$$= \sum_{j \in 2N+1 \leq 2n+1} c_j \text{Tr} A^j$$
$$= 0.$$

Analogously, it follows for even $n$ that

$$\alpha_{n+1} = \text{Tr} U_n U_n^* A$$
$$= \text{Tr} \left( \sum_{j \in 2N_0 \leq n} c_j A^j \right) \left( \sum_{j \in 2N_0 \leq n} c_j A^{*j} \right) A$$
$$= \sum_{j \in 2N-1 \leq 2n+1} c_j \text{Tr} A^j$$
$$= 0.$$

From this finding, we finally obtain the following corollary.

**Corollary 4.** For $A \in \mathbb{C}^{N \times N}$ having a spectrum point-wise symmetric around zero, Algorithm 1 produces a bidiagonal matrix

$$T_K = \begin{bmatrix}
0 & \beta_1 & 0 \\
\beta_1 & 0 & \ddots \\
& \ddots & \ddots & \beta_K \\
0 & & \beta_K & 0
\end{bmatrix}.$$

This yields a more efficient version of the algorithm as each $U_i$ is in this case guaranteed to be orthogonal to $U_{i-1}$ and hence only one orthogonalization has to be performed in each iteration of the algorithm. Note that the orthogonalization of two MPOs requires solving an optimization problem and is hence significantly more computationally demanding than the orthogonalization of full matrices. From these insights we also obtain yet another means of checking for the effect of truncation errors by monitoring the magnitude of the $\alpha_i$ when it is known they must be zero.

**4. Spectra of Hamiltonians.** The results obtained in the previous section naturally raise the question what kinds of matrices exhibit the required spectral property and how many useful cases there are. While we cannot give a general answer to this question, we can provide a partial answer for a specific application, namely spin systems in quantum physics. These systems are often studied analytically and numerically because they exhibit interesting physical phenomena while still allowing for the derivation of mathematically rigorous results and comparably efficient simulations by tensor network approaches.
Spin systems are described by their corresponding Hamiltonians which for open boundaries and interactions between direct neighbours take the form

\[ H_{\text{OBC}} = \sum_{(i, \alpha) \in \mathcal{I}} h_{ij} (I \otimes \sigma_{\alpha} \otimes I) \otimes I^{L-i-j} \]

where \( L \in \mathbb{N} \) is the number of spin particles and \( \mathcal{I} \) is a set of tuples \((i, \alpha) \in \mathbb{N}_L \times \{x, y, z\}\) denoting the number of consecutive applications of \( \sigma_{\alpha} \). In this case, \( \sigma_{x,y,z} \) denote the Pauli matrices

\[
\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},
\]

and the \( h_{ij} \in \mathbb{R} \) simply are scaling constants. Similarly, the case of closed or periodic boundaries is expressed as

\[ H_{\text{PBC}} = \sum_{(i, \alpha) \in \mathcal{I}} h_{ij} (I \otimes \sigma_{\alpha} \otimes I) \otimes I^{L-i-j} + \sum_{(i, \alpha) \in \mathcal{I}} \sum_{k=1}^{i-1} h_{i+k} \sigma_{\alpha} \otimes I^{L-i} \otimes \sigma_{\alpha}^{i-k}. \]

We will in the following denote the individual terms in the sums of the Hamiltonians as interaction terms and refer to the products of multiple Pauli matrices inside these interaction terms as blocks. This terminology is derived from the fact that each term describes the interaction between the particles at whose position there is a Pauli operator in the product. While the formulations introduced above naturally do not describe all possible Hamiltonians, they cover many interesting cases which are furthermore treatable via tensor network methods. This typically gets much more difficult for cases of arbitrary and long-range interaction patterns, which are not covered by the above expressions.

Now, one way of formally characterizing a point-wise symmetric spectrum around zero looks as follows: for a given \( H \in \mathbb{C}^{2^L \times 2^L} \), does there exists a unitary and Hermitian matrix \( R \) of equal size, such that

\[ RH = -HR \]

and consequently by the standard eigenvalue formulation \( Hv = \lambda v \) it holds that

\[ H(Rv) = -\lambda(Rv)? \]

In the following, we will make statements about the existence of such an \( R \) for several classes of spin Hamiltonians. Although absence of such an \( R \) does not imply that the Hamiltonian in question does not have a point symmetric spectrum around zero, the above formulation still captures a large class of possible symmetries. Note that in quantum physics it is already known that one can make use of the rotation transformation properties of spin operators to change the sign of particular terms in a Hamiltonian \([43]\). However, here we tackle the problem of changing all terms, from now on also called interaction terms, in a Hamiltonian to relate different eigenvalues/-states to each other and our focus lies on formally defining classes of spin Hamiltonians for which such an \( R \) exists and which hence are valid inputs for our improved algorithm.

Before we start, we remind ourselves that the Pauli matrices are Hermitian and unitary and that each pair of Pauli matrices anticommutes such that for \( \alpha, \beta \in \{x, y, z\} \) it holds

\[ \{\sigma_{\alpha}, \sigma_{\beta}\} = 2\delta_{\alpha,\beta} I. \]
Furthermore, we note that the Kronecker product of Hermitian and unitary matrices is again Hermitian and unitary. These properties will be used in all following proofs.

We start by considering Hamiltonians with open boundaries and neighbour interactions of arbitrary length for a single Pauli operator.

**Theorem 6.** For every spin Hamiltonian with open boundaries of the form

\[ H_{OBC,\alpha,i} = \sum_{j=0}^{L-i} h_j I^{\otimes j} \otimes \sigma_{\alpha}^{\otimes i} \otimes I^{\otimes L-i-j} \]

where \( \alpha \in \{x, y, z\} \) and \( i, L \in \mathbb{N} \) and \( i \leq L \), there exists a unitary \( R \in \mathbb{C}^{2^L \times 2^L} \) such that \( RH_{OBC,\alpha,i} = -H_{OBC,\alpha,i} R \).

**Proof.** We can construct \( R = (I^{\otimes i-1} \otimes \sigma_{\alpha'})^{\otimes L/i} \otimes I^{\otimes L/i} \) with \( \alpha' \in \{x, y, z\} \setminus \{\alpha\} \) as we need only apply one \( \sigma_{\alpha'} \) for each block \( \sigma_{\alpha}^{\otimes i} \) to change the sign in every term of the sum in \( H_{\alpha,i} \) and thereby ultimately the sign of \( H_{\alpha,i} \) itself. Hereby, \( \otimes^{L/i} \) denotes the repetition of the given expression for \( L/i \) times whereas \( I^{\otimes L/i} \) simply refers to a ‘padding’ of \( R \) to the required length \( L \).

While for the case of open boundaries and a single Pauli matrix the statement is quite universal, the additional structure introduced by periodic boundaries forces us to restrict the statement to odd interactions lengths.

**Theorem 7.** For every spin Hamiltonian with periodic boundaries of the form

\[ H_{PBC,\alpha,i} = \sum_{j=0}^{L-i} h_j I^{\otimes j} \otimes \sigma_{\alpha}^{\otimes i} \otimes I^{\otimes L-i-j} + \sum_{k=1}^{i-1} h_k \sigma_{\alpha}^{\otimes k} \otimes I^{\otimes L-i} \otimes \sigma_{\alpha}^{i-k} \]

where \( \alpha \in \{x, y, z\} \) and \( i \in 2\mathbb{N} - 1 \), \( L \in \mathbb{N} \) and \( i \leq L \), there exists a unitary \( R \in \mathbb{C}^{2^L \times 2^L} \) such that \( RH_{PBC,\alpha,i} = -H_{PBC,\alpha,i} R \).

**Proof.** By defining \( R = \sigma_{\alpha'}^{\otimes L} \) with \( \alpha' \in \{x, y, z\} \setminus \{\alpha\} \) we obtain an odd number of sign changes in every term of the sum in \( H_{PBC,\alpha,i} \) inducing a sign change of \( H_{PBC,\alpha,i} \). □

These two statements together show that a large subset of spin Hamiltonians with interaction terms involving only one particular Pauli matrix exhibit a point symmetric spectrum around zero. Not surprisingly, the situation becomes more involved when considering Hamiltonians with up to two different Pauli operators and differing interaction lengths. We first examine the case of interaction terms involving two differing Pauli operators.

**Theorem 8.** For every spin Hamiltonian with open boundaries of the form

\[ H_{OBC,\alpha,\beta,i,k} = \sum_{j=0}^{L-i} h_{\alpha j} I^{\otimes j} \otimes \sigma_{\alpha}^{\otimes i} \otimes I^{\otimes L-i-j} + \sum_{l=0}^{L-k} h_{\beta l} I^{\otimes l} \otimes \sigma_{\beta}^{\otimes k} \otimes I^{\otimes L-k-l} \]

where \( \alpha, \beta \in \{x, y, z\}, \alpha \neq \beta, i, k, L \in \mathbb{N} \) and \( i, k \leq L \), there exists a unitary \( R \in \mathbb{C}^{2^L \times 2^L} \) such that \( RH_{OBC,\alpha,\beta,i,k} = -H_{OBC,\alpha,\beta,i,k} R \).

**Proof.** We have to distinguish two cases regarding the relation of \( i \) and \( k \).

**Case** \( i = k \)

In this case there is a \( \gamma \in \{x, y, z\} \setminus \{\alpha, \beta\} \) such that \( \sigma_{\alpha} \sigma_{\gamma} = -\sigma_{\gamma} \sigma_{\alpha} \) and \( \sigma_{\beta} \sigma_{\gamma} = -\sigma_{\gamma} \sigma_{\beta} \). Hence, we can again define \( R = (I^{\otimes i-1} \otimes \sigma_{\gamma})^{\otimes L/i} \otimes I^{\otimes L/i} \) to obtain a unitary that induces a sign change in every block \( \sigma_{\alpha}^{\otimes i} \) and \( \sigma_{\beta}^{\otimes k} \) and hence changes the sign of \( H_{OBC,\alpha,\beta,i,k} \).

**Case** \( i \neq k \)
Let w.l.o.g. \( i > k \). Then we can construct \( R \) as the Kronecker product of \( L \) matrices such that at every \( k \)-th position we apply \( \sigma_\alpha \) and at every \( i \)-th position we apply \( \sigma_\beta \). In the case where multiples of \( i \) and \( k \) coincide, we again choose \( \gamma \in \{ x, y, z \} \setminus \{ \alpha, \beta \} \) and apply it in these positions. The remaining free factors are again chosen to be the identity. It is evident from the construction of \( R \) that it induces exactly one sign change in every block \( \sigma_\alpha \otimes I \) and \( \sigma_\beta \otimes I \) respectively.

A different situation presents itself when we again restrict the interaction terms in the Hamiltonian to involve only one Pauli operator but allow two different interaction lengths.

**Theorem 9.** For every spin Hamiltonian with open boundaries of the form

\[
H_{OBC,\alpha,i,k} = \sum_{j=0}^{L-i} h_{ij} I \otimes \sigma_\alpha \otimes I \otimes L^{-i-j} + \sum_{l=0}^{L-k} h_{kl} I \otimes \sigma_\beta \otimes I \otimes L^{-k-l}
\]

where \( \alpha \in \{ x, y, z \} \), \( i, k \in \mathbb{N} \), and \( i, k \leq L \), there exists a unitary \( R \in \mathbb{C}^{2L \times 2L} \) such that \( RH_{OBC,\alpha,i,k} = -H_{OBC,\alpha,i,k} R \).

**Proof.** We again have to distinguish two cases regarding the relation of \( i \) and \( k \).

**Case** \( i = k \)

In this case, the Hamiltonian is a member of the class considered in Theorem 6.

**Case** \( i \neq k \)

In this case, we can again choose an \( \alpha' \in \{ x, y, z \} \setminus \{ \alpha \} \) and define \( R = \sigma_\alpha^{\otimes L} \). \( R \) then induces an odd number of sign changes in every term of \( H_{OBC,\alpha,i,k} \) and consequentially a sign change in the whole Hamiltonian.

This result can now easily be generalized to the case of more than two interaction lengths for a fixed Pauli operator.

**Corollary 5.** By a straightforward generalization of the above proof we obtain that for all Hamiltonians with open boundaries and one Pauli operator of the form

\[
H_{PBC,\alpha} = \sum_{i=1}^{L-i} \sum_{j=0}^{L-i} h_{ij} I \otimes \sigma_\alpha \otimes I \otimes L^{-i-j}
\]

where \( \alpha \in \{ x, y, z \} \) and \( I \subset 2\mathbb{N} - 1 \), there exists a unitary \( R \in \mathbb{C}^{2^k \times 2^k} \) such that \( RH_{PBC,\alpha} = -H_{PBC,\alpha} R \).

While we restricted the interaction lengths to be odd for the statements above, we find that there exists another case for arbitrary interaction lengths with a certain relation between them.

**Theorem 10.** For every spin Hamiltonian with open boundaries of the form

\[
H_{OBC,\alpha,i,k} = \sum_{j=0}^{L-i} h_{ij} I \otimes \sigma_\alpha \otimes I \otimes L^{-i-j} + \sum_{l=0}^{L-k} h_{kl} I \otimes \sigma_\beta \otimes I \otimes L^{-k-l}
\]

where \( \alpha \in \{ x, y, z \} \), \( i, k \in \mathbb{N} \), \( i/k \in 2\mathbb{N} - 1 \), \( L \in \mathbb{N} \), and \( i, k \leq L \), there exists a unitary \( R \in \mathbb{C}^{2^k \times 2^k} \) such that \( RH_{OBC,\alpha,i,k} = -H_{OBC,\alpha,i,k} R \).

**Proof.** Also here, we have to distinguish two cases regarding the relation of \( i \) and \( k \).

**Case** \( i = k \)

In this case, the Hamiltonian is a member of the class considered in Theorem 6.

**Case** \( i \neq k \)
We can construct \( R = (I^\otimes k - \otimes \sigma_\alpha')^\otimes L/k \otimes I^\otimes \%k \) with \( \alpha' \in \{x, y, z\} \setminus \{\alpha\} \). Since \( i/k \in 2\mathbb{N} - 1 \) we find that \( R \) induces an odd number of sign changes in all terms of \( H_{OBC, \alpha, i, k} \) and thus in the overall Hamiltonian. \( \Box \)

What is now left to discuss for Hamiltonians involving up to two different Pauli operators is the case of periodic boundaries, which again introduces more constraints. Hence we find that we can only make a positive statement about odd interaction lengths as follows.

**Theorem 11.** For every spin Hamiltonian with periodic boundaries of the form

\[
H_{PBC, \alpha, \beta, i, l} = \sum_{j=0}^{L-i} h_{ij} I^\otimes j \otimes \sigma_\alpha^\otimes I^\otimes L-i-j + \sum_{k=1}^{i-1} h_{ik} \sigma_\alpha^\otimes I^\otimes L-i - \sum_{m=0}^{L-l} h_{jm} I^\otimes m \otimes \sigma_\beta^\otimes I^\otimes L-l-m + \sum_{n=1}^{l-1} h_{jn} \sigma_\beta^\otimes I^\otimes L-l - \sigma_\alpha^\otimes
\]

where \( \alpha, \beta \in \{x, y, z\} \), \( i, l \in 2\mathbb{N} - 1 \), \( L \in \mathbb{N} \) and \( i, l \leq L \), there exists a unitary \( R \in \mathbb{C}^{2^L \times 2^L} \) such that \( RH_{PBC, \alpha, i} = -H_{PBC, \alpha, i}R \).

**Proof.** As before we can choose \( \gamma \in \{x, y, z\} \setminus \{\alpha, \beta\} \) and define \( R = \sigma_\gamma^\otimes \). Since \( i, l \in 2\mathbb{N} - 1 \), \( R \) induces and odd number of sign changes in ever term of and consequently in \( H_{PBC, \alpha, i, l} \). This statement can again be readily generalized to multiple interaction lengths and hence more complex Hamiltonians.

**Corollary 6.** By a straightforward generalization of the above proof we obtain that for all Hamiltonians with periodic boundaries and at most two different Pauli operators of the form

\[
H_{PBC, \alpha, \beta} = \sum_{i,j} \sum_{i,j} h_{i,j} I^\otimes j \otimes \sigma_\alpha^\otimes I^\otimes L-i-j + \sum_{i,k} \sum_{i,k} h_{i,k} \sigma_\alpha^\otimes I^\otimes L-i - \sum_{j,m} \sum_{l,m} h_{j,m} I^\otimes m \otimes \sigma_\beta^\otimes I^\otimes L-l-m + \sum_{k,n} \sum_{l,n} h_{k,n} \sigma_\beta^\otimes I^\otimes L-l - \sigma_\alpha^\otimes
\]

where \( \alpha, \beta \in \{x, y, z\} \) and \( I, J \subset 2\mathbb{N} - 1 \), there exists a unitary \( R \in \mathbb{C}^{2^L \times 2^L} \) such that \( RH_{PBC, \alpha, \beta} = -H_{PBC, \alpha, \beta}R \).

Now, we finally come to the case of Hamiltonians consisting of interaction terms generated by up to three Pauli operators which is clearly the most complicated setting. We begin by inspecting Hamiltonians with open boundaries involving all three Pauli matrices.

**Theorem 12.** For every spin Hamiltonian with open boundaries of the form

\[
H_{OBC, \alpha, \beta, \gamma, i, k, m} = \sum_{j=0}^{L-i} h_{ij} I^\otimes j \otimes \sigma_\alpha^\otimes I^\otimes L-i-j + \sum_{l=0}^{L-k} h_{il} I^\otimes l \otimes \sigma_\beta^\otimes I^\otimes L-k-l + \sum_{n=0}^{L-m} h_{im} I^\otimes m \otimes \sigma_\gamma^\otimes I^\otimes L-m-n
\]

where \( \alpha, \beta, \gamma \in \{x, y, z\} \), \( \alpha \neq \beta \neq \gamma \neq \alpha, k, L \in \mathbb{N}, i, m \in 2\mathbb{N} - 1, i < k \) and \( i, k, m \leq L \), there exists a unitary \( R \in \mathbb{C}^{2^L \times 2^L} \) such that \( RH_{OBC, \alpha, \beta, \gamma, i, k, m} = -H_{OBC, \alpha, \beta, \gamma, i, k, m}R \).

**Proof.** We define \( R = (\sigma_\alpha^{k-1} \otimes \sigma_\beta^k) I^\otimes L/k \otimes \sigma_\beta^L \). It is clear that \( R \) induces an odd number of sign changes in all blocks \( \sigma_\alpha^\otimes \) since \( i \leq k - 1 \) is odd. Similarly, it is obvious that \( R \) causes exactly one sign change in every block \( \sigma_\beta^\otimes \) through the single \( \sigma_\alpha \) in the
product. As both $\sigma_\alpha$ and $\sigma_\beta$ cause sign changes in the blocks $\sigma\otimes^m_\gamma$ and $m$ is odd, it is evident that $R$ also induces and odd number of sign changes in this case. Hence it holds that $RH_{OBC,\alpha,\beta,\gamma,i,k,m} = -H_{OBC,\alpha,\beta,\gamma,i,k,m}R$.

Finally, we examine the case of two Pauli matrices and three different interaction lengths for open boundary conditions.

**Theorem 13.** For every spin Hamiltonian with open boundaries of the form

\[
H_{OBC,\alpha,\beta,i,k,m} = \sum_{j=0}^{L-i} h_{\alpha j} I^{\otimes j} \otimes \sigma^{\otimes i}_\alpha \otimes I^{\otimes L-i-j} + \sum_{l=0}^{L-k} h_{\beta kl} I^{\otimes l} \otimes \sigma^{\otimes k}_\beta \otimes I^{\otimes L-k-l} + \sum_{n=0}^{L-m} h_{\gamma mn} I^{\otimes n} \otimes \sigma^{\otimes m}_\gamma \otimes I^{\otimes L-m-n}
\]

where $\alpha, \beta \in \{x, y, z\}, \alpha \neq \beta, L \in \mathbb{N}, i, k, m \in 2\mathbb{N} - 1, i < k$ and $i, k, m \leq L$, there exists a unitary $R \in \mathbb{C}^{2^L \times 2^L}$ such that $RH_{OBC,\alpha,\beta,i,k,m} = -H_{OBC,\alpha,\beta,i,k,m}R$.

**Proof.** As before we can choose $\gamma \in \{x, y, z\} \setminus \{\alpha, \beta\}$ and define $R = \sigma^{\otimes L}_\gamma$. Since $i, k, l \in 2\mathbb{N} - 1$, $R$ induces and odd number of sign changes in every term of and consequentially in $H_{PBC,\alpha,\beta,i,l}$.

This statement can now again be generalized to multiple interaction terms.

**Corollary 7.** Again by a straightforward generalization of the above proof we find that for all Hamiltonians with open boundaries and two Pauli operators of the form

\[
H_{PBC,\alpha,\beta} = \sum_{i \in \mathcal{I}} \sum_{j=0}^{L-i} h_{ij} I^{\otimes j} \otimes \sigma^{\otimes i}_\alpha \otimes I^{\otimes L-i-j} + \sum_{k \in \mathcal{J}} \sum_{j=0}^{L-k} h_{kj} I^{\otimes j} \otimes \sigma^{\otimes k}_\beta \otimes I^{\otimes L-k-j}
\]

where $\alpha, \beta \in \{x, y, z\}$ and $\mathcal{I} \subset 2\mathbb{N} - 1$, there exists a unitary $R \in \mathbb{C}^{2^L \times 2^L}$ such that $RH_{PBC,\alpha,\beta} = -H_{PBC,\alpha,\beta}R$.

To the best of our knowledge, we cannot make a positive statement for periodic boundaries and interaction terms involving all three Pauli operators. As a remark, we would like to point out that in addition to the Hamiltonians treated in this section, positive statements about the existence of an $R$ as considered here should be easy to proof in a very similar way for arbitrary interactions, i.e. interactions not between nearest neighbours but arbitrary particles, and odd numbers of particles affected by the interaction terms.

We have shown in this section that a significant subset of all spin Hamiltonians exhibits a point symmetric spectrum around zero according to the introduced characterization and that consequently there exists a strong use case of our improvement of Algorithm 1 in quantum mechanical simulations. In the next section, we will now use a well known Hamiltonian belonging to this subset to numerically illustrate the advantage of the improved algorithm in this case.

**5. Numerical Evidence.** To provide numerical evidence of the correctness of our statements in Sections 3 and 4, we will now state results obtained by conducting some numerical experiments for the well known Ising Hamiltonian with a transverse field. The Hamiltonian is given by

\[
H = J \sum_{i=1}^{L-1} I^{\otimes i-1} \otimes \sigma_x \otimes I^{\otimes L-(i+1)} + g \sum_{i=1}^{L} I^{\otimes i-1} \otimes \sigma_z \otimes I^{\otimes L-i}
\]

where $\sigma_{x,z}$ are again the Pauli matrices. As we have seen in Section 4, the transverse field Ising Hamiltonian clearly has the spectral property required to apply the improved version of the algorithm. It also has the additional advantage that it can be diagonalized analytically to obtain reference results. Given a Hamiltonian, its thermal equilibrium, or Gibbs, state is described by

$$\rho(\beta) = \frac{e^{-\beta H}}{Z}$$

where $\beta$ is the inverse temperature and

$$Z = \text{Tr} e^{-\beta H}$$

is the so called partition function or simply the normalization constant of the distribution. As our goal in this section is to compare both versions of the algorithm and not to provide physically relevant results, we will simply approximate $Z$ by chosing

$$f(H) = e^{-\beta H}$$

FIG. 5.1. Comparisons of the runtime in seconds between the improved and the vanilla version of the algorithm. Left: Comparison of average runtime of one iteration over $L$ with $D_{\text{max}} = 50$. Right: Comparison of average runtime of one iteration over $D_{\text{max}}$ with $L = 50$.

FIG. 5.2. Comparisons of the relative error in $Z$ between the improved and the vanilla version of the algorithm. Left: Comparison of the relative error over $L$ with $D_{\text{max}} = 50$. Right: Comparison over the relative error over $D_{\text{max}}$ and $L = 50$.  

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where we set the scaling coefficients of the Hamiltonian and the inverse temperature to $J = g = \beta = 1$.

To provide a thorough comparison between the vanilla, i.e. standard, and the improved version of our algorithm in terms of runtime and accuracy, we have conducted two sets of experiments. Firstly, we fixed the maximal bond dimension to be $D_{\text{max}} = 50$ and computed the average runtime for one iteration of the algorithm over a run of 50 iterations for $L$, i.e., the system size, increasing from 10 to 100. Secondly, we set $L = 50$ and increased $D_{\text{max}}$ from 10 to 100 and again computed the average runtime of one iteration over a run of 50 iterations. The comparison of the runtimes is depicted in Figure 5.1.

For both of these settings, we also evaluated the approximation accuracy as the relative error in $Z$ when we let the algorithm run until the relative difference between approximations
results became smaller than $10^{-6}$. These results are illustrated in Figure 5.2. All results reported here were obtained for a C++ implementation of our algorithm on an Intel i5-5200U mobile CPU.

The results in Figure 5.1 clearly show an advantage in runtime for the improved version of the algorithm for all considered settings. On average over all conducted experiments this advantage is around 20%, which seems like only a modest improvement but can easily amount to several hours of runtime less for large systems and large values of $D_{\text{max}}$. The results additionally illustrate the linear complexity in $L$ and cubic dependence on $D_{\text{max}}$ we have claimed in [2] and which is not affected by the improvement introduced in this work.

In Figure 5.2 we can furthermore observe that for the case of an input that exhibits the required spectral symmetry the accuracy of both versions of the algorithm is similar with slight advantages for the improved variant. This might be due to the fact that the unnecessarily computed partial results in the vanilla version of the algorithm are not exactly zero and hence introduce a small amount of additional error into the approximation.

Finally, in Figure 5.3 we show heatmaps of the first six computed basis matrices in a run of the algorithm without approximations for $L = 10$. While the first basis matrix is simply the scaled transverse field Ising Hamiltonian, the following matrices represent its orthogonalized powers. Although this naturally does not constitute a rigorous argument, we can find by simple visual inspection that the basis matrices inherit the symmetric properties of the Hamiltonian, providing some intuition for the statements made in Section 3.

6. Conclusion. In this work we have tried to shed some more light on the analytic properties of the matrix product function approximation algorithm by analyzing the characteristics of the partial results computed during a full run.

As a result, we have found that the basis matrices as computed by the algorithm inherit a range of properties from the input matrix. We have also seen that these properties then yield a more efficient version of the algorithm for a particular kind of input class, namely the class of matrices with point symmetric spectrum around zero.

We then went on to show for the application of quantum physics that a variety of spin Hamiltonians exhibits this spectral symmetry property and that hence in this field of application the discovered improvement can be successfully applied in many cases.

Finally, we demonstrated and verified our findings in numerical experiments conducted for the example of the Ising Hamiltonian with a transverse magnetic field.

While we were able to improve our understanding of the algorithm, more remains to be done, especially with respect to the influence of the introduced truncation errors on the overall approximation accuracy. In addition to his, it would be interesting to see further applications of the algorithm outside of numerical quantum physics.

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REFERENCES

[1] W. Arnoldi, The principle of minimized iterations in the solution of the matrix eigenvalue problem, Quarterly of applied mathematics, 9 (1951), pp. 17–29.

[2] M. August, M. C. Bañuls, and T. Huckle, On the approximation of functionals of very large hermitian matrices represented as matrix product operators, Electronic Transactions on Numerical Analysis, 46 (2017), pp. 215–232.

[3] M. Bachmayr, R. Schneider, and A. Uschmajew, Tensor networks and hierarchical tensors for the solution of high-dimensional partial differential equations, Foundations of Computational Mathematics, (2016), pp. 1–50.
[4] J. Baglama, C. Fenu, L. Reichel, and G. Rodriguez, Analysis of directed networks via partial singular value decomposition and gauss quadrature, Linear Algebra and its Applications, 456 (2014), pp. 93–121.

[5] Z. Bai, G. Fahey, and G. Golub, Some large-scale matrix computation problems, Journal of Computational and Applied Mathematics, 74 (1996), pp. 71–89.

[6] C. Bekas, E. Kokologiannou, and Y. Saad, An estimator for the diagonal of a matrix, Applied numerical mathematics, 57 (2007), pp. 1214–1229.

[7] M. Bellalij, L. Reichel, G. Rodriguez, and H. Sadok, Bounding matrix functionals via partial global block lanczos decomposition, Applied Numerical Mathematics, 94 (2015), pp. 127–139.

[8] D. Calvetti, L. Reichel, and D. Sorensen, An implicitly restarted lanczos method for large symmetric eigenvalue problems, Electronic Transactions on Numerical Analysis, 2 (1994), p. 21.

[9] J. Cullum and W. Donath, A block lanczos algorithm for computing the q algebraically largest eigenvalues and a corresponding eigenspace of large, sparse, real symmetric matrices, in Decision and Control including the 13th Symposium on Adaptive Processes, 1974 IEEE Conference on, IEEE, 1974, pp. 505–509.

[10] P. Davis and P. Rabinowitz, Methods of numerical integration, Courier Corporation, 2007.

[11] V. Druiskin, On monotonicity of the lanczos approximation to the matrix exponential, Linear Algebra and its Applications, 429 (2008), pp. 1679–1683.

[12] L. Elbouyahyaoui, A. Messaoudi, and H. Sadok, Algebraic properties of the block gmres and block arnoldi methods, Electronic Transactions on Numerical Analysis, 33 (2009), p. 4.

[13] E. Estrada and D. Higham, Network properties revealed through matrix functions, SIAM review, 52 (2010), pp. 696–714.

[14] M. Fannes, B. Nachtergaele, and R. F. Werner, Finitely correlated states on quantum spin chains, Communications in mathematical physics, 144 (1992), pp. 443–490.

[15] C. Fenu, D. Martin, L. Reichel, and G. Rodriguez, Block gauss and anti-gauss quadrature with application to networks, SIAM Journal on Matrix Analysis and Applications, 34 (2013), pp. 1655–1684.

[16] J. J. García-Ripoll, Time evolution of matrix product states, New Journal of Physics, 8 (2006), p. 305.

[17] G. Golub, F. Luk, and M. Overton, A block lanczos method for computing the singular values and corresponding singular vectors of a matrix, ACM Transactions on Mathematical Software (TOMS), 7 (1981), pp. 149–169.

[18] G. Golub and G. Meurant, Matrices, moments and quadrature, Pitman Research Notes in Mathematics Series, (1994), pp. 105–105.

[19] ———, Matrices, moments and quadrature with applications, Princeton University Press, 2009.

[20] S. Goreinov, I. Oseledec, and D. Savostyanov, Wedderburn rank reduction and krylov subspace method for tensor approximation, part 1: Tucker case, SIAM Journal on Scientific Computing, 34 (2012), pp. A1–A27.

[21] L. Grasedyck, D. Kressner, and C. Tobler, A literature survey of low-rank tensor approximation techniques, GAMM-Mitteilungen, 36 (2013), pp. 53–78.

[22] R. Grimes, J. Lewis, and H. Simon, A shifted block lanczos algorithm for solving sparse symmetric generalized eigenproblems, SIAM Journal on Matrix Analysis and Applications, 15 (1994), pp. 228–272.

[23] M. Hastings, An area law for one-dimensional quantum systems, Journal of Statistical Mechanics: Theory and Experiment, 2007 (2007), p. P08024.

[24] T. Huckle, K. Waldherr, and T. Schulte-Herbrüggen, Computations in quantum tensor networks, Linear Algebra and its Applications, 438 (2013), pp. 750–781.

[25] M. Hutchinson, A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines, Communications in Statistics-Simulation and Computation, 19 (1990), pp. 433–450.

[26] K. Jbilou, A. Messaoudi, and H. Sadok, Global fom and gmres algorithms for matrix equations, Applied Numerical Mathematics, 31 (1999), pp. 49–63.

[27] D. Karevski, Ising quantum chains, arXiv preprint cond-mat/0611327, (2006).

[28] B. Khoromskij, O (dlog n)-quantics approximation of nd tensors in high-dimensional numerical modeling, Constructive Approximation, 34 (2011), pp. 257–280.

[29] D. Kressner and C. Tobler, Low-rank tensor krylov subspace methods for parametrized linear systems, SIAM Journal on Matrix Analysis and Applications, 32 (2011), pp. 1288–1316.

[30] A. Krylov, On the numerical solution of the equation by which the frequency of small oscillations is determined in technical problems, Izv. Akad. Nauk SSSR Ser. Fiz.-Mat, 4 (1931), pp. 491–539.

[31] C. Lanczos, An iteration method for the solution of the eigenvalue problem of linear differential and integral operators, United States Governm. Press Office Los Angeles, CA, 1930.

[32] D. Martin, Quadrature approximation of matrix functions, with applications, PhD thesis, Kent State University, 2012.

[33] C. Meyer, The idea behind krylov methods, The American mathematical monthly, 105 (1998), pp. 889–899.

[34] P. Montgomery, A block lanczos algorithm for finding dependencies over gf (2), in International Confer-
ence on the Theory and Applications of Cryptographic Techniques, Springer, 1995, pp. 106–120.

[35] M. Newman, Networks: an introduction, Oxford university press, 2010.

[36] I. Osieck, Tensor-train decomposition, SIAM Journal on Scientific Computing, 33 (2011), pp. 2295–2317.

[37] D. Perez-Garcia, F. Verstraete, M. Wolf, and I. Cirac, Matrix product state representations, arXiv preprint quant-ph/0608197, (2006).

[38] B. Pirvu, V. Murg, I. Cirac, and F. Verstraete, Matrix product operator representations, New Journal of Physics, 12 (2010), p. 025012.

[39] L. Reichel, M. Spalević, and T. Tang, Generalized averaged gauss quadrature rules for the approximation of matrix functionals, BIT Numerical Mathematics, (2015), pp. 1–23.

[40] Y. Saad, Numerical methods for large eigenvalue problems, vol. 158, SIAM, 1992.

[41] Y. Saad and M. Schultz, Gmres: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM Journal on scientific and statistical computing, 7 (1986), pp. 856–869.

[42] S. Sachdev, Quantum phase transitions, Wiley Online Library, 2007.

[43] J. J. Sakurai and E. D. Commins, Modern quantum mechanics, revised edition, AAPT, 1995.

[44] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, Annals of Physics, 326 (2011), pp. 96–192.

[45] S. Suzuki, J. Inoue, and B. Chakrabarti, Quantum Ising phases and transitions in transverse Ising models, vol. 862, Springer, 2012.

[46] J. Tang and Y. Saad, A probing method for computing the diagonal of a matrix inverse, Numerical Linear Algebra with Applications, 19 (2012), pp. 485–501.

[47] L. Trefethen and D. Bau III, Numerical linear algebra, vol. 50, Siam, 1997.

[48] F. Verstraete and I. Cirac, Matrix product states represent ground states faithfully, Physical Review B, 73 (2006), p. 094423.

[49] F. Verstraete, J. García-Ripoll, and I. Cirac, Matrix product density operators: simulation of finite-temperature and dissipative systems, Physical review letters, 93 (2004), p. 207204.

[50] F. Verstraete, V. Murg, and I. Cirac, Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems, Advances in Physics, 57 (2008), pp. 143–224.

[51] F. Verstraete, D. Porras, and I. Cirac, Density matrix renormalization group and periodic boundary conditions: a quantum information perspective, Physical review letters, 93 (2004), p. 227205.

[52] G. Vidal, Efficient classical simulation of slightly entangled quantum computations, Physical Review Letters, 91 (2003), p. 147902.

[53] G. Vidal, Efficient simulation of one-dimensional quantum many-body systems, Physical review letters, 93 (2004), p. 040502.

[54] K. Waldherr, Numerical Linear and Multilinear Algebra in Quantum Control and Quantum Tensor Networks, Verlag Dr. Hut, 2014.

[55] M. Zwolak and G. Vidal, Mixed-state dynamics in one-dimensional quantum lattice systems: a time-dependent superoperator renormalization algorithm, Physical review letters, 93 (2004), p. 207205.