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## Problem 10.1: The AKLT state - A prime example for a MPS

[**Written** | 11 pt(s)]

ID: ex_aklt_mps_part_1:tqp25

**Learning objective**

The goal of this exercise is to gain a better understanding of *matrix product states* (MPS). To this end, you first construct the exact ground state wave function of the famous Affleck–Kennedy–Lieb–Tasaki (AKLT) model in the MPS framework. You then study local order parameters and find that these can be expressed as a product of two local expectation values. Combining these results, you can evaluate the ferromagnetic order parameter for the AKLT state.

In the lecture, you learned that every state $|\psi\rangle \in \mathcal{H} = \bigotimes_{i=1}^{L} \mathbb{C}_i^d$ can be written as matrix product state (MPS) with periodic boundary conditions

$$|\psi\rangle \equiv \sum_{\boldsymbol{s}} \psi_{\boldsymbol{s}} |\boldsymbol{s}\rangle = \sum_{\boldsymbol{s}} \sum_{\boldsymbol{\alpha}} M^{[1]s_1}_{\alpha_0,\alpha_1} M^{[2]s_2}_{\alpha_1,\alpha_2} \dots M^{[L-1]s_{L-1}}_{\alpha_{L-2},\alpha_{L-1}} M^{[L]s_L}_{\alpha_{L-1},\alpha_0} |s_1, s_2, \dots, s_{L-1}, s_L\rangle \,. \quad (1)$$

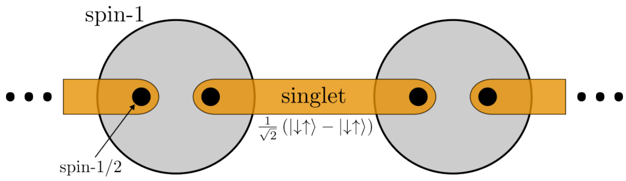
Here $\boldsymbol{s} = (s_1, \dots, s_L)$ where $s_i \in \{1, \dots, d\}$ labels the local states in $\mathbb{C}_i^d$ on site $i \in \{1, \dots, L\}$, and $\alpha_i \in \{1, \dots, D_i\}$ (including $\alpha_0$ due to periodic boundary conditions) denotes the virtual indices with bond dimension $D_i$. The sums over $\alpha_i$ are the "matrix products" (and sum over $\alpha_0$ corresponds to taking the trace). Note that for each $i$ and each $s_i$ the $M^{[i]s_i}$ is a $D_{i-1} \times D_i$-matrix.

Furthermore, you introduced the Affleck–Kennedy–Lieb–Tasaki (AKLT) model as an exactly solvable point in the symmetry-protected topological Haldane phase of the antiferromagnetic spin-1 Heisenberg chain. The AKLT Hamiltonian with periodic boundary conditions reads

$$H_{\text{AKLT}} = \sum_{i=1}^{L} P^{S=2}_{i,i+1} = \sum_{i=1}^{L} \left[ \frac{1}{2} \boldsymbol{S}_i \boldsymbol{S}_{i+1} + \frac{1}{6} \left( \boldsymbol{S}_i \boldsymbol{S}_{i+1} \right)^2 + \frac{1}{3} \right] , \quad (2)$$

where $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$ are spin operators on site $i \in \{1, \dots, L\}$ in the spin-1 representation (so that the dimension of the local Hilbert spaces is $d = 3$). $P^{S=2}_{i,i+1}$ denotes the projector onto the spin-2 representation on sites $i$ and $i+1$ (remember that $1 \otimes 1 = 0 \oplus 1 \oplus 2$).

The structure of the ground state $|\psi_{\text{AKLT}}\rangle$ of this Hamiltonian is most transparent if one starts with two (artificial) spin-$\frac{1}{2}$ representations on each site and forms a valence bond (singlet state) between the spins of adjacent sites (figure on the right). The AKLT ground state is then obtained by projecting the four-dimensional on-site Hilbert space into the three-dimensional spin-1 representation (remember that $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$).




In this exercise, you derive the representation of this AKLT state in the MPS framework and use it to evaluate correlation functions.

a) We start by considering two spin-$\frac{1}{2}$ forming a singlet state **2**pt(s)

$$\left|\psi_{\text{singlet}}\right\rangle = \tfrac{1}{\sqrt{2}}\left(|\downarrow_1\uparrow_2\rangle - |\uparrow_1\downarrow_2\rangle\right) . \tag{3}$$

Show that the matrix product state representation of this state reads

$$\left|\psi_{\text{singlet}}\right\rangle = \sum_{s_1,s_2,\alpha_1} M^{[1]s_1}_{\alpha_1} M^{[2]s_2}_{\alpha_1} |s_1, s_2\rangle \tag{4}$$

with matrices

$$M^{[1]\downarrow} = \begin{pmatrix}\frac{1}{\sqrt{2}}, & 0\end{pmatrix} , \; M^{[1]\uparrow} = \begin{pmatrix}0, & \frac{1}{\sqrt{2}}\end{pmatrix} \quad \text{and} \quad M^{[2]\downarrow} = \begin{pmatrix}0\\-1\end{pmatrix} , \; M^{[2]\uparrow} = \begin{pmatrix}1\\0\end{pmatrix} .$$

What is the bond dimension of this state? What is the entanglement entropy of this state?

**Note:** Since we only consider two spins, the bond index $\alpha_0$ is not needed (or alternatively $D_0 = 1$), thus the matrices $M^{[1]s_1}$ (and $M^{[2]s_2}$) are in this case $1 \times D_1$ row (and $D_1 \times 1$ column) vectors. Moreover, we have $D_1 = 2$, thus each $M^{[i]s_i}$ has two entries. Note however, that these two entries live in the virtual bond space, and not in the physical Hilbert space.

We now consider a *chain* of $2L$ spin-$\frac{1}{2}$ in a product of $L$ such singlet states:

$$\begin{aligned}\left|\psi_{\text{singlet-chain}}\right\rangle &= \tfrac{1}{\sqrt{2}}\left(|\downarrow_1\uparrow_2\rangle - |\uparrow_1\downarrow_2\rangle\right) \otimes \tfrac{1}{\sqrt{2}}\left(|\downarrow_3\uparrow_4\rangle - |\uparrow_3\downarrow_4\rangle\right) \otimes \dots \\ &\qquad \dots \otimes \tfrac{1}{\sqrt{2}}\left(|\downarrow_{2L-1}\uparrow_{2L}\rangle - |\uparrow_{2L-1}\downarrow_{2L}\rangle\right) \\ &\equiv \sum_{\boldsymbol{s}} M^{[1]s_1} M^{[2]s_2} M^{[1]s_3} M^{[2]s_4} \dots M^{[1]s_{2L-1}} M^{[2]s_{2L}} |\boldsymbol{s}\rangle .\end{aligned} \tag{5}$$

**Note:** Note that we reuse the matrices $M^{[1]}$ and $M^{[2]}$ on every other site!

b) Draw the MPS pictorially (e.g. for $L = 3$). What are the bond dimensions at each bond? **1**pt(s)

c) Next, consider an even site $2i$ and its neighbor $2i + 1$ (these belong to different singlets!). **1**pt(s)

Calculate the projection of these two sites onto the spin-1 subspace

$$\sum_{s_{2i},s_{2i+1}} P^{S=1}_{2i,2i+1} \underbrace{M^{[2]s_{2i}} M^{[1]s_{2i+1}}}_{2\times 2\text{-matrix}} |s_{2i}, s_{2i+1}\rangle \equiv \sum_{j_i} A^{j_i} |j_i\rangle , \tag{6}$$

where $j_i \in \{+, 0, -\}$ denotes the three possible spin-1 states and $A^{j_i}$ are the MPS matrices for the spin-1 AKLT state (which do not depend on the site index $i$ due to translation invariance).

The projection operator is given by (we omit site indices)

$$P^{S=1} = |-\rangle\langle\downarrow\downarrow| + |0\rangle \frac{\langle\downarrow\uparrow| + \langle\uparrow\downarrow|}{\sqrt{2}} + |+\rangle\langle\uparrow\uparrow| . \tag{7}$$

By now, you have shown that the AKLT state (with periodic boundary conditions) can be written as a matrix product state

$$|\psi_{\text{AKLT}}\rangle = \sum_{\boldsymbol{j}} \sum_{\boldsymbol{\alpha}} A^{j_1}_{\alpha_0,\alpha_1} \dots A^{j_L}_{\alpha_{L-1},\alpha_0} |\boldsymbol{j}\rangle = \sum_{\boldsymbol{j}} \text{tr}\left(A^{j_1} \cdots A^{j_L}\right) |\boldsymbol{j}\rangle , \tag{8}$$

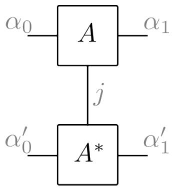
with the $2 \times 2$-matrices $A^{j_i}$ (after normalization)

$$A^+ = \sqrt{\tfrac{2}{3}}\,\sigma^+\,, \quad A^0 = \sqrt{\tfrac{1}{3}}\,\sigma^z \quad \text{and} \quad A^- = -\sqrt{\tfrac{2}{3}}\,\sigma^-\,. \tag{9}$$

**Note:** The trace is taken to contract the indices of the first and last matrices to implement periodic boundary conditions.

Now that we have an MPS representation of the AKLT ground state, we are interested in evaluating expectation values $\langle\psi|\, O_i\,|\psi\rangle$ and local order parameters like $\langle\psi|\, O_i O_k\,|\psi\rangle$. To this end, it is useful to introduce the *transfer matrix*, which is given by

$$T_{(\alpha_0,\alpha_0'),(\alpha_1,\alpha_1')} \equiv$$




$$= \sum_j \left(A^j\right)_{\alpha_0,\alpha_1} \left(A^j_{\alpha_0',\alpha_1'}\right)^* = \sum_j A^j \otimes \left(A^j\right)^*\,. \tag{10}$$

d) Calculate the transfer matrix $T$ of the AKLT state (8). Then diagonalize it to find its eigenvalues $\eta_i$ and eigenvectors $\boldsymbol{\phi}_i$. Thus, you can write the transfer matrix in its spectral decomposition as **2**pt(s)

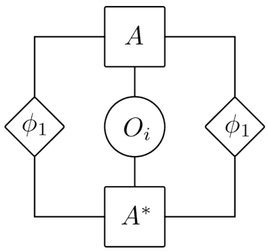
$$T = \sum_i \eta_i \boldsymbol{\phi}_i \boldsymbol{\phi}_i^\dagger\,, \tag{11}$$

where $\boldsymbol{\phi}_i\boldsymbol{\phi}_i^\dagger$ is the outer product of the 4-component column vector $\boldsymbol{\phi}_i$ and the row vector $\boldsymbol{\phi}_i^\dagger$.

**Note:** The transfer matrix is a tensor with four indices, $\alpha_0, \alpha_1, \alpha_0', \alpha_1'$. However, we can combine the indices $\alpha_0$ and $\alpha_0'$ ($\alpha_1$ and $\alpha_1'$) into a single index $\beta_0$ ($\beta_1$) which leaves us with a $4 \times 4$ matrix that can be diagonalized as usual.

e) Use the spectral decomposition of the transfer matrix to show that the expectation value can be written in the limit $L \to \infty$ as **2**pt(s)

$$\langle\psi|\, O_i\,|\psi\rangle = \operatorname{tr}\left(\mathbb{O}_i T^{L-1}\right) \overset{L\to\infty}{=} \boldsymbol{\phi}_1^\dagger \mathbb{O}_i \boldsymbol{\phi}_1 \equiv \tag{12}$$




where $\boldsymbol{\phi}_1$ is the eigenvector of the transfer matrix with the largest eigenvalue $\eta_1 = 1$. Determine the $4 \times 4$ matrix

$$\mathbb{O}_i = \sum_{j,j'} A^j_{\alpha_0,\alpha_1} O_i^{j,j'} \left(A^{j'}_{\alpha_0',\alpha_1'}\right)^* \tag{13}$$

and calculate the expectation value for $O_i \in \{S_i^z, S_i^x\}$, where

$$S_i^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad S_i^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\,. \tag{14}$$

f) Similarly, show that the correlation function of a local order parameter $O_i$ in the limit $L \to \infty$ and for large distances $|i-k|$ is given by **2pt(s)**

$$\langle\psi| O_i O_k |\psi\rangle = \text{tr}\left(\mathbb{O}_i T^{|i-k|-1} \mathbb{O}_i T^{L-|i-k|-1}\right) = \langle\psi| O_i |\psi\rangle \cdot \langle\psi| O_k |\psi\rangle + \mathcal{O}(e^{-|i-k|/\xi}) \,. \quad (15)$$

What is the *correlation length* $\xi$ for the AKLT state?

g) Finally, use Eq. (15) and your previous results to calculate the ferromagnetic order parameter $\langle\psi| S_i^z S_k^z |\psi\rangle$ and $\langle\psi| S_i^x S_k^x |\psi\rangle$ in the limit $|i-k| \to \infty$. **1pt(s)**

## Problem 10.2: The AKLT state - A symmetry protected topological phase [**Oral** | 8 pt(s)]

ID: ex_aklt_mps_part_2:tqp25

> **Learning objective**
>
> In Problem 10.1 you constructed the AKLT state as a matrix product state (MPS), and showed that the correlations of the ferromagnetic order parameter vanish. This demonstrates that symmetry protected topological (SPT) phases – such as the Haldane phase realized by the AKLT Hamiltonian – cannot be characterized by local order parameters. In this exercise, you characterize the AKLT state by the transformation of its matrices under symmetry transformations. Furthermore, you show that a non-local *string-order parameter* can be used to characterize the topological Haldane phase.

The MPS representation of the AKLT state, derived in Problem 10.1, has the form

$$|\psi_{\text{AKLT}}\rangle = \sum_{\boldsymbol{j}} \sum_{\boldsymbol{\alpha}} A^{j_1}_{\alpha_0,\alpha_1} \dots A^{j_N}_{\alpha_{L-1},\alpha_0} |\boldsymbol{j}\rangle = \sum_{\boldsymbol{j}} \text{tr}\left(A^{j_1} \cdots A^{j_L}\right) |\boldsymbol{j}\rangle \,, \quad (16)$$

with spin-1 states $|j_i\rangle \in \mathbb{C}^3_i$ on each site $i = 1, \dots, L$ with $j_i \in \{+, 0, -\}$, and matrices $A^{j_i}$

$$A^+ = \sqrt{\tfrac{2}{3}}\,\sigma^+ \,, \quad A^0 = \sqrt{\tfrac{1}{3}}\,\sigma^z \quad \text{and} \quad A^- = -\sqrt{\tfrac{2}{3}}\,\sigma^- \,. \quad (17)$$

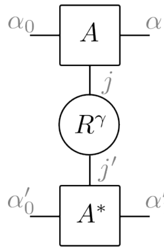
In the lecture, you learned that the Haldane phase is protected by the dihedral symmetry group $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$. This symmetry group is realized by local $\pi$-rotations of the spins about any of the three axes $\gamma \in \{x, y, z\}$ and has four elements $\{\mathbb{1}, R^x, R^y, R^z\}$. The rotations $R_i^\gamma = e^{i\pi S_i^\gamma}$ operate on the spin-1 Hilbert spaces $\mathbb{C}^3_i$ and read explicitly (on each site $i$)

$$R_i^x = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \,, \quad R_i^y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad R_i^z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \,. \quad (18)$$

The $D_2$ symmetry on the complete system then acts as $R^\gamma = \bigotimes_{i=1}^L R_i^\gamma$. Since the ground state of the AKLT Hamiltonian is uniquely given by $|\psi_{\text{AKLT}}\rangle$ for periodic boundary conditions, it cannot break the $D_2$ symmetry so that $R^\gamma |\psi_{\text{AKLT}}\rangle = \alpha(\gamma) |\psi_{\text{AKLT}}\rangle$ for some phase $\alpha(\gamma)$.

a) To understand in detail how the symmetries act on the AKLT state, we study the *generalized* **3pt(s)** *transfer matrix* $T^{R^\gamma}$ defined as

$$T^{R^\gamma}_{(\alpha_0,\alpha_0'),(\alpha_1,\alpha_1')} \equiv$$



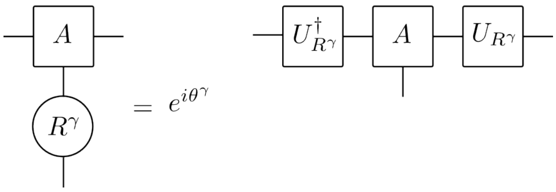

$$= \sum_{j,j'} A^j_{\alpha_0,\alpha_1} R^\gamma_{jj'} \left(A^{j'}_{\alpha_0',\alpha_1'}\right)^* = \sum_{j,j'} R^\gamma_{jj'} \cdot A^j \otimes \left(A^{j'}\right)^* . \tag{19}$$

Calculate the generalized transfer matrices $T^{R^\gamma}$ for $\gamma = x, z$ explicitly for the AKLT state. Compute also their eigenvalues $\eta_i^\gamma$ and eigenvectors $\boldsymbol{\phi}_i^\gamma$.

Then show that the dominant eigenvector (corresponding to the largest eigenvalue) of $T^{R^x}$ can be interpreted as a $2 \times 2$ matrix $(\phi_1^x)_{\alpha,\alpha'} = \sigma^x_{\alpha,\alpha'}$ (up to normalization).

Show analogously that the dominant eigenvector of $T^{R^z}$ reads $(\phi_1^z)_{\alpha,\alpha'} = \sigma^z_{\alpha,\alpha'}$.

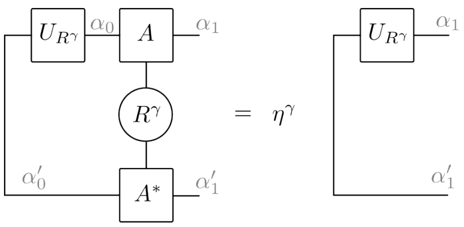
In the lecture, it was argued (under some technical assumptions) that the physical action of symmetries can be "pulled through" on the virtual indices




(20)

where the unitaries $U_{R^\gamma}$ form a *projective* representation of the symmetry group $D_2$.

b) Use Eq. (20) to show that the unitary $U_{R^\gamma}$ is necessarily a left-eigenvector with eigenvalue $|\eta^\gamma| = 1$ of the generalized transfer matrix. I.e., show that **2**pt(s)




$$\Leftrightarrow \quad U^{R^\gamma}_{(\alpha_0,\alpha_0')} \cdot T^{R^\gamma}_{(\alpha_0,\alpha_0'),(\alpha_1,\alpha_1')} = \eta^\gamma \cdot U^{R^\gamma}_{(\alpha_1,\alpha_1')} . \tag{21}$$

**Hint:** Show and use that $\sum_{j,\beta} A^j_{\beta\alpha_0} A^{*j}_{\beta\alpha_1} = \delta_{\alpha_0,\alpha_1}$.

Use this, in combination with your results from subtask (a), to identify the projective representations $U_{R^x}$ and $U_{R^z}$.

As discussed in the lecture, a map $U : G \to \mathrm{GL}(\mathcal{H}) : g \mapsto U_g$ from a symmetry group $G$ into the general linear group of the Hilbert space $\mathcal{H}$ that satisfies

$$U_f \cdot U_g = \chi(f,g)\, U_{fg} \tag{22}$$

is called a *projective representation* of $G$ in $\mathcal{H}$. (Here it is $G = D_2$ and $f, g \in \{\mathbb{1}, R^x, R^y, R^z\}$.)

The function $\chi : G \times G \to \mathrm{U}(1)$ is called *2-cocycle* and characterizes the projective representation. Associativity of the group demands that it satisfies the *cocycle condition*

$$\chi(f,g)\chi(fg,h) = \chi(g,h)\chi(f,gh)\,, \tag{23}$$

i.e., $\chi$ is not arbitrary.

Two cocycles $\chi_1$ and $\chi_2$ describe equivalent projective representations if and only if there is a function $\varphi : G \to \mathrm{U}(1)$ such that

$$\chi_1 \sim \chi_2 \quad :\Leftrightarrow \quad \chi_1(f,g) = \chi_2(f,g)\frac{\varphi(f)\varphi(g)}{\varphi(fg)}\,. \tag{24}$$

A representation with $\chi \sim 1$ is *linear* and labels the trivial phase; by contrast, a representation with $\chi \nsim 1$ labels non-trivial SPT phases.

c) In subtask (b) you identified the projective representation of $D_2$ that acts on the virtual bonds: **1**pt(s)

$$U_{\mathbb{1}} = \mathbb{1}_{2\times 2}\,, \quad U_{R^x} = \sigma^x\,, \quad U_{R^z} = \sigma^z\,, \quad \text{and} \quad U_{R^y} = U_{R^z}\cdot U_{R^x} = i\sigma^y\,. \tag{25}$$

**Note:** Note that this definition is not unique (e.g., the order in the definition of $U_{R^y}$ is arbitrary). Why does this not matter for the classification of the SPT phase?

Evaluate the 2-cocycle explicitly for the following products

$$U_{R^x}U_{R^x} = \chi(R^x,R^x)\,U_{\mathbb{1}} \tag{26a}$$
$$U_{R^z}U_{R^z} = \chi(R^z,R^z)\,U_{\mathbb{1}} \tag{26b}$$
$$U_{R^x}U_{R^z} = \chi(R^x,R^z)\,U_{R^y} \tag{26c}$$
$$U_{R^y}U_{R^y} = \chi(R^y,R^y)\,U_{\mathbb{1}} \tag{26d}$$

and use this [and Eq. (24)] to show that $\chi$ is non-trivial.

This shows that the AKLT state belongs to a non-trivial SPT phase protected by $D_2$.

The non-triviality of the 2-cocycle $\chi$ also manifests in non-local order parameters, so-called *string order parameters*. The $z$-string order parameter is defined as

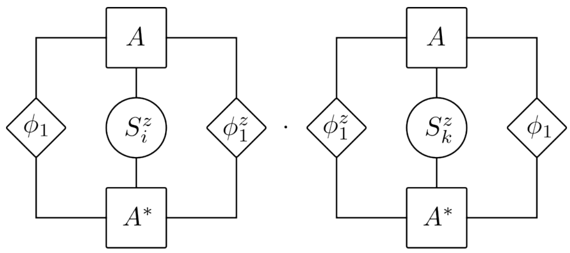
$$\mathcal{S}_{i,k}(S^z) := \langle\psi|\, S_i^z \left(\prod_{i<l<k} R_l^z\right) S_k^z\,|\psi\rangle \tag{27}$$

for any given state $|\psi\rangle$.

d) Argue similar to subtask (f) and (g) in Problem 10.1 that in the limit $L, |i-k| \to \infty$ the string order parameter can be evaluated as **1**pt(s)

$$\mathcal{S}_{i,k}(S^z) = \mathrm{tr}\left(\mathbb{O}_i^z (T^{R^z})^{|i-k|-1}\mathbb{O}_k^z T^{L-|i-k|-1}\right)$$

$$= \boldsymbol{\phi}_1^\dagger \mathbb{O}_i^z \boldsymbol{\phi}_1^z (\boldsymbol{\phi}_1^z)^\dagger \mathbb{O}_k^z \boldsymbol{\phi}_1 = \tag{28}$$




where $\boldsymbol{\phi}_1 = 1/\sqrt{2}(1,0,0,1)^T$ was the dominant eigenvector of normal transfer matrix $T$ and $\boldsymbol{\phi}_1^z$ is the dominant eigenvector of the generalized transfer matrix $T^{R^z}$ from subtask (a).

e) Evaluate the $z$-string order parameter (27) explicitly for the AKLT state (16). **1**pt(s)

**Note:** The string order of the AKLT state is sometimes also referred to as *hidden antiferromagnetic order*. This nomenclature is warranted because when looking at the allowed spin configurations of the state $|\psi_{\text{AKLT}}\rangle$, one finds an antiferromagnetic pattern (i.e., alternating $|+\rangle$ and $|-\rangle$ states) which is "hidden" in a sea of $|0\rangle$ states (and therefore cannot be detected by local 2-point correlation functions).