The Hubbard Star

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The Hubbard model is solved exactly on a cluster, which consists of a central site connected to Z neighboring sites. For $Z \to \infty$ this "Hubbard Star" can be viewed as the elementary structural element of the Hubbard model on a lattice in high dimensions, since in this case the Hubbard model is known to reduce to an effective single-site problem. It is found that in this limit a novel type of mean field description becomes exact. Both the groundstate energy and the full thermodynamics for $T > 0$ is derived.

1. Introduction

Although the Hubbard model has an extremely simple form, it describes a quantum mechanical many-body problem of great complexity. In one dimension an exact solution for the ground state energy, based on the Bethe-Ansatz, has been obtained already some time ago [1]. However, for dimensions $d > 1$ there exist no analytic methods to derive exact results systematically – except for limiting cases where, for example, perturbation theory may be applied. The opposite extreme to $d = 1$ is the limit of *high* dimensions, $d = \infty$. This limit, which has only recently been introduced for the study of fermionic lattice models [2], has since been found to be very useful in a number of different applications [3–10]. In this limit many investigations become tractable, which are prohibitively difficult in lower dimensions. In particular, essential features of systems in $d = 3$, and even lower dimensions, are well described by the results in $d = \infty$ or expansions around it [3, 4, 11]. The simplifications arising in this approach have made possible the exact solution of a simplified Hubbard model (where only one spin species can hop) in $d = \infty$ [6]. In this case one can show that the solution has mean field character [7], albeit of a novel kind.

In spite of the simplifications mentioned above an exact solution of the full Hubbard model in $d = \infty$ has not been possible sofar – neither on a regular lattice, nor even on a Bethe lattice, which is known to give rise to further simplifications. In classical models (e.g. the Ising model) the solution in $d = \infty$, or on a Bethe lattice, is known to yield "the" mean field solution. On the other hand, in fermionic models with Hubbard interaction the situation is much more complex [3, 7], and one can no longer speak of a unique mean field solution. In fact, for the Hubbard model itself a non-trivial, controlled mean field solution (i.e. which one can be systematically improved by expansion in some small parameter and which is correct for all densities and interaction strengths) does not even exist yet. In this situation one may *define* the exact solution of a fermionic lattice model in $d = \infty$ as mean field solution with the above mentioned properties.

To gain insight into the yet unknown solution of the Hubbard model in $d = \infty$, and hence derive the first step towards a mean field theory for this model, we consider in this paper the essential structural element of a lattice in high dimensions: namely a (central) site, which is connected to Z otherwise unconnected neighbors (see Fig. 1a). This model, which we refer to as the "Hubbard Star", may be viewed as the elementary building block of the Hubbard model *both* on a regular, e.g. hypercubic, lattice in $d = Z/2$ dimensions and on a Bethe lattice with connectivity $K = Z - 1$. In view of the fact that for $Z \to \infty$ lattice models such as the Hubbard model reduce to a purely *local*, "atomic" problem [2, 3, 5–7] (the irreducible self-energy becomes site-*diagonal*, i.e. $\mathbf{k}$-independent), the Hubbard Star obviously captures some of the essential features of the infinite-dimensional Hubbard model, since it models a typical site in the high dimensional lattice. An obvious generalization of the Hubbard star is a double-star (Fig. 1b), which even allows one to study magnetic (e.g. antiferromagnetic) correlations between the two central sites.

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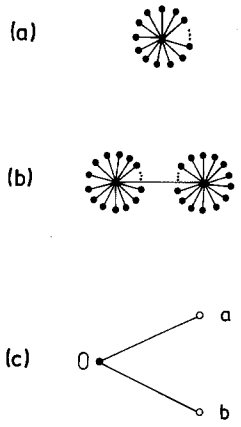

Fig. 1. a Schematic representation of the Hubbard Star studied in this paper; **b** Hubbard Double Star; **c** effective 3-site Hamiltonian that models the Hubbard Star for $T \neq 0$ (see Sect. 3 and 4)

In this paper we will mainly focus on the single Star, but the methods developed here can be straightforwardly extended to related models like the Double Star. One of the questions to be investigated is whether for $Z \to \infty$ this model can also be solved exactly by a mean-field description as was possible for the simplified Hubbard model [7].

The organization of this paper is as follows. The Hubbard Star Hamiltonian is introduced and discussed in some detail in Sect. 2. In Sect. 3 we show that in the limit $Z \to \infty$ a mean field description becomes exact and in Sect. 4 we calculate the thermodynamics of this model. In Sect. 5, the ground state energy is calculated exactly. A discussion of the results in Sect. 6 closes the presentation.

2. The Hubbard Star

We consider the Hubbard model for a star-like structure, which consists of a central site connected to Z otherwise unconnected sites (Fig. 1a). The corresponding Hamiltonian for the "Hubbard Star" is

$$\hat{H} = \hat{H}_t + \hat{H}_U \tag{1}$$

with the kinetic energy $\hat{H}_t$ and the interaction energy $\hat{H}_U$ given by

$$\hat{H}_t = -2t \sum_{\substack{i=1 \\ \sigma}}^{Z} (\hat{c}_{0\sigma}^{+} \hat{c}_{i\sigma} + \hat{c}_{i\sigma}^{+} \hat{c}_{0\sigma}) \tag{2a}$$

$$\hat{H}_U = U \sum_{i=0}^{Z} \hat{D}_i; \quad \hat{D}_i = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \tag{2b}$$

Here the operator $\hat{c}_{i\sigma}$ annihilates an electron at the central site $i=0$ or at the boundary ($1 \leqq i \leqq Z$), and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{+} \hat{c}_{i\sigma}$ denotes the number operator for spin-σ electrons at site i. As in the case of the Hubbard model with infinite range hopping [13], the kinetic energy $\hat{H}_t$ in (2a) can be diagonalized by introducing new fermions

$$\hat{A}_\sigma \equiv Z^{-1/2} \sum_{i=1}^{Z} \hat{c}_{i\sigma} \tag{3a}$$

whereby

$$\hat{H}_t = -2tZ^{1/2} \sum_{\sigma} (\hat{c}_{0\sigma}^{+} \hat{A}_\sigma + \hat{A}_\sigma^{+} \hat{c}_{0\sigma}) \tag{3b}$$

Obviously the non-interacting part of the Hamiltonian (1) is completely determined by only *two* fermionic degrees of freedom. With the definitions

$$\hat{\gamma}_{1\sigma} \equiv \frac{1}{\sqrt{2}} (\hat{c}_{0\sigma} + \hat{A}_\sigma) \tag{4a}$$

$$\hat{\gamma}_{2\sigma} \equiv \frac{1}{\sqrt{2}} (\hat{c}_{0\sigma} - \hat{A}_\sigma) \tag{4b}$$

and $\hat{\nu}_{k\sigma} \equiv \hat{\gamma}_{k\sigma}^{+} \hat{\gamma}_{k\sigma} (k = 1, 2)$, one finds that $\hat{H}_t$ assumes the form

$$\hat{H}_t = 2tZ^{1/2} \sum_{\sigma} (\hat{\nu}_{2\sigma} - \hat{\nu}_{1\sigma}) = \sum_{\substack{k=1,2 \\ \sigma}} \varepsilon_k \hat{\nu}_{k\sigma} \tag{5}$$

with $\varepsilon_1 = -\varepsilon_2 = -2tZ^{1/2}$. The ground state is given by $\hat{\nu}_{1\sigma} = 1$ and $\hat{\nu}_{2\sigma} = 0$ ($\sigma = \uparrow, \downarrow$), yielding a ground state energy of $2\varepsilon_1$. Note that the ground state is highly degenerate, since the kinetic energy is determined by only 2 out of a total of $Z+1$ degrees of freedom.

An interesting special case, that will be discussed in Sect. 3, is obtained in the limit $Z \to \infty$. This limit is very similar to the limit of high dimensions ($d \to \infty$), since in both cases the number of nearest neighbors becomes large. In high dimensions each site on a hypercubic lattice is connected to $Z = 2d$ neighboring sites via hopping processes with hopping amplitude $t \propto Z^{-1/2}$. Since the main motivation for studying the Hubbard Star is to model the influence of high dimensions, we choose the same scaling here. More precisely, we choose $t = \bar{t}/(2Z^{1/2})$, with $\bar{t}$ fixed as $Z \to \infty$. All energies are measured in terms of $\bar{t}$. For convenience we set $\bar{t} = 1$ below.

3. Exact mean field theory for the Hubbard Star

We will now show that the thermodynamics of the Hubbard Star becomes relatively simple in the limit of many boundary sites ($Z \to \infty$). In this limit the properties of the central site ($i=0$) can be calculated *exactly* from a novel mean field description [7].

The Hubbard Star at positive temperatures ($T > 0$) shows both trivial and highly non-trivial features if one considers the limit $Z \to \infty$. The trivial aspect appears when one considers the Star *as a whole*. At positive temperatures the free energy is extensive, proportional to Z, so that the kinetic energy and the interaction energy of the central site (which are of the order of unity) can be neglected. The remaining boundary sites are effectively uncoupled. The situation is then identical to that known from the Hubbard model with infinite range hopping, which can be solved exactly, too [13]. In this model

the kinetic energy is found to commute with the interaction part, i.e. they decouple [14]. Hence the grand-canonical partition function of the Hubbard Star is given by

$$\Xi_{HS} \sim C \prod_{i=1}^{Z} \mathrm{Tr}[\mathrm{e}^{-\beta(U\hat{D}_i - \mu\hat{n}_i)}]$$
$$\sim C(1+2\mathrm{e}^{\beta\mu}+\mathrm{e}^{2\beta\mu-\beta U})^Z, \quad Z\to\infty \tag{6}$$

where $\hat{n}_i = \hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}$ and $C>0$ is some constant. The grand potential and all thermodynamic quantities of interest then follow automatically.

The highly non-trivial aspects appear when one focusses on the central site ($i=0$). This site allows for a Hubbard interaction and is coupled to a bath of Z other sites with Hubbard interaction via hopping processes with hopping amplitude of order $Z^{-1/2}$ (as $Z\to\infty$). All this is familiar from the usual Hubbard model in high dimensions. The quantities of interest are therefore not the properties of the bath, but rather those of the central site. Since all these quantities (the double occupancy, kinetic energy, entropy and others) can be expressed in terms of Green functions, we shall consider these in the remainder of this section.

Therefore we consider Green functions of the form

$$G_{ij}(\tau) \equiv \langle T_\tau \hat{c}_{i\sigma}(\tau)\hat{c}^+_{j\sigma}(0)\rangle \tag{7}$$

where $0\leqq i,j\leqq Z$ and $\hat{c}_{i\sigma}(\tau)$ is a Heisenberg operator. The Green function G_{ij} is not the most general one, but the extension of the considerations presented below to other Green functions is straightforward. To obtain an impression of the order of magnitude of G_{ij} as $Z\to\infty$, we consider first $i=j$ and then $i\neq j$. For $i=j$, $G_{ij}(\tau)$ is clearly of order unity for all values of Z and all sites i. Let us therefore assume that $1\leqq i\leqq Z$ but $j=0$. By expanding the exponentials (such as $\mathrm{e}^{\tau\hat{H}}$), occurring in the definition of $\hat{c}_{i\sigma}(\tau)$, in a power series in $\hat{H}$, one finds that non-zero contributions to the trace in (7) require at least one hopping process from site i to site 0. The amplitude for this process is of order $t=1/2Z^{1/2}$, so that the Green function G_{i0} is of order $Z^{-1/2}$. Similarly G_{ij} with $i\neq 0$ and $j\neq 0$ (but $i\neq j$) requires at least two jumps, implying that this Green function is of order Z^{-1}.

Since we are mainly interested in the properties of the central site, we focus on the Green function $G_{00}(\tau)$. For $Z\to\infty$ the central site is surrounded by infinitely many other sites. It is intuitively clear that this site experiences only some *average* influence of the bath. One therefore expects that the central site can be described *exactly* by a mean-field description. This expectation will now shown to be correct.

The construction of the exact mean field theory for the central site proceeds in two steps. In the first step we show that the Green function $G_{00}(\tau)$ is coupled only to a finite number of other Green functions by the equations of motion. In the second step we show that the equations of motion may equally be obtained from a simple effective Hamiltonian containing only a few new quantum mechanical degrees of freedom. These new degrees of freedom will then be interpreted as mean field variables.

To show that $G_{00}(\tau)$ is coupled only to a finite number of other Green functions, we consider its equation of motion:

$$\frac{\partial}{\partial\tau}G_{00}(\tau) = \delta(\tau) + \langle T_\tau[\hat{H}(\tau)-\mu\hat{N},\, \hat{c}_{0\sigma}(\tau)]\,\hat{c}^+_{0\sigma}(0)\rangle \tag{8a}$$
$$= \delta(\tau) + \langle T_\tau \hat{A}_\sigma(\tau)\hat{c}^+_{0\sigma}(0)\rangle - U\langle T_\tau \hat{n}_{0-\sigma}(\tau)\hat{c}_{0\sigma}(\tau)\hat{c}^+_{0\sigma}(0)\rangle + \mu G_{00}(\tau) \tag{8b}$$

where $\hat{N}=\sum_{i\sigma}\hat{n}_{i\sigma}$. In (8b) we worked out the commutator in (8a). Equation (8b) is interesting because it shows that the only new dynamical degree of freedom entering in $\partial G_{00}/\partial\tau$ is the collective variable $\hat{A}_\sigma(\tau)$. In turn $\hat{A}_\sigma(\tau)$ also gives rise to new degrees of freedom. This may be seen from

$$\frac{\partial}{\partial\tau}\langle T_\tau \hat{A}_\sigma\hat{c}^+_{0\sigma}(0)\rangle = \langle T_\tau[\hat{c}_{0\sigma}(\tau) - U\hat{B}_\sigma(\tau)+\mu\hat{A}_\sigma(\tau)]\,\hat{c}^+_{0\sigma}(0)\rangle \tag{9a}$$

which introduces the new variable

$$\hat{B}_\sigma = Z^{-1/2}\sum_{i=1}^{Z}\hat{n}_{i-\sigma}\hat{c}_{i\sigma}. \tag{9b}$$

The basic point is that the equation of motion for $\langle T_\tau \hat{B}_\sigma(\tau)\hat{c}^+_{0\sigma}(0)\rangle$ does *not* lead to new terms, i.e., the proliferation of dynamical degrees of freedom stops here. This may be seen from

$$\frac{\partial}{\partial\tau}\langle T_\tau \hat{B}_\sigma(\tau)\hat{c}^+_{0\sigma}(0)\rangle$$
$$= \left\langle T_\tau\left\{\left(\frac{1}{Z}\sum_{i=1}^{Z}\hat{n}_{i-\sigma}(\tau)\right)\hat{c}_{0\sigma}(\tau) + (\mu-U)\,\hat{B}_\sigma(\tau)\right\}\hat{c}^+_{0\sigma}(0)\right\rangle$$
$$+ \text{corrections} \tag{10a}$$

where the corrections are given by

$$-\frac{1}{Z}\sum_i\langle T_\tau(\hat{c}^+_{0-\sigma}(\tau)\hat{c}_{i-\sigma}(\tau)+\hat{c}_{0-\sigma}(\tau)\hat{c}^+_{i-\sigma}(\tau))\,\hat{c}_{i\sigma}(\tau)\hat{c}^+_{0\sigma}(0)\rangle. \tag{10b}$$

Arguments similar to those sketched below (7) show that the corrections, (10b), are of relative order Z^{-1} compared to the dominant terms and can hence be neglected as $Z\to\infty$. Furthermore, apart from corrections of order Z^{-1}, the sum $Z^{-1}\sum_i\hat{n}_{i-\sigma}$ in (10a) can be replaced by the density (c-number!) $n_{-\sigma}=n/2$, so that, to leading order, the r.h.s. of (10a) reduces to

$$\frac{\partial}{\partial\tau}\langle T_\tau \hat{B}_\sigma(\tau)\hat{c}^+_{0\sigma}(0)\rangle = \tfrac{1}{2}nG_{00}(\tau) + (\mu-U)\langle T_\tau \hat{B}_\sigma(\tau)\hat{c}^+_{0\sigma})0)\rangle. \tag{11}$$

In summary: the dynamics of $G_{00}(\tau)$ involves only 3 dynamical degrees of freedom, namely $\hat{c}_{0\sigma}$, $\hat{A}_\sigma$ and $\hat{B}_\sigma$. Apart from corrections of order Z^{-1} the commutator algebra of $\hat{c}_{0\sigma}$, $\hat{A}_\sigma$ and $\hat{B}_\sigma$ is *closed*.

Next we address the second step: the derivation of an effective Hamiltonian that yields the same equations of motion as the original Hamiltonian for the Hubbard Star [7]. As a first requirement we impose that the variables occurring in the effective Hamiltonian are proper fermionic variables. Note that $\hat{A}_\sigma$ and $\hat{B}_\sigma$ are *not* properly normalized. We therefore transform to new variables:

$$\hat{a}_\sigma \equiv \left(1-\frac{n}{2}\right)^{-1/2}(\hat{A}_\sigma - \hat{B}_\sigma) \tag{12a}$$

$$\hat{b}_\sigma \equiv \left(\frac{n}{2}\right)^{-1/2}\hat{B}_\sigma. \tag{12b}$$

The interpretation of $\hat{a}_\sigma$ and $\hat{b}_\sigma$ is that they annihilate a σ-electron on a boundary site, provided that this site is ($\hat{b}_\sigma$) or is not ($\hat{a}_\sigma$) doubly occupied. The variables $\hat{a}_\sigma$, $\hat{b}_\sigma$ and $\hat{c}_{0\sigma}$ satisfy proper fermionic commutation relations apart from negligible corrections of order Z^{-1}.

The time evolution of the Green functions involving $\hat{a}_\sigma$, $\hat{b}_\sigma$ and $\hat{c}_{0\sigma}$ is completely determined by the commutators between these operators and the grand canonical Hamiltonian $(\hat{H}-\mu\hat{N})$. The important point is now, that these commutators can equally be calculated from the following effective Hamiltonian, depending only on $\hat{a}_\sigma$, $\hat{b}_\sigma$ and $\hat{c}_{0\sigma}$:

$$\hat{H}_{\mathrm{MF}} = \hat{H}_t^{\mathrm{MF}} + \hat{H}_U^{\mathrm{MF}} + \hat{H}_\mu^{\mathrm{MF}} \tag{13a}$$

where

$$\begin{aligned}
\hat{H}_t^{\mathrm{MF}} &= \\
&-\sum_\sigma \left\{ \sqrt{1-\frac{n}{2}}\,(\hat{a}_\sigma^+ \hat{c}_{0\sigma} + \hat{c}_{0\sigma}^+ \hat{a}_\sigma) + \sqrt{\frac{n}{2}}\,(\hat{b}_\sigma^+ \hat{c}_{0\sigma} + \hat{c}_{0\sigma}^+ \hat{b}_\sigma) \right\} \\
\hat{H}_U^{\mathrm{MF}} &= U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} \\
\hat{H}_\mu^{\mathrm{MF}} &= -\mu\sum_\sigma (\hat{n}_{0\sigma}+\hat{n}_{a\sigma}) - (\mu-U)\sum_\sigma \hat{n}_{b\sigma}
\end{aligned} \tag{13b}$$

and $\hat{n}_{a\sigma} \equiv \hat{a}_\sigma^+ \hat{a}_\sigma$ and similarly for $\hat{n}_{b\sigma}$. Note that $\hat{H}_{\mathrm{MF}}$ is an effective Hamiltonian for a 3-site model (see Fig. 1c) with a Hubbard interaction only on the central site. The Hamiltonian $\hat{H}_{\mathrm{MF}}$ carries the label MF since it shows all the familiar characteristics of a mean field Hamiltonian, where $\hat{a}_\sigma$ and $\hat{b}_\sigma$ play the role of mean field *operators* [7]. The interpretation of (13) is that the influence of the bath on the central site enters only through the two collective (mean field) variables $\hat{a}_\sigma$ and $\hat{b}_\sigma$ describing sites that are ($\hat{b}_\sigma$) or are not ($\hat{a}_\sigma$) doubly occupied. Note that the Hubbard interaction U modifies the chemical potential of the $\hat{b}$-variables.

Stated differently, Eq. (13) shows that non-zero contributions to thermodynamic quantities come only from a very small subspace of the total Hilbert space. The mean field Hamiltonian is therefore nothing but a projection of the original Hamiltonian onto that small subspace. Since $\hat{H}_{\mathrm{MF}}$ in (13) is a Hamiltonian for a finite (3-site) system, it is clear that all thermodynamic quantities of interest can readily be calculated from (13). This will be done in the following section.

4. Thermodynamics of the Hubbard Star

We restrict our evaluation to the half-filled case, with $N_\uparrow = N_\downarrow$. The partition function $\mathscr{Z}$ of the three-site model, on which the effective Hamiltonian (13) operates, is given by

$$\mathscr{Z} = \mathrm{Tr}\, \mathrm{e}^{-\beta\hat{H}_{\mathrm{MF}}} = \sum_{N=0}^{6} Z_N \tag{14}$$

where $Z_N = \mathrm{Tr}_N \exp(-\beta\hat{H}_{\mathrm{MF}})$ involves the trace over states with $N(=0, 1, \ldots, 6)$ electrons. Since $n=1$, the chemical potential is $\mu = U/2$; in this case

$$\hat{H}_\mu^{\mathrm{MF}} = -\frac{U}{2}\sum_\sigma (\hat{n}_{0\sigma}+\hat{n}_{a\sigma}-\hat{n}_{b\sigma}) \tag{15a}$$

$$\equiv \hat{\mathscr{H}}_\mu - \frac{U}{2}\hat{N} \tag{15b}$$

with $\hat{N} = \sum_\sigma (\hat{n}_{0\sigma}+\hat{n}_{a\sigma}+\hat{n}_{b\sigma})$ and $\hat{\mathscr{H}}_\mu = U\sum_\sigma \hat{n}_{b\sigma}$. For $n=1$ the Hamiltonian (13) is invariant under the particle-hole (ph) transformation

$$\begin{aligned}
&\hat{a}_\sigma^+ \to \hat{b}_\sigma, && \hat{a}_\sigma \to \hat{b}_\sigma^+ \\
&\hat{b}_\sigma^+ \to \hat{a}_\sigma, && \hat{b}_\sigma \to \hat{a}_\sigma^+ \\
&\hat{c}_{0\sigma}^+ \to -\hat{c}_{0\sigma}, && \hat{c}_{0\sigma} \to -\hat{c}_{0\sigma}^+
\end{aligned} \tag{16}$$

which interchanges $\hat{a}_\sigma$ and $\hat{b}_\sigma$. This implies $Z_0 = Z_6$, $Z_1 = Z_5$ and $Z_2 = Z_4$, whereby the problem simplifies:

$$\mathscr{Z} = Z_3 + 2\sum_{N=0}^{2} Z_N. \tag{17}$$

Furthermore, it is more convenient to work with the Hamiltonian

$$\hat{\mathscr{H}} \equiv \hat{H}_t^{\mathrm{MF}} + \hat{H}_U^{\mathrm{MF}} + \hat{\mathscr{H}}_\mu = \hat{H}_{\mathrm{MF}} + \frac{U}{2}\hat{N} \tag{18}$$

referring to a fixed particle number, whereby

$$\mathscr{Z} = \mathrm{e}^{\frac{3}{2}\beta U}\mathscr{Z}_3 + 2\sum_{N=0}^{2} \mathrm{e}^{\frac{1}{2}\beta UN}\mathscr{Z}_N \tag{19}$$

with $\mathscr{Z}_n = \mathrm{Tr}_N \exp(-\beta\hat{\mathscr{H}})$. The explicit calculation of $\mathscr{Z}_N$ is tedious, but straight-forward, and is described in Appendix A.

The expectation value of an operator $\hat{\mathcal{O}}$ is then given by

$$\langle\hat{\mathcal{O}}\rangle = \sum_{N=0}^{6} p_N \langle\mathcal{O}\rangle_N \tag{20a}$$

with $p_N = Z_N/\mathscr{Z}$ and

$$\langle\hat{\mathcal{O}}\rangle_N = \frac{1}{Z_N}\mathrm{Tr}_N(\hat{\mathcal{O}}\mathrm{e}^{-\beta\hat{H}_{\mathrm{MF}}}). \tag{20b}$$

Under the ph-transformation (16) one has $p_N \to p_{6-N}$ and $\hat{\mathcal{O}} \to \hat{\mathcal{O}}'$, such that

$$\langle \hat{\mathcal{O}} \rangle = \tfrac{1}{2} p_3 \langle \hat{\mathcal{O}} + \hat{\mathcal{O}}' \rangle_3 + \sum_{N=0}^{2} p_N \langle \hat{\mathcal{O}} + \hat{\mathcal{O}}' \rangle_N . \tag{20c}$$

4.1. Double occupancy of central site

Under the ph-transformation (16) the number operator for double occupancy at the central site, $\hat{D}_c \equiv \hat{H}_U^{\mathrm{MF}}/U$, (13b), transforms into $\hat{E}_c \equiv \hat{D}_c'$, the operator for an empty site ("hole"). Once the matrix representation of $\hat{\mathscr{D}} \equiv \hat{D}_c + \hat{E}_c$ for different N is known, $\langle \hat{D}_c \rangle$ can be calculated from (20c). We now calculate $\langle \hat{\mathscr{D}} \rangle_N$ using the results for the Hamiltonian $\hat{\mathscr{H}}$ derived in Appendix A:

(i) $N=0$: $\hat{\mathscr{D}}=1$, such that $\langle \hat{\mathscr{D}} \rangle_0 = 1$.
(ii) $N=1$: There are $2 \times 3 = 6$ states. For $\sigma = \uparrow$ one has $\hat{\mathscr{D}}_\uparrow = \mathrm{diag}(1, 0, 1)$, where $\mathrm{diag}(a, b, c, \ldots)$ is a diagonal matrix with elements $a, b, c, \ldots$ etc. Hence

$$\langle \hat{\mathscr{D}} \rangle_1 = 2 \mathscr{Z}_1^{-1} \mathrm{Tr}(\hat{\mathscr{D}}_\uparrow \mathrm{e}^{-\beta \hat{\mathscr{H}}_\uparrow}) \tag{21}$$

(iii) $N=2$: For $(\uparrow\uparrow)$ we have $\hat{\mathscr{D}}_{\uparrow\uparrow} = \mathrm{diag}(0, 1, 0)$, while for $(\uparrow\downarrow)$
$\hat{\mathscr{D}}_{\uparrow\downarrow} = \mathrm{diag}(1, 0, 1, 0, 1, 0, 1, 0, 1)$. Hence

$$\langle \hat{\mathscr{D}} \rangle_2 = \mathscr{Z}_2^{-1} [2 \mathrm{Tr}(\hat{\mathscr{D}}_{\uparrow\uparrow} \mathrm{e}^{-\beta \hat{\mathscr{H}}_\uparrow}) + \mathrm{Tr}(\hat{\mathscr{D}}_{\uparrow\downarrow} \mathrm{e}^{-\beta \hat{\mathscr{H}}_\downarrow})]. \tag{22}$$

(iv) $N=3$: For $(\uparrow\uparrow\uparrow)$ one has $\hat{\mathscr{D}}_{\uparrow\uparrow\uparrow} = 0$ and for $(\uparrow\uparrow\downarrow)$
$\hat{\mathscr{D}}_{\uparrow\uparrow\downarrow} = \mathrm{diag}(0, 1, 0, 1, 0, 1, 0, 1, 0)$; hence

$$\langle \hat{\mathscr{D}} \rangle_3 = 2 \mathscr{Z}_3^{-1} \mathrm{Tr}(\hat{\mathscr{D}}_{\uparrow\uparrow\downarrow} \mathrm{e}^{-\beta \hat{\mathscr{H}}_{\uparrow\uparrow\downarrow}}) \tag{23}$$

The U-dependence of the double occupancy of the central site is shown in Fig. 2 for different temperatures.

4.2. Kinetic energy

The kinetic energy is given by

$$E_{\mathrm{kin}} = \langle \hat{H}_t^{\mathrm{MF}} \rangle \tag{24a}$$
$$= \langle \hat{H}_{\mathrm{MF}} \rangle - \langle \hat{\mathscr{H}}_\mu \rangle + \tfrac{3}{2} U - U \langle \hat{D}_c \rangle . \tag{24b}$$

The invariance of $\hat{H}_{\mathrm{MF}}$ under ph-transformation implies

$$\langle \hat{H}_{\mathrm{MF}} \rangle = p_3 \langle \hat{H}_{\mathrm{MF}} \rangle_3 + 2 \sum_{N=0}^{2} p_N \langle \hat{H}_{\mathrm{MF}} \rangle_N \tag{25a}$$

where

$$\langle \hat{H}_{\mathrm{MF}} \rangle_N = \frac{1}{\mathscr{Z}_N} \sum_\nu E_\nu \mathrm{e}^{-\beta E_\nu} - \frac{U}{2} N \tag{25b}$$

with E_ν as the eigenvalues of $\hat{\mathscr{H}}$ in the subspace with N electrons (see Appendix A). It remains to calculate $\langle \hat{\mathscr{H}}_\mu \rangle$ in (24b).

We note that the ph-transformation implies the following changes: $\hat{\mathscr{H}}_\mu = U \sum_\sigma \hat{n}_{b\sigma} \to \hat{\mathscr{H}}_\mu' = \sum_\sigma (1 - \hat{n}_{a\sigma})$ and hence $\langle \hat{\mathscr{H}}_{\mu} \rangle_N \to \langle \hat{\mathscr{H}}_\mu' \rangle_{6-N}$. For convenience we introduce the number operator

$$\hat{M} = \sum_\sigma (1 - \hat{n}_{a\sigma} + \hat{n}_{b\sigma}) \tag{26a}$$

such that

$$\langle \hat{\mathscr{H}}_\mu + \hat{\mathscr{H}}_\mu' \rangle_N = U \langle \hat{M} \rangle_N . \tag{26b}$$

We now calculate $\langle \hat{M} \rangle_N$.

(i) $N=0$: Since $\hat{M}=2$ we find $\langle \hat{M} \rangle_0 = 2$.
(ii) $N=1$: For $\sigma = \uparrow$ one finds $\hat{M}_\uparrow = \mathrm{diag}(1, 2, 3)$ and hence $\langle \hat{M} \rangle_1$ is given by (21) with $\hat{\mathscr{D}}_\uparrow$ replaced by $\hat{M}_\uparrow$.
(iii) $N=2$: For $(\uparrow\uparrow)$ we have $\hat{M}_{\uparrow\uparrow} = \mathrm{diag}(1, 2, 3)$, while for $(\uparrow\downarrow)$

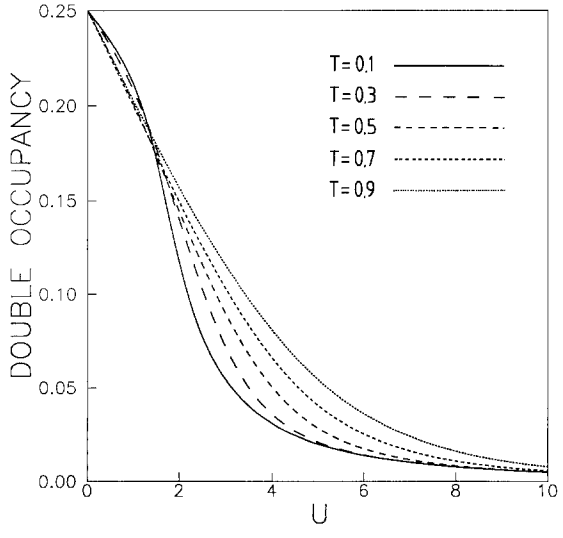

Fig. 2. Double occupancy of central site vs. interaction U for various temperatures T; here $k_B = 1$ and all energies are measured in units of $\bar{t} = 1$

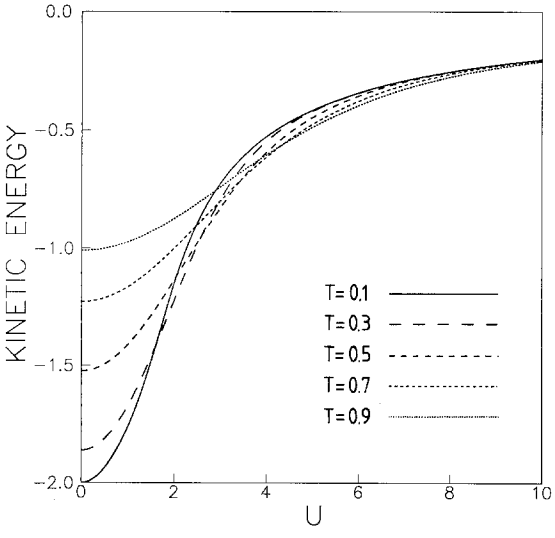

Fig. 3. Kinetic energy vs. interaction U for various temperatures T; here $k_B = 1$ and all energies are measured in units of $\bar{t} = 1$

$\hat{M}_{\uparrow\downarrow}=\mathrm{diag}(0,1,2,3,4,3,2,1,2)$, so that $\langle\hat{M}\rangle_2$ is given by (22) with the $\hat{\mathscr{D}}$-operators replaced by the corresponding $\hat{M}$-operators.

(iv) $N=3$: For $(\uparrow\uparrow\uparrow)$ one finds $\hat{M}_{\uparrow\uparrow\uparrow}=2$, while for $(\uparrow\uparrow\downarrow)$ $\hat{M}_{\uparrow\uparrow\downarrow}=\mathrm{diag}(0,1,2,3,4,1,2,3,2)$, so that

$$\langle\hat{M}\rangle_3=2\mathscr{Z}_3^{-1}[2\mathrm{e}^{-\beta U}+\mathrm{Tr}(\hat{M}_{\uparrow\uparrow\downarrow}\mathrm{e}^{-\beta\hat{\mathscr{H}}_{\uparrow\uparrow\downarrow}})]. \tag{27}$$

Thereby $\langle\hat{\mathscr{H}}_u\rangle$ is provided via (20c) and E_{kin} in (24) is fully determined.

The kinetic energy is shown in Fig. 3 as a function of U for different temperatures.

5. Ground state energy of the Hubbard Star

The properties of the Hubbard Star in the ground state ($T=0$) differ strongly from those for $T>0$. Most notably, for a fixed average density N/Z the free energy is *extensive* as $Z\to\infty$ for $T>0$, whereas the ground state energy remains *finite* for large Z. This may be seen directly from (5), where ε_1 and ε_2 are finite ($\varepsilon_1=-\varepsilon_2=-1$) due to our choice $t=1/(2Z^{1/2})$. In the following we show that the ground state energy of the Hubbard Star can be calculated exactly, at least for the half-filled case. With this restriction the result is valid for an arbitrary number of sites in the Hubbard Star ($Z+1$) and for arbitrary numbers of $\uparrow$- and $\downarrow$-spins.

In order to derive an explicit expression for the ground state wave function, we first construct a fully symmetric wave function $|\psi_0\rangle$ for $N_\uparrow$ up- and $N_\downarrow$ down-electrons on the $Z=N\equiv N_\uparrow+N_\downarrow$ boundary sites. This wave function should satisfy two conditions:

i) all sites on the boundary should be equivalent and,
ii) no double occupancy is allowed.

Whereas the first condition is introduced in order to preserve the symmetry of the Hamiltonian, the second one ensures the search for the state of lowest energy, i.e., the ground state. Let us substantiate the second point. In the large U limit, states can be classified in accord with the total number of double occupancies. In particular, the ground state belongs to the subspace of total energy approaching 0 (absence of double occupancy). Then, a continuity argument shows that the ground state wave function has to be related to this subspace also for finite U values.

The wave function satisfying the previously discussed conditions is:

$$|\psi_0\rangle=\sqrt{\frac{N_\uparrow!\,N_\downarrow!}{N!}}\sum_{\{\sigma_i\}}\hat{c}^+_{1\sigma_1}\hat{c}^+_{2\sigma_2}\ldots\hat{c}^+_{N\sigma_N}|0\rangle, \tag{28}$$

where the sum is over all permutations of N integers. Note that $|\psi_0\rangle$ is properly normalized:

$$\langle\psi_0|\psi_0\rangle=1.$$

Next, we construct a wave function $|\psi_1\rangle=\hat{c}^+_{0\uparrow}|\psi_0\rangle$ describing $N+1$ electrons on the Star, and repeatedly apply the Hamiltonian $\hat{H}$ (1) to this wave function to produce new wave functions. The procedure ends when a closed subspace is arrived. In this case, the following set of orthonormal wave functions forms a basis of the subspace:

$$\begin{aligned}
|\psi_1\rangle&=\hat{c}^+_{0\uparrow}|\psi_0\rangle\\
|\psi_2\rangle&=\frac{1}{\sqrt{4N_\uparrow N_\downarrow}}\hat{c}^+_{0\uparrow}\sum_{1\le i\ne j\le N}(\hat{c}^+_{i\uparrow}\hat{c}_{j\uparrow}-\hat{c}^+_{i\downarrow}\hat{c}_{j\downarrow})|\psi_0\rangle\\
|\psi_3\rangle&=\frac{1}{\sqrt{N_\downarrow(N_\downarrow-1)}}\hat{c}^+_{0\downarrow}\sum_{1\le i\ne j\le N}\hat{c}^+_{i\uparrow}\hat{c}_{j\downarrow}|\psi_0\rangle\\
|\psi_4\rangle&=\frac{1}{\sqrt{N_\downarrow(N_\uparrow+1)}}\hat{c}^+_{0\downarrow}\sum_{i=1}^{N}\hat{c}^+_{i\uparrow}\hat{c}_{i\downarrow}|\psi_0\rangle\\
|\psi_5\rangle&=\frac{1}{\sqrt{2N_\downarrow}}\sum_{i=1}^{N}(\hat{c}^+_{i\uparrow}+\hat{c}^+_{0\uparrow}\hat{c}^+_{0\downarrow}\hat{c}_{i\downarrow})|\psi_0\rangle.
\end{aligned} \tag{29}$$

The representation of $\hat{H}$ in this basis takes the form:

$$\hat{H}=\begin{pmatrix}0&0&0&0&\beta_1\\0&U&0&0&\beta_2\\0&0&U&0&\beta_3\\0&0&0&0&\beta_4\\\beta_1&\beta_2&\beta_3&\beta_4&U\end{pmatrix} \tag{30a}$$

where the matrix elements $\beta_1,\ldots,\beta_4$ are given by

$$\begin{aligned}
\beta_1&=-\sqrt{\frac{2N_\downarrow}{N}};\qquad \beta_2=\sqrt{\frac{2N_\uparrow}{N}};\\
\beta_3&=\sqrt{\frac{2(N_\downarrow-1)}{N}};\qquad \beta_4=\sqrt{\frac{2(N_\uparrow+1)}{N}}.
\end{aligned} \tag{30b}$$

The formulae needed to check the orthonormality of the basis and to obtain the Hamiltonian matrix elements are given and proved, in some cases, in Appendix B.

Matrix (30a) can be reduced noting that an appropriate linear combination of $|\psi_1\rangle$ and $|\psi_4\rangle$ gives an eigenstate of constant energy equal to 0 whereas a combination of $|\psi_2\rangle$ and $|\psi_3\rangle$ produces a second eigenstate of constant energy equal to U. The remaining three-dimensional subspace is spanned by:

$$\begin{aligned}
|\tilde{\psi}_1\rangle&=\frac{1}{\sqrt{\beta_1^2+\beta_4^2}}(\beta_1|\psi_1\rangle+\beta_4|\psi_4\rangle)\\
|\tilde{\psi}_2\rangle&=\frac{1}{\sqrt{\beta_2^2+\beta_3^2}}(\beta_2|\psi_2\rangle+\beta_3|\psi_3\rangle)\\
|\tilde{\psi}_3\rangle&=|\psi_5\rangle.
\end{aligned} \tag{31}$$

Within the basis, the Hamiltonian takes the form:

$$\hat{H}=\begin{pmatrix}0&0&\gamma_1\\0&U&\gamma_2\\\gamma_1&\gamma_2&U\end{pmatrix}, \tag{32a}$$

where the matrix elements γ_1 and γ_2 are:

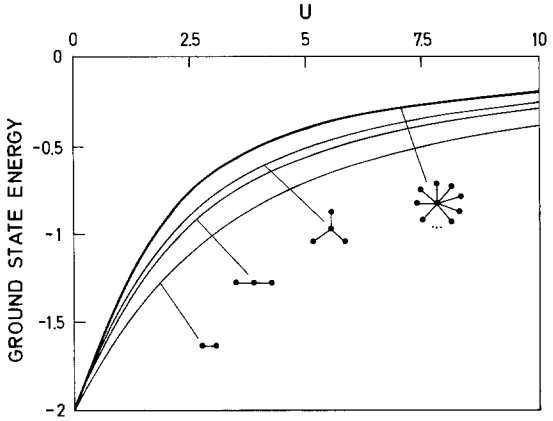

Fig. 4. U-dependence of the groundstate energy of Hubbard Stars with increasing number ($Z=2, 3, 4, \infty$) of boundary sites

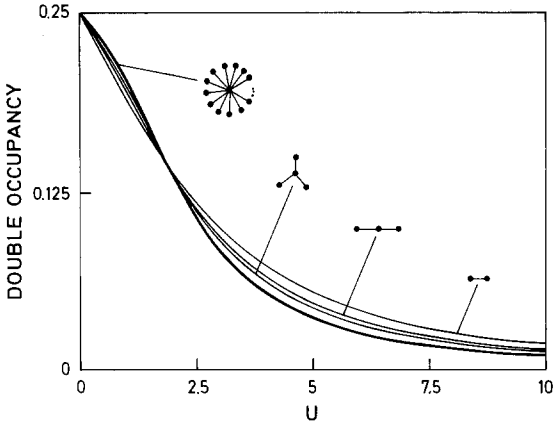

Fig. 5. U-dependence of the double occupancy of the central site of Hubbard Stars with increasing number ($Z=2, 3, 4, \infty$) of boundary sites (ground state)

$$\gamma_1=\sqrt{\frac{2(N+1)}{N}}$$
$$\gamma_2=\sqrt{\frac{2(N-1)}{N}}. \tag{32b}$$

One important property of (32) should be mentioned at this point: the Hamiltonian matrix does not depend on $N_\uparrow$ and $N_\downarrow$ separately, but only on the sum of both $N_\uparrow+N_\downarrow=N$. In particular, the lowest eigenvalue of (32a) is the same for all $N_\uparrow=0, 1, \ldots, N-1$ values, i.e., the ground state is N-fold degenerate. This result might be surprising at first sight but it is in accord with Lieb's theorem on the ground state of the Hubbard model with positive U on a biparticle cluster [15]. In our case the central atom is of one type whereas all the surface atoms are of the other type. This implies a "non-degenerate" ground state except for the trivial spin degeneracy that equals

$$2S+1=2[\tfrac{1}{2}(N-1)]+1=N. \tag{33}$$

Moreover, the fact that the total spin is $\frac{1}{2}(N-1)$ can be understood on physical grounds: due to the topology of the cluster, only two electrons (see (3b)) are allowed to form a bond, reducing an initial total spin of $\frac{1}{2}(N+1)$ to $\frac{1}{2}(N-1)$.

The eigenvalues of (32a) are given by the roots of the characteristic equation:

$$E(E-U)^2-4E+\frac{2(N+1)}{N}U=0. \tag{34}$$

The ground state energy as a function of U is given in Fig. 4 for several values of N. Once the energy is known, also the double occupancy of the central site can be obtained by noting that only $|\tilde{\psi}_3\rangle=|\psi_5\rangle$ contributes to the mean value $\langle\hat{c}^+_{0\uparrow}\hat{c}_{0\uparrow}\hat{c}^+_{0\downarrow}\hat{c}_{0\downarrow}\rangle$. It is given by:

$$D_{GS}(U)=\frac{1}{2}\left[1+\frac{2(N+1)}{N}\frac{1}{E_{GS}^2}+\frac{2(N-1)}{N}\frac{1}{(E_{GS}-U)^2}\right]^{-1} \tag{35}$$

and has been plotted in Fig. 5.

It is easy to obtain some limiting cases. For small U one finds:

$$E_{GS}(U)=-2+\frac{3N-1}{4N}U-\frac{5N^2+2N-3}{64N^2}U^2+\mathcal{O}(U^3)$$
$$|\psi_{GS}\rangle\propto\frac{1}{2}\gamma_1\left(1+\frac{3N-1}{8N}U\right)|\tilde{\psi}_1\rangle \tag{36}$$
$$+\frac{1}{2}\gamma_2\left(1-\frac{N+1}{8N}U\right)|\tilde{\psi}_2\rangle-|\tilde{\psi}_3\rangle+\mathcal{O}(U^2),$$

whereas for large U:

$$E_{GS}(U)=-\frac{2(N+1)}{N}U^{-1}+\mathcal{O}(U^{-2})$$
$$|\psi_{GS}\rangle=|\tilde{\psi}_1\rangle+\mathcal{O}(U^{-1}). \tag{37}$$

The explicit expression of the ground state energy in the limit $N\to\infty$ is:

$$E_{GS}(U)=\frac{2}{3}U-\frac{2}{3}\sqrt{12+U^2}$$
$$\cdot\cos\left\{\frac{1}{3}\cos^{-1}\left[\frac{(9-U^2)U}{(12+U^2)^{3/2}}\right]-\frac{\pi}{3}\right\}. \tag{38}$$

We have checked the small U limit by perturbation theory around $U=0$. Both linear and quadratic terms of the ground state energy are correctly recovered. On the other hand, the large U limit is easily checked owing to Lieb's theorem [15]. In this limit the total spin is the only degree of freedom of wavefunctions with energy going to zero and our solution shows the spin degeneracy (or total spin) predicted by the theorem.

6. Discussion

In this paper we considered the Hubbard Star (Fig. 1a) as a simple model for a lattice site in a high dimensional lattice surrounded by a bath of many other sites. In

Sect. 3 we showed that for $Z \to \infty$ (i.e., in the thermodynamic limit) the central site experiences only an average field from the surrounding sites. We showed that only few degrees of freedom contribute to thermodynamic quantities and that these degrees of freedom have a clear interpretation in terms of mean field variables. The thermodynamic properties of interest can be calculated by exact diagonalization of an effective Hamiltonian for a 3-site model. We also found that the ground state energy of the entire Star (not just of the central site) is similarly determined by only a few degrees of freedom. Within this subspace the Hamiltonian can be explicitly diagonalized, showing that the ground state energy is determined as the root of a simple cubic equation.

The star-shaped cluster investigated here also allows for exact solutions of quite different models and/or physical situations. For example, in the absence of interactions the Anderson disorder problem can be solved exactly [16]. It is hoped that this opens a new avenue to the investigation of the simultaneous influence of disorder and correlations, e.g. on a Bethe lattice.

In this paper we considered only the single Hubbard Star. However, along completely similar lines one can solve also other models, such as the Double Star sketched in Fig. 1b. For this particular model one finds that the effective Hamiltonian describes a 6-site model, instead of the 3-site model of Sect. 3: the six sites are the two central sites, with an a- and a b-site attached to each one of them. Extension of these techniques to more complicated models is possible in principle.

Finally we add a remark concerning symmetry breaking. Obviously the Star and the Double Star do not give rise to spontaneous phase transitions. In this respect the Stars reflects the properties of the high-temperature phase of the (standard) Hubbard model, rather than the low-temperature phase. However, it is possible to use these models to study the consequences of symmetry breaking, e.g., on the double occupancy or the kinetic energy, by modifying the chemical potentials. The chemical potentials of the Star can be tuned such that the boundary sites are predominantly occupied by $\downarrow$-spins and the central site by an $\uparrow$-spin. Similarly one can choose the chemical potentials of the Double Star such that the boundary sites connected to one of the two central sites carry predominantly $\uparrow$-spins, and those connected to the other carry predominantly $\downarrow$-spins.

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Appendix A. Calculation of $\mathscr{Z}_N$

(i) $N=0$: There is only one state, with zero energy, i.e. $\mathscr{Z}_0 = 1$.

(ii) $N=1$: There are three states for given σ, namely $(\sigma=\uparrow)\,|\psi_1\rangle = \hat{a}_\uparrow^+ |0\rangle$, $|\psi_2\rangle = \hat{c}_{0\uparrow}^+ |0\rangle$, $|\psi_3\rangle = \hat{b}_\uparrow^+ |0\rangle$. In this basis $\hat{\mathscr{H}}_\uparrow$ is given by

$$\hat{\mathscr{H}}_\uparrow = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & U \end{pmatrix}. \tag{A.1}$$

If the eigenvalues of $\hat{\mathscr{H}}_\uparrow$ are $E_{\uparrow\nu}(\nu=1, 2, 3)$, then

$$\mathscr{Z}_1 = 2\mathscr{Z}_\uparrow = 2\sum_{\nu=1}^{3} \mathrm{e}^{-\beta E_{\uparrow\nu}} \tag{A.2}$$

where the factor 2 is due to $\sigma=\uparrow$ or $\downarrow$.
(iii) $N=2$: Here the spins can be $(\uparrow\uparrow)$, $(\uparrow\downarrow)$, and $(\downarrow\downarrow)$ so that

$$\mathscr{Z}_2 = \mathscr{Z}_{\uparrow\downarrow} + 2\mathscr{Z}_{\uparrow\uparrow}. \tag{A.3}$$

We first consider $\mathscr{Z}_{\uparrow\uparrow}$. There are three states

$$\begin{aligned} |\psi_1\rangle &= \hat{a}_\uparrow^+ \hat{c}_{0\uparrow}^+ |0\rangle \\ |\psi_2\rangle &= \hat{a}_\uparrow^+ \hat{b}_\uparrow^+ |0\rangle \\ |\psi_1\rangle &= \hat{c}_{0\uparrow}^+ \hat{b}_\uparrow^+ |0\rangle. \end{aligned} \tag{A.4}$$

In this basis $\mathscr{H}_{\uparrow\uparrow}$ is given by $\mathscr{H}_\uparrow$, (A.1), however, with $(\hat{\mathscr{H}}_{\uparrow\uparrow})_{22} = U$, rather than zero. Hence $\mathscr{Z}_{\uparrow\uparrow} = \sum_{\nu=1}^{3} \mathrm{e}^{-\beta E_{\uparrow\uparrow\nu}}$, where $E_{\uparrow\uparrow\nu}$ are the eigenvalues of $\mathscr{H}_{\uparrow\uparrow}$. – Next we consider $\mathscr{Z}_{\uparrow\downarrow}$. There are 9 states possible, yielding a 9×9 matrix for $\mathscr{H}_{\uparrow\downarrow}$. In the basis

$$\begin{aligned} |\psi_1\rangle &= \hat{a}_\uparrow^+ \hat{a}_\downarrow^+ |0\rangle \\ |\psi_2\rangle &= \frac{1}{\sqrt{2}}(\hat{a}_\uparrow^+ \hat{c}_{0\downarrow}^+ - \hat{a}_\downarrow^+ \hat{c}_{0\uparrow}^+)|0\rangle \\ |\psi_3\rangle &= \frac{1}{\sqrt{6}}(2\hat{c}_{0\uparrow}^+ \hat{c}_{0\downarrow}^+ + \hat{a}_\uparrow^+ \hat{b}_\downarrow^+ - \hat{a}_\downarrow^+ \hat{b}_\uparrow^+)|0\rangle \\ |\psi_4\rangle &= \frac{1}{\sqrt{2}}(\hat{c}_{0\uparrow}^+ \hat{b}_\downarrow^+ - \hat{c}_\downarrow^+ \hat{b}_\uparrow^+)|0\rangle \\ |\psi_5\rangle &= \hat{b}_\uparrow^+ \hat{b}_\downarrow^+ |0\rangle \\ |\psi_6\rangle &= \frac{1}{\sqrt{2}}(\hat{c}_{0\uparrow}^+ \hat{b}_\downarrow^+ + \hat{c}_{0\downarrow}^+ \hat{b}_\uparrow^+)|0\rangle \\ |\psi_7\rangle &= \frac{1}{\sqrt{2}}(\hat{a}_\uparrow^+ \hat{b}_\downarrow^+ + \hat{a}_\downarrow^+ \hat{b}_\uparrow^+)|0\rangle \\ |\psi_8\rangle &= \frac{1}{\sqrt{2}}(\hat{a}_\uparrow^+ \hat{c}_{0\downarrow}^+ + \hat{a}_\downarrow^+ \hat{c}_{0\uparrow}^+)|0\rangle \\ |\psi_9\rangle &= \frac{1}{\sqrt{3}}(\hat{c}_{0\uparrow}^+ \hat{c}_{0\downarrow}^+ - \hat{a}_\uparrow^+ \hat{b}_\downarrow^+ + \hat{a}_\downarrow^+ \hat{b}_\uparrow^+)|0\rangle. \end{aligned} \tag{A.5}$$

$\hat{\mathscr{H}}_{\uparrow\downarrow}\,(=\hat{\mathscr{H}}_{\uparrow\downarrow}^T)$ assumes as block diagonal form

$$\hat{\mathscr{H}}_{\uparrow\downarrow}=\begin{pmatrix}\hat{\mathscr{H}}_{(5)} & & \\ & \hat{\mathscr{H}}_{(3)} & \\ & & U\end{pmatrix} \tag{A.6a}$$

where

$$\hat{\mathscr{H}}_{(5)}=\begin{pmatrix}0 & -1 & 0 & 0 & 0\\ -1 & 0 & -\sqrt{\frac{3}{2}} & 0 & 0\\ 0 & -\sqrt{\frac{3}{2}} & U & -\sqrt{\frac{3}{2}} & 0\\ 0 & 0 & -\sqrt{\frac{3}{2}} & U & -1\\ 0 & 0 & 0 & -1 & 2U\end{pmatrix} \tag{A.6b}$$

$$\hat{\mathscr{H}}_{(3)}=\begin{pmatrix}U & -\frac{1}{\sqrt{2}} & 0\\ -\frac{1}{\sqrt{2}} & U & -\frac{1}{\sqrt{2}}\\ 0 & -\frac{1}{\sqrt{2}} & 0\end{pmatrix} \tag{A.6c}$$

and $\hat{\mathscr{Z}}_{\uparrow\downarrow}=\sum_{\nu=1}^{9}\mathrm{e}^{-\beta E_{\uparrow\downarrow\nu}}$, where $E_{\uparrow\downarrow\nu}$ are the eigenvalues of $\hat{\mathscr{H}}_{\uparrow\downarrow}$.

(iv) $N=3$. The possible states are $(\uparrow\uparrow\uparrow)$, $(\uparrow\uparrow\downarrow)$, $(\uparrow\downarrow\downarrow)$, $(\downarrow\downarrow\downarrow)$, so that

$$\hat{\mathscr{Z}}_{(3)}=2\hat{\mathscr{Z}}_{\uparrow\uparrow\uparrow}+\hat{\mathscr{Z}}_{\uparrow\uparrow\downarrow}. \tag{A.7}$$

Here $\hat{\mathscr{Z}}_{\uparrow\uparrow\uparrow}=\mathrm{e}^{-\beta U}$, so that only $\hat{\mathscr{Z}}_{\uparrow\uparrow\downarrow}$ needs consideration. There are 9 states, and it is convenient to choose the basis

$$\begin{aligned}
|\psi_1\rangle&=\hat{a}_\uparrow^+\,\hat{a}_\downarrow^+\,\hat{c}_{0\uparrow}^+|0\rangle\\
|\psi_2\rangle&=\frac{1}{\sqrt{2}}(\hat{a}_\uparrow^+\,\hat{a}_\downarrow^+\,\hat{b}_\uparrow^+-\hat{a}_\uparrow^+\,\hat{c}_{0\uparrow}^+\,\hat{c}_{0\downarrow}^+)|0\rangle\\
|\psi_3\rangle&=\frac{1}{\sqrt{6}}(2\hat{a}_\uparrow^+\,\hat{c}_{0\downarrow}^+\,\hat{b}_\uparrow^+-\hat{a}_\downarrow^+\,\hat{c}_{0\uparrow}^+\,\hat{b}_{0\uparrow}^+-\hat{a}_\uparrow^+\,\hat{c}_{0\uparrow}^+\,\hat{b}_\downarrow^+)|0\rangle\\
|\psi_4\rangle&=\frac{1}{\sqrt{2}}(\hat{c}_{0\uparrow}^+\,\hat{c}_{0\downarrow}^+\,\hat{b}_\uparrow^+-\hat{a}_\uparrow^+\,\hat{b}_\uparrow^+\,\hat{b}_\downarrow^+)|0\rangle\\
|\psi_5\rangle&=\hat{c}_{0\uparrow}^+\,\hat{b}_\uparrow^+\,\hat{b}_\downarrow^+|0\rangle\\
|\psi_6\rangle&=\frac{1}{\sqrt{2}}(\hat{a}_\uparrow^+\,\hat{a}_\downarrow^+\,\hat{b}_\uparrow^++\hat{a}_\uparrow^+\,\hat{c}_{0\uparrow}^+\,\hat{c}_{0\downarrow}^+)|0\rangle\\
|\psi_7\rangle&=\frac{1}{\sqrt{2}}(\hat{a}_\uparrow^+\,\hat{c}_{0\uparrow}^+\,\hat{b}_\downarrow^+-\hat{a}_\downarrow^+\,\hat{c}_{0\uparrow}^+\,\hat{b}_\uparrow^+)|0\rangle\\
|\psi_8\rangle&=\frac{1}{\sqrt{2}}(\hat{c}_{0\uparrow}^+\,\hat{c}_{0\downarrow}^+\,\hat{b}_\uparrow^++\hat{a}_\uparrow^+\,\hat{b}_\uparrow^+\,\hat{b}_\downarrow^+)|0\rangle\\
|\psi_9\rangle&=\frac{1}{\sqrt{3}}(\hat{a}_\uparrow^+\,\hat{c}_{0\downarrow}^+\,\hat{b}_\uparrow^++\hat{a}_\downarrow^+\,\hat{c}_{0\uparrow}^+\,\hat{b}_\uparrow^++\hat{a}_\uparrow^+\,\hat{c}_{0\uparrow}^+\,\hat{b}_\downarrow^+)|0\rangle.
\end{aligned} \tag{A.8}$$

In this basis the 9×9 matrix $\hat{\mathscr{H}}_{\uparrow\uparrow\downarrow}(=\hat{\mathscr{H}}_{\uparrow\downarrow}^T)$ is given by (A.6a), however, with $(\hat{\mathscr{H}}_{(5)})_{22}=U$, $(\hat{\mathscr{H}}_{(5)})_{44}=2U$, $(\hat{\mathscr{H}}_{(5)})_{45}=1$, and $(\hat{\mathscr{H}}_{(3)})_{33}=2U$. Hence $\hat{\mathscr{Z}}_{\uparrow\uparrow\downarrow}=\sum_{\nu=1}^{9}\mathrm{e}^{-\beta E_{\uparrow\uparrow\downarrow\nu}}$, where $E_{\uparrow\uparrow\downarrow\nu}$ are the eigenvalues of $\hat{\mathscr{H}}_{\uparrow\uparrow\downarrow}$.

Combination of the results for $N=0$, 1, 2, 3 yields the full partition function $\mathscr{Z}$, (19).

Appendix B. Ground state wave function

In this Appendix the expressions needed to normalize the wave functions given in (29), and to calculate matrix elements with them, are calculated. In (3a) new fermion operators are defined as the sum over all the fermion operators on the star surface. They are normalized and satisfy the standard requirements:

$$\hat{A}_\sigma\hat{A}_\sigma=\hat{A}_\sigma^+\,\hat{A}_\sigma^+=0 \tag{B.1}$$

$$[\hat{A}_\sigma^+,\hat{A}_{\sigma'}]_+=\delta_{\sigma\sigma'}. \tag{B.2}$$

The most important property of these operators appears in connection with the totally symmetric wave function $|\psi_0\rangle$ defined in (28). Creation or annihilation of a doubly occupied site destroys the symmetric state:

$$\hat{A}_\sigma^+\,\hat{A}_{-\sigma}^+|\psi_0\rangle=\hat{A}_\sigma\hat{A}_{-\sigma}|\psi_0\rangle=0. \tag{B.3a}$$

Let us prove the first one:

$$\hat{A}_\uparrow^+\,\hat{A}_\downarrow^+|\psi_0\rangle=\frac{1}{Z}\sum_{\substack{i,j=1\\ i<j}}^{Z}(\hat{c}_{i\uparrow}^+\,\hat{c}_{j\downarrow}^++\hat{c}_{j\uparrow}^+\,\hat{c}_{i\downarrow}^+)|\psi_0\rangle \tag{B.3b}$$

because diagonal terms like $\hat{c}_{i\uparrow}^+\,\hat{c}_{i\downarrow}^+$ give zero when applied to $|\psi_0\rangle$ due to the single occupation of *all* sites on the surface. Using now the explicit form of $|\psi_0\rangle$ we get:

$$\hat{A}_\uparrow^+\,\hat{A}_\downarrow^+|\psi_0\rangle=\frac{1}{Z}\sum_{\substack{i,j=1\\ i<j}}^{Z}(\hat{c}_{i\uparrow}^+\,\hat{c}_{j\downarrow}^+-\hat{c}_{i\downarrow}^+\,\hat{c}_{j\uparrow}^+)|\psi_0\rangle \tag{B.3c}$$

$$\begin{aligned}
&=\frac{1}{Z}\sqrt{\frac{N_\uparrow!\,N_\downarrow!}{N!}}\sum_{\substack{i,j=1\\ i<j}}^{Z}(-)^{j-i-1}\sum_{\{\sigma_k\}}(\hat{c}_{i\uparrow}^+\,\hat{c}_{j\downarrow}^+-\hat{c}_{i\downarrow}^+\,\hat{c}_{j\uparrow}^+)\\
&\cdot\hat{c}_{i\sigma_i}^+\,\hat{c}_{j\sigma_j}^+[\hat{c}_{1\sigma_1}^+\ldots\hat{c}_{N\sigma_N}^+|0\rangle]
\end{aligned} \tag{B.3d}$$

where the second sum is over all permutations of N integers and the operators $\hat{c}_{i\sigma_i}^+$ and $\hat{c}_{j\sigma_j}^+$ have been moved to the very left of the product that defines $|\psi_0\rangle$. But

$$\begin{aligned}
&(\hat{c}_{i\uparrow}^+\,\hat{c}_{j\downarrow}^+-\hat{c}_{i\downarrow}^+\,\hat{c}_{j\uparrow}^+)\hat{c}_{i\sigma_i}^+\,\hat{c}_{j\sigma_j}^+\\
&=(\hat{c}_{i\uparrow}^+\,\hat{c}_{i\sigma_i}^+)(\hat{c}_{j\sigma_j}^+\,\hat{c}_{j\downarrow}^+)-(\hat{c}_{i\sigma_i}^+\,\hat{c}_{i\downarrow}^+)(\hat{c}_{j\uparrow}^+\,\hat{c}_{j\sigma_j}^+).
\end{aligned} \tag{B.3e}$$

When these operator products are inserted back into the sum over all spin permutations, they act as projection operators that eliminate some permutations from the sum. For example, the term $(\hat{c}_{i\uparrow}^+\,\hat{c}_{i\sigma_i}^+)(\hat{c}_{j\sigma_j}^+\,\hat{c}_{j\downarrow}^+)$ eliminates those terms having σ_i equal to $\uparrow$ or σ_j equal to $\downarrow$. At the end, both projection operators produce exactly the same sum of permutations but with opposite signs. Thus an overall cancellation follows. In a similar way $\hat{A}_\sigma\hat{A}_{-\sigma}|\psi_0\rangle=0$ is proved.

Let us now introduce an average spin-flip operator on the surface:

$$\hat{F}\equiv\sum_{i=1}^{Z}\hat{c}_{i\uparrow}^+\,\hat{c}_{i\downarrow}. \tag{B.4}$$

Notice that $\hat{F}$ is nothing but the sum over the boundary sites of the corresponding spin raising operators. It shows the following properties:

$$\hat{A}_{\downarrow}^{+}\hat{F}|\psi_0\rangle=-(N_{\uparrow}+1)\hat{A}_{\uparrow}^{+}|\psi_0\rangle \tag{B.5a}$$

$$\hat{A}_{\uparrow}^{+}\hat{F}|\psi_0\rangle=(N_{\uparrow}+1)\hat{A}_{\downarrow}^{+}|\psi_0\rangle. \tag{B.5b}$$

Similar properties are verified by $\hat{F}^{+}$, the sum of spin lowering operators, but they are not neccessary for the development of Sect. 4. Let us prove (B.5a):

$$\hat{A}_{\downarrow}^{+}\hat{F}|\psi_0\rangle=\frac{1}{\sqrt{Z}}\sum_{i=1}^{Z}\hat{c}_{i\downarrow}^{+}\sum_{j=1}^{Z}\hat{c}_{j\uparrow}^{+}\hat{c}_{j\downarrow}|\psi_0\rangle \tag{B.5c}$$

$$=-\hat{A}_{\uparrow}^{+}|\psi_0\rangle+\frac{1}{\sqrt{Z}}\sum_{\substack{i,j=1\\ i\neq j}}^{Z}\hat{c}_{i\downarrow}^{+}\hat{c}_{j\uparrow}^{+}\hat{c}_{j\uparrow}|\psi_0\rangle, \tag{B.5d}$$

where the fact that $\hat{c}_{i\uparrow}^{+}\hat{c}_{i\downarrow}^{+}|\psi_0\rangle=0$ has been used once more. Defining

$$C\equiv\frac{1}{\sqrt{Z}}\sqrt{\frac{N_{\uparrow}!\,N_{\downarrow}!}{N!}} \tag{B.6a}$$

we have for the second term in the previous sum:

$$C\sum_{\substack{i,j=1\\ i\neq j}}^{Z}\hat{c}_{i\downarrow}^{+}\hat{c}_{j\uparrow}^{+}\hat{c}_{j\downarrow}\sum_{\{\sigma_k\}}[\hat{c}_{1\sigma_1}^{+}\ldots\hat{c}_{i\sigma_i}^{+}\ldots\hat{c}_{j\sigma_j}^{+}\ldots\hat{c}_{N\sigma_N}^{+}|0\rangle] \tag{B.6b}$$

$$=C\sum_{\substack{i,j=1\\ i\neq j}}^{Z}(-)^{i}\sum_{\substack{\{\sigma_k\}\\ \sigma_i=\uparrow,\sigma_j=\downarrow}}[\hat{c}_{1\sigma_1}^{+}\ldots(\hat{c}_{i\uparrow}^{+}\hat{c}_{i\downarrow}^{+})\ldots\hat{c}_{j\uparrow}^{+}\ldots\hat{c}_{N\sigma_N}^{+}|0\rangle] \tag{B.6c}$$

$$=N_{\uparrow}C\sum_{i=1}^{Z}(-)^{i}\sum_{\substack{\{\sigma_k\}\\ \sigma_i=\downarrow}}[\hat{c}_{1\sigma_1}^{+}\ldots(\hat{c}_{i\uparrow}^{+}\hat{c}_{i\downarrow}^{+})\ldots\hat{c}_{N\sigma_N}^{+}|0\rangle] \tag{B.6d}$$

$$=-N_{\uparrow}\hat{A}_{\uparrow}^{+}|\psi_0\rangle. \tag{B.6e}$$

Equation (B.5a) is obtained after adding both contributions.

Mean values with respect to $|\psi_0\rangle$ are easily computed with the help of (B.1)–(B.4). For example:

$$\langle\psi_0|\hat{A}_{\sigma}^{+}\hat{A}_{\sigma}|\psi_0\rangle=\frac{1}{Z}\sum_{i,j=1}^{Z}\langle\psi_0|\hat{c}_{i\sigma}^{+}\hat{c}_{j\sigma}|\psi_0\rangle \tag{B.7a}$$

$$=\frac{1}{Z}\sum_{i=1}^{Z}\langle\psi_0|\hat{c}_{i\sigma}^{+}\hat{c}_{i\sigma}|\psi_0\rangle=\frac{N_{\sigma}}{Z}=\frac{N_{\sigma}}{N} \tag{B.7b}$$

$$\langle\psi_0|(\hat{A}_{\uparrow}^{+}\hat{A}_{\uparrow}-\hat{A}_{\downarrow}^{+}\hat{A}_{\downarrow})^{2}|\psi_0\rangle=1. \tag{B.7c}$$

Equations (B.6) are neccessary to prove the normalization of the wavefunction $|\psi_2\rangle$.

Finally, we list below the rest of the formulae needed to normalize wave functions and calculate matrix elements of the Hamiltonian or other operators:

$$\langle\psi_0|\hat{F}^{+}\hat{F}|\psi_0\rangle=N_{\downarrow}(N_{\uparrow}+1) \tag{B.8a}$$

$$\langle\psi_0|\hat{A}_{\downarrow}^{+}\hat{A}_{\uparrow}\hat{F}|\psi_0\rangle=\frac{(N_{\uparrow}+1)N_{\downarrow}}{N} \tag{B.8b}$$

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