Low-energy states for correlated-electron models in the strong-coupling limit

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I. INTRODUCTION

The theoretical description of electronic correlations in solids is still a challenge. Even one of the simplest models for correlated electrons, the Hubbard model, exhibits enormous mathematical complexity. Its analysis is far from being complete.

Recently, a new class of models for tight-binding electrons with infinitely strong on-site repulsion has been discovered. For particle numbers of two or more particles per unit cell, one can construct the ground states of these models. These ground states are spin-singlets and have the structure of resonating-valence-bond states for certain cases.

The class of models which are solvable by this method has been generalized by several authors. One-dimensional models of this class are allowed for the calculation of equal-time correlation functions using a transfer-matrix technique. All equilibrium correlations studied so far decay exponentially. Dynamical correlations obtained numerically for the one-dimensional Hubbard chain indicate dispersionless excitation spectra for an electron density of two per cell. The propagation of one hole, however, shows dispersive delocalized features.

The regime of particle numbers below two per unit cell has not been accessible by analytical methods so far. The main result of this paper is an analytical upper bound on the ground state energy of systems containing $2N-1$ particles ($N$ denotes the number of cells). The trial state and the corresponding upper bound on the ground-state energy are discussed for two examples. The first example is a hypercubic Hubbard model as introduced in Ref. [2]. It is shown that the trial state becomes an asymptotically exact eigenstate of this particular $(2N-1)$-particle system in the thermodynamic limit. For the second system, a linear Hubbard chain, the upper bound on the ground-state energy may be calculated analytically as well. A comparison to exact numerical results is presented.

II. THE CLASS OF SOLVABLE MODEL HAMILTONIANS

In this section we recall the most general description of the class of solvable models. This class contains Hubbard, Anderson and Emery models in the limit of infinitely strong interaction ($U = \infty$). The solution presented below requires certain lattice structures. (In the following, the term graph is used, because lattice implies translational invariance which needs not be assumed.)

The models are defined on graphs, where each of the $N$ vertices contains a cell of sites. (The cells need not be identical either.) The cells are labeled by an index $i = 1, \ldots, N$. Let the set of all sites within the cell $i$ be called $\mathcal{N}_i$. (It is mentioned in passing that $\mathcal{N}_i$ is not a unit cell if the graph is translationally invariant, because neighboring cells may share some sites.) The sites (or electronic orbitals) within a cell $i$ are labeled by an index $\alpha$. Some of those orbitals (not necessarily all) may carry an infinitely strong on-site repulsion, e.g. a cell may contain “d-sites” which may be empty or occupied by one particle only (with spin up or down) and “p-sites” which can be occupied by up to two particles. The set of d-sites is called $\mathcal{U}_i$. The repulsion is incorporated into the model by a projection operator

$$ P = \prod_i \prod_{\alpha \in \mathcal{U}_i} \left( 1 - n_{i,\alpha,\uparrow} n_{i,\alpha,\downarrow} \right) $$

which strictly excludes double occupancy on all sites $i, \alpha \in \mathcal{U}_i$, where $n_{i,\alpha,\sigma} = c_{i,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma}$. The Fermi operators $c_{i,\alpha,\sigma}^\dagger (c_{i,\alpha,\sigma})$ denote creation (annihilation) operators and are defined as usual. The connection between cells is established by common sites. We denote the set of common sites by the intersection $\mathcal{C}_{ij} = \mathcal{N}_i \cap \mathcal{N}_j$. Examples for some models are given in Ref. [2]. Figure 1 illustrates the two cases discussed below.

In order to construct the ground state of the models defined above consider the linear combination of Fermi operators

$$ \Psi_{i,\sigma}^\dagger := \sum_{\alpha \in \mathcal{N}_i} \lambda_{i,\alpha,\sigma} c_{i,\alpha,\sigma}^\dagger. $$
They obey the following algebra:

\[
[\Psi_{i,\sigma}^\dagger, \Psi_{j,\sigma'}^\dagger]_+ = [\Psi_{i,\sigma}, \Psi_{j,\sigma'}]_+ = 0
\] (3)

\[
[\Psi_{i,\sigma}, \Psi_{j,\sigma'}]_+ = \delta_{\sigma,\sigma'}
\]

\[
\times \left\{ \begin{array}{ll}
\sum_{\alpha \in N_i} |\lambda_{i,\alpha,\sigma}\|^2 & \text{for } i = j \\
\sum_{\alpha,\beta \in C_{ij}} \delta_{(i\alpha),(j\beta)} \lambda_{i,\alpha,\sigma}^* \lambda_{j,\beta,\sigma} & \text{otherwise}
\end{array} \right.
\]

(The Kronecker symbol \(\delta_{(i\alpha),(j\beta)}\) assumes the value one if the indices \(i\alpha\) and \(j\beta\) label the same site and equals zero otherwise.) The coefficients \(\lambda_{i,\alpha,\sigma}\) define the parameters of the Hamiltonian which will be constructed below.

The \(\Psi\)-operators allow to write down a positive semidefinite Hamiltonian in a very concise way:

\[
H = \sum_{\sigma} H_{\sigma} \quad \text{with} \quad H_{\sigma} = \sum_{i} \Psi_{i,\sigma}^\dagger \Psi_{i,\sigma}.
\] (4)

However, the physical meaning of this Hamiltonian becomes more transparent if it is rewritten in terms of the Fermion \(c\)-operators by using the relation

\[
\Psi_{i,\sigma}^\dagger P = P \Psi_{i,\sigma}^\dagger + \sum_{\alpha \in U_i} \lambda_{i,\alpha,\sigma} c_{i,\alpha,\sigma}^\dagger n_{i,\alpha,-\sigma} P
\] (5)

and the definition of the \(\Psi\) operators as defined in Eq. (3).

The Hamiltonian (4) is transformed into the following form:

\[
H_{\sigma} = -P \sum_{i} \left\{ \sum_{\alpha \neq \beta \in N_i} \lambda_{i,\alpha,\sigma}^* \lambda_{i,\beta,\sigma} c_{i,\alpha,\sigma}^\dagger c_{i,\beta,\sigma} + \sum_{\alpha \in N_i} |\lambda_{i,\alpha,\sigma}|^2 (n_{i,\alpha,\sigma} - 1) + \sum_{\alpha \in U_i} |\lambda_{i,\alpha,\sigma}|^2 n_{i,\alpha,-\sigma} \right\} P.
\] (6)

The first term in \(H_{\sigma}\) describes particle hopping within a cell where each site (orbital) is connected to all others. (Particle transfer between interacting orbitals and orbitals without interaction is usually called a hybridization. In that case, the model would describe e.g. an Anderson model.) The remaining terms contain trivial constants and sums over occupation numbers which add up to the total particle-number operator for the case of the \(D\)-dimensional Hubbard model as discussed below. If the sets \(U_i\) and \(N_i\) are not identical or if not every site within a cell is connected to a neighbor cell, the sums over occupation number operators may add up to an additional field which shifts the energy of certain sites. Such a model then contains more than one parameter and the exact ground state as derived below is only valid on a parameter surface defined by the quantities \(\lambda\). In the following, all \(\lambda\)-coefficients are assumed to be real.

**III. THE GROUND STATE FOR \(2N\) OR MORE PARTICLES**

The models as defined above allow to write down an exact ground state if the system contains two or more particles per cell. The ground state is a Gutzwiller projected Slater determinant:

\[
|\Phi_0\rangle := P \prod_i \Psi_{i,\uparrow}^\dagger \Psi_{i,\downarrow}^\dagger |\chi\rangle.
\] (7)

The expression \(H|\Phi_0\rangle\) always contains a factor \((P \Psi_{i,\sigma}^\dagger)^2\). Because of the equation \((P \Psi_{i,\sigma}^\dagger)^2 = 0\), the state Eq. (7) is an eigenstate of \(H\), the corresponding eigenvalue equals zero.

Further, \(H\) is positive semi-definite. Therefore the state (7) belongs to the ground-state manifold. In Ref. 7 Tasaki provides a proof of the uniqueness of the ground state if the state \(|\chi\rangle\) is equal to the vacuum state \(|0\rangle\) (2\(N\) particles). Larger fillings can be discussed if \(|\chi\rangle\) contains additional particles, for that case it immediately follows by construction that the state (7) is degenerate.

If all sites carry an infinitely strong on-site repulsion and, e.g. the \(\lambda\)-coefficients are set to unity, the state (7) exhibits a structure often called resonating-valence-bond state. In that case the ground state consists of a linear combination of local singlet bonds:

\[
P \Psi_{i,\uparrow}^\dagger \Psi_{i,\downarrow} = P \sum_{\alpha \neq \beta} (c_{i,\alpha,\uparrow}^\dagger c_{i,\beta,\downarrow} + c_{i,\alpha,\downarrow}^\dagger c_{i,\beta,\uparrow}).
\]

The projector ensures that no two singlet bonds have a site in common.

**IV. UPPER BOUND ON THE GROUND-STATE ENERGY FOR \(2N-1\) PARTICLES**

Although the ground state is known for two or more particles per cell, the only analytical result that has been obtained for particle numbers \(N_e\) below the “magic” number \(N_e = 2N\) so far is the trivial lower bound on the ground state energy \(E_0(N_e) \geq 0\) which is valid for any number of particles. [The Hamiltonian (4) is non-negative.] The present section provides an upper bound on the ground state energy of \(H\) for one additional hole, e.g. a particle number of \(N_e = 2N-1\) using a variational state. The quality of variational methods is not very well controlled, there exists no small parameter, only an inequality for the energies. Therefore the method requires some intuition in order to “hit” the correct physics by guessing a good state. The first guess of a variational state, the state

\[
|\varphi_i\rangle := P \Psi_{i,\uparrow}^\dagger \prod_{j, j \neq i} \Psi_{j,\uparrow}^\dagger \Psi_{j,\downarrow}^\dagger |0\rangle,
\] (8)

is led by the idea to leave as much of the \(2N\) particle physics unchanged as possible. The state is constructed in a way that most terms of the Hamiltonian generate zero-states due to the relation \((P \Psi_{i,\sigma}^\dagger)^2 = 0\). From
If the norm of the states $|\varphi_i\rangle$ and $|\Phi_0\rangle$ were known, the expectation value of $H$ could be evaluated. Unfortunately, this is not possible in general. However, the following orthogonal and normalized [see Eq. (1)] trial states

$$|\chi_i\rangle := \frac{\sqrt{H}}{\langle \Phi_0 | \Phi_0 \rangle} |\varphi_i\rangle$$

allow us to calculate the desired expectation value. (The positive square root of $H$ is well defined because $H \geq 0$.) Surprisingly, the Hamiltonian matrix elements $\langle \chi_j | H | \chi_i \rangle$ of the $(2N - 1)$ particle system can be expressed in terms of occupation-number expectation-values of the $2N$-particle system in the following way:

$$\langle \chi_j | H | \chi_i \rangle = \delta_{i,j} \left( \sum_{\alpha \in \mathcal{N}_i} \lambda_{i,\alpha,\uparrow}^2 - \sum_{\alpha \in \mathcal{U}_i} \lambda_{i,\alpha,\downarrow}^2 \langle n_{i,\alpha,\uparrow} \rangle \right)$$

$$+ (1 - \delta_{i,j}) \left( \sum_{\alpha,\beta \in \mathcal{C}_i} \delta_{(i\alpha),(j\beta)} \lambda_{i,\alpha,\uparrow} \lambda_{j,\beta,\downarrow} \right.$$

$$\left. - \sum_{\alpha,\beta \in \mathcal{C}_i \cap \mathcal{U}_i} \delta_{(i\alpha),(j\beta)} \lambda_{i,\alpha,\downarrow} \lambda_{j,\beta,\downarrow} \langle n_{i,\alpha,\uparrow} \rangle \right),$$

where

$$\langle n_{i,\alpha,\sigma} \rangle = \frac{\langle \Phi_0 | n_{i,\alpha,\sigma} | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}.$$  

(12)

In the following section, the upper bound Eq. (11) on the ground-state energy is discussed for two examples which allow us to calculate the expectation value $\langle n_{i,\alpha,\sigma} \rangle$.

V. RESULTS

A. $D$-dimensional Hubbard model

The first example, where the upper bound on the ground-state energy of the $(2N - 1)$ particle system may be evaluated is the Hubbard model as introduced in Ref. 2, where all $\lambda$s are set to unity and the spatial dimension is larger than one. For the three-dimensional case, the cells have the topology of octahedra with $2D = 6$ sites. All sites carry interaction, therefore the sets $\mathcal{U}_i$ and $\mathcal{N}_i$ are identical. Further, every site in $\mathcal{N}_i$ is shared by exactly one neighboring cell, forming a $D$ dimensional (hyper)cubic lattice of cells. Periodic boundary conditions are assumed. The corresponding lattice is visualized in Fig. 3a. The Hamiltonian of this system reads

$$H = \sum_{i,\sigma} \Psi_{i,\sigma} \Psi_{i,\sigma}^\dagger$$

$$= \sum_{i,\sigma} \left( - \sum_{\alpha \neq \beta} \epsilon_{i,\alpha,\sigma} c_{i,\beta,\sigma}^\dagger \right) P + 4 P \left( ND - \tilde{N}_e \right).$$

The last term in (13) contains a trivial constant $4ND$ and the total electron-number operator $\tilde{N}_e$ (with eigenvalue $N_c$) which is a conserved quantity.

With the Fourier transform

$$|\chi_k\rangle = \frac{1}{\sqrt{N}} \sum_j e^{i k j} |\chi_j\rangle$$

and $\langle n_{i,\alpha,\sigma} \rangle = D^{-1}$ (the occupation probabilities for all sites are equal for symmetry reasons) one obtains an upper bound on the $(2N - 1)$ particle ground state energy

$$\langle \chi_k | H | \chi_k \rangle = 2(1 - \frac{1}{D})(D + \sum_{\mu=1}^{D} \cos k_{\mu})$$

(15)

The minimum $E_{>}(2N - 1) = \min \langle \chi_k | H | \chi_k \rangle$ with respect to the $k$-vector is obvious: For ($k_1, k_2, \ldots, k_D$) = ($\pi, \pi, \ldots, \pi$) the right hand side of (15) becomes zero. However, this $k$-vector has to be excluded for this particular model, because it can be shown that the state $|\Phi_0\rangle$ vanishes if $\vec{k} = (\pi, \ldots, \pi)$ is allowed. That particular $k$-vector can be excluded by the restriction to systems where one of the $D$ system dimensions contains an odd number of cells. Then the $k$-vector component corresponding to this particular direction cannot equal $\pi$.

This result indicates that the state $|\chi_k\rangle$ becomes an asymptotically exact $(2N - 1)$ particle ground state of $H$ for the thermodynamic limit. The upper bound on the ground state energy vanishes as

$$E_{<}(2N - 1) = O(N^{-\delta})$$

and asymptotically approaches the lower bound $E_{<}(2N - 1) = 0$. This result is even relevant for $D = 2$, where the asymptotically exact state describes one hole in a half filled RVB-background. The absence of ferromagnetism does not contradict Nagaoka’s theorem because the present lattice is not bipartite. (For a bipartite lattice, the state would be a ferromagnet, i.e. the total spin would assume its maximum value.) Unfortunately, no rigorous statements on the uniqueness of this ground state can be made.

Further, it can be seen that for $D > 2$ the chemical potential of the system for particle numbers of $N_e = 2N - 1, \ldots, ND$ remains constant. The non-interacting tight-binding analogue exhibits quite similar behavior: The band structure of this particular lattice consists of one cosine band with $\epsilon(k) = 2 - 2(D + \sum \cos k_{\mu})$ and $D - 1$ flat bands at the upper band edge of the extended
band. However, the “bandwidth” of the interacting system is reduced by a factor \((1 - 1/D)\), which may be interpreted as an increased mass. This result sheds new light on the conductivity in the system. It might be that the many-particle state describes a dispersive delocalized hole which may contribute to conduction. Unfortunately, no results on hole densities have been obtained and the dispersive state is not exact except in the vicinity of \(k = (\pi, \ldots, \pi)\).

B. Linear Hubbard chain

As a second example, we study a linear chain with \(N\) cells and 4 sites per cell \(N_s\) (3 sites per unit cell). The topology of this chain is illustrated in Fig. 2; it may be interpreted as a chain of connected tetrahedra. Again, periodic boundary conditions and the case of infinite on-site repulsion on every site are assumed, and thus the sets \(N_s\) and \(N_t\) are identical. The cells \(i\) and \(i + 1\) are connected by one site (backbone site): the sites with indices \((i, \alpha = 1)\) and \((i + 1, \beta = 4)\) are identical. All \(\lambda\)'s are set to unity. The Hamiltonian of this particular chain reads

\[
H = \sum_{i, \sigma} \Psi_{i, \sigma} \Psi_{i, \sigma}^\dagger
\]

\[
= P \left( - \sum_{i, \sigma} \sum_{\alpha, \beta = 1, \alpha \neq \beta}^4 c_{i, \alpha, \sigma}^\dagger c_{i, \beta, \sigma} - 2 \sum_{i, \sigma} n_{i, 1, \sigma} \right) P
\]

\[
+ P \left( 8N - 2\bar{N}_e \right).
\]

In addition to the hopping terms, one obtains a local field which shifts the energy of the backbone sites \((\alpha = 1)\).

For this model, the upper bound Eq. (13) reduces to the simple expression:

\[
\langle \chi_k | H | \chi_k \rangle = 3 - \langle n_{i, \alpha = 1, \uparrow} \rangle + 2(1 - \langle n_{i, \alpha = 1, \uparrow} \rangle) \cos k
\]

\[(18)\]

The right hand side of Eq. (18) assumes a minimum for \(k = \pi\) (which is allowed for this model). This leads to the following upper bound on the ground state energy:

\[
E_g (N - 1) = 1 + \langle n_{i, \alpha = 1, \uparrow} \rangle.
\]

\[(19)\]

The occupation probability on the backbone sites may be calculated by a transfer-matrix technique for the thermodynamic limit. This calculation is briefly outlined in appendix B and yields

\[
\lim_{N \to \infty} E_g (2N - 1) = \frac{1}{2} \left( 3 - \frac{1}{\sqrt{13}} \right) \approx 1.361325
\]

\[(20)\]

In contrast to the previous example this result indicates a gap in the \((2N - 1)\) particle spectrum. Equation (20) estimates this gap from above. Therefore the upper bound is compared to numerically obtained exact results as described in Ref. [5].

The numerical results have been obtained by the conjugate-gradient algorithm. [4] The energies are listed in Tab. II. For chain lengths up to four unit cells, the ground state is calculated without applying symmetry restrictions. In order to check for ground-state degeneracy, the determination of the lowest eigenstate is repeated in the subspace orthogonal to the ground state. For an even number of unit cells, the energies of these orthogonal eigenstates do not coincide with the ground-state energy, therefore the ground states for even chain length are non-degenerate. (Chains with an odd number of unit cells are degenerate because of reflection symmetry which induces degeneracy with respect to \(\pm k\).)

As a second step, the same calculations have been performed assuming site-interchange symmetry as described in Ref. [8] and translational invariance with \(k = \pi\). The energies of the symmetrized states coincide with the previously calculated non-degenerate ground-state energies, therefore the symmetry of the ground state is uniquely determined.

The chain with six cells is numerically treated by application of site interchange symmetry only and the result for \(N = 8\) is obtained assuming translational invariance in addition to site-interchange symmetry.

The numerically obtained exact ground-state energies \(E_g (2N - 1)\) are shown in Tab. II. The upper bound Eq. (21) of the infinite system deviates from the numerical result for \(N = 8\) by \(\approx 13\%\). This agreement is not very close. However, the symmetries of the variational state and the numerically exact state coincide. Better quantitative agreement may be obtained by the expectation value of \(H\) with respect to the state

\[
| \varphi_k \rangle = \frac{1}{\sqrt{N}} \sum_j e^{ikj} | \varphi_j \rangle,
\]

\[(21)\]

The state \(| \varphi_k \rangle\) is defined by Eq. (8), which may be evaluated numerically. For a chain with \(N = 4\) one obtains \(\langle \varphi_{k = \pi} | H | \varphi_{k = \pi} \rangle = 1.2555\). This result deviates from the numerically exact result by \(\approx 4\%\) only. The state \(| \chi_k \rangle\) is proportional to \(\sqrt{\Pi} | \varphi_k \rangle\), therefore a difference in the expectation values \(\langle \varphi_{k = \pi} | H | \varphi_{k = \pi} \rangle\) and \(\langle \chi_{k = \pi} | H | \chi_{k = \pi} \rangle\) simply reflects the fact that \(| \chi_{k = \pi} \rangle\) (and hence \(| \varphi_{k = \pi} \rangle\)) is not an eigenstate. The operator \(\sqrt{\Pi}\) “amplifies” the deviation from the exact ground state.

The single-particle band-structure of this particular chain is illustrated in Fig. 3 and consists of two extended bands, one broad band separated from a narrower one by a gap of the size of one energy unit. The highest energy band collapses to one dispersionless flat band which is again separated by a small gap. For \(2N\) particles the non-interacting system would have a completely filled lower valence band describing an insulator. It is obvious that the interacting system shows different behavior here: In the framework of the one-particle language, one would expect a gap if the particle number is changed from \(N_e = 2N\) to \(N_e = 2N + 1\), however, for that case the chemical potential of the interacting system remains
constant. In contrast to the one-particle picture, the chemical potential of the interacting system changes if the particle number is changed from \( N_e = 2N - 1 \) to \( N_e = 2N \). This contradiction illustrates the breakdown of one-particle physics in this particular model.

VI. SUMMARY

For a class of models describing strongly interacting Fermions it is possible to write down the exact ground state if the particle number equals 2 per unit cell or more. The particle number regime below this threshold has not been accessible by rigorous methods so far. We present a tractable variational state for systems with one additional hole. The corresponding expectation value of the Hamiltonian approaches a lower bound for the case of a particular \( D \)-dimensional Hubbard model in the thermodynamic limit. We conclude that the presented variational state approaches the ground state or an eigenstate which is degenerate to the ground state if the ground state is not unique.

For a second model, a special Hubbard chain, the analytical expectation value deviates significantly from the numerically calculated ground state energy. Although it is shown that the numerical ground state and the variational state exhibit the same symmetries, it remains unclear, how well the ground-state physics of the chain is described by our variational ansatz.

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APPENDIX A:

This appendix provides a proof that the state \(|\Phi_0\rangle\) [Eq. (A3)] of the 2\(N\)-particle \(D\)-dimensional system vanishes, if the system extends an even number of unit cells in each direction.

The state and the Hamiltonian are expressed in terms of creation (annihilation) operators \(\Psi_{i,\sigma}^\dagger\) (\(\Psi_{i,\sigma}\)) referring to non-orthogonal one-particle states. However, they must be linear independent, otherwise the corresponding Slater determinant vanishes.

There is no problem for models with non-equivalent sites, however, the \(D\)-dimensional Hubbard model requires some care. Consider the Slater determinant

\[
|\Phi\rangle = \prod_i \Psi_{i,\uparrow,\sigma}^\dagger \Psi_{i,\downarrow,\sigma}^\dagger |0\rangle.
\] (A1)

The norm of \(|\Phi\rangle\) can be expressed in terms of a determinant

\[
\sqrt{\langle \Phi | \Phi \rangle} = \det M
\] (A2)

The matrix \(M\) has the elements

\[
M_{ij} = 2D\delta_{ij} + \delta_{<ij>},
\] (A3)

where \(\delta_{<ij>}\) equals one if \(i\) and \(j\) are nearest neighbors and zero otherwise. The structure of \(M\) is similar to a \(D\)-dimensional hypercubic tight-binding problem with periodic boundary conditions.

The determinant is equal to the product over all eigenvalues of the above tridiagonal matrix. The eigenvalues are given by the familiar cosine bands \(2(D + \sum_{\nu=1}^D \cos k_\nu)\). If all system length contain an even number of unit cells, one of the eigenvalues vanishes, because one of all possible \(k\)-vectors equals \((\pi, \pi, \pi, \ldots, \pi)\).

Therefore, the state \(|\Phi\rangle = 0\) and the projected state \(|\Phi_0\rangle = P|\Phi\rangle\) vanishes as well. The condition that at least one system length must be odd is a necessary condition for this model.

APPENDIX B:

We briefly recall the transfer matrix calculation of the occupation probability for certain sites of the Hubbard chain. This calculation requires open boundary conditions. However, the influence of the boundary conditions decreases with increasing system size.

The ground state of this chain can be decomposed into a sum over all possible configurations of \(N\) singlet bonds (dimers). Every component of the ground state has exactly one dimer in each cell. Let the singlets (dimers) be written as \(b_{i\sigma} \alpha \eta|0\rangle = \frac{1}{2} (\Psi_{i,\sigma}^\dagger \Psi_{i,\eta}^\dagger + \Psi_{i,\eta}^\dagger \Psi_{i,\sigma}^\dagger)|0\rangle\).

For every cell there exist six possible contributions:

\[
|1\rangle = b_{12}^\dagger |0\rangle, \quad |2\rangle = b_{13}^\dagger |0\rangle, \quad |3\rangle = b_{14}^\dagger |0\rangle
\] (B1)

\[
|4\rangle = b_{42}^\dagger |0\rangle, \quad |5\rangle = b_{43}^\dagger |0\rangle, \quad |6\rangle = b_{23}^\dagger |0\rangle
\]

The interaction excludes any double occupancy. Therefore the indices \(\alpha\) and \(\beta\) have to be different within a cell. This condition is not sufficient, because double occupancy on the backbone sites could occur due to certain configurations of neighbor cells: If e.g. cell \(i\) contains the singlet \(|1\rangle\) and cell \(i+1\) the singlets \(|3\rangle\), \(|4\rangle\), or \(|5\rangle\) the connection site would be occupied by two particles. These neighbor configurations have to be excluded. The restriction to allowed neighbor configurations is coded by the transfer matrix:

\[
T = \begin{pmatrix}
1 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}.
\] (B2)
With these definitions, the norm of the ground state \( \langle \Phi_0 | \Phi_0 \rangle \) for a chain with \( N \) cells may be written as

\[
\langle \Phi_0 | \Phi_0 \rangle = \sum_{i,j} (T^{N-1})_{ij} .
\]  
(B3)

The occupation of one \( \alpha = 2 \)-site well within the chain (the cell index \( m \) should be \( \approx 1/2N \)) is given by the expression

\[
\langle (n_{i,2,\uparrow} + n_{i,2,\downarrow}) \rangle = \frac{1}{\langle \Phi_0 | \Phi_0 \rangle} \sum_{i,j} \sum_{l=1,4,6} (T^m)_{ij} (T^{N-m-1})_{lj} \]  
(B4)

which may be simplified by using a spectral representation of the matrix \( T \). The eigenvalues of \( T \) are \( \epsilon_+ = \frac{1}{2}(5 + \sqrt{13}) \), \( \epsilon_- = \frac{1}{2}(5 - \sqrt{13}) \) and a fourfold degenerate eigenvalue \( \epsilon = 0 \). The right and left eigenstates may be calculated by \( T^N r_\pm = 1/2 (r_\pm) \) and \( (l_\pm | T = \epsilon l_\pm) \). They are mutually orthogonal and have to be normalized according to \( (l_\pm | l_\pm) = 1 \). Then the matrix \( T^N \) reads

\[
T^N = |r_+|^N (l_+) + |r_-|^N (l_-) \]  
(B5)

As usual, the contribution of the largest eigenvalue dominates the results with growing system size. In the thermodynamic limit the total occupation of the \( \alpha = 2 \)-sites becomes

\[
\langle (n_{i,2,\uparrow} + n_{i,2,\downarrow}) \rangle = \sum_{i=1,4,6} \langle l_+ | i \rangle \langle i | r_+ \rangle = \frac{1}{2}(1 + \frac{1}{\sqrt{13}})
\]  
(B6)

The backbone occupation may be calculated analogously or simply by applying \( \sum_\sigma \sum_{\alpha=1}^3 \langle n_{i,\alpha,\sigma} \rangle = 2 \).

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10. It is possible to construct a model with periodic boundary conditions, where not all phases of the \( \lambda \)-coefficients can be removed by a gauge transformation. The implications of this fact are disregarded here.
Figure 1
