Density Matrix Renormalization Group of Gapless Systems

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(November 17, 2021)

We investigate convergence of the density matrix renormalization group (DMRG) in the thermodynamic limit for gapless systems. Although the DMRG correlations always decay exponentially in the thermodynamic limit, the correlation length at the DMRG fixed-point scales as $\xi \sim m^{1.3}$, where $m$ is the number of kept states, indicating the existence of algebraic order for the exact system. The single-particle excitation spectrum is calculated, using a Bloch-wave ansatz, and we prove that the Bloch-wave ansatz leads to the symmetry $E(k) = E(\pi - k)$ for translationally invariant half-integer spin-systems with local interactions. Finally, we provide a method to compute overlaps between ground states obtained from different DMRG calculations.

I. INTRODUCTION

Since White constructed the density matrix renormalization group (DMRG) technique about five years ago, numerical renormalization techniques have become very useful. The DMRG has by now been applied to a wide range of different problems beyond quantum spin systems, where it was originally used. Today, people use it to compute, for instance, properties of two-dimensional classical lattice systems, thermodynamics of one-dimensional quantum systems, etc. The DMRG and matrix product states have proven to be computationally very efficient and to determine properties of many systems with unusually high accuracy.

This paper aims at a better understanding of the underlying structure and the fundamental limitations of the DMRG. It has been reported that the DMRG is less accurate for gapless systems than for gapped systems. This has motivated us to analyse the DMRG of gapless systems in more detail, which we do in two steps: first, we investigate the correlation functions (which pertain to the wavefunction), and second, we study the excitation spectrum. We have chosen to study free fermions on a one-dimensional lattice as a paradigm of gapless systems.

In this work, we show that the DMRG of a gapless system converges, for each choice of the number of kept states, to a fixed-point. The corresponding correlation functions are calculated by using an eigenvalue technique, and the results show that this fixed-point describes with increasing accuracy the exact system. In particular, we address the question of how the DMRG handles algebraic correlations (infinite correlation lengths), which is characteristic of gapless systems, in contrast to gapped systems having finite correlation lengths and determine a scaling formula for how the DMRG correlation length depends on the number of kept states. In DMRG applications, this scaling formula may serve as a guide for how many states that is necessary to keep in order to accurately calculate correlations. We perform calculations for the particle-hole and the density-density correlation functions. In addition, we derive conditions for which types of operators that can give truly long ranged DMRG correlations. By introducing a gap, we also investigate how the DMRG correlation lengths change as the critical point (free fermions) is approached.

A matrix product Bloch-wave ansatz has been proposed for describing the excited states of a system. In this paper, we have used the Bloch-wave ansatz to calculate the excitation spectrum. In particular, we look at the spectrum close to the Fermi points, where the gap closes. Furthermore, it was recently shown that many half-integer spin systems have the symmetry $E(k) = E(\pi - k)$. We prove that this symmetry is inherent also in the Bloch-wave ansatz.

In DMRG calculations, it is important to check convergence with respect to the only source of error (except from round off errors), namely the truncation of the Hilbert space. A commonly used measure of the truncation error is the truncation of the density matrix. However, that measure is algorithm dependent and therefore not universal. It would be desirable to instead calculate and use the overlap between states from different DMRG calculations as a measure. The problem is then that the states will refer to differently renormalized Hilbert spaces. In this work, we demonstrate how the matrix product formalism can be used to handle this problem.

The organization of the paper is as follows: the system we have studied is defined in Section II A; a brief introduction to matrix product states and the Bloch-wave ansatz is given in Section II B; we describe how we calculate correlation functions and overlaps in Section II C and II D; computational methods are outlined in Section II E. The results are presented and discussed in Section II F; convergence of the projection operator (to a fixed-point) and of the ground state is demonstrated in Section II G.
correlation functions and the scaling formula are treated in Section III A. Appendix A contains an important result for the determination of correlation lengths in a fermionic system; conditions for true long range correlations are derived in Appendix B. The excitation spectra is presented in Section III C and a proof of the symmetry of the spectra is given in Appendix D. Finally, the results and conclusions are summarized in Section IV.

II. METHODOLOGY

A. Hamiltonian

We have studied a system of non-interacting spinless fermions on a one-dimensional lattice. The Hamiltonian is:

\[ H = -\frac{t}{2} \sum_{j=1}^{N} [c_{j}^{\dagger} c_{j+1} + \text{h.c.}] + \epsilon \sum_{j=1}^{N} (-1)^{j} c_{j}^{\dagger} c_{j}, \]

where \( N \) is the size of the lattice, \( c_{j}^{\dagger} \) creates a fermion on site \( j \), and \( t \) is the hopping amplitude \( t \) ( \( t = 2 \) throughout this work). We have added a staggered on-site potential \( \epsilon \) to the lattice since we want to compare DMRG of the gapless system \( (\epsilon = 0) \) to that of gapped systems \( (\epsilon \neq 0) \). The simple Hamiltonian gives us the advantage of having access to exact solutions when evaluating the DMRG. In the remaining part of this section, we will state exact results used in our analysis.

The Hamiltonian is particle-number conserving and is invariant under the transformation \( c_{j} \rightarrow (-1)^{j} c_{j}^{\dagger} \) for all \( \epsilon \). In addition, when \( \epsilon = 0 \), the Hamiltonian has particle-hole symmetry, i.e. it is invariant under the transformation

\[ c_{j} \rightarrow (-1)^{j} c_{j}^{\dagger}. \]

We will only consider chains of length \( N = 4n + 2 \) in order to have a unique ground state, which corresponds to a half filled system. The gap between the valence band and the conduction band at the Fermi points is \( 2|\epsilon| \). The correlation functions \( C(l) \) decay algebraically for the gapless system and exponentially for a gapped system. When \( \epsilon = 0 \) we have

\[ C_{ph}(l) = \langle c_{j}^{\dagger} c_{j+l} \rangle = \frac{1}{\pi t} \sin \pi l/2, \]

and

\[ C_{dd}(l) = \langle n_{j} n_{j+l} \rangle - \langle n_{j} \rangle \langle n_{j+l} \rangle = -\frac{1}{\pi t^2} \sin^2 \pi l/2, \]

for the particle-hole and density-density correlation functions respectively, where \( n_{j} = c_{j}^{\dagger} c_{j} \).

When \( \epsilon \neq 0 \), the correlation length for the ground state particle-hole correlation function can be calculated analytically to be

\[ \xi_{ph}(t, \epsilon) = \frac{1}{\ln \left[ \frac{\epsilon}{t} + \sqrt{1 + \left( \frac{\epsilon}{t} \right)^2} \right]}. \]

Similarly, the exact density-density correlation length is given by \( \xi_{dd} = \xi_{ph}/2 \).

Finally, we note that there is a well-known connection to spin-systems. We associate a spin-1/2 with each site in the lattice and consider an occupied site as spin up and an empty site as spin down. Using the spin raising and lowering operators we may rewrite the Hamiltonian (after a Jordan-Wigner transformation) as

\[ H = -\frac{t}{2} \sum_{j=1}^{N} [S_{j}^{+} S_{j+1}^{-} + \text{h.c.}] + \epsilon \sum_{j=1}^{N} (-1)^{j} (S_{j}^{x} + S_{j}^{y} + 1/2), \]

where as usual \( S^{z} = S^{x} \pm i S^{y} \). The number operator \( n_{j} \) in fermionic terminology is identified as \( S_{j}^{z} + 1/2 \) in the spin terminology.

B. Matrix Product States

We refer to previous work for a derivation of the ansatz and for details concerning the calculations in this section. A general matrix product state takes the form

\[ |Q\rangle = \sum_{\{s_{j}\}} \text{tr} [Q A[s_{N}] \cdots A[s_{1}]] |s_{N} \cdots s_{1}\rangle, \]

where \( Q \) is an \( m \times m \) matrix containing the boundary conditions on the chain, \( A[s] \) is an \( m \times m \) projection matrix obtained either from a DMRG calculation or variationally, and \( s_{j} \) is the quantum number associated with site \( j \). The projection matrix \( A \) contains the information about states to keep when the lattice is augmented with one site. The number of degrees of freedom in \( A \) is reduced by preservation of orthonormal bases:

\[ \sum_{s} A[s] A^\dagger[s] = \mathbb{I}_{m}. \]

Further reduction of the number of free parameters is possible by exploiting symmetries of the system. In our variational calculations we have used particle-hole symmetry and conservation of the number of particles. Generally, the projection matrix \( A[s] \) is built up from states that form irreducible representations of the symmetry group of the Hamiltonian.

In terms of the spin Hamiltonian Eq. (B), each factor \( A[s] \) in Eq. (B) adds a spin-1/2, hence taking a half-integer (\( n_{j} \)) total spin into an integer (\( n \)) total spin and vice versa. This implies that we can define our projection matrix \( A \) with an off-diagonal block structure

\[ A[s] = \begin{pmatrix} 0 & A_{s_{1} \rightarrow s_{1}+1} \[s] \\ A_{s_{1} \rightarrow n_{1} \[s]} & 0 \end{pmatrix} \].
It is convenient to introduce the following mapping, denoted $\widehat{\sim}$, from a local $s \times s$ matrix $M$ to an $m^2 \times m^2$ matrix $\widehat{M}$:

$$\widehat{M} = \sum_{s',s} M_{s',s} A^*[s'] \otimes A[s].$$

(8)

Just using the block structure of $A[s]$, one can show\footnote{Note that if we use a different sign convention in the Hamiltonian, the ground state would have momentum $\pi$ and hence we would have to choose a $Q$ that anticommutes with $A[s]$, $\{Q, A[s]\} = 0$ for all $s$. From this it follows that we must choose $Q$ as the generalized (right) eigenvector corresponding to the eigenvalue $-1$ of $\widehat{1}$. Let us denote this generalized eigenvector by $R$ for future purposes. This indicates that $R$ is associated with momentum $\pi$. Further evidence for this is given in connection to the section of the single particle excitation spectrum, see Section III C.} that the eigenvalues of an operator $\widehat{M}$ appear in pairs $\pm \lambda$. We will frequently interpret the eigenvectors of $\widehat{M}$ (of length $m^2$) as matrices of size $m \times m$.

The matrix $\widehat{1}$, i.e. the $\widehat{\sim}$-image of the identity matrix, plays an important role in the theory. Since $\widehat{1}$ is guaranteed to have an eigenvalue 1, due to the orthonormalization condition, there also exists an eigenvalue $\sqrt{1}$, due to the orthonormalization condition, there also exists an eigenvalue $\sqrt{-1}$. The block structure of the projection matrix also implies that there may occur eigenvalues due to mixing of the integer and half-integer representations. However, these eigenvalues are spurious (unphysical), in the sense that they do not affect the correlation functions, and can be removed simply by working with two different $A$ matrices formed of the two off-diagonal blocks in Eq. (7). For this reason we leave these spurious eigenvalues aside in the subsequent discussion.

For a translationally invariant system Eq. (1) can be generalized to a Bloch-wave ansatz:

$$|Q,k\rangle_N = \sum_{j,s} e^{ijk} \mathrm{tr}[A[s_N] \cdots A[s_{j+1}]Q \cdots A[s_1]] |s_N \cdots s_1\rangle,$$

where $k$ is the momentum.

The ground state of our model is translationally invariant. This implies that the matrix $Q$ in Eq. (1) should satisfy $\{Q, A[s]\} = 0$ for all $s$, or equivalently, $Q$ must be a generalized right eigenvector\footnote{Further evidence for this is given in connection to the section of the single particle excitation spectrum, see Section III C.} of $\widehat{1}$ corresponding eigenvalue 1 (provided that this eigenvalue is non-degenerate). This means that $Q \sim 1_m$ and hence our ground state ansatz takes the form,

$$|1\rangle_N = \sum_{\{s\}} \mathrm{tr}[A[s_N] \cdots A[s_1]] |s_N \cdots s_1\rangle.$$

(10)

C. Correlation functions

Suppose we want to compute the ground state correlation function $C(l)$ between two local operators $M^1_j$ and $M^2_{j+l}$ acting on sites $j$ and $j+l$ respectively. Since we are working with a fermionic model it is necessary to distinguish between local operators depending on whether they commute or anticommute on different sites. We refer to these operators as bosonic and fermionic respectively. For example, the density-density correlation is expressed in terms of two bosonic operators, while the particle-hole correlation is expressed in terms of two fermionic operators. We will use the superscripts $B$ and $F$ to denote bosonic and fermionic operators respectively. For bosonic operators the correlation function is given by

$$C(l) = \langle M^B_j M^B_{j+l} \rangle = (1|1)^{-1} \mathrm{tr}[(\widehat{M}^B_1 \widehat{1}^{-1} \widehat{M}^B_2 \widehat{1}^{-1})].$$

(11)

If we instead are interested in a correlation function between fermionic operators, we have to keep track of the number of fermions between the sites $j$ and $j+l$ in order to get the phases correct. Defining $\widehat{F}$ as a diagonal matrix with diagonal elements $(-1, 1)$, we find the expression to be

$$C(l) = \langle M^F_j M^F_{j+l} \rangle = (1|1)^{-1} \mathrm{tr}[(\widehat{M}^F_1 \widehat{F}^{-1} \widehat{M}^F_2 \widehat{F}^{-1})].$$

(12)

Eqs. (11) and (12) imply\footnote{Further evidence for this is given in connection to the section of the single particle excitation spectrum, see Section III C.} that in general a correlation function takes the analytical form

$$C(l) = \sum_{i=1}^{m^2} \alpha_i \mathrm{sgn} \lambda_i^l \exp[-l/\xi_i],$$

(13)

where $\xi_i = -1/\ln |\lambda_i|$, and $\lambda_i$ are the eigenvalues of $\widehat{1}$ or $\widehat{F}$, depending on the statistics of the operators. The $\alpha_i$’s are coefficients that depend on the operators in the correlation function. Thus, the eigenvalues of $\lambda_i$ determine the possible correlation lengths in the system and it is therefore important to investigate the spectrum of $\widehat{1}$ and $\widehat{F}$. Eigenvalues that fulfill $|\lambda_i| = 1$ can potentially give rise to true long-range order. Due to normalization, $\widehat{1}$ is guaranteed to have eigenvalues $\pm 1$, which potentially could give long-range order in the bosonic correlation functions. In Appendix A we show that the spectrum of $\widehat{F}$ differs from that of $\widehat{1}$ only by a factor $i$. Hence, fermionic and bosonic operators have the same set of possible correlation lengths, which means that $\widehat{F}$ has eigenvalues $\pm i$ and these can give rise to true long-range order in the fermionic correlation functions. Finally, we note that negative and imaginary eigenvalues correspond to oscillating correlation functions.
D. Overlap of DMRG states

Suppose we perform two different DMRG calculations, keeping $m_1$ and $m_2$ states respectively. The overlap \( N(1_{m_1}|1_{m_2})_N \), where \( |1_{m_2}\rangle_N \) is the normalized ground state obtained by keeping \( m_2 \) states etc., can be computed as follows,

\[
N(1_{m_1}|1_{m_2})_N = \text{tr}\left[ \hat{1}_{m_1,m_2}^N \right], \tag{14}
\]

where we have defined the mixed \((m_1m_2) \times (m_1m_2)\) matrix \( \hat{1}_{m_1,m_2} \) as

\[
\hat{1}_{m_1,m_2} = \sum_s A^*_{m_1}[s] \otimes A_{m_2}[s]. \tag{15}
\]

Note that this overlap would be difficult to compute without the matrix product formalism since we have no mapping between the different basis states of the two DMRG calculations due to renormalization. In contrast, all matrix product states are formulated in terms of the fixed \( \{|s_N\cdots\rangle_1\} \) basis (rather than renormalized basis sets), with the projection matrix just providing the amplitudes.

Using Eq. (14) we find that the overlap decays exponentially as \( \lambda^r \), where \( \lambda \) is the (in absolute value) leading eigenvalue of \( \hat{1}_{m_1,m_2} \).

The overlap between DMRG states for different number of kept states gives a measure of the gain in accuracy obtained by increasing the number of kept states. We consider this measure to be more universal and relevant than the usual measure used, namely the truncation of the density matrix, \( 1 - \text{tr}\rho_c \), where \( \rho_c \) is the truncated density matrix. The old measure is algorithm-dependent and can, for instance, be made equal to zero despite the fact that an exact calculation is not performed, simply by using a superblock configuration.

E. Computational methods

Due to the large dimensions of \( \hat{1}_{m_1,m_2} \), namely \((m_1m_2) \times (m_1m_2)\), it becomes necessary to use iterative eigenvalue routines that require no explicit construction or storage of \( \hat{1}_{m_1,m_2} \). Moreover, \( \hat{1}_{m_1,m_2} \) is non-symmetric. We have used the Arnoldi algorithm to handle these problems.

Furthermore, the computations become much more efficient if we rewrite the operation of \( \hat{1}_{m_1,m_2} \) on an \((m_1m_2)\) vector \( v \) as a matrix product with \( v \) interpreted as an \( m_1 \times m_2 \) matrix:

\[
\hat{1}_{m_1,m_2} v = \sum_s A^*_{m_1}[s]v A^T_{m_2}[s].
\]

In this way we only need to operate with \( m_1 \times m_2 \) matrices, and the eigenvalues of \( \hat{1}_{m_1,m_2} \) can easily be obtained.

In order to calculate the projection operators \( A[s] \), we have performed standard DMRG calculations by using a superblock of the form:

\[
\begin{array}{c}
\bullet \\
B \quad \bullet \\
B' \quad \bullet
\end{array}
\]

the infinite lattice algorithm, and by adding a single site per iteration to each block. When we have an on-site potential \( \epsilon \) present in the problem we have to keep four projection matrices in order to completely describe the system, see Fig. 1. From these four matrices we form two projection operators \( A^+ \) and \( A^- \) taking us from positive to negative on-site potential and vice versa. Explicitly:

\[
A^\pm[s] = \begin{pmatrix} 0 & A^\pm_1[s] \\ A^\pm_2[s] & 0 \end{pmatrix}.
\]

FIG. 1. The figure shows the four projection matrices needed to describe the system. Filled discs denote sites with positive on-site potential and circles denote sites with negative on-site potential, \( \hbar i \) denotes half-integer representations and \( i \) denotes integer representations. Andersson et. al.

In each DMRG iteration we update either the \( \hbar i \rightarrow i \) or the \( i \rightarrow \hbar i \) matrices.

III. RESULTS AND DISCUSSION

A. Convergence of the DMRG

In this section we will discuss the convergence of the DMRG. First, we demonstrate that the DMRG projection operator of the critical system converges to a fixed-point, and thus, justifying the matrix product ansatz when studying the thermodynamic limit of the DMRG. Second, we check the convergence of the ground state with respect to the number of kept states by using the overlap measure.

The fundamental assumption of the matrix product approach is that the projection matrix converges to a fixed-point with respect to \( N \), i.e. \( \lim_{N \to \infty} A_N[s] = A[s] \). In order to show this, we define the matrix norm \( \| \cdot \|_{\text{max}} \) via,

\[
\|A\|_{\text{max}} = \max_{i,j,s} |A_{i,j}[s]|. \tag{16}
\]
In addition, we make a consistent enumeration (with respect to quantum numbers) and use a fixed sign convention of the states in the system blocks. It is then easy to study the convergence of the projection operator by measuring the quantity \( r(N) = (\|A_{N+1} - A_N\|_{\text{max}} + \|A_N - A_{N-1}\|_{\text{max}})/2 \), where \( N \) is the number of DMRG iterations. In Fig. 2 we have shown results from such calculations. From the figure we see that the convergence of the projection operator seems to be exponential with respect to the number of DMRG iterations and that the convergence rate decreases when the number of kept states is increased. We have also found that the ground state energy per site converges much faster than the projection matrices and is therefore not a good indicator on whether or not a fixed-point has been reached.

![Figure 2](image.png)

**FIG. 2.** The norm \( r(N) \) is shown as a function of the number of DMRG iterations, \( N \), for the gapless case. It is clear from the figure that the DMRG projection operator converges with respect to \( N \). Furthermore, the convergence seems to be exponential with respect to \( N \). The peaks in the (36,32) curve indicate that either the DMRG has changed the states kept in the Hilbert space basis or our sign-fixing procedure of the states has failed. The notation \((m_1, m_2)\) means \( m_1 \) states in the integer representation and \( m_2 \) states in the half-integer representation.

| \((m_1, m_2)\) | (4,6) | (12,12) | (21,20) | (36,32) |
|-----------------|-------|-------------|------------|-----------|
| (4,6)           | 0     | 0.00231     | 0          | 0.00381   |
| (12,12)         | 0     | 0.00277     | 0.000644   | 0         |
| (21,20)         | 0.00328| 0.000277   | 0          | 0.00134   |
| (36,32)         | 0.00381| 0.000644   | 0.000134   | 0         |

**TABLE I.** Leading eigenvalues \( 1 - \lambda \), governing the overlap between different DMRG ground state wavefunctions. The notation \((m_1, m_2)\) means \( m_1 \) states in the integer representation and \( m_2 \) states in the half-integer representation.

In Table. I we have presented the eigenvalues that govern the overlap in the thermodynamic limit between ground states obtained by keeping different numbers of states. We have chosen to write out \( 1 - \lambda \) instead of \( \lambda \) since this gives a more direct measure of the error.

### B. The spectrum of \( \hat{\mathcal{T}} \) and correlation lengths

Since the DMRG projection operator converges to a fixed-point, the correlation functions of the DMRG in the thermodynamic limit are given by Eq. (11) and the correlation lengths are determined by the eigenvalues of \( \hat{\mathcal{T}} \) (the correlation lengths obtained from \( \hat{F} \) are identical). An analysis of the spectrum of \( \hat{\mathcal{T}} \) is therefore pivotal.

We have found that the eigenvalues \( \pm 1 \) are non-degenerate, and that all the other eigenvalues fulfill \( |\lambda| < 1 \). Only the eigenvalues \( \pm 1 \) can give rise to infinite correlations lengths. However, it turns out that that the density-density and the particle-hole operators are orthogonal to the corresponding eigenvectors, and hence the correlation lengths will be determined by other eigenvalues.

An interesting question is which local operators \( \mathcal{M} \) that potentially can give true long-range order in the correlation functions Eqs. (11) and (12). We show in Appendix B that true long-range order for bosonic operators is not possible if \( \text{tr}[\mathcal{M}^B] = 0 \). For fermionic operators we find that true long-range order is not possible for off-diagonal operators. This explains why there is no true long-range order in the density-density and particle-hole correlation functions. The proof exploits that the Hamiltonian conserves the number of particles and that it is particle-hole symmetric. If we break the particle-hole symmetry, we are only guaranteed that the particle-hole correlation function can not be truly long-ranged.

Thus, the DMRG will approximate infinite correlation lengths by finite, and it is interesting to investigate how the DMRG correlation lengths depend on the number of kept states and on the gap of the system.

First of all we need to identify the leading eigenvalues of \( \hat{\mathcal{T}} \) and \( \hat{\mathcal{F}} \) governing the particle-hole and density-density correlations respectively. These eigenvalues can be identified either by a matrix product calculation of the respective correlation function, or by measuring the correlation length directly in the DMRG calculation. Degeneracies in the spectrum are also instrumental in identifying the leading eigenvalue. For instance, if we want to compute the particle-hole correlation function, we expect this correlation to couple to an eigenvalue that is two-fold degenerate since the hole-particle correlation function has an equal correlation length. The density-density correlation function, on the other hand, will couple to a non-degenerate eigenvalue since there is no symmetry related correlation function that demand an equal eigenvalue.

Using the analytical result for the correlation length given by Eq. (13) together with \( \lambda = \exp[-1/\xi] \), we find that the exact expression for the eigenvalue dominating the particle-hole correlation is:
\[ \lambda^*_{\text{ph}}(t, \epsilon) = \sqrt{1 + \frac{\epsilon^2}{t^2}} - \frac{\epsilon}{t}. \]  

The * is used to indicate that this is an exact value. The expression will be used as a reference when we evaluate our numerical data.

![Figure 3](image.png)

**FIG. 3.** The eigenvalues of \( \hat{F} \) governing the particle-hole correlation length versus \( \epsilon \) for different numbers of kept states. The solid line corresponds to the exact result from Eq. (13). From the bottom to the top, the point sets correspond to the following numbers of kept states: (4, 6), (12, 12), (21, 20), (36, 32). Due to numerical problems, we can not continue the set with \( m_1 \) or \( m_2 \) > 12 to larger \( \epsilon \) values.

![Figure 4](image.png)

**FIG. 4.** Convergence of the eigenvalue \( \lambda \) of \( \hat{F} \) governing the particle-hole correlation length. In the figure we show \( 1 - |\lambda| \) versus the number of kept states, \( m = m_1 + m_2 \), in the gapless \( (\epsilon = 0) \) case.

In Fig. 3 our results for the particle-hole correlation length are shown. It is clear that as we increase the number of kept states in our truncated Hilbert space, the accuracy of the correlation length increases. For the case \( \epsilon = 0 \) we see that the eigenvalue \( |\lambda_{\text{ph}}| \) approaches the exact value 1, i.e. an infinite correlation length, as the number of states is increased. The convergence of \( |\lambda_{\text{ph}}| \) towards 1 is more clearly seen in Fig. 4, where we consider the gapless case and plot \( 1 - |\lambda_{\text{ph}}| \) versus the number of kept states, \( m = m_1 + m_2 \). Thus, we conclude that the DMRG gives exponentially decaying correlation functions in the gapless case, but as the number of states is increased the correlation length grows towards infinity.

We can actually make this conclusion more quantitative. As is seen in Fig. 4 the eigenvalue \( |\lambda_{\text{ph}}| \) behaves as \( |\lambda_{\text{ph}}| \approx 1 - km^{-\beta} \). Thus the correlation length behaves as

\[ \xi_{\text{ph}} \approx \frac{1}{\ln|1 - km^{-\beta}|} \approx \frac{1}{km^{\beta}}. \]  

That is, the correlation length scales as a power of \( m \). We find the exponent \( \beta \approx 1.3 \) and \( k \approx 0.45 \). The density-density correlation function gives similar results.

In any realistic DMRG computation, the correlation function will be given by a sum of a finite (even if large) number of exponentially decaying functions according to Eq. (13). Keeping only a few states, we have seen that the correlation function approximates the true power-law (Eq. (2)) for short correlations, but as we increase \( l \) we eventually end up with an exponential decay. Increasing the number of kept states will make the correlation function look like a power-law for rather large \( l \), but in the end, when \( l \to \infty \), it will always behave as an exponentially decaying function with correlation length given by Eq. (13).

### C. The single-particle excitation spectrum

In order to study the single particle excitation spectrum, we have used the Bloch-wave ansatz of Eq. (3) and the pole-expansion technique to calculate the spectrum. The result is shown in Fig. 5. The curve shows a pair of excitations corresponding to a single particle/hole (or spin \( S^z = \pm 1 \)). We can see that the dispersion relation obtained from the Bloch-wave ansatz is in good agreement with the exact dispersion \( E(k) = \sin k \), except close to the Fermi points, where the gap closes. Instead of having a linear form, the calculated dispersion relation has the form \( E(k) \approx \Delta_0 + \left( \frac{\epsilon_0}{\sqrt{1 - \epsilon^2}} \right) k^2 \) close to \( k = 0 \). Furthermore, our excitations have negative energies close to the Fermi points, a consequence of a defect ground state. Such a negative energy gap was also found to appear for the biquadratic spin-1 chain somewhere between the Heisenberg point and the Takhtajan-Babujian point. We have investigated how the size of this negative energy gap depends on the number of kept states in the truncated Hilbert space. These calculations are computationally demanding and also sensitive to numerical
effects. However, the results we have indicate that the
size of the negative energy gap decreases as the number of
states is increased, but the numerical control was poor
for \( m_1 + m_2 > 12 \).

A possible explanation of this defect ground state could
be that the DMRG has an instability of some sort. We
have investigated whether the DMRG at \( \epsilon = 0 \) is unstable
against breaking the translational symmetry of ground
state by starting the DMRG calculation with a non-zero
staggered on-site potential and then, after about 20 iter-
ations, turning the potential off. We then let the projec-
tion operator converge and compare it with the projection
operator obtained by a DMRG calculation with the
on-site potential turned off all the time. However, the two
converge to the same limit (within the numerical accu-
ry) with only one exception. If we keep 3 states in the
integer representation and 6 states in the half-integer rep-
resentation, we find that the DMRG is actually unstable
and we obtain an energetically more favorable state by
breaking the translational symmetry. However, it is suffi-
cient to add a single state in the integer representation in
order to remove this instability. In addition, we have also
performed variational calculations allowing for a ground
state with periodicity two, but the energetically lowest state
turns out to be translationally invariant. Thus, it
seems like the DMRG is stable against forming a ground
state which is not translationally invariant.

Thus, we have shown that \( E(k) = E(k + \pi) \), but this also
proves that \( E(k) = E(\pi - k) \) since we have the sequence of
mappings:

\[
E(k) \xrightarrow{\mathcal{P}} E(-k) \xrightarrow{R} E(\pi - k),
\]

where \( \mathcal{P} \) is a parity transformation, an exact symmetry
of our model. The details of the proof can be found in
Appendix C. This symmetry is true in general for trans-
lationally invariant half-integer spin systems with local
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by Kladko, without any reference to the Bloch-wave
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Kladko explicitly constructs a state with momentum \( k + \pi \)
from a state with momentum \( k \) and then shows that these
states have equal energy.

\[
E(k) \xrightarrow{\mathcal{P}} E(-k) \xrightarrow{R} E(\pi - k),
\]

where \( \mathcal{P} \) is a parity transformation, an exact symmetry
of our model. The details of the proof can be found in
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energy gap decreases as the number of kept states is increased. In addition, we have shown that the Bloch-wave ansatz for the excitation spectrum exhibits the symmetry \( E(k) = E(\pi - k) \) for translationally invariant half-integer spin systems with local interactions.

**ACKNOWLEDGMENTS**

The authors would like to thank Stefan Rommer for fruitful discussions. We acknowledge the support of the Swedish Research Council for Engineering Sciences (TFR) and the Swedish Natural Science Research Council (NFR).

**APPENDIX A: SPECTRUM OF \( \hat{F} \)**

Since \( \hat{F} \) determines the possible correlation lengths of fermionic operators, it is important to understand the eigenvalue spectrum of this operator. We will in this appendix show that the eigenvalues of \( \hat{F} \) are related to those of \( \hat{1} \) by a factor \( i \). That is, \( \lambda F = i\lambda 1 \). To show this, we will start by constructing an eigenvector of \( \hat{F} \) with eigenvalue \( i \). This construction is similar to the one used by Román et al. Using \( F[s,s'] = \delta_{s,s'}i^{2k+1} \), we may write the matrix elements of the operator \( \hat{F} \) as

\[
\hat{F}(\gamma',m'_{\gamma'i}) = \sum_s i^{2(m'_\gamma - m_\gamma) + 1} A(\gamma',m'_{\gamma'i})[s]A(\gamma,m_{\gamma'i})[s],
\]

where we have used that since the projection operator conserves the particle number, the element \( A(\gamma,m')[s] \) is zero unless \( m' = m + s \). Next, we define the vector \( |u_F\rangle(\gamma_2,m_2)[\gamma_1,m_1] = \delta_{\gamma_2,\gamma_1}\delta_{m_2,\gamma_1}i^{2m_2} \).

We will now show that \( |u_F\rangle \) is an eigenvector of \( \hat{F} \) with eigenvalue \( i \). We have

\[
(\hat{F}|u_F\rangle)(\gamma',m'_{\gamma'i}) = \sum_{\gamma_1,\gamma_2} \sum_{m_1,m_2,s} i^{2(m'_\gamma - m_\gamma) + 1} A(\gamma',m'_{\gamma'i})[\gamma_2,m_2][s]A(\gamma,m_{\gamma'i})[\gamma_1,m_1][s],
\]

which proves the claim. In the third line we have used the identity \( \sum_s A[s]A^T[s] = 1 \). Let us now show that the entire eigenvalue spectrum of \( \hat{F} \) is related to that of \( \hat{1} \) by a factor \( i \). First of all we note that \( | \det u_F \rangle = 1 \), which implies that the inverse \( u_F^{-1} \) exists. In fact \( u_F^{-1} = u_F^\dagger \), i.e., \( u_F \) is unitary. Furthermore, \( u_F \) satisfies the equation

\[
iu_F A[s] = F[s,s']A[s]u_F,
\]

since this equation is equivalent to \( \hat{F}|u_F\rangle = i|u_F\rangle \), as can be seen by simply multiplying Eq. (A1) by \( \hat{A}^\dagger[s] \) and summing over \( s \). Define the unitary operator \( \xi = (u_F \otimes 1) \) and consider

\[
i\xi\hat{1}\xi^\dagger = i(u_F \otimes 1)\left( \sum_s A[s] \otimes A[\gamma,m_{\gamma'i}] \right)(u_F \otimes 1)
\]

\[
= i \sum_s (u_F A[s]u_F^\dagger) \otimes A[s]
\]

\[
= \sum_s F[s,s']A[s] \otimes A[s](u_F u_F^\dagger \otimes 1) = \hat{F}.
\]

This implies that \( \hat{F} \) has exactly the same spectrum as \( i\hat{1} \), which was our claim. In the third line we have used Eq. (A1).

**APPENDIX B: CONDITIONS FOR TRUE LONG-RANGE ORDER**

In this appendix, we show how symmetries of the Hamiltonian determine which local operators that potentially can give true long-range order in correlation functions. In order for a local bosonic operator \( M^B \) to give true long-range order it must hold that at least one of the following expectation values is non-zero: \( \langle 1|M^B|1 \rangle \), \( \langle 1|M^B|R \rangle \) and \( \langle R|M^B|R \rangle \), where \( |1 \rangle \) and \( |R \rangle \) denote the eigenvectors of \( \hat{1} \) with eigenvalues 1 and \( -1 \) respectively. These expectation values will be determined if we can determine the expectation values of \( A^\dagger[s]A[s] \) for all combinations of \( s \) and \( s' \). We will frequently interpret the \( m^2 \) state-vectors \( |1 \rangle \) and \( |R \rangle \) as \( m \times m \) matrices denoted by \( 1 \) and \( R \). The matrix \( R \) has the block-form \( 1 \oplus -1 \) which implies that \( R^2 = 1 \). A subscript \( L \) on the matrix denotes that it represents the left eigenvector. Furthermore, we will consider the projection matrix \( A[s] \) to be real.

Let us start by relating different expectation values. We have

\[
\langle R|A[s] \otimes A[s']|R \rangle = \mathrm{tr}[R^T_LA[s]RA^T[s']]
\]

\[
= -\mathrm{tr}[R^T_LA[s]AT[s']]
\]

\[
= -\langle 1|A[s] \otimes A[s']|1 \rangle,
\]

and similarly,

\[
\langle R|A[s] \otimes A[s']|R \rangle = -\langle 1|A[s] \otimes A[s']|R \rangle.
\]

The indices of \( A[s] \) correspond to different states and we will label these states as \( \gamma, m \), where \( m \) is the particle number measured from half-filling and \( \gamma \) is an integer labeling particle-hole representations. The transformation of the state \( |\gamma, m \rangle \) under a particle-hole transformation \( B \) is

\[
B|\gamma, m \rangle = \phi(\gamma, m)|\gamma, -m \rangle.
\]
where $\phi(\gamma, m) = \pm 1$. That is, the state $|\gamma, m\rangle$ transforms within the $\gamma$ representation of the particle-hole symmetry group. Note also that $B^2 = 1$, which implies that $\phi$ is independent of $m$, since $B^2|\gamma, m\rangle = \phi(\gamma, m)\phi(\gamma, -m)|\gamma, m\rangle$.

We are now going to show that $I_L|\gamma', m\rangle, (\gamma, m)\rangle$ is zero unless $m' = m$. To see this we write the equation (1) = (1|I) as

$$I_L|\gamma_1, m_1\rangle, (\gamma_2, m_2\rangle = \sum_s \sum_{\gamma_3, \gamma_4, m_3, m_4} A_{\gamma_3, m_3, \gamma_4, m_4} |s\rangle A_{\gamma_4, m_4, \gamma_2, m_2\rangle} [s].$$

Using the fact that $A$ conserves the particle number (see Appendix [A]), we conclude that $m_1 - m_2 = m_3 - m_4$. Since the difference between the $m$-values of $I_L|\gamma_1, m_1\rangle, (\gamma_2, m_2\rangle$ is conserved under the action of $I$, we can write $I_L = I_L^0 + I_L^{rest}$ where $I_L^0$ only has non-zero matrix elements between states of equal particle number and $I_L^{rest}$ is the remainder, mixing particle numbers. This decomposition will not be mixed under the action of $I$ and hence both matrices must be eigenstates of $I$ with eigenvalue 1. This eigenvalue is, however, non-degenerate, which means that either of $I_L^0$ and $I_L^{rest}$ is zero. Since $\text{tr} I_L = (1|1) = 1$, $I_L$ must contain $I_L^0$ and hence $I_L^{rest} = 0$. This means that $I_L$ only connects states containing an equal number of particles.

Furthermore, since $R_L = I_L R$ and $R$ also conserves the number of particles (it is diagonal), we conclude that $R_L$ conserves the number of particles.

Let us now consider the following expectation value:

$$\langle 1|A|s\rangle \otimes A(s')|1\rangle = \text{tr} I_L^T A|s\rangle A^T(s')\rangle = \sum_{\gamma_1, m_1} (I_L^T|\gamma_1, m_1\rangle, (\gamma_2, m_2\rangle \times A_{\gamma_2, m_2\rangle} |s\rangle A_{\gamma_1, m_1\rangle, (\gamma_3, m_3\rangle\rangle}.$$

Using particle number conservation of $A$ and $I_L$, we conclude that the expectation value is zero unless $s = s'$, i.e.

$$\langle 1|A|s\rangle \otimes A(s')|1\rangle \sim \delta_{s, s'}. \quad \text{(B2)}$$

Similarly, using $R_L$ instead of $I_L$, one finds

$$\langle 1|A|s\rangle \otimes A(s')|R\rangle \sim \delta_{s, s'}. \quad \text{(B3)}$$

To summarize, Eqs. (B2) and (B3) follow from the particle-number conserving property of the Hamiltonian together with the uniqueness of the eigenvalue 1 of $I$. In the next paragraph, we will investigate the expectation values when $s = s'$. Note that the Pauli matrix $\sigma_3$ and 1 form a complete basis for all diagonal operators $M^B$, which according to the above results are the only operators that can give true long-range order.

Recall the defining relation of the projection operator:

$$|\gamma', m\rangle = \sum_{(\gamma, m), s_j} A_{\gamma', m', (\gamma, m)}(s_j) |\gamma, m\rangle \otimes |s_j\rangle. \quad \text{(B4)}$$

Applying the particle-hole transformation to the defining relation Eq. (B4), we find that $A$ has the following symmetry:

$$A_{\gamma', m', (\gamma, m)}(s_j) = \phi(\gamma')\phi(\gamma)(-1)^j A_{\gamma', -m', (\gamma, -m)}(-s_j). \quad \text{(B5)}$$

Let us write down the operator form of $A[s]$

$$A[s] = \sum_{(\gamma', m'), (\gamma, m)} A_{\gamma', m', (\gamma, m)}(s_j) |\gamma', m\rangle \langle \gamma, m|. \quad \text{(B6)}$$

Using the definition of $I$ we find the transformation property of $I$ under particle-hole transformations:

$$(B \otimes B) \sum_s A|s\rangle \otimes A(s)|B \otimes B\rangle = \sum_s A[-s] \otimes A[-s].$$

That is, $I$ is invariant under particle-hole transformations. Let us also consider the transformation of $\sigma_3$, where $\sigma_3$ is a Pauli matrix. Using exactly the same technique, we find that $(B \otimes B) \sigma_3 = \sigma_3$. Since $I$ is invariant under particle-hole transformations. Using the non-degeneracy of this eigenvalue, we conclude that $(1|B \otimes B) = e^{-i\theta} |1\rangle$ and similarly $(B \otimes B)|1\rangle = e^{i\theta} |1\rangle$.

Let us now compute the expectation value of $\sigma_3$

$$\langle 1|\sigma_3|1\rangle = \langle 1|B \otimes B\rangle \sigma_3 = \langle 1|B \otimes B\rangle^2 = (-1|\sigma_3|1),$$

and thus $\langle 1|\sigma_3|1\rangle = 0$. Since $\langle 1|I|1\rangle = 1$ we arrive at

$$\langle 1|A|s\rangle \otimes A(s')|1\rangle = -\langle R|A|s\rangle \otimes A(s')|R\rangle = \frac{1}{2} \delta_{s, s'}. \quad \text{(B7)}$$

It only remains to consider expectation values of $I$ and $\sigma_3$ between $(1|1)$ and $(1|R)$. Trivially, $(1|1) = 0$, since $(1|1)$ and $(1|R)$ are eigenvectors of $I$ with different eigenvalues. Using the structure of $(1|1)$ and $(1|R)$, let us show that they must transform with the same phase factor. Noting that $B$ must be block-diagonal, it follows that $|B, R\rangle = 0$. Assuming $(B \otimes E)|1\rangle = BB^T = e^{i\theta}|1\rangle$ we find

$$(B \otimes B)|R\rangle = BB^T = BB^T = Re^{i\theta} = e^{i\theta}|R\rangle.$$ 

Using this property we find

$$\langle 1|\sigma_3|R\rangle = -\langle 1|\sigma_3|R\rangle = 0$$

and we conclude

$$\langle 1|A|s\rangle \otimes A(s')|1\rangle = -\langle R|A|s\rangle \otimes A(s')|1\rangle = 0. \quad \text{(B8)}$$
Using the derived expressions for the expectation values, a general bosonic operator $\hat{M}^B$ can couple to the eigenstates with corresponding eigenvalues $\pm 1$ only if $\text{tr}\hat{M}^B \neq 0$. In particular, the density-density correlation function can not be truly long-ranged when the Hamiltonian has particle-hole symmetry and conserves the number of particles.

Let us also investigate correlation functions between fermionic operators, $\hat{M}^F$, in order to be able to draw conclusions concerning the particle-hole correlation function. We will now show that off-diagonal fermionic operators can not give rise to truly long-ranged correlation functions. From Eq. (12) we see that true long-range order is possible only if some expectation value of the form $\langle \hat{S}^+ \rangle$ is possible. Hence, an expectation value of the above form will be

$$\langle \hat{S}^+ \rangle \sim \sum \delta_{m,m'} \delta_{m,1} \delta_{m',1/2} \delta_{m',-1/2} \hat{M}^F \equiv 0,$$

where the second and third delta-functions come from the particle-number conserving property of $\hat{A}[s]$. Thus we can not have true long-range order in the particle-hole correlation function.

Note that we have not proved that the correlation function between two traceless fermionic operators (like $\sigma_3$) can not be long ranged. On the contrary, this is the structure of the string order correlation function in the spin-1 chain, which is long-ranged.

**APPENDIX C: PROOF OF THE BLOCH-STATE SYMMETRY**

In this appendix, we prove that the energy spectrum obtained from the Bloch-state ansatz exhibits the symmetry $E(k) = E(\pi - k)$. Since the symmetry $E(k) = E(-k)$ follows from parity being a good quantum number, we only need to show that $E(k) = E(k + \pi)$. The strategy used in the proof is to construct a Bloch-state of momentum $k + \pi$ from a state of momentum $k$ and to show that expectation values of these two states are equal in the thermodynamic limit.

Let us first recall some properties of the eigenvector $\hat{R}$ of $\hat{\Pi}$. We will use the convention that $|R\rangle$ is an $m^2$ vector and $R$ is an $m \times m$ matrix and similarly we will write the eigenvector of $\hat{\Pi}$ corresponding to the eigenvalue 1 as $|1\rangle$ or $1$. Using the block-diagonal structure of $R$ it follows that $[\{1 \otimes R\}, \hat{M}] = 0$ and that $[\{R \otimes R\}, \hat{M}] = 0$ for all local operators $M$.

We also need the property $(R \otimes R) \lim_{n \to \infty} \hat{\Pi}^n = \lim_{n \to \infty} \hat{\Pi}^n$. To show this we recall that all but two eigenvalues of $\hat{\Pi}$ have absolute value less than one. The corresponding eigenvectors will be annihilated by $\lim_{n \to \infty} \hat{\Pi}^n$. Hence we may write

$$\lim_{n \to \infty} \hat{\Pi}^n = |1\rangle \langle 1| + (1/n)|R\rangle \langle R|.$$ 

If we let this operator act on a general state $|\psi\rangle = \sum \psi_i |i\rangle$ we obtain

$$\lim_{n \to \infty} \hat{\Pi}^n |\psi\rangle = |1\rangle \langle 1| + (1/n)\psi_R |R\rangle.$$ 

Now, if we act on the resulting vector with $(R \otimes R)$, we obtain (now we use the matrix form of the vectors)

$$(R \otimes R) \lim_{n \to \infty} \hat{\Pi}^n |\psi\rangle = (R \otimes R) \psi_R |R\rangle = |1\rangle \langle 1| + (1/n)\psi_R |R\rangle.$$ 

Thus we have shown that $(R \otimes R) \lim_{n \to \infty} \hat{\Pi}^n$ and $\lim_{n \to \infty} \hat{\Pi}^n$ act equally on a general state and hence the operators must be identical.

We are now ready to show that for all local operators $M$, it holds that

$$\text{LHS} = (RQ', k | M | RQ, k) = (Q', k + \pi | M | Q, k + \pi) = \text{RHS}, \quad (C1)$$

where the Bloch-states are defined in Eq. (1). If we apply this result to the Hamiltonian operator and the normalization, we obtain the result that the states $|RQ, k\rangle$ and $|Q, k + \pi\rangle$ have equal energy. That is, we have a mapping from a state of momentum $k$ to a state of momentum $k + \pi$ with equal energy, which proves the symmetry $E(k) = E(k + \pi)$.

In order to prove Eq. (C1), we begin by writing the Bloch-state $|RQ,k\rangle$ as

$$|RQ,k\rangle = \sum_{j_{\cdot \{s_i\}}} e^{i(j(k + \pi)} \text{tr}[RA[s_N \cdots A[s_{j+1}]Q \cdots A[s_1]] \times |s_N \cdots s_1\rangle,$$

where we have used $\{R, A[s]\} = 0$ to move the $R$ to the left side of the trace. Thus we may write the left-hand side of Eq. (C1) as

$$\text{LHS} = \sum_{j \cdot j'} e^{i(j(k + \pi)} e^{-i(j'(k + \pi)} \times \text{tr}[(R \otimes R)\hat{\Pi}^{N-j} \times (1 \otimes Q)\hat{P}^{j-1} \hat{M}\hat{P}^{-1}] (Q' \otimes 1)\hat{P}^j\]$$

where we have assumed that $M$ acts on the site $l$. Now, when we go to the thermodynamic limit $N \to \infty$, we will always have a factor $\hat{\Pi}^\infty$ somewhere in the trace. If we could move $(R \otimes R)$ through the trace until it reaches the $\hat{\Pi}^\infty$ factor, the $(R \otimes R)$ would be annihilated and we would be left with an expression that is
\[
\sum_{j,j'} e^{ij(k+\pi)}e^{-ij'(k+\pi)} \text{tr}[\hat{M}^{N-j}(\mathbb{1} \otimes Q) \\
\times \hat{j}^{j-l} \hat{M}^{l-j'-1}(Q^* \otimes \mathbb{1}) \hat{j}^{j'}] = \text{RHS}
\]

and our proof would be complete. It turns out that it is always possible to perform such a move. If the factor \(\hat{M}^\infty\) is not between the factors \((\mathbb{1} \otimes Q)\) and \((Q^* \otimes \mathbb{1})\), we just commute \((R \otimes R)\) through the \(\hat{M}\)-operators until it reaches \(\hat{M}^\infty\) and gets annihilated. If the factor \(\hat{M}^\infty\) is between \((\mathbb{1} \otimes Q)\) and \((Q^* \otimes \mathbb{1})\) we can make the split \((R \otimes R) = (\mathbb{1} \otimes R)(R \otimes \mathbb{1})\) and move these factors in different directions until they meet between \((\mathbb{1} \otimes Q)\) and \((Q^* \otimes \mathbb{1})\) and get annihilated by \(\hat{M}^\infty\). During the movements we will pick up a factor \((-1)^{j''+(N-j''')}\), and since we are only considering chains of even length, this factor is equal to 1. Note that the proof works even if the operator \(\hat{M}\) does not act on a single site, but, as for example the Hamiltonian, acts on a couple of neighboring sites. The important thing is that the operator is local, so that a factor of \(\hat{M}^\infty\) always can be found in the trace.

This completes the proof.

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17. In the thermodynamic limit \(N \rightarrow \infty\), the ground state energy per site is given by

\[
E_0 = \frac{\epsilon}{\pi} E \left[ -\frac{t^2}{\epsilon^2} , \frac{\pi}{2} \right],
\]

where \(E\) is an elliptic integral of the second kind.
18. The result is derived by introducing periodic boundary conditions, letting \(N \rightarrow \infty\), and studying the asymptotic behavior of \(C(l)\) for large \(l\).
19. From the block-structure of \(A[s]\) it follows that \(\tilde{M}\) has the block-form

\[
\tilde{M} = \begin{pmatrix} 0 & M_b \\ M_a & 0 \end{pmatrix}.
\]

Assuming that \(u = u_a \oplus u_b\) is an eigenvector of \(\tilde{M}\) with corresponding eigenvalue \(\lambda\), it follows that \(M_a u_a = \lambda u_a\) and \(M_b u_a = \lambda u_b\). Defining \(\bar{u} = u_a - u_b\) we find

\[
\tilde{M} \bar{u} = \begin{pmatrix} M_a u_b \\ -M_b u_a \end{pmatrix} = \begin{pmatrix} \lambda u_a \\ -\lambda u_b \end{pmatrix} = -\lambda \bar{u},
\]

i.e. \(\bar{u}\) is an eigenvector of \(\tilde{M}\) corresponding to the eigenvalue \(-\lambda\).
20. Generally the matrix \(\hat{M}\) is non-symmetric, which forces us to distinguish between right and left eigenvectors.
21. We have used the ARPACK library available on Netlib. See also: D. C. Sorensen, SIAM J. Matrix. Anal. Appl. 13, 357 (1992).
22. J. M. Román, G. Sierra, J. Dukelsky and M. A. Martín-Delgado, Preprint [cond-mat/9802150].