# Structure of the Hilbert-space of the infinite-dimensional Hubbard model 

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#### Abstract

An iterative procedure for the explicit construction of the nontrivial subspace of all symmetryadapted configurations with non-zero weight in the ground-state of the $\infty$-dimensional Hubbard model is developed on the basis of a symmetrized representation of the transition operators on a sequence of Bethe-Lattices of finite depth. The relationship between these operators and the well-known mapping of the $\infty$-dimensional Hubbard model onto an effective impurity problem coupled to a (self-consistent) bath on non-interacting electrons is given. As an application we calculate the properties of various Hubbard stars and give estimates for the half-filled Hubbard model with up to $0.1 \%$ accuracy.


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## 1 Introduction

The Hamiltonian of the half-filled Hubbard model is given by

$$
\begin{aligned}
H= & \frac{-t^{*}}{\sqrt{2 Z}} \sum_{\langle i, j\rangle, \sigma} f_{i, \sigma}^{\dagger} f_{j, \sigma} \\
& +U \sum_{i}\left(f_{i, \uparrow}^{\dagger} f_{i, \uparrow}-1 / 2\right)\left(f_{i, \downarrow}^{\dagger} f_{i, \downarrow}-1 / 2\right),
\end{aligned}
$$

where $Z$ is the coordination number of the lattice, i.e. $Z=2 D$ on a simply hypercubic lattice. The model is well defined and nontrivial in the limit $D \rightarrow \infty$ [1]. In this limit all correlations are local $[1,2]$ and the Hubbard model can be solved iteratively by mapping it to an effective Anderson impurity model [3], which reads for the $n$th iteration as

$$
\begin{align*}
H^{(n)} & =\sum_{l=1, \sigma}^{M_{\sigma}^{(n-1)}}\left[V_{l, \sigma}^{(n-1)} f_{\sigma}^{\dagger} c_{l, \sigma}+\text { H.C. }\right] \\
& +\sum_{l=1, \sigma}^{M_{\sigma}^{(n-1)}} \epsilon_{l, \sigma}^{(n-1)} c_{l, \sigma}^{\dagger} c_{l, \sigma}+U\left(f_{\uparrow}^{\dagger} f_{\uparrow}-1 / 2\right)\left(f_{\downarrow}^{\dagger} f_{\downarrow}-1 / 2\right), \tag{1}
\end{align*}
$$

where $n=0,1,2, \ldots$ denotes the number of iterations. The $f_{\sigma}^{\dagger}$ is the creation operator of the central (impurity) site and $M_{\sigma}^{(n-1)}$ the number of state of the bath obtained from the previous $(n-1)$ iterations. The 'onsite' energies $\epsilon_{l, \sigma}^{(n-1)}$ and hybridization matrix elements $V_{l, \sigma}^{(n-1)}$ may

[^0]be obtained from the local (impurity) Green's function of the previous iteration, $G_{\sigma}^{(n-1)}(\omega)$. For the $\infty$-dimensional Bethe lattice this relation is given by [4]
\[

$$
\begin{equation*}
G_{\sigma}^{(n-1)}(\omega)=\sum_{l=1}^{M_{\sigma}^{(n-1)}} \frac{2\left(V_{l, \sigma}^{(n-1)} / t^{*}\right)^{2}}{\omega-\epsilon_{l, \sigma}^{(n-1)}} . \tag{2}
\end{equation*}
$$

\]

The spin-dependence, $\sigma=\uparrow, \downarrow$, has been explicitly retained in above formulas, in order include the antiferromagnetically ordered state.

Once the parameters $\epsilon_{l, \sigma}^{(n-1)}$ and $V_{l, \sigma}^{(n-1)}$ have been extracted from (2) one needs to calculate $G_{\sigma}^{(n)}(\omega)$ by solving (1). The relevant Hilbert-space is of the order of

$$
\begin{equation*}
M_{\sigma}^{(n)} \approx 4 \cdot 2^{M_{\uparrow}^{(n-1)}} \cdot 2^{M_{\downarrow}^{(n-1)}} \tag{3}
\end{equation*}
$$

The number of poles in $G_{\sigma}(n)(\omega)$ will of the same order of magnitude as (3), exponentially larger than $M_{\sigma}^{(n-1)}$. In any numerical treatment of it is therefore necessary to throw away an exponentially large part of the Hilbertspace $[5,6]$.

Above route to solve the infinite-D Hubbard model is aimed to determine the one-particle Green's function and it is not obvious from (1) how to construct the eigenstates in the original Hilbert-space, in particular of the ground-state wavefunction. Here we show, that it is possible to construct the ground-state wavefunction iteratively, taking the half-filled Bethe lattice as an example.

## 2 Transition operators on the Hubbard-Star

A natural approach to solve (1) iteratively is to consider the series of generalized Hubbard stars [7], which are


Fig. 1. Illustration of the Hubbard star $S(1)$ and the star of the stars $S(2)$.
truncated Bethe-lattices. We denote with $S(0)$ the single site, with $S(1)$ the Hubbard star, with $S(2)$ the star of stars, etc., see Figure 1. This approach has previously been applied successfully to the study of the Mott-Hubbard transition [4] and allows to determine the ground-state of the infinite-D Hubbard model iteratively. In following we restrict ourselves to the case of the antiferromagnetic state at half filling, generalization to other fillings and frustrated models are straightforward.

We write the Hamiltonian of $S(n)$ as

$$
\begin{gather*}
H^{(n)}=\sum_{i=1}^{Z} H_{i}^{(n-1)}-\frac{t^{*}}{\sqrt{2}} \sum_{\sigma=\uparrow, \downarrow}\left[f_{\sigma}^{\dagger} A_{\sigma}+A_{\sigma}^{\dagger} f_{\sigma}\right] \\
+U\left(f_{\uparrow}^{\dagger} f_{\uparrow}-1 / 2\right)\left(f_{\downarrow}^{\dagger} f_{\downarrow}-1 / 2\right), \tag{4}
\end{gather*}
$$

where the $f_{\sigma}^{\dagger}$ are the electron creation operators at the central site and

$$
\begin{equation*}
A_{\sigma}^{\dagger}=\frac{1}{\sqrt{Z}} \sum_{i=1}^{Z} c_{i, \sigma}^{\dagger} \tag{5}
\end{equation*}
$$

Here the $c_{i, \sigma}^{\dagger}$ are the electron creation operators of the respective central sites of $S_{i}(n-1)$. The $H_{i}^{(n-1)}$ in (4) are the Hamiltonians of the $\mathrm{S}_{i}(n-1), i=1, \ldots, Z$.

We will show next that the knowledge of the exact eigenstates of $H_{i}^{(n-1)}$ allows for the construction of the exact eigenstates of $H^{(n)}$ with a finite number of operations, despite the fact that $Z \rightarrow \infty$ stars of order $(n-1)$ couple to the central site.

We now introduce a notation for the eigenstates of $H_{i}^{(n-1)}$. Let $\left|k_{\mathbf{m}}, i\right\rangle$ designate the $k$ th state in the sector $\mathbf{m}=\left(m_{+}, m_{-}\right)$containing $m_{\sigma}$-particles of spin- $\sigma$ on subsystem $i$. We measure $m_{\sigma}$ relative to the ground-state of $H_{i}^{(n-1)}$. For the enumeration of the accessible states in the Hilbert space it is useful to define many-body transition operators

$$
\begin{equation*}
\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. k_{\mathbf{m}}^{\prime}\right|_{i}=\bigotimes_{j<i} \mathbf{1}_{j} \otimes \mid k_{\mathbf{m}+\mathbf{s}}, i\right\rangle\left\langle i, k_{\mathbf{m}}^{\prime}\right| \otimes \bigotimes_{i<j} \mathbf{1}_{j} \tag{6}
\end{equation*}
$$

for the subsystem $i$ with $\mathbf{s}=(\mathbf{1}, \mathbf{0})$ or $\mathbf{s}=(\mathbf{0}, \mathbf{1})$ respectively. We note that these operators obey the anticommutation relations

$$
\begin{gather*}
\left\{\left|k_{\mathbf{m}+\mathbf{s}^{\prime}}\right\rangle\left\langle k_{\mathbf{m}}^{\prime}\right| i,\left|q_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. q_{\mathbf{m}}^{\prime}\right|_{j}\right\}=\delta_{i, j} \delta_{k_{\mathbf{m}}^{\prime}, q_{\mathbf{m}+\mathbf{s}}}\left|k_{\mathbf{m}+\mathbf{s}^{\prime}}\right\rangle\left\langle q_{\mathbf{m}}^{\prime}\right| i\right. \\
\left.+\delta_{i, j} \delta_{q_{\mathbf{m}}^{\prime}, k_{\mathbf{m}+\mathbf{s}^{\prime}}\left|q_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. k_{\mathbf{m}}^{\prime}\right|_{i} .\right.} .7\right) \tag{7}
\end{gather*}
$$

Since $A_{\sigma}^{\dagger}$ creates only symmetrized combinations of states on the periphery of the star, it is useful to rewrite $A_{\sigma}^{\dagger}$ as

$$
\begin{equation*}
A_{\sigma}^{\dagger}=\sum_{k, k^{\prime}, \mathbf{m}} a\left(k_{\mathbf{m}+\mathbf{s}}, k_{\mathbf{m}}^{\prime}\right)\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle k_{\mathbf{m}}^{\prime}\right| \tag{8}
\end{equation*}
$$

where we introduced the symmetrized transition operator

$$
\begin{equation*}
\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle k_{\mathbf{m}}^{\prime}\right|=\frac{1}{\sqrt{Z}} \sum_{i}\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. k_{\mathbf{m}}^{\prime}\right|_{i}\right. \tag{9}
\end{equation*}
$$

The coupling matrix elements in equation (8) are given as

$$
\begin{equation*}
a\left(k_{\mathbf{m}+\mathbf{s}}, k_{\mathbf{m}}^{\prime}\right) \equiv\left\langle k_{\mathbf{m}+\mathbf{s}}, i\right| c_{i, \sigma}^{\dagger}\left|i, k_{\mathbf{m}}^{\prime}\right\rangle \tag{10}
\end{equation*}
$$

independent of $i$.
Using equation (7), commutation rules for the symmetrized operators are easily derived:

$$
\begin{align*}
\left(\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle k_{\mathbf{m}}^{\prime}\right|\right)^{2} & =\frac{1}{Z} \sum_{i, j}\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. k_{\mathbf{m}}^{\prime}\right|_{i} \mid k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. k_{\mathbf{m}}^{\prime}\right|_{j}\right. \\
& =0 \tag{11}
\end{align*}
$$

Similarly we find:

$$
\begin{align*}
\left|k_{\mathbf{m}}^{\prime}\right\rangle\left\langle k_{\mathbf{m}+\mathbf{s}^{\prime}}\right|\left|q_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle q_{\mathbf{m}}^{\prime}\right| & =\frac{1}{Z} \sum_{i j}\left|k_{\mathbf{m}}^{\prime}\right\rangle\left\langle\left. k_{\mathbf{m}+\mathbf{s}^{\prime}}\right|_{i} \mid q_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle\left. q_{\mathbf{m}}^{\prime}\right|_{j}\right. \\
& =\frac{1}{Z} \delta_{k_{\mathbf{m}+\mathbf{s}^{\prime}}, q_{\mathbf{m}+\mathbf{s}}} \sum_{i}\left|k_{\mathbf{m}}^{\prime}\right\rangle\left\langle\left. q_{\mathbf{m}}^{\prime}\right|_{i}\right. \\
& =\frac{1}{\sqrt{Z}} \delta_{k_{\mathbf{m}+\mathbf{s}^{\prime}}, q_{\mathbf{m}+\mathbf{s}}}\left|k_{\mathbf{m}}^{\prime}\right\rangle\left\langle q_{\mathbf{m}}^{\prime}\right| \tag{12}
\end{align*}
$$

Note that operators of type $\left|k_{\mathbf{m}}^{\prime}\right\rangle\left\langle q_{\mathbf{m}}^{\prime}\right|$, which do not change the number of particles on periphery, are bosonic in nature, while the $\left|k_{\mathbf{m}+\mathbf{s}}\right\rangle\left\langle k_{\mathbf{m}}^{\prime}\right|$ are fermionic in nature, see (7).

## 3 Construction of the Hilbert space

We define the vacuum $|0\rangle$ of $S(n)$ by

$$
\begin{equation*}
|0\rangle=|0\rangle_{\mathrm{c}} \bigotimes_{i}\left|0_{(0,0)}, i\right\rangle \tag{13}
\end{equation*}
$$

where $|0\rangle_{\mathrm{c}}$ designates the vacuum of the central site and $\left|0_{(0,0)}, i\right\rangle$ the (many-body) ground-state on the $i$ th leg of the peripheral sites. We define

$$
\begin{equation*}
|\sigma\rangle=f_{\sigma}^{\dagger}|0\rangle, \quad \quad|\uparrow \downarrow\rangle=f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger}|0\rangle \tag{14}
\end{equation*}
$$



Fig. 2. Distribution of the $\left|a\left(k_{ \pm \mathbf{s}}, 0_{(0,0)}\right)\right|^{2}$ for $\mathrm{S}(2)$ as a function of $t^{*}$. Solid bars: $\mathbf{s}=(\mathbf{0}, \pm \mathbf{1})$, dashed bars: $\mathbf{s}=( \pm \mathbf{1}, \mathbf{0})$. For $U=2 t^{*}+|a|^{2}$ are shown, for $U=8-|a|^{2}$ are shown. The formation of the lower and upper Hubbard band for $U=8 t^{*}$ can be seen. Here $t^{*}=1$ has been used.

In order to iteratively construct the overall Hilbert space with nonzero coupling to the vacuum state defined above, we concentrate on the accessible states. Suppose for simplicity that the central site is occupied by an electron with spin $\sigma=\uparrow$. The Hamiltonian $H^{(n)}$ then couples the state $|\uparrow\rangle$ directly to the normalized states

$$
\begin{equation*}
\left|k_{(1,0)}\right\rangle\left\langle 0_{(0,0)}\right||0\rangle \quad \text { and } \quad\left|k_{(0,-1)}\right\rangle\left\langle 0_{(0,0)}\right||\uparrow \downarrow\rangle . \tag{15}
\end{equation*}
$$

The matrix elements of above states with $|\uparrow\rangle$ are

$$
-t^{*} a\left(k_{(1,0)}, 0_{(0,0)}\right) / \sqrt{2} \quad \text { and } \quad-t^{*} a\left(k_{(0,-1)}, 0_{(0,0)}\right) / \sqrt{2}
$$

respectively, i.e. they are of order one in the limit $Z \rightarrow \infty$.
To construct the next set of states in the hierarchy of accessible configuration, we must act with $A_{\sigma}$ on the periphery and re populate the central site. Without loss of generality we consider $\sigma=\downarrow$. For the first state in equation (15), $\left|k_{(1,0)}\right\rangle\left\langle 0_{(0,0)}\right||0\rangle$, we have only one possibility,

$$
\begin{equation*}
\left|q_{(0,-1)}\right\rangle\left\langle 0_{(0,0)}\right|\left|k_{(1,0)}\right\rangle\left\langle 0_{(0,0)}\right||\downarrow\rangle, \tag{16}
\end{equation*}
$$

which is a normalized state. The normalization of
$\left|q_{(1,-1)}\right\rangle\left\langle k_{(1,0)}\right|\left|k_{(1,0)}\right\rangle\left\langle 0_{(0,0)}\right||\downarrow\rangle=\frac{1}{\sqrt{Z}}\left|q_{(1,-1)}\right\rangle\left\langle 0_{(0,0)}\right||\downarrow\rangle$
is $1 / Z$ and therefore vanishes in the limit $Z \rightarrow \infty$ (here we have used (12)). States with overturned spins on the same subsystem therefore do not couple to the groundstate of $H^{(n)}$. Generalizing this result one can show that only states on the periphery with

$$
\begin{equation*}
\left|m_{\uparrow}\right|+\left|m_{\downarrow}\right| \leq 1 \tag{18}
\end{equation*}
$$

on the same subsystem contribute to the ground-state of $H^{(n)}$.

The other state, $\left|k_{(0,-1)}\right\rangle\left\langle 0_{(0,0)}\right||\uparrow \downarrow\rangle$, in equation (15) couples to $|0\rangle$ and to the normalized state

$$
\begin{equation*}
\left|q_{(0,1)}\right\rangle\left\langle 0_{(0,0)}\right|\left|k_{(0,-1)}\right\rangle\left\langle 0_{(0,0)}\right||\uparrow\rangle . \tag{19}
\end{equation*}
$$

The normalization of the state
$\left|q_{(0,0)}\right\rangle\left\langle k_{(0,-1)}\right|\left|k_{(0,-1)}\right\rangle\left\langle 0_{(0,0)}\right||\uparrow\rangle=\frac{1}{\sqrt{Z}}\left|q_{(0,0)}\right\rangle\left\langle 0_{(0,0)}\right||\downarrow\rangle$
does again vanish for $Z \rightarrow \infty$.
We therefore conclude that of all states on the periphery with $m_{\uparrow}=0=m_{\downarrow}$ only the ground-state $\left|0_{(0,0)}\right\rangle$ couples to the ground-state of $H^{(n)}$. The complete Hilbert space is therefore spanned by

$$
\begin{equation*}
\prod_{\left\{k_{( \pm 1,0)}\right\}}\left|k_{( \pm 1,0)}\right\rangle\left\langle 0_{(0,0)}\right| \prod_{\left\{k_{(0, \pm 1)}\right\}}\left|k_{(0, \pm 1)}\right\rangle\left\langle 0_{(0,0)}\right||x\rangle \tag{21}
\end{equation*}
$$

where $|x\rangle=|0\rangle,|\sigma\rangle$ or $|\uparrow \downarrow\rangle$ and where all $\left\{k_{( \pm 1,0)}\right\}$ and $\left\{k_{(0, \pm 1)}\right\}$ are mutually distinct, due to equation (11).

## 4 Mapping to the Anderson model

Let us define with $M_{\mathrm{s}}^{(n-1)}$ the number of non-zero matrix elements $a\left(k_{\mathbf{s}}, k_{(0,0)}\right)$. The $M_{\mathbf{s}}^{(n-1)}$ are related to the $M_{\sigma}^{(n-1)}$ occurring in (1) via

$$
\begin{equation*}
M_{\uparrow}^{(n-1)}=M_{(1,0)}^{(n-1)}+M_{(-1,0)}^{(n-1)} \tag{22}
\end{equation*}
$$

and

$$
\begin{equation*}
M_{\downarrow}^{(n-1)}=M_{(0,1)}^{(n-1)}+M_{(0,-1)}^{(n-1)} . \tag{23}
\end{equation*}
$$

The hybridization matrix elements $V_{l, \sigma}^{(n-1)}$ of (1) are given by

$$
\begin{equation*}
V_{l, \uparrow}^{(n-1)}=\frac{-t^{*}}{\sqrt{2}} a\left(l_{( \pm 1,0)}, 0_{(0,0)}\right) \tag{24}
\end{equation*}
$$

and respectively for $\sigma=\downarrow$. The onsite energies $\epsilon_{l, \sigma=\uparrow}^{(n-1)}$ of (1) are given by

$$
\begin{equation*}
\pm \epsilon_{l, \uparrow}^{(n-1)}=E\left(l_{( \pm 1,0)}\right)-E\left(0_{(0,0)}\right) \tag{25}
\end{equation*}
$$

where the $E\left(l_{\mathbf{s}}\right)$ are the diagonal energies of $H_{i}^{(n-1)}$,

$$
\begin{equation*}
E\left(l_{\mathbf{s}}\right) \equiv\left\langle l_{\mathbf{s}}, i\right| H_{i}^{(n-1)}\left|i, l_{\mathbf{s}}\right\rangle \tag{26}
\end{equation*}
$$

independent of $i$. Note, that all energies are measured with respect to the Fermi-energy $U / 2$, which is absorbed in equation (1) in the interaction term.

Let's us see how things work out for $S(1)$ and $S(2)$. The half-filled ground state of $S(0)$ is single occupied, let's say with an up-electron. We have then

$$
M_{(1,0)}^{(0)}=0=M_{(0,-1)}^{(0)}, \quad M_{(-1,0)}^{(0)}=1=M_{(0,1)}^{(0)}
$$

Table 1. The ground-state expectation values for the number of doubly occupied sites, $\langle d\rangle$, the local moment, $\langle m\rangle$ and of the kinetic energy, $\langle T\rangle$ (in units of $t^{*}$ ), see equation (28). The values are for $U=8$ and various Hubbard stars. $Z$ is the weight of the states retained, see equation (27). $L$ is the effective cluster size used.

|  | $\langle d\rangle$ | $\langle m\rangle$ | $\langle T\rangle$ | $Z$ | $L$ |
| :--- | :---: | ---: | ---: | :--- | :--- |
| $\mathrm{~S}(1)$ | 0.007687 | -0.492080 | -0.249824 | 1.0 | 2 |
| $\mathrm{~S}(2)$ | 0.007797 | 0.491952 | -0.249810 | 1.0 | 5 |
| $\mathrm{~S}(3)$ | 0.007807 | -0.491941 | -0.249896 | 0.99993 | 7 |
| $\mathrm{~S}(4)$ | 0.007807 | -0.491940 | -0.249901 | 0.99995 | 15 |

with

$$
\epsilon_{\uparrow}^{(0)}=-U / 2, \quad \epsilon_{\downarrow}^{(0)}=U / 2, \quad V_{\uparrow}^{(0)}=\frac{-t^{*}}{\sqrt{2}}=V_{\downarrow}^{(0)} .
$$

The Anderson model for Hubbard star S(1) corresponds therefore to a two-site cluster [8] and the number of states contributing to the ground-state (which has one $\uparrow$ - and one $\downarrow$-electron) is ( $\left.\begin{array}{l}2 \\ 1\end{array}\right)\binom{2}{1}=4$. The numbers of one-particle and one-hole excited states for $S(1)$ are all

$$
M_{( \pm 1,0)}^{(1)}=2=M_{(0, \pm 1)}^{(1)}
$$

and $S(2)$, the star of the stars, corresponds to a 5 -site cluster. The ground-state is realized for three $\uparrow$ - and two $\downarrow$-electrons (the state with two $\uparrow$ - and three $\downarrow$-electrons is higher in energy). One has therefore

$$
M_{(-1,0)}^{(2)}=50=M_{(0,1)}^{(2)}, \quad M_{(1,0)}^{(2)}=100=M_{(0,-1)}^{(2)}
$$

$\mathrm{S}(3)$ corresponds therefore to a 151 -site cluster.
Above considerations are valid for constructing the exact ground-state and one-particle Green's function in the antiferromagnetic state. Effective Anderson models for $S(1)$ and $S(2)$ can although be constructed for the paramagnetic state, though with an increased size [4].

## 5 Discussion

In view of the fact that the Hilbert-space increases exponentially with every iteration one needs to discuss the feasibility of truncation schemes. From the anticommutation rule

$$
c_{i, \sigma} c_{i, \sigma}^{\dagger}+c_{i, \sigma}^{\dagger} c_{i, \sigma}=1
$$

for every $i=1, \ldots, Z$ and $\sigma=\uparrow, \downarrow$ one can easily derive the sum-rule

$$
\begin{equation*}
\sum_{k_{\mathbf{s}}}\left|a\left(k_{\mathbf{s}}, 0_{(0,0)}\right)\right|^{2}+\sum_{k_{-\mathbf{s}}}\left|a\left(k_{-\mathbf{s}}, 0_{(0,0)}\right)\right|^{2}=1 \tag{27}
\end{equation*}
$$

which hold for both $\mathbf{s}=(\mathbf{1}, \mathbf{0})$ and $\mathbf{s}=(\mathbf{0}, \mathbf{1})$. Truncation schemes become feasible, when an exponentially large number of the matrix-elements (24) become small due to the sum-rule (27). An indication of whether this is the

Table 2. The same as in Table 1, for $U=4$.

|  | $\langle d\rangle$ | $\langle m\rangle$ | $\langle T\rangle$ | $Z$ | $L$ |
| :--- | :---: | ---: | :--- | :--- | :--- |
| $\mathrm{~S}(1)$ | 0.029127 | -0.467646 | -0.495066 | 1.0 | 2 |
| $\mathrm{~S}(2)$ | 0.030323 | 0.465713 | -0.493618 | 1.0 | 5 |
| $\mathrm{~S}(3)$ | 0.030728 | -0.465060 | -0.495726 | 0.99994 | 15 |

Table 3. The same as in Table 1, for $U=2$.

|  | $\langle d\rangle$ | $\langle m\rangle$ | $\langle T\rangle$ | $Z$ | $L$ |
| :--- | :---: | ---: | ---: | :--- | :--- |
| $\mathrm{~S}(1)$ | 0.091221 | -0.379144 | -0.905348 | 1.0 | 2 |
| $\mathrm{~S}(2)$ | 0.092159 | 0.372893 | -0.855795 | 1.0 | 5 |
| $\mathrm{~S}(3)$ | 0.097549 | -0.359257 | -0.878246 | 0.99953 | 15 |

case or not may be seen by studying the distribution of the $\left|a\left(k_{ \pm \mathbf{s}}, 0_{(0,0)}\right)\right|^{2}$ for $\mathrm{S}(2)$, which is given in Figure 2.

Due to the formation of a local moment the matrixelements shown in Figure 2 are different for $\sigma=\downarrow$ (solid bars) and $\sigma=\uparrow$ (dashed bars). Note, that Figure 2 can also be interpreted as the one-particle Green's function of $S(2)$ [4]. We observe that only a limited number of the transition matrix elements shown in Figure 2 has an appreciable weight. The number of relevant poles increases with cluster size.

We now consider in detail the ground-state properties of various Hubbard stars for $U=8,4$ and $U=2$ (see Tabs. 1, 2 and 3). For $S(1)$ and $S(2)$ we have constructed the exact ground-state wavefunctions and calculated the ground-state expectation values of the doubly-occupancy $\langle d\rangle$, the local moment, $\langle m\rangle$ and of the kinetic energy, $\langle T\rangle$, with (see Eq. (4))

$$
\begin{array}{r}
d=f_{\uparrow}^{\dagger} f_{\uparrow} f_{\downarrow}^{\dagger} f_{\downarrow}, \quad m=\left(f_{\uparrow}^{\dagger} f_{\uparrow}-f_{\downarrow}^{\dagger} f_{\downarrow}\right) / 2 \\
T=\frac{t^{*}}{\sqrt{2}} \sum_{\sigma=\uparrow, \downarrow}\left[f_{\sigma}^{\dagger} A_{\sigma}+A_{\sigma}^{\dagger} f_{\sigma}\right] . \tag{28}
\end{array}
$$

Since $S(3)$ corresponds to a cluster with $L=151$ sites we cannot diagonalize $\mathrm{S}(3)$ exactly. For $U=2$ and $U=4$ we have approximated $\mathrm{S}(3)$ with a $L=14+1$ site cluster, i.e. we have retained only the largest 14 transition matrix elements (per spin) $a\left(k_{\mathbf{s}}, 0_{(0,0)}\right)$ in equation (8) (all other matrix elements are set to zero). We also give in Tables 2 and 3 the accuracy of this approximation, i.e. the contribution $Z$ of the largest 14 matrix elements per spin to the sum-rule equation (27). We observe that the truncation is better for larger values of $U$. For $U=8$ it is possible to approximate $\mathrm{S}(3)$ already with by a $L=6+1$ site cluster and $S(4)$ by a $L=14+1$ site cluster, see Table 1 .

By setting the transition matrix elements to certain excited states on the periphery to zero a variational approximation is obtained. It turns out that all the neglected excitations (those with very small $a\left(k_{\mathbf{s}}, 0_{(0,0)}\right)$ ) are high in energy in the sense that they are either above the upper Hubbard band or below the lower Hubbard band, they contribute only to the tails of the respective Hubbard bands. One can therefore estimate the contribution
of these excitations to the ground-state of $S(3)$ by perturbation theory, their weight is $<10^{-3}$ for $U=2$ and $<10^{-4}$ for $U=4,8$. Inspecting the data presented in Tables 1, 2 and 3 for various $\mathrm{S}(n)$ one sees that convergence with $n$ is good, especially for $U=4$ and $U=8$. For $U=8$ the data has converged to within $0.01 \%$ for $\langle m\rangle$, to within $0.1 \%$ for $\langle T\rangle$ and to within $1 \%$ for $\langle d\rangle$.

In summary we have shown how the finite dimensional, minimal interacting Hilbert-Space of the Hubbard model on the infinite-D Bethe-lattice can be constructed iteratively on the basis of symmetry adapted transition operators. We explicitly provided the close relationship to the recursive construction of the one-particle Green's function based on the mapping to a self-consistent Anderson model. We have discussed the feasibility of truncation schemes in the iteration process, which are necessary due to the exponential increase of the Hilbert-space at every step of the iteration. We have found that the sum-rule for the transition-matrix elements leads to a natural truncation criterion. We have applied the truncation scheme to various Hubbard stars and estimated the ground-state
properties of the half-filled Hubbard model up to $0.1 \%$ accuracy.

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