Density-matrix renormalization group for a gapless system of free fermions

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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. [S0163-1829(99)05315-1]

I. INTRODUCTION

Since White constructed the density-matrix renormalization group (DMRG) technique about five years ago,[1,2] 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,[3] thermodynamics of one-dimensional quantum systems,[4] etc. The DMRG and matrix product states[5–10] 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.[2,11,12] This has motivated us to analyze the DMRG of gapless systems in more detail, which we do in two steps: first, we investigate the correlation functions (which pertain to the wave function), 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,[13,14] 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 are 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-range 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[13,14] 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[15] 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.[1,2] 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 Sec. II A; a brief introduction to matrix product states and the Bloch-wave ansatz is given in Sec. II B; we describe how we calculate correlation functions and overlaps in Secs. II C and II D; computational methods are outlined in Sec. II E. The results are presented and discussed in Sec. III: convergence of the projection operator (to a fixed point) and of the ground state is demonstrated in Sec. III A; correlation functions and the scaling formula are treated in Sec. III B; 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 Sec. III C and a proof of the symmetry of the spectra is given in Appendix C. Finally, the results and conclusions are summarized in Sec. IV.

II. METHODOLOGY

A. Hamiltonian

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

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

where N is the size of the lattice, $c_j^\dagger$ creates a fermion on site j, and t is the hopping amplitude[16] ($t=2$ throughout this work). We have added a staggered on-site potential ϵ 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 $c_j\rightarrow(-1)^j c_{j+1}^\dagger$ for all ϵ. 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.[17] 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

$$C_{ph}(l)=\langle c_j^\dagger c_{j+l}\rangle=\frac{1}{\pi l}\sin \pi l/2, \qquad (2)$$

and

$$C_{dd}(l)=\langle n_j n_{j+l}\rangle-\langle n_j\rangle\langle n_{j+l}\rangle=-\frac{1}{\pi^2 l^2}\sin^2 \pi l/2 \qquad (3)$$

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[18] to be

$$\xi_{ph}(t,\epsilon)=\frac{1}{\ln[\epsilon/t+\sqrt{1+(\epsilon/t)^2}]}. \qquad (4)$$

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

$$\begin{aligned}H&=-\frac{t}{2}\sum_{j=1}^{N}\left[S_j^+ S_{j+1}^-+\text{H.c.}\right]+\epsilon\sum_{j=1}^{N}(-1)^j(S_j^z+1/2)\\&=-t\sum_{j=1}^{N}\left[S_j^x S_{j+1}^x+S_j^y S_{j+1}^y\right]+\epsilon\sum_{j=1}^{N}(-1)^j(S_j^z+1/2),\end{aligned} \qquad (5)$$

where as usual $S^\pm=S^x\pm iS^y$. 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[13,14] for a derivation of the ansatz and for details concerning the calculations in this section. A general matrix product state takes the form

$$|Q\rangle_N=\sum_{\{s_j\}}\text{tr}(QA[s_N]\cdots A[s_1])\times|s_N\cdots s_1\rangle, \qquad (6)$$

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 which 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: $\Sigma_s A[s]A^\dagger[s]=\mathbb{1}$. 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. (5), each factor $A[s]$ in Eq. (6) adds a spin-1/2, hence taking a half-integer (hi) total spin into an integer i total spin and vice versa. This implies that we can define our projection matrix A with an off-diagonal block structure

$$A[s]=\begin{pmatrix}0 & A_{\text{hi}\rightarrow\text{i}}[s]\\ A_{\text{i}\rightarrow\text{hi}}[s] & 0\end{pmatrix}. \qquad (7)$$

It is convenient to introduce the following mapping, denoted $\hat{}$, from a local $s\times s$ matrix M to an $m^2\times m^2$ matrix $\hat{M}$:

$$\hat{M}=\sum_{s',s}M_{s',s}A^*[s']\otimes A[s]. \qquad (8)$$

Just using the block structure of $A[s]$, one can show[19] that the eigenvalues of an operator $\hat{M}$ appear in pairs $\pm\lambda$. We will frequently interpret the eigenvectors of $\hat{M}$ (of length m^2) as matrices of size $m\times m$.

The matrix $\hat{1}$, i.e., the $\hat{}$ image of the identity matrix, plays an important role in the theory. Since $\hat{1}$ is guaranteed to have an eigenvalue of 1, due to the orthonormalization condition, there also exists an eigenvalue -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. (6) can be generalized to a Bloch-wave ansatz:

$$|Q,k)_N=\sum_{j,\{s\}} e^{ijk}\mathrm{tr}(A[s_N]\cdots A[s_{j+1}]Q\cdots A[s_1]) \times|s_N\cdots s_1\rangle, \tag{9}$$

where k is the momentum.

The ground state of our model is translationally invariant. This implies that the matrix Q in Eq. (6) should satisfy $[Q,A[s]]=0$ for all s, or equivalently, Q must be a generalized right eigenvector[20] of $\hat{1}$ with corresponding eigenvalue 1. Provided that this eigenvalue is nondegenerate, this means that $Q\sim\mathbb{1}_m$ and hence our ground-state ansatz takes the form

$$|1)_N=\sum_{\{s_j\}} \mathrm{tr}(A[s_N]\cdots A[s_1])\times|s_N\cdots s_1\rangle. \tag{10}$$

Note that if we use a different sign convention in the Hamiltonian[16] the ground state would have momentum π 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 $\hat{1}$. Let us denote this generalized eigenvector by R for future purposes. This indicates that R is associated with momentum π. Further evidence for this is given in connection to the discussion of the single-particle excitation spectrum, see Sec. III C.

C. Correlation functions

Suppose we want to compute the ground-state correlation function $C(l)$ between two local operators M_j^1 and M_{j+l}^2 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

$$C(l)=\langle M_j^{B_1}M_{j+l}^{B_2}\rangle=(1|1)^{-1}\mathrm{tr}[\hat{M}^{B_1}\hat{1}^{l-1}\hat{M}^{B_2}\hat{1}^{N-l-1}]. \tag{11}$$

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 F as the diagonal matrix

$$F=\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{12}$$

we find the expression to be

$$C(l)=\langle M_j^{F_1}M_{j+l}^{F_2}\rangle=(1|1)^{-1}\mathrm{tr}[\hat{M}^{F_1}\hat{F}^{l-1}\hat{M}^{F_2}\hat{1}^{N-l-1}]. \tag{13}$$

Equations (11) and (13) imply[14] that in general a correlation function takes the analytical form

$$C(l)=\sum_{i=1}^{m^2}\alpha_i\left(\frac{\lambda_i}{|\lambda_i|}\right)^l\exp[-l/\xi_i], \tag{14}$$

where $\xi_i=-1/\ln|\lambda_i|$, and λ_i are the eigenvalues of $\hat{1}$ or $\hat{F}$, depending on the statistics of the operators. The α_i's are coefficients that depend on the operators in the correlation function. Thus, the eigenvalues λ_i determine the possible correlation lengths in the system and it is therefore important to investigate the spectrum of $\hat{1}$ and $\hat{F}$. Eigenvalues that fulfill $|\lambda_i|=1$ can potentially give rise to true long-range order. Due to normalization, $\hat{1}$ is guaranteed to have eigenvalues ±1, which potentially could give long-range order in the bosonic correlation functions. In Appendix A we show that the spectrum of $\hat{F}$ differs from that of $\hat{1}$ only by a factor i. Hence, fermionic and bosonic operators have the same set of possible correlation lengths, which means that $\hat{F}$ 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 and m' states, respectively. The overlap ${}_N(1_m|1_{m'})_N$, where $|1_{m'})_N$ is the normalized ground state obtained by keeping m' states etc., can be computed as follows:

$${}_N(1_m|1_{m'})_N=\mathrm{tr}[\hat{1}^N_{m,m'}]=\sum_{i=1}^{mm'}\lambda_i^N, \tag{15}$$

where we have defined the mixed $(mm')\times(mm')$ matrix $\hat{1}_{m,m'}$ as

$$\hat{1}_{m,m'}=\sum_s A_m^*[s]\otimes A_{m'}[s], \tag{16}$$

and the λ_i's are the eigenvalues of the matrix $\hat{1}_{m,m'}$. 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 $\{|s_N\cdots s_1\rangle\}$ basis (rather than renormalized basis sets), with the projection matrix just providing the amplitudes.

Using Eq. (15), we find that for large chain lengths N, the overlap is

$${}_N(1_m|1_{m'})_N\simeq\lambda^N, \tag{17}$$

where λ is the (in absolute value) leading eigenvalue of $\hat{1}_{m,m'}$. 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. So far, this gain in accuracy has often been described by the weight of the truncated density matrix, $\mathrm{tr}\,\rho_e$. $1-\mathrm{tr}\,\rho_e$ is then interpreted as the error introduced in a single DMRG iteration, while $(\mathrm{tr}\,\rho_e)^N$ is considered a measure of the accumulated weight after N iterations. We note that the structure of this

accumulated weight is identical to that of the overlap in Eq. (17), and that $1-\lambda$ is the loss in overlap due to the truncation in a single iteration.

One advantage of using $1-\lambda$ rather than $1-\mathrm{tr}\,\rho_e$ as a measure of the error is that the overlap measure has a well-defined reference state, whereas the truncation error of the density matrix is computed with respect to an approximate target state obtained in terms of states from the previous iteration.

Moreover, we consider the $1-\lambda$ measure to be more universal than the truncation of the density matrix, $1-\mathrm{tr}\,\rho_e$. First, the truncation error of the density matrix is algorithm dependent. For example, the error estimate $1-\mathrm{tr}\,\rho_e$ can be made equal to zero,[2] despite the fact that an exact calculation is not performed, simply by using a superblock configuration

$$\boxed{\mathrm{B}} \bullet \boxed{\mathrm{B}^r}$$

In contrast, the $1-\lambda$ measure depends only on the states themselves, and not on the method (algorithm) used to obtain the states.

Second, the truncation error of the density matrix is peculiar to the DMRG, whereas the overlap can be calculated by other methods. This allows, in principle, for a direct comparison of the DMRG with other methods.

However, we would like to emphasize that the overlap is not as easy to compute as the ordinary truncation error, since it is not a by-product of the calculation.

E. Computational methods

Due to the large dimensions of $\hat{1}_{m,m'}$, namely $(mm')\times(mm')$, it becomes necessary to use iterative eigenvalue routines that require no explicit construction or storage of $\hat{1}_{m,m'}$. Moreover, $\hat{1}_{m,m'}$ is nonsymmetric. We have used the Arnoldi algorithm[21] to handle these problems.

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

$$\hat{1}_{m,m'}v=\sum_s A_m^*[s]vA_{m'}^T[s].$$

In this way we only need to operate with $m\times m'$ matrices, and the eigenvalues of $\hat{1}_{m,m'}$ can easily be obtained. Moreover, by representing the projection operator as a sparse matrix, it is possible to compute eigenvalues of $\hat{1}_{m,m'}$ where a large number of states have been kept.

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

$$\boxed{\mathrm{B}} \bullet\bullet \boxed{\mathrm{B}^r}$$

the infinite lattice algorithm, and by adding a single site per iteration to each block. When we have an on-site potential ϵ 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:

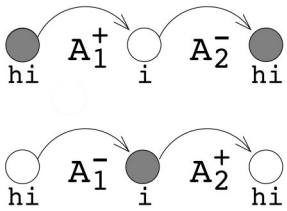

FIG. 1. The figure shows the four projection matrices needed to describe the system. Filled disks denote sites with positive on-site potential and circles denote sites with negative on-site potential; hi denotes half-integer representations and *i* denotes integer representation.

$$A^+[s]=\begin{pmatrix} 0 & A_1^+[s] \\ A_2^+[s] & 0 \end{pmatrix}$$

and

$$A^-[s]=\begin{pmatrix} 0 & A_1^-[s] \\ A_2^-[s] & 0 \end{pmatrix}.$$

In each DMRG iteration we update either the hi$\rightarrow$i or the $i\rightarrow$hi matrices. When we talk about the number of kept states, what we mean is the sum of the number of kept states in the integer and half-integer representations.

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., $\lim_{N\rightarrow\infty}A_N[s]=A[s]$. In order to show this, we define the matrix norm $\|\cdot\|_{max}$ via

$$\|A\|_{max}=\max_{i,j,s}|A_{i,j}[s]|. \tag{18}$$

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 $r(N)=(\|A_{N+1}-A_N\|_{max}+\|A_N-A_{N-1}\|_{max})/2$, 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-

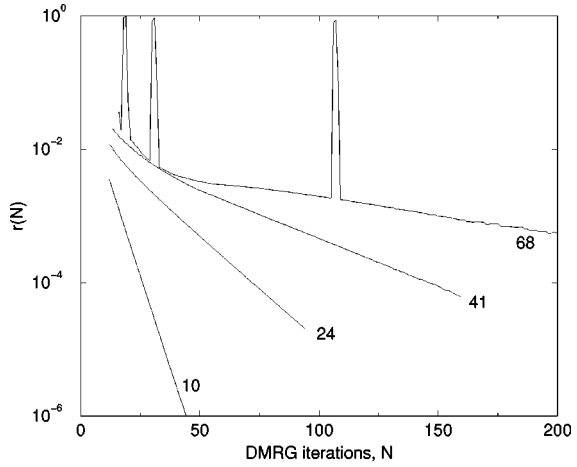

FIG. 2. The norm $r(N)=(\|A_{N+1}-A_N\|_{max}+\|A_N-A_{N-1}\|_{max})/2$ is shown as a function of the number of DMRG iterations, N, for the gapless case. It is clear from the figure that the DMRG projection operator converges with respect to N. Furthermore, the convergence seems to be exponential with respect to N. The peaks in the 68 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.

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.

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 λ since this gives a more direct measure of the error. One way to use such a table is to focus on the change in the wave function due to the addition of extra states. For example, using the table, we see that comparing the wave functions obtained by keeping 10 and 24 states, respectively, the difference $1-\lambda$ is 0.002 31, this being a measure of the change in the wave function due to the additional 14 states. Moving on by comparing we see that the change when going from 24 to 41 states is 0.000 277 and so on. The relevant information here is the change in the wave function per added state. Computing this quantity for a large number of different m values, it might be possible to fit these values to a functional form, which can then be used to predict how many states are needed to obtain a certain accuracy. However, since this lies beyond the scope of this article, we will not deal with this question here.

B. The spectrum of $\hat{1}$ 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. (14) and the correlation lengths are determined by the eigenvalues of $\hat{1}$ (the correlation lengths obtained from $\hat{F}$ are identical). An analysis of the spectrum of $\hat{1}$ is therefore pivotal.

TABLE I. Leading eigenvalues $1-\lambda$, governing the overlap between different DMRG ground-state wave functions. The number m is the sum of the number of kept states in the integer and half-integer representations.

m	10	24	41	68
10	0	0.002 31	0.003 28	0.003 81
24	0.002 31	0	0.000 277	0.000 644
41	0.003 28	0.000 277	0	0.000 134
68	0.003 81	0.000 644	0.000 134	0

We have found that the eigenvalues ± 1 are nondegenerate, and that all the other eigenvalues fulfill $|\lambda|<1$. Only the eigenvalues ± 1 can give rise to infinite correlations lengths. However, it turns out 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 M that potentially can give true long-range order in the correlation functions Eqs. (11) and (13). We show in Appendix B that true long-range order for bosonic operators is not possible if $\mathrm{tr}[M^B]=0$. 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 cannot be truly long range.

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 $\hat{F}$ and $\hat{1}$ 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 twofold 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 nondegenerate 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. (4) together with $\lambda=\exp[-1/\xi]$, we find that the exact expression for the eigenvalue dominating the particle-hole correlation is

$$\lambda^*_{ph}(t,\epsilon)=\sqrt{1+\frac{\epsilon^2}{t^2}}-\frac{\epsilon}{t}. \tag{19}$$

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.

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 $|\lambda_{ph}|$ approaches the exact value 1, i.e., an infinite correlation length, as the number of states is increased. The convergence of $|\lambda_{ph}|$ towards 1 is more clearly

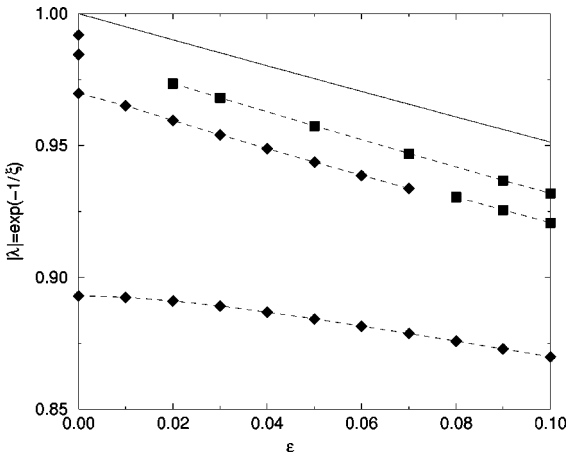

FIG. 3. The eigenvalues of $\hat{F}$ governing the particle-hole correlation length vs ϵ for different numbers of kept states. The solid line corresponds to the exact result from Eq. (19). From the bottom to the top, the point sets correspond to the following numbers of kept states: 10,24,41,68. Due to numerical problems with the eigenvalue routines, we cannot continue the set with $m>24$ to larger ϵ values. Instead, in these cases we have computed the correlation lengths directly from the DMRG correlation functions. Data points computed using the eigenvalue methods are indicated by diamonds, while those obtained from the correlation functions are indicated by squares.

seen in Fig. 4, where we consider the gapless case and plot $1-|\lambda_{ph}|$ versus the number of kept states, m. 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 $|\lambda_{ph}|$ behaves as $|\lambda_{ph}| \simeq 1-km^{-\beta}$. Thus the correlation length behaves as

$$\xi_{ph} \simeq -\frac{1}{\ln|1-km^{-\beta}|} \simeq \frac{1}{k} m^{\beta}. \tag{20}$$

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

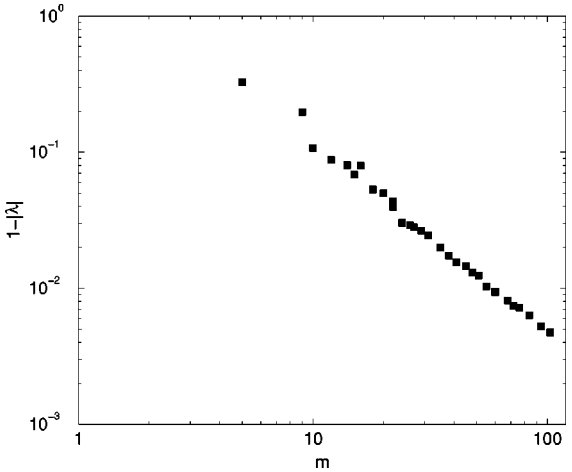

FIG. 4. Convergence of the eigenvalue λ of $\hat{F}$ governing the particle-hole correlation length. In the figure we show $1-|\lambda|$ versus the number of kept states, m, in the gapless ($\epsilon=0$) case.

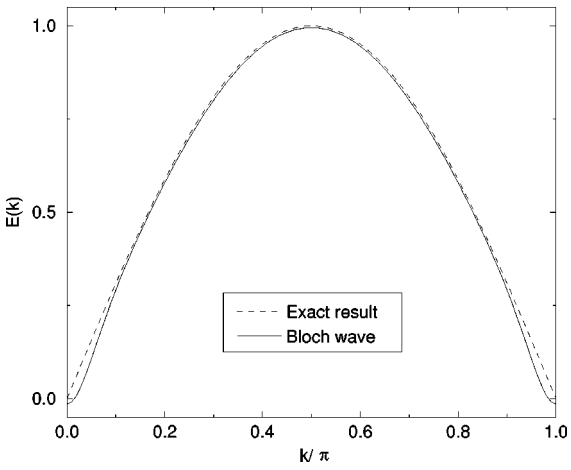

FIG. 5. Single-particle energy dispersion relation $E(k)$. The Bloch-wave result deviates from the exact result only close to the Fermi points. The number of kept states in $m=8$.

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. (14). 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. (20).

C. The single-particle excitation spectrum

In order to study the single particle excitation spectrum, we have used the Bloch-wave ansatz of Eq. (9) and the pole-expansion technique[14] 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 $E(k)\simeq\Delta_0+v_0^2k^2$ 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[13] 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 errors. 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 $m>12$.

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 start-

ing the DMRG calculation with a nonzero staggered on-site potential and then, after about 20 iterations, turning the potential off. We then let the projection 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 accuracy) with only one exception. If we keep three states in the integer representation and six states in the half-integer representation, we find that the DMRG is actually unstable and we obtain an energetically more favorable state by breaking the translational symmetry. However, it is sufficient 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 that is not translationally invariant.

There is an interesting symmetry concerning the dispersion relation in Fig. 5. We find that the dispersion relation has the symmetry $E(\pi-k)=E(k)$ in the thermodynamic limit. This is in fact a consequence of the block structure of $A[s]$, and should therefore be a characteristic feature of many half-integer spin systems. To prove this we use the R matrix to explicitly construct a Bloch state of momentum $k+\pi$ from a state of momentum k and show that these two states have equal energy. 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

$$E(k)\overset{\mathcal{P}}{\rightarrow}E(-k)\overset{R}{\rightarrow}E(\pi-k), \tag{21}$$

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 translationally invariant half-integer spin systems with local interactions. As a test, we have checked numerically that it is true also for the isotropic antiferromagnetic spin-1/2 Heisenberg chain. Furthermore, calculations on the spin-1 chain, as expected, lack this symmetry. The symmetry has recently been studied on more general grounds by Kladko,[15] without any reference to the Bloch-wave ansatz. Similarly to our proof for the Bloch-wave ansatz, Kladko explicitly constructs a state with momentum $k+\pi$ from a state with momentum k and then shows that these states have equal energy.

IV. CONCLUSIONS

We have investigated fundamental properties of the DMRG when applied to a gapless system of free fermions. We find that the DMRG projection operator converges to a fixed point. This convergence means that states of a matrix-product form are identical to the DMRG states in the thermodynamic limit. By using the matrix-product formalism, we have found that DMRG calculations give qualitatively wrong particle-hole and density-density correlation functions: the DMRG correlations decay exponentially, while the true correlations decay algebraically. However, for short distances, the DMRG correlation function agrees with the exact result. The finite correlation length of the DMRG particle-hole correlation function scales as $\xi\sim m^{1.3}$, where m is the number of kept states. In addition, we have derived conditions for whether a general operator potentially can give rise to truly long-range correlations or not. These conditions are found to be determined by symmetries of the Hamiltonian.

We have demonstrated that the matrix product formalism can be used to calculate overlaps between differently renormalized states. This makes it possible to directly compare states obtained from DMRG calculations, using different numbers of kept states. We propose this overlap as a criterion of convergence of DMRG states.

From the matrix-product ansatz we obtain accurate values for the ground-state energy. Furthermore, using a Bloch-wave ansatz, we find a dispersion relation for the excitations that is close to the exact result. Despite this, close to the Fermi points, where the gap closes, our excitations have negative energies, indicating that the ground state is defective. We have not yet been able to trace the origin of these negative energy excitations, although our calculations indicate that the magnitude of this negative 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.

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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.*[22] We denote a block state by $|\gamma,m\rangle$, where m is the particle number measured from half-filling and γ is an integer labeling particle-hole representations. Using $F[s,s']=\delta_{s,s'}i^{2s+1}$ [see Eq. (12)], we may write the matrix elements of the operator $\hat{F}$ as

$$\hat{F}^{(\gamma_2',m_2')(\gamma_1',m_1'),(\gamma_2,m_2)(\gamma_1,m_1)}$$

$$=\sum_s i^{2(m_2'-m_2)+1}A^{(\gamma_2',m_2')(\gamma_2,m_2)}[s]A^{(\gamma_1',m_1')(\gamma_1,m_1)}[s],$$

where we have used that the element $A^{(\gamma',m'),(\gamma,m)}[s]$ is zero unless $m'=m+s$, since the projection operator conserves the particle number. Next, we define the vector $|u_F\rangle^{(\gamma_2,m_2)(\gamma_1,m_1)}=\delta_{\gamma_2,\gamma_1}\delta_{m_2,m_1}i^{2m_2}$. We will now show that $|u_F\rangle$ is an eigenvector of $\hat{F}$ with eigenvalue i. We have

$$
\begin{aligned}
&(\hat{F}|u_F\rangle)^{(\gamma_2',m_2')(\gamma_1',m_1')} \\
&= \sum_{\gamma_1,\gamma_2} \sum_{m_1,m_2,s} i^{2(m_2'-m_2)+1} A^{(\gamma_2',m_2')(\gamma_2,m_2)}[s] \\
&\quad \times A^{(\gamma_1',m_1')(\gamma_1,m_1)}[s] i^{2m_2} \delta_{m_1,m_2} \delta_{\gamma_1,\gamma_2} \\
&= i i^{2m_2'} \sum_{\gamma_1,m_1,s} A^{(\gamma_2',m_2')(\gamma_1,m_1)}[s] A^{(\gamma_1',m_1')(\gamma_1,m_1)}[s] \\
&= i i^{2m_2'} \delta_{m_2',m_1'} \delta_{\gamma_2',\gamma_1'} \\
&= i|u_F\rangle^{(\gamma_2',m_2')(\gamma_1',m_1')},
\end{aligned}
$$

which proves the claim. In the third line we have used the identity $\Sigma_s A[s]A^T[s]=\mathbb{1}$. 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 $|\det u_F|=1$, 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

$$
i u_F A[s] = F[s,s] A[s] u_F, \tag{A1}
$$

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 $A^\dagger[s]$ and summing over s. Define the unitary operator $\xi=(u_F\otimes\mathbb{1})$ and consider

$$
\begin{aligned}
i\xi\hat{1}\xi^\dagger &= i(u_F\otimes\mathbb{1})\left(\sum_s A[s]\otimes A[s]\right)(u_F^\dagger\otimes\mathbb{1}) \\
&= i\sum_s (u_F A[s] u_F^\dagger)\otimes A[s] \\
&= \sum_s F[s,s] A[s]\otimes A[s](u_F u_F^\dagger\otimes\mathbb{1}) \\
&= \hat{F}.
\end{aligned}
$$

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 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 nonzero: $\langle 1|\hat{M}^B|1\rangle$, $\langle 1|\hat{M}^B|R\rangle$, and $\langle R|\hat{M}^B|R\rangle$, 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 $A^*[s]\otimes A[s']$ 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 $\mathbb{1}$ and R. The matrix R has the block-form $\mathbb{1}\oplus-\mathbb{1}$, which implies that $R^2=\mathbb{1}$. 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

$$
\begin{aligned}
&\langle R|A[s]\otimes A[s']|R\rangle \\
&\quad = \mathrm{tr}(R_L^T A[s] R A^T[s']) = -\mathrm{tr}(R_L^T R A[s] A^T[s']) \\
&\quad = -\mathrm{tr}(\mathbb{1}_L^T A[s] A^T[s']) = -\langle 1|A[s]\otimes A[s']|1\rangle,
\end{aligned}
$$

and similarly,

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

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

$$
\mathcal{B}|\gamma,m\rangle = \phi(\gamma,m)|\gamma,-m\rangle, \tag{B1}
$$

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

We are now going to show that $\mathbb{1}_L^{(\gamma',m'),(\gamma,m)}$ is zero unless $m'=m$. To see this we write the equation $\langle 1|=\langle 1|\hat{1}$ as

$$
\begin{aligned}
\mathbb{1}_L^{(\gamma_1,m_1),(\gamma_2,m_2)} &= \sum_s \sum_{\gamma_3,\gamma_4,m_3,m_4} \mathbb{1}_L^{(\gamma_3,m_3),(\gamma_4,m_4)} \\
&\quad \times A^{(\gamma_3,m_3),(\gamma_1,m_1)}[s] A^{(\gamma_4,m_4),(\gamma_2,m_2)}[s].
\end{aligned}
$$

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 $\mathbb{1}_L^{(\gamma_1,m_1),(\gamma_2,m_2)}$ is conserved under the action of $\hat{1}$, we can write $\mathbb{1}_L=\mathbb{1}_L^0+\mathbb{1}_L^{rest}$ where $\mathbb{1}_L^0$ only has nonzero matrix elements between states of equal particle number and $\mathbb{1}_L^{rest}$ is the remainder, mixing particle numbers. This decomposition will not be mixed under the action of $\hat{1}$ and hence both matrices must be eigenstates of $\hat{1}$ with eigenvalue 1. This eigenvalue is, however, nondegenerate, which means that either of $\mathbb{1}_L^0$ and $\mathbb{1}_L^{rest}$ is zero. Since $\mathrm{tr}\mathbb{1}_L=\langle 1|1\rangle=1$, $\mathbb{1}_L$ must contain $\mathbb{1}_L^0$ and hence $\mathbb{1}_L^{rest}=0$. This means that $\mathbb{1}_L$ only connects states containing an equal number of particles.

Furthermore, since $R_L=\mathbb{1}_L R$ 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:

$$
\begin{aligned}
\langle 1|A[s]\otimes A[s']|1\rangle &= \mathrm{tr}(\mathbb{1}_L^T A[s] A^T[s']) \\
&= \sum_{\{\gamma_i,m_i\}} (\mathbb{1}_L^T)^{(\gamma_1,m_1),(\gamma_2,m_2)} \\
&\quad \times A^{(\gamma_2,m_2),(\gamma_3,m_3)}[s] \\
&\quad \times A^{(\gamma_1,m_1),(\gamma_3,m_3)}[s'].
\end{aligned}
$$

Using particle number conservation of A and $\mathbb{1}_L$ we conclude that the expectation value is zero unless $s=s'$, i.e.,

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

Similarly, using R_L instead of $\mathbb{1}_L$, one finds

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

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 $\hat{1}$. In the next paragraph, we will investigate the expectation values when $s=s'$. Note that the Pauli matrix σ_3 and $\mathbb{1}$ 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:

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

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

$$A[s_j] = \sum_{(\gamma',m'),(\gamma,m)} A^{(\gamma',m'),(\gamma,m)}[s_j]\,|\gamma',m'\rangle\langle\gamma,m|.$$

Applying a particle-hole transformation to $A[s]$, making use of the symmetry Eq. (B5), one finds that

$$\mathcal{B}A[s_j]\mathcal{B} = (-1)^j A[-s_j]. \quad \text{(B6)}$$

Using the definition of $\hat{1}$ we find the transformation property of $\hat{1}$ under particle-hole transformations,

$$(\mathcal{B}\otimes\mathcal{B})\sum_s A[s]\otimes A[s](\mathcal{B}\otimes\mathcal{B}) = \sum_s A[-s]\otimes A[-s].$$

That is, $\hat{1}$ is invariant under particle-hole transformations. Let us also consider the transformation of $\hat{\sigma}_3$, where σ_3 is a Pauli matrix. Using exactly the same technique, we find that $(\mathcal{B}\otimes\mathcal{B})\hat{\sigma}_3(\mathcal{B}\otimes\mathcal{B}) = -\hat{\sigma}_3$.

$\langle 1|$ and $\langle 1|(\mathcal{B}\otimes\mathcal{B})$ must both have eigenvalue 1 of $\hat{1}$, since $\hat{1}$ is invariant under particle-hole transformations. Using the nondegeneracy of this eigenvalue, we conclude that $\langle 1|(\mathcal{B}\otimes\mathcal{B}) = e^{-i\theta}\langle 1|$ and similarly $(\mathcal{B}\otimes\mathcal{B})|1\rangle = e^{i\theta}|1\rangle$.

Let us now compute the expectation value of $\hat{\sigma}_3$,

$$\langle 1|\hat{\sigma}_3|1\rangle = \langle 1|(\mathcal{B}\otimes\mathcal{B})^2\hat{\sigma}_3(\mathcal{B}\otimes\mathcal{B})^2|1\rangle = -\langle 1|\hat{\sigma}_3|1\rangle,$$

and thus $\langle 1|\hat{\sigma}_3|1\rangle = 0$. Since $\langle 1|\hat{1}|1\rangle = 1$ we arrive at

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

It only remains to consider expectation values of $\hat{1}$ and $\hat{\sigma}_3$ between $\langle 1|$ and $|R\rangle$. Trivially, $\langle 1|\hat{1}|R\rangle = 0$, since $\langle 1|$ and $|R\rangle$ are eigenvectors of $\hat{1}$ with different eigenvalues. Using the structure of $|1\rangle$ and $|R\rangle$, let us show that they must transform with the same phase factor. Noting that $\mathcal{B}$ must be block diagonal, it follows that $[\mathcal{B},R]=0$. Assuming $(\mathcal{B}\otimes\mathcal{B})|1\rangle = \mathcal{B}\mathcal{B}^T = e^{i\theta}|1\rangle$ we find

$$(\mathcal{B}\otimes\mathcal{B})|R\rangle = \mathcal{B}R\mathcal{B}^T = R\mathcal{B}\mathcal{B}^T = Re^{i\theta}\mathbb{1} = e^{i\theta}|R\rangle.$$

Using this property we find

$$\langle 1|\hat{\sigma}_3|R\rangle = -\langle 1|\hat{\sigma}_3|R\rangle = 0$$

and we conclude that

$$\langle 1|A[s]\otimes A[s']|R\rangle = -\langle R|A[s]\otimes A[s']|1\rangle = 0. \quad \text{(B8)}$$

Using the derived expressions for the expectation values, a general bosonic operator $\hat{M}^B$ can couple to the eigenstates with corresponding eigenvalues ± 1 only if $\mathrm{tr}\,M^B \neq 0$. In particular, the density-density correlation function cannot be truly long range when the Hamiltonian has particle-hole symmetry and conserves the number of particles.

Let us also investigate correlation functions between fermionic operators, M^F, in order to be able to draw conclusions concerning the particle-hole correlation function. We will only show that off-diagonal fermionic operators cannot give rise to truly long-range correlation functions. From Eq. (13) we see that true long-range order is possible only if some expectation value of the form $\langle 1|\hat{S}^+|u_F\rangle$ is nonzero; that is, $\hat{S}^+$ must connect eigenstates of $\hat{1}$ and $\hat{F}$ with the corresponding eigenvalues having absolute value 1. We will now show that this is impossible due to the particle-number conserving property of $A[s]$. Note that all the important eigenvectors are proportional to $\delta_{m,m'}$. Hence, an expectation value of the above form will be

$$\langle 1|\hat{S}^+|u_F\rangle \sim \sum \delta_{m,m'}\delta_{m,1/2+m''}\delta_{m',-1/2+m'''}\delta_{m'',m'''} = 0,$$

where the second and third δ functions come from the particle-number conserving property of $A[s]$. Thus we cannot 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 σ_3) cannot be long range. On the contrary, this is the structure of the string order correlation function in the spin-1 chain, which is long range.

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 R of $\hat{1}$. 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 $\hat{1}$ corresponding to the eigenvalue 1 as $|1\rangle$ or $\mathbb{1}$. Using

the block-diagonal structure of R it follows that $\{(\mathbb{1}\otimes R),\hat{M}\}=0$ and that $[(R\otimes R),\hat{M}]=0$ for all local operators M.

We also need the property $(R\otimes R)\lim_{n\to\infty}\hat{1}^n=\lim_{n\to\infty}\hat{1}^n$. To show this we recall that all but two eigenvalues of $\hat{1}$ have absolute value less than one. The corresponding eigenvectors will be annihilated by $\lim_{n\to\infty}\hat{1}^n$. Hence we may write

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

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

$$\lim_{n\to\infty}\hat{1}^n|\psi\rangle=\psi_1|1\rangle+(-1)^n\psi_R|R\rangle.$$

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

$$\begin{aligned}(R\otimes R)\lim_{n\to\infty}\hat{1}^n|\psi\rangle&=(R\otimes R)[\psi_1|1\rangle+(-1)^n\psi_R|R\rangle]\\&=\psi_1R\mathbb{1}R^T+(-1)^n\psi_RRRR^T\\&=\psi_1\mathbb{1}+(-1)^n\psi_RR\\&=\lim_{n\to\infty}\hat{1}^n|\psi\rangle.\end{aligned}$$

Thus we have shown that $(R\otimes R)\lim_{n\to\infty}\hat{1}^n$ and $\lim_{n\to\infty}\hat{1}^n$ 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

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

where LHS and RHS are left- and right-hand side, respectively, and the Bloch states are defined in Eq. (9). If we apply this result to the Hamiltonian operator and the normalization, we obtain the result that the states $|RQ,k)$ and $|Q,k+\pi)$ 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 $|RQ,k)$ as

$$|RQ,k)=\sum_{j,\{s_j\}}e^{ij(k+\pi)}\times\mathrm{tr}(RA[s_N]\cdots A[s_{j+1}]Q\cdots A[s_1])|s_N\cdots s_1\rangle,$$

where we have used $\{R,A[s]\}=0$ to move the R to the left side of the trace. Thus we may write[14] the left-hand side of Eq. (C1) as

$$\mathrm{LHS}=\sum_{j,j'}e^{ij(k+\pi)}e^{-ij'(k+\pi)}\times\mathrm{tr}[(R\otimes R)\hat{1}^{N-j}(\mathbb{1}\otimes Q)\hat{1}^{j-l}\hat{M}\hat{1}^{l-j'-1}(Q'^*\otimes\mathbb{1})\hat{1}^{j'}],$$

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 $\hat{1}^\infty$ somewhere in the trace. If we could move $(R\otimes R)$ through the trace until it reaches the $\hat{1}^\infty$ factor, the $(R\otimes R)$ would be annihilated and we would be left with an expression that is

$$\sum_{j,j'}e^{ij(k+\pi)}e^{-ij'(k+\pi)}\times\mathrm{tr}[\hat{1}^{N-j}(\mathbb{1}\otimes Q)\hat{1}^{j-l}\hat{M}\hat{1}^{l-j'-1}(Q'^*\otimes\mathbb{1})\hat{1}^{j'}]=\mathrm{RHS}$$

and our proof would be complete. It turns out that it is always possible to perform such a move. If the factor $\hat{1}^\infty$ is not between the factors $(\mathbb{1}\otimes Q)$ and $(Q'^*\otimes\mathbb{1})$, we just commute $(R\otimes R)$ through the $\hat{}$ operators until it reaches $\hat{1}^\infty$ and gets annihilated. If the factor $\hat{1}^\infty$ 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 $\hat{1}^\infty$. 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 M does not act on a single site, but, can easily be generalized to operators describing local correlations. The important thing is that the operator is local, so that a factor of $\hat{1}^\infty$ always can be found in the trace.

This completes the proof.

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[16] We have chosen to include a factor of -1 in the hopping term of the Hamiltonian in order to have a translationally invariant ground state, but this is only a matter of convenience. By simply

making the canonical transformation $c_j \to (-1)^j c_j$, we can remove this sign from H.

[17] In the thermodynamic limit $N \to \infty$, the ground-state energy per site is given by

$$E_0 = -\frac{1}{\pi}\int_0^{\pi/2} \sqrt{\epsilon^2 + t^2 \cos^2 k}\, dk,$$

which is a complete elliptic integral of the second kind.

[18] The result is derived by introducing periodic boundary conditions, letting $N \to \infty$, and studying the asymptotic behavior of $C(l)$ for large l.

[19] From the block structure of $A[s]$ it follows that $\hat{M}$ has the block form

$$\hat{M} = \begin{pmatrix} 0 & M_a \\ M_b & 0 \end{pmatrix}.$$

Assuming that $u = u_a \oplus u_b$ is an eigenvector of $\hat{M}$ with corresponding eigenvalue λ, it follows that $M_a u_b = \lambda u_a$ and $M_b u_a = \lambda u_b$. Defining $\overline{u} = u_a \oplus -u_b$ we find

$$\hat{M}\overline{u} = \begin{pmatrix} M_a u_b \\ -M_b u_a \end{pmatrix} = \begin{pmatrix} \lambda u_a \\ -\lambda u_b \end{pmatrix} = -\lambda \overline{u},$$

i.e., $\overline{u}$ is an eigenvector of $\hat{M}$ corresponding to the eigenvalue $-\lambda$.

[20] Generally the matrix $\hat{1}$ is nonsymmetric, 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, J. Phys. A **31**, 9729 (1998).