Hubbard Hamiltonian in the dimer representation. Large $U$ limit

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Abstract

We formulate the Hubbard model for the simple cubic lattice in the representation of interacting dimers applying the exact solution of the dimer problem. By eliminating from the considerations unoccupied dimer energy levels in the large $U$ limit (it is the only assumption) we analytically derive the Hubbard Hamiltonian for the dimer (analogous to the well-known $t-J$ model), as well as, the Hubbard Hamiltonian for the crystal as a whole by means of the projection technique. Using this approach we can better visualize the complexity of the model, so deeply hidden in its original form. The resulting Hamiltonian is a mixture of many multiple ferromagnetic, antiferromagnetic and more exotic interactions competing one with another. The interplay between different competitive interactions has a decisive influence on the resulting thermodynamic properties of the model, depending on temperature, model parameters and assumed average number of electrons per lattice site. A simplified form of the derived Hamiltonian

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can be obtained using additionally Taylor expansion with respect to $x = \frac{1}{U}$ ($t$-hopping integral between nearest neighbours, $U$-Coulomb repulsion). As an example, we present the expansion including all terms proportional to $t$ and to $\frac{t^2}{U}$ and we reproduce the exact form of the Hubbard Hamiltonian in the limit $U \to \infty$.

The nonperturbative approach, presented in this paper, can, in principle, be applied to clusters of any size, as well as, to another types of model Hamiltonians.

1 Introduction

The single-band Hubbard model, Ref. [1], plays in the solid state physics a similar principal role as the hydrogen atom in the atomic physics. This explains a continuous interest in its properties. The Hubbard Hamiltonian reads

$$H = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^+ c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \quad (1)$$

Here $c_{i,\sigma}$ ($c_{i,\sigma}^+$) are annihilation (creation) operators of an electron with spin $\sigma = \uparrow, \downarrow$ in the Wannier representation at the lattice site $\mathbf{R}_i$ and $n_{i,\sigma} = c_{i,\sigma}^+ c_{i,\sigma}$. Moreover, $t_{i,j}$ is the hopping integral between different lattice sites $i$ and $j$ ($t_{i,i} = 0$) and $U$ is the intrasite Coulomb repulsion. The Bloch conduction band energy $\varepsilon_k$ is given by

$$\varepsilon_k = \sum_{i-j} t_{i,j} e^{-i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \quad (2)$$

In the following we restrict ourselves to the simple cubic (sc) lattice and assume that

$$t_{i,j} = \begin{cases} -t & \text{i, j-nearest neighbours} \\ 0 & \text{otherwise.} \end{cases}$$

Then

$$\varepsilon_k = -2t(\cos k_x a + \cos k_y a + \cos k_z a). \quad (3)$$

The hopping parameter $t$ is simply related to the bandwidth $W$ of the Bloch band (2), e. g. $W = 12t$ for the sc lattice. The interplay between the two model parameters, $W$ and $U$, is decisive for the properties of the model.
resulting in strong electron correlations, leading to band magnetism (see e.g. Refs [2], [3] for a review), insulator-to-metal transition (see e.g. Refs [3], [4] and papers cited therein) and high-$T_c$ superconductivity (negative $U$-model, see e.g. Ref. [5]). The Hubbard model very often plays also a role of a submodel for many other more complicated models (as e.g. Anderson model (see Ref. [6]), s-f model (see Refs [7,8]) and so on). Especially interesting, but difficult to handle are the properties of the Hubbard model in such a regime of the model parameters where the bandwidth $W$ is comparable to the Coulomb repulsion $U$. In a large number of papers [9-30] the authors tried to solve this model using many sophisticated methods. The exact solution, however, does not exist till now. Many authors tried to change the situation in this field by introducing the expansion parameter $x = t/U$ ($x \ll 1$). This idea (cf Refs [31,32]) consists in replacing ”difficult physics” connected with the model by ”difficult mathematics” obtained by a laborious expansion with respect to $x$. Different methods connected with this problem have been applied as e.g. the perturbation expansion (see Refs [18], [21]), canonical transformation (see Refs [9], [12], [17], [22], [23]) or ab initio derivations (see Refs [25], [28-30]). Most of the methods, leading to the $t-J$ model (or generalized $t-J$ model) are also summarized in Refs [27], [4].

The goal of the present paper is just to show that we can take another, nonperturbative way. In the first step we divide the crystal lattice into a set of interacting dimers. In other words, we can rewrite the Hubbard Hamiltonian (1) for the sc lattice (see Fig. 1) in the equivalent form

$$H = \sum_I H_I^d - t \sum_{I,\sigma} (c_{I,1,\sigma}^+ c_{I+1,1,\sigma} + c_{I+1,1,\sigma}^+ c_{I,2,\sigma} + c_{I,1,\sigma}^+ c_{I,1,\sigma} + c_{I,2,\sigma}^+ c_{I,2,\sigma})$$

(4)

where

$$H_I^d = -t \sum_{\sigma} (c_{I,1,\sigma}^+ c_{I,2,\sigma}^+ c_{I,1,\sigma} c_{I,2,\sigma}) + U (n_{I,1,\uparrow} n_{I,1,\downarrow} + n_{I,2,\uparrow} n_{I,2,\downarrow}).$$

(5)

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1The dimer Fourier transformation

c_{I,1,\sigma} = \frac{1}{\sqrt{N}} \sum_k \epsilon_{k,\sigma} e^{i k \cdot R_I}, c_{I,2,\sigma} = \frac{1}{\sqrt{N}} \sum_k \epsilon_{k,\sigma} e^{i k \cdot R_{I,2}}

where $N$ is the number of lattice points, applied to (4), gives the well known result

$$H = \sum_{k,\sigma} \epsilon_k n_{k,\sigma} + \frac{U}{N} \sum_{k,k',q} c_{k+q,\uparrow}^+ c_{k',\downarrow}^+ c_{k,\uparrow} c_{k,\downarrow}$$

with $\epsilon_k$ given by (3).
The indices $I$ and $J$ enumerate the dimers and $H_d^I$ is the dimer Hamiltonian. The second term in (4) describes the hopping between nearest dimers in the $z$-direction, the third one represents the hopping between nearest dimers ($(y, z)$-plane) and between different dimer planes (see Fig. 1).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure1.png}
\caption{A plane of the Hubbard dimers. The crystal is considered as a collection of parallel lying dimer planes.}
\end{figure}

The equivalent form of the Hubbard Hamiltonian (4) is especially suitable because we can apply in the following the exact solution of the dimer problem (5). In the next step we express the construction operators $a_\sigma$ ($a_\sigma^+$) as linear combinations of the transition operators between different dimer states. This, in turn, allows to find the exact dimer representation of the whole Hamiltonian (4). The space of the dimer eigenvectors consists, however, of two subspaces. One of them corresponds to the lowest lying energy levels, the second one contains the levels with energies which in the large $U$ limit take on large, positive values. These levels in a reasonable temperature range cannot be occupied by electrons and therefore we can exclude them from further considerations. It is interesting to note that this approach, without any additional assumptions, applied to the dimer Hamiltonian (5)
produces the analogy of the well known $t - J$ model (cf Refs [31], [32]). A similar approach can be applied to the Hamiltonian (4), describing the crystal as a whole. By eliminating from the considerations the unoccupied dimer energy levels in the large $U$ limit (it is the only assumption) with the use of the projection technique we can find in a straightforward way the final form of the Hamiltonian in this limit without using perturbation expansion or canonical transformation. The resulting Hamiltonian, obtained in this way, is very complicated. It, however, explicitly shows all possible magnetic, nonmagnetic or more complex competitive interaction processes very deeply hidden in the original Hamiltonian written in the site representation (1). It is the aim of this paper just to reveal these important but normally invisible elementary interactions. One important advantage might be that a given approach to the unsolvable Hubbard problem can be tested with respect to the types of neglected interaction processes. Besides, the new and straightforward method, presented in this paper, can easily be adopted to clusters of any size and also to another types of model Hamiltonians.

The paper is organized as follows. In Sec. 2 we find the exact solution of the Hubbard dimer (5) and give the exact expressions for the annihilation operators $c_{i,1(2),\sigma}$ in the dimer representation. In Sec. 3 we derive the Hubbard dimer Hamiltonian (5) in the large $U$ limit. With the use of the projection technique onto the lowest lying dimer states we derive in Sec. 4 the Hubbard Hamiltonian for the crystal in this limit (central formula of this paper). A simplified version of the derived Hamiltonian with the use of the Taylor expansion with respect to $x = \frac{t}{U} (x \ll 1)$ and the case $U \to \infty$ is discussed in Sec. 5.

### 2 Exact solution of the Hubbard dimer

The eigenvalues and eigenvectors of the dimer Hamiltonian (5) can be found by using a standard procedure (cf Refs [33-35]). We start with the vectors $|n_{1,\uparrow}, n_{1,\downarrow}; n_{2,\uparrow}, n_{2,\downarrow}\rangle (n_{i,\sigma} = 0, 1; i = 1, 2; \sigma = \uparrow, \downarrow)$ which constitute the Fock
basis of the single-dimer space of states:

\[
\begin{align*}
|0\rangle &= |0; 0; 0, 0\rangle, & |21\rangle &= |1, 1; 0, 0\rangle, & |31\rangle &= |0, 1; 1, 1\rangle, \\
|11\rangle &= |1, 0; 0, 0\rangle, & |22\rangle &= |1, 0; 1, 0\rangle, & |32\rangle &= |1, 0; 1, 1\rangle, \\
|12\rangle &= |0, 1; 0, 0\rangle, & |23\rangle &= |1, 0; 0, 1\rangle, & |33\rangle &= |1, 1; 0, 1\rangle, \\
|13\rangle &= |0, 0; 1, 0\rangle, & |24\rangle &= |0, 1; 1, 0\rangle, & |34\rangle &= |1, 1; 1, 0\rangle, \\
|14\rangle &= |0, 0; 0, 1\rangle, & |26\rangle &= |0, 0; 1, 1\rangle, & |4\rangle &= |1, 1; 1, 1\rangle.
\end{align*}
\]

(6)

Starting with the vectors (6) we easily get the eigenvalues \(E_\alpha\) and the eigenvectors \(|E_\alpha\rangle\) of the Hubbard dimer (5). Here, we only mention that the space of 16 eigenvectors \(|E_\alpha\rangle\) can be divided into some subspaces numbered by \(n = \sum_i n_{i,\sigma}\). The subspace, belonging to \(n = 0\) and \(n = 4\) is 1-dimensional (\(E_0 = 0\), \(|E_0\rangle = |0\rangle\); \(E_4 = 2U\), \(|E_4\rangle = |4\rangle\)). There are, however, two 2-dimensional subspaces corresponding to \(n = 1\) (as e.g. \(E_{11} = -t\), \(|E_{11}\rangle = \frac{1}{\sqrt{2}}(|11\rangle + |13\rangle\)), etc.) and two 2-dimensional subspaces corresponding to \(n = 3\) (as e.g. \(E_{31} = t + U\), \(|E_{31}\rangle = \frac{1}{\sqrt{2}}(|31\rangle + |33\rangle\)), etc.). The subspace, belonging to \(n = 2\) consists of one 4-dimensional subspace (as e.g. \(E_{21} = 0\), \(|E_{21}\rangle = \frac{1}{\sqrt{2}}(|23\rangle + |24\rangle\)), etc.) and two 1-dimensional subspaces (\(E_{25} = E_{26} = 0\), \(|E_{25}\rangle = |22\rangle\), \(|E_{26}\rangle = |25\rangle\)). The complete set of the eigenvalues \(E_\alpha\) and eigenvectors \(|E_\alpha\rangle\) of the Hubbard dimer is given in the Appendix A. It allows to express the dimer Hamiltonian (5) in the equivalent form

\[
H^d = \sum_\alpha E_\alpha |E_\alpha\rangle \langle E_\alpha|.
\]

(7)

The next important step in our calculations is the possibility to express the annihilation operators \(c_{1(2),\sigma}\) as linear combinations of transition operators between dimer states \(\hat{P}_{\alpha,\beta} = \langle E_\alpha|E_\beta\rangle\). This procedure can easily be performed when acting with the annihilation operators on the basis vectors (6) and using the reciprocal relations to (A.1). In this way we can obtain the dimer representation of the annihilation (creation) operators, given in Appendix B. After this operation we can insert so prepared \(c_{I,1(2),\sigma}\) \((c_{I,1(2),\sigma}^+)\) into the Hubbard Hamiltonian (4) to obtain the Hubbard model in the dimer representation for the SC lattice. This representation will be used later to derive the Hubbard Hamiltonian in the large \(U\) limit (see Sec. 4).
Looking at the eigenvalues (A.1) of the Hubbard dimer it is easy to see that for large $U$ ($U \gg t$) the energies $E_\alpha = E_{22}, E_{23}, E_{31}, E_{32}, E_{33}, E_{34}$ and $E_4$ take on large, positive values, producing in the partition function the terms which can practically be neglected. It means that the mentioned energies are not occupied in the reasonable temperature range ($1 \text{ eV} \sim 11604.5 \text{ K}$) and can be excluded from our considerations. Therefore the dimer Hamiltonian, given by (7), reduces to

\begin{equation}
\mathcal{H}_d = -tP_{11,11} + tP_{12,12} - tP_{13,13} + tP_{14,14} + \left(-C + \frac{U}{2}\right) P_{24,24}.
\end{equation}

To bring this expression into a compact (second quantization) form we introduce the Hubbard operators

\begin{align}
a_{i,\sigma} &= c_{i,\sigma}(1 - n_{i,-\sigma}), \\
b_{i,\sigma} &= c_{i,\sigma} n_{i,-\sigma}
\end{align}

and spin operators

\begin{align}
S_z^i &= \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow}) = \frac{1}{2}(n_{i,\uparrow}^a - n_{i,\downarrow}^a), \\
S^+_i &= c_{i,\downarrow}^a c_{i,\uparrow} = a_{i,\uparrow}^a a_{i,\downarrow}, \\
S^-_i &= c_{i,\uparrow}^a c_{i,\downarrow} = a_{i,\uparrow}^a a_{i,\downarrow}
\end{align}

where $n_{i,\sigma}^a = a_{i,\sigma}^a a_{i,\sigma}$ ($i = 1, 2; \sigma = \uparrow, \downarrow$).

With the use of (9)-(13) the Hamiltonian of the Hubbard dimer (8) for large $U$ can be presented in the form (we introduce the omitted earlier dimer index $I$)
\[ H_d^I = -t \sum_{\sigma} [a_{I,1,\sigma}^+ a_{I,2,\sigma} + a_{I,2,\sigma}^+ a_{I,1,\sigma}] \]
\[ + \frac{4t^2}{U} \left[ \vec{S}_{I,1} \cdot \vec{S}_{I,2} - \frac{n_{I,1}^a n_{I,2}^b}{4} \right] \]
\[ + \frac{t^2(1 - \sqrt{1 + \left(\frac{4t}{U}\right)^2})}{U(1 + \sqrt{1 + \left(\frac{4t}{U}\right)^2} \sqrt{1 + \left(\frac{4t}{U}\right)^2})} [2(b_{I,1,\uparrow}^+ a_{I,1,\downarrow}^+ a_{I,2,\downarrow} b_{I,2,\uparrow}^+) + b_{I,2,\downarrow}^+ a_{I,1,\downarrow}^+ a_{I,1,\uparrow} b_{I,1,\uparrow}] \]
\[ + (1 - n_{I,1}^a) n_{I,2}^b + (1 - n_{I,2}^b) n_{I,1}^a - n_{I,1}^a n_{I,2}^b \]
\[ + \frac{t(1 - \sqrt{1 + \left(\frac{4t}{U}\right)^2})}{2\sqrt{1 + \left(\frac{4t}{U}\right)^2}} \sum_{\alpha=1,2} \sum_{\sigma} [a_{I,\alpha,\sigma}^+ b_{I,\sigma} + b_{I,\alpha,\sigma}^+ a_{I,\sigma}] \]  

where \( n_{I,\alpha}^{a,b} = \sum_{\sigma} n_{I,\alpha,\sigma}^{a,b}, n_{I,\alpha,\sigma}^{b} = b_{I,\alpha,\sigma}^+ b_{I,\alpha,\sigma} = n_{I,\alpha,\sigma} n_{I,\alpha,-\sigma} \) (\( \alpha = 1, 2 \)), \( \alpha = 1 \) when \( \alpha = 2 \) and \( \alpha = 2 \) when \( \alpha = 1 \). It is very important to stress that the formula (14) has been obtained in a nonperturbative way, starting from the exact form of the dimer Hamiltonian (see (5) or (7)), and excluding from the considerations unoccupied dimer energy levels in the large \( U \) limit. Let us note that using the Taylor expansion in (14) with respect to \( x = \frac{t}{U} \) and retaining the terms proportional to \( t^2 \) we obtain

\[ H_d^I = -t \sum_{\sigma} [a_{I,1,\sigma}^+ a_{I,2,\sigma} + a_{I,2,\sigma}^+ a_{I,1,\sigma}] + \frac{4t^2}{U} \left[ \vec{S}_{I,1} \cdot \vec{S}_{I,2} - \frac{n_{I,1}^a n_{I,2}^b}{4} \right]. \]  

The formula (15) is the well-known \( t-J \) model for the Hubbard dimer where the first part in (15), similarly to (14), represents the exact form of the dimer Hamiltonian (5) in the limit \( U \to \infty \).

The same result (14) can also be obtained applying a more general approach which will be used later to derive the Hubbard Hamiltonian for large
$U$ in the case of a crystal. Let us note that after elimination of the unoccupied levels the subspace of the eigenvectors of the Hubbard dimer (A.1) for large $U$ consists of the following eigenvectors: $|E_0\rangle$, $|E_{11}\rangle$, $|E_{12}\rangle$, $|E_{13}\rangle$, $|E_{14}\rangle$, $|E_{21}\rangle$, $|E_{24}\rangle$, $|E_{25}\rangle$, and $|E_{26}\rangle$. It means that we can define a projection operator onto this subspace

$$P_I = P_{0,0}^{(I)} + P_{11,11}^{(I)} + P_{12,12}^{(I)} + P_{13,13}^{(I)} + P_{14,14}^{(I)} + P_{21,21}^{(I)} + P_{24,24}^{(I)} + P_{25,25}^{(I)} + P_{26,26}^{(I)}$$

which, in the second quantization form, reads

$$P_I = 1 - \frac{1}{4}(n_{I,1}^b + n_{I,2}^b) + \frac{1}{4}n_{I,1}^an_{I,2}^a$$

$$+ \frac{1}{8}(1 - \frac{1}{\sqrt{1+(\frac{t}{U})^2}})[4(\vec{S}_{I,1} \cdot \vec{S}_{I,2} - \frac{1}{4}n_{I,1}^an_{I,2}^a)$$

$$+ 2(b_{I,1,\uparrow}^+ a_{I,1,\uparrow}^+ a_{I,2,\downarrow} b_{I,2,\uparrow} + b_{I,2,\downarrow}^+ a_{I,2,\downarrow}^+ a_{I,1,\uparrow} b_{I,1,\uparrow})$$

$$+ (1 - n_{I,1}^a)n_{I,2}^b + (1 - n_{I,2}^a)n_{I,1}^b$$

$$+ \frac{t}{U}\sqrt{1+(\frac{t}{U})^2} \sum_{\alpha=1,2} \sum_{\sigma} (a_{I,\alpha,\sigma}^+ b_{I,\sigma} + b_{I,\alpha,\sigma}^+ a_{I,\sigma})]$$

Now, the Hamiltonian (14) can also be obtained from (5) (or (7)) with the use of the projection operator (16) or (17) using the relation

$$\hat{\Pi}_I^d = P_I \hat{H}_I^d P_I$$

and applying a straightforward but laborious algebraic calculation.

### 4 Hubbard model for large $U$

The Hamiltonian of the whole crystal (4) can be expressed (similar to (7)) in the form

$$H = \sum_{\gamma} E_{\gamma}|E_{\gamma}\rangle\langle E_{\gamma}|$$
with unknown energies $\overline{E}_\gamma$ and eigenvectors $|\overline{E}_\gamma\rangle$. We can, however, expand the eigenvectors $|\overline{E}_\gamma\rangle$ in the series of the dimer eigenvectors (see (A.1))

$$|\overline{E}_\gamma\rangle = \sum_{\gamma_1...\gamma_M} c^\gamma_{\gamma_1...\gamma_M} |E_{\gamma_1}\rangle...|E_{\gamma_M}\rangle$$ \hspace{1cm} (20)

assuming that the crystal consists of $M$ dimers. Using (19) and (20) we obtain

$$H = \sum_\gamma \overline{E}_\gamma \sum_{\gamma_1...\gamma_M} c^\gamma_{\gamma_1...\gamma_M} c^{\gamma*}_{\gamma_1...\gamma_M} |E_{\gamma_1}\rangle...|E_{\gamma_M}\rangle \langle E_{\gamma_1}|...\langle E_{\gamma_M}|.$$ \hspace{1cm} (21)

It is clear that to obtain the Hubbard Hamiltonian for large $U$ we have to project (21) onto the subspace of the lowest lying dimer states with the use of the projection operator

$$P = P_1P_2...P_M$$ \hspace{1cm} (22)

where $P_I$ is given by (16) or (17). In analogy to (14) we denote the Hubbard Hamiltonian in the large $U$ limit by $\overline{H}$. Similar to (18) we write

$$\overline{H} = PHP$$ \hspace{1cm} (23)

and instead of the form (21) for the Hamiltonian $H$ we can use (4). Taking into account that $P^2 = P$ ($P^2_I = P_I$, $[P_I, P_J] = 0$) we obtain

$$\overline{H} = P \sum_I \overline{H}^d_I - t \sum_{I,\sigma} \left( \overline{c}^+_I,2,\sigma \overline{c}_{I+1,1,\sigma} + \overline{c}^+_I,1,\sigma \overline{c}_{I,2,\sigma} \right) - t \sum_{I \neq J,\sigma} \left( \overline{c}^+_I,1,\sigma \overline{c}_{J,1,\sigma} + \overline{c}^+_I,2,\sigma \overline{c}_{J,2,\sigma} \right) \equiv P\overline{H}$$ \hspace{1cm} (24)

where $\overline{H}^d_I$ is given by (14) and $(\alpha = 1, 2)$

$$\overline{c}_{I,\alpha,\sigma} = c_{I,\alpha,\sigma} P_I,$$ \hspace{1cm} (25)

$$\overline{c}^+_I,\alpha,\sigma = P_I c^+_{I,\alpha,\sigma}.$$ \hspace{1cm} (26)

Applying the projection operator (16) or (17) to (B.1) - (B.4) and introducing Hubbard- and spin operators (9) - (13) we obtain

$$\overline{c}_{I,1,\uparrow} = \overline{a}_{I,1,\uparrow} + \beta \left[ S^z_{I,2} a_{I,1,\uparrow} + S_{I,2}^- a_{I,1,\downarrow} \right] - \delta \left[ S^z_{I,1} a_{I,2,\uparrow} + S^-_{I,1} a_{I,2,\downarrow} \right],$$ \hspace{1cm} (27)
\[ \overline{c}_{\downarrow,1,\downarrow} = \overline{a}_{\downarrow,1,\downarrow} - \beta \left[ S_{\downarrow,2}^z a_{\downarrow,1,\downarrow} - S_{\downarrow,1}^+ a_{\downarrow,1,\uparrow} \right] + \delta \left[ S_{\downarrow,1}^z a_{\downarrow,2,\downarrow} - S_{\downarrow,1}^+ a_{\downarrow,2,\uparrow} \right] \]  

(28)

where the corresponding expressions for \( \overline{c}_{\downarrow,2,\sigma} \) (\( \sigma = \uparrow, \downarrow \)) can easily be obtained by changing the internal dimer index 1 \( \leftrightarrow \) 2 in (27) and (28).

The new operators \( \overline{a}_{\downarrow,\alpha,\sigma} \) (\( \alpha = 1, 2; \sigma = \uparrow, \downarrow \)) are introduced to obtain a relatively compact form of (27) and (28). They are defined as follows

\[ \overline{a}_{\downarrow,\alpha,\sigma} = a_{\downarrow,\alpha,\sigma} + \beta \left( b_{\downarrow,\alpha,\sigma} + a_{\downarrow,\alpha,-\sigma}^+ a_{\downarrow,\pi,-\sigma} b_{\downarrow,\pi,\sigma} \right) + \delta \left[ b_{\downarrow,\pi,\sigma} + a_{\downarrow,\pi,-\sigma}^+ a_{\downarrow,\alpha,-\sigma} b_{\downarrow,\alpha,\sigma} + a_{\downarrow,\pi,\sigma} n_{\downarrow,\pi}^2 / 2 \right] \]  

(29)

where

\[ a_{\downarrow,\alpha,\sigma} = a_{\downarrow,\alpha,\sigma} \left( 1 - \frac{\beta}{2} n_{\downarrow,\pi}^a - \frac{1}{2} n_{\downarrow,\pi}^b \right), \]  

(30)

\[ b_{\downarrow,\alpha,\sigma} = b_{\downarrow,\alpha,\sigma} \left( 1 - n_{\downarrow,\pi}^a - \frac{1}{2} n_{\downarrow,\pi}^b \right) \]  

(31)

and

\[ \beta = \frac{1}{4} \left( 1 - \frac{1}{\sqrt{1 + (4t/U)^2}} \right), \]  

(32)

\[ \delta = \frac{t}{U} \frac{1}{\sqrt{1 + (4t/U)^2}}. \]  

(33)

To write down the explicit form of the Hubbard Hamiltonian \( \overline{H} \) (see (24)) we have to insert (27) and (28) into \( \overline{H} \). This operation leads, however, to a very complicated form of \( \overline{H} \), given in the Appendix C (a simplified form of this Hamiltonian is discussed in the next Section). Here again the only assumption made to derive \( \overline{H} \) was the reduction of the whole dimer space (A.1) to the subspace of the dimer eigenvectors \( |E_0\rangle, |E_{11}\rangle, |E_{12}\rangle, |E_{13}\rangle, |E_{14}\rangle, |E_{21}\rangle, |E_{24}\rangle, |E_{25}\rangle \) and \( |E_{26}\rangle \), corresponding to the lowest lying dimer energy levels because in the large \( U \) limit only these levels can be occupied. The Hamiltonian \( \overline{H} \), obtained in this way, contains many competing, magnetic, nonmagnetic and more complex interactions. Among them we can
find a direct antiferromagnetic interaction generated by the term $\vec{S}_{I,1} \cdot \vec{S}_{I,2}$ (Heisenberg exchange interaction) multiplied by the positive coupling constant. Such a term appears in $\mathcal{H}^I$ (see (C.6) and (14)). Inside of $\mathcal{H}$ (see (C.6) and (C.2) - (C.5)) a kind of ferromagnetic interactions between spins from different dimers, represented by (C.3), appears within the terms proportional to $\beta^2$ and $\delta^2$ (negative coupling constants). The antiferromagnetic interactions, however, appear again in terms proportional to $\beta \delta$. There are also many other magnetic, more exotic interactions, represented by (C.2), (C.4) and (C.5), entering into (C.6). The situation is, however, much more complicated when we consider the total Hamiltonian $\mathcal{H}$ (see (24)) in the large $U$ limit. $\mathcal{H}$ differs from $\overline{\mathcal{H}}$ by the multiplicative factor $P$ (a product of the projection operators $P_I$ (see (22) and (17)), standing on the left. Inside of each $P_I$ the mentioned antiferromagnetic interaction also appears (see (17)). In other words, the total Hamiltonian $\mathcal{H}$, we are interested in, is actually a sum of the products of many competitive ferromagnetic, antiferromagnetic and more exotic interactions. The thermodynamic properties of the system, described by the Hamiltonian $\mathcal{H}$ (24), are then a result of the competition between all of them. Which interaction wins in such a competition certainly depends on temperature, model parameters ($t, U$) and on the average number of electrons per lattice site, determining the chemical potential of the system.

The formalism presented in this paper is also applicable to a more complicated decomposition of the Hubbard Hamiltonian (1) into a set of interacting clusters consisting e.g. of one central atom and $z$ its nearest neighbours. We, however, know (see e.g. Refs [36]-[39] and papers cited therein) that, unfortunately, the mathematical problems in this case exponentially grows up with the size of the cluster.

5 Taylor expansion

The complicated form of the Hubbard Hamiltonian $\overline{\mathcal{H}}$ in the large $U$ limit (see (24), (C.6)) where $P$ is given by (22) (see also (17)) can essentially be reduced when applying the Taylor expansion with respect to the parameter $x = \frac{t}{U} \ll 1$. To do it we have to expand all the coefficients in (14), (17) and (C.6) including also $\beta$ and $\delta$ (see (32), (33)). Such an expansion can be performed to any power of $x$, however, the most simple form we obtain when we restrict ourselves to the linear approximation, resulting in the terms
proportional to $t$ and $\frac{t^2}{U}$. The accuracy of this expansion can easily be verified assuming e.g. a typical value of the ratio $\frac{W}{U} = \frac{1}{5}$ (or less). Because the bandwidth of the conduction band for the sc lattice is $W = 12t$, it results in a small value of the expansion parameter $x = \frac{t}{U} = \frac{1}{60}$ in this case. It, however, means that the linear approximation is quite reasonable because all higher terms in the expansion, proportional to $x^n$ ($n = 2, 3, ...$), produce 60 times smaller contribution.

To present the results of the Taylor expansion including all the terms proportional to $t$ and $\frac{t^2}{U}$ let us first define several auxiliary quantities

$$P^{(1)} = \prod_{I=1}^{M} P^{(1)}_I,$$  \hspace{1cm} (34)$$

$$P^{(2)} = \frac{t}{U} \sum_{I=1}^{M} P^{(1)}_I \cdot \ldots \cdot P^{(1)}_{I-1} P^{(2)}_I P^{(1)}_{I+1} \cdot \ldots \cdot P^{(1)}_M$$  \hspace{1cm} (35)$$

where

$$P^{(1)}_I = 1 - \frac{1}{2} \left( n^{b}_{I,1} + n^{b}_{I,2} \right) + \frac{1}{4} n^{b}_{I,1} n^{b}_{I,2}.$$  \hspace{1cm} (36)$$

$$P^{(2)}_I = \sum_{\sigma} \sum_{\alpha=1}^{2} \left( a^{\dagger}_{I,\alpha,\sigma} b_{I,\pi,\sigma} + b^{\dagger}_{I,\alpha,\sigma} a_{I,\pi,\sigma} \right)$$  \hspace{1cm} (37)$$

and ($\alpha = 1, 2$)

$$\tilde{a}_{I,\alpha,\sigma} = a_{I,\alpha,\sigma} \left( 1 - \frac{1}{2} n^{b}_{I,\pi} \right),$$  \hspace{1cm} (38)$$

$$\tilde{a}_{I,\alpha,\sigma} = b_{I,\pi,\sigma} + a^{\dagger}_{I,\alpha,-\sigma} a_{I,\alpha,-\sigma} b_{I,\alpha,\sigma} + a_{I,\pi,\sigma} n^{a}_{I,\alpha} \frac{1}{2}$$  \hspace{1cm} (39)$$

where $b_{I,\alpha,\sigma}$ is given by (31).

The Hamiltonian $\overline{H}$ (C.6), including all the terms proportional to $t$ and $\frac{t^2}{U}$, takes on the form

$$\overline{H} = \overline{H}^{(1)} + \overline{H}^{(2)}$$  \hspace{1cm} (40)$$
where

$$\overline{H}^{(1)} = -t \sum_{I,\sigma} [a_{I,1,\sigma} a_{I,2,\sigma} + a_{I,2,\sigma} a_{I,1,\sigma}] - t \sum_{I,\sigma} [\tilde{a}_{I,1,\sigma} \tilde{a}_{I+1,1,\sigma} + \tilde{a}_{I,1,\sigma} \tilde{a}_{I+1,2,\sigma}]$$

$$- t \sum_{I \neq J,\sigma} [\tilde{a}_{I,\alpha,\sigma} \tilde{a}_{J,\beta,\sigma}]$$

(41)

and

$$\overline{H}^{(2)} = \frac{4t^2}{U} \sum_{I} [\vec{S}_{I,1} \cdot \vec{S}_{I,2} - \frac{1}{4} n_{I,1} n_{I,2}] - \frac{t^2}{U} \sum_{I,\sigma} [\tilde{a}_{I,2,\sigma} \tilde{a}_{I+1,1,\sigma} + \tilde{a}_{I,2,\sigma} \tilde{a}_{I+1,1,\sigma}]$$

$$+ \tilde{a}_{I+1,1,\sigma} \tilde{a}_{I,2,\sigma} + \tilde{a}_{I+1,1,\sigma} \tilde{a}_{I,2,\sigma}]$$

$$- \frac{t^2}{U} \sum_{I \neq J,\sigma} \sum_{\alpha=1}^{2} [\tilde{a}_{I,\alpha,\sigma} \tilde{a}_{J,\beta,\sigma} + \tilde{a}_{I,\alpha,\sigma} \tilde{a}_{J,\beta,\sigma}]$$

$$+ \frac{2t^2}{U} \sum_{I} [\vec{S}_{I,2} \cdot (\vec{S}_{I+1,1,1} + \frac{1}{2} \vec{S}_{I+1,1,1})$$

$$+ \vec{S}_{I+1,1,1} \cdot (\vec{S}_{I+2,1,2} + \vec{S}_{I+2,1,2})]$$

$$+ \frac{2t^2}{U} \sum_{I \neq J} [\vec{S}_{I,1} \cdot (\vec{S}_{I+2,2,1} + \vec{S}_{I+2,2,1})$$

$$+ \frac{2t^2}{U} \sum_{I \neq J} [\vec{S}_{I,2} \cdot (\vec{S}_{I+2,2,1} + \vec{S}_{I+2,2,1})]$$

(42)

The operators $s_{I,\mu;J,\nu}^{\pm}$ and $s_{I,\mu;J,\nu}^{\pm}$ in (42) retain their forms introduced in (C.1) but $a_{I,\mu,\sigma} (a_{I,\mu,\sigma}^{\dagger})$ in (C.1) should actually be replaced by $\tilde{a}_{I,\mu,\sigma} (\tilde{a}_{I,\mu,\sigma}^{\dagger})$, defined by (38). The total Hamiltonian $\overline{H}$ in the large $U$ limit (24) including all terms proportional to $t$ and $t^2$ can thus be written in the form

$$\overline{H} = P^{(1)} (\overline{H}^{(1)} + \overline{H}^{(2)}) + P^{(2)} \overline{H}^{(1)} = P^{(1)} \overline{H}^{(1)} + (P^{(1)} \overline{H}^{(2)} + P^{(2)} \overline{H}^{(1)}).$$

(43)
The first part, \( P^{(1)} H^{(1)} \), contains the terms proportional to \( t \) whereas the term in the parentheses is proportional to \( t^2 \) (see (35) and (42)). In the expression for \( H^{(2)} \) (see (42)) the first term describes the antiferromagnetic, Heisenberg intradimer interaction (see also the second term in (15)). The appearance of this term may suggest that such an interaction should also arise between different dimers. This is of course the case. However, because of applied procedure such terms do not appear explicitly. In the last analysis our method treats all interactions within and between dimers, on the same quality level, i.e. all interactions are taken into account. The magnetic interdimer interactions, represented by the fourth and fifth term in (42), have formally the same structure as the Heisenberg interactions but instead of the scalar products of spin operators there are the products of spin operators and "hopping spin" operators (defined in C.1). All the terms presented in (42) are correct because they originate from the exact decomposition of the Hubbard Hamiltonian (1) into a set of interacting dimers (4) where each dimer problem has been exactly solved (exact dimer representation of the construction operators after applying the projection procedure, given by (27) and (28)). The total Hamiltonian \( H \) (43), we are interested in, is much more complicated than \( H^{(1)} \) and \( H^{(2)} \) alone (see (41)-(43)) because of the presence of the projection operators \( P^{(1)} \) and \( P^{(2)} \) (see (34)-(37)) in the expression (43). 

It is also interesting to see what happens in the special case when taking the limit \( U \to \infty \). The second term in the parentheses of Eq.(43) vanishes in this limit (cf (35) and (42)). Besides, each lattice site cannot be at the same time occupied by two electrons what is equivalent to the assumption \( (\alpha = 1, 2) \)

\[
\begin{align*}
    n^b_{I,\alpha,\sigma} &= b^+_I\alpha,\sigma b_{I,\alpha,\sigma} = n_{I,\alpha,\sigma} n_{I,\alpha,-\sigma} = 0, \\
    n^b_{I,\alpha} &= \sum_{\sigma} n^b_{I,\alpha,\sigma} = 0 \\
\end{align*}
\]

and (cf (38))

\[
\tilde{a}_{I,\alpha,\sigma} = a_{I,\alpha,\sigma}.
\]
The total Hamiltonian (43) is thus given by a simple formula

$$H = P^{(3)}\mathcal{H} = -t \sum_{I,\sigma} \left[ a_{I,1,\sigma}^+ a_{I,2,\sigma} + a_{I,2,\sigma}^+ a_{I,1,\sigma} \right]$$

(47)

$$-t \sum_{I,\sigma} \left[ a_{I,2,\sigma}^+ a_{I+1,1,\sigma} + a_{I+1,1,\sigma}^+ a_{I,2,\sigma} \right]$$

$$-t \sum_{J \neq I,\sigma} \sum_{\alpha=1}^2 a_{J,\alpha,\sigma}^+ a_{J,\alpha,\sigma}.$$ 

Going back to the original lattice (cf (4),(5) and (1)) it is easy to see that the exact Hubbard Hamiltonian in the limit $U \to \infty$ takes on the form

$$H = -t \sum_{i,j,\sigma} a_{i,\sigma}^+ a_{j,\sigma}$$

(48)

where $i$ and $j$ (as before) number the lattice points and $a_{i,\sigma}$ ($a_{i,\sigma}^+$) are the Hubbard operators, defined by (9).

6 Conclusions

Using a new, nonperturbative approach, basing on the equivalent form of the Hubbard Hamiltonian, represented by the collection of interacting dimers (4) where each dimer problem has been exactly solved, we have expressed the annihilation (creation) operators (B.1)-(B.4) as linear combinations of transition operators between different dimer states (dimer representation). This method made it possible to exclude from the considerations the unoccupied dimer energy levels in the large $U$ limit by means of the projection technique resulting in the final Hamiltonian for the dimer itself (14), as well as, for the crystal as a whole (see (23), (24) and (C.6)). It is important to stress that the elimination of the unoccupied dimer energy levels was the only assumption to derive the Hubbard Hamiltonian (24) in the large $U$ limit. Therefore we can be sure that expanding (24) with respect to $x = \frac{t}{U}$ (Taylor expansion) we obtain absolutely all terms proportional to $x^n$ ($n = 1, 2, ...$). In other words all the coefficients proportional to $x^n$ are easy to control what is not always the case when using another methods. The final form of the obtained Hamiltonian in the large $U$ limit (see (23), (24) and (C.6)) visualizes high
degree of complexity of the model, deeply hidden in its original version, forming a mixture of many multiple ferromagnetic, antiferromagnetic and more complex interactions competing one with another. This fact seems to be decisive for our final conclusion. Because we are still dealing with the approximate solutions of the model (the exact solution does not exist till now) it may happen that we underestimate in this way some important interactions and overestimate the others. It is the reason why the resulting thermodynamic properties of the Hubbard model, obtained in an approximate way, so strongly depend on the quality of applied approximations.

We note in passing that the exact dimer solution may serve as a novel alloy analogy for the Hubbard model, which could be treated by coherent potential approximation (CPA). It is well-known that the standard alloy analogy, based on the atomic limit, does not allow for ferromagnetism in the Hubbard model. This may change by application of the dimer solution which already accounts for a restricted hopping of the band electrons. A corresponding study is in preparation.

Another example of a dimer approach to Hubbard-like models is the bond operator theory as an extension of the slave bosonic and fermionic operators (see Refs [40], [41] and papers cited therein).
Appendix A

The exact solution of the dimer eigenvalue problem (5) reads:

\[ E_0 = 0; \quad |E_0\rangle = |0\rangle, \]

\[ E_{11} = -t; \quad |E_{11}\rangle = \frac{1}{\sqrt{2}}(|11\rangle + |13\rangle), \]
\[ E_{12} = t; \quad |E_{12}\rangle = \frac{1}{\sqrt{2}}(|11\rangle - |13\rangle), \]
\[ E_{13} = -t; \quad |E_{13}\rangle = \frac{1}{\sqrt{2}}(|12\rangle + |14\rangle), \]
\[ E_{14} = t; \quad |E_{14}\rangle = \frac{1}{\sqrt{2}}(|12\rangle - |14\rangle), \]

\[ E_{21} = 0; \quad |E_{21}\rangle = \frac{1}{\sqrt{2}}(|23\rangle + |24\rangle), \]
\[ E_{22} = U; \quad |E_{22}\rangle = \frac{1}{\sqrt{2}}(|21\rangle - |26\rangle), \]
\[ E_{23} = C + \frac{U^2}{2}; \quad |E_{23}\rangle = a_1(|21\rangle + |26\rangle) - a_2(|23\rangle - |24\rangle), \]  
(A.1)
\[ E_{24} = -C + \frac{U^2}{2}; \quad |E_{24}\rangle = a_2(|21\rangle + |26\rangle) + a_1(|23\rangle - |24\rangle), \]
\[ E_{25} = 0; \quad |E_{25}\rangle = |22\rangle, \]
\[ E_{26} = 0; \quad |E_{26}\rangle = |25\rangle, \]

\[ E_{31} = t + U; \quad |E_{31}\rangle = \frac{1}{\sqrt{2}}(|31\rangle + |33\rangle), \]
\[ E_{32} = -t + U; \quad |E_{32}\rangle = \frac{1}{\sqrt{2}}(|31\rangle - |33\rangle), \]
\[ E_{33} = t + U; \quad |E_{33}\rangle = \frac{1}{\sqrt{2}}(|32\rangle + |34\rangle), \]
\[ E_{34} = -t + U; \quad |E_{34}\rangle = \frac{1}{\sqrt{2}}(|32\rangle - |34\rangle), \]

\[ E_4 = 2U; \quad |E_4\rangle = |4\rangle \]

where

\[ C = \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}, \]  
(A.2)
\[ a_1 = \frac{1}{2} \sqrt{1 + \frac{U}{2C}}, \]  
(A.3)
\[ a_2 = \frac{1}{2} \sqrt{1 - \frac{U}{2C}}. \]  
(A.4)
Appendix B

The exact dimer representation of the construction operators is given by the following expressions:

\[ c_{1,\uparrow} = \frac{1}{\sqrt{2}} (P_{0,11} + P_{0,12}) + \frac{1}{\sqrt{2}} P_{11,25} - \frac{1}{\sqrt{2}} P_{12,25} \]
\[ + \frac{1}{2} (P_{13,21} + P_{13,22}) + \frac{1}{\sqrt{2}} (bP_{13,23} + aP_{13,24}) \]
\[ - \frac{1}{2} (P_{14,21} - P_{14,22}) + \frac{1}{\sqrt{2}} (aP_{14,23} - bP_{14,24}) \]
\[ + \frac{1}{2} (P_{21,33} - P_{21,34}) - \frac{1}{2} (P_{22,33} + P_{22,34}) \]
\[ + \frac{1}{\sqrt{2}} (aP_{23,33} + bP_{23,34}) - \frac{1}{\sqrt{2}} (bP_{24,33} - aP_{24,34}) \]
\[ + \frac{1}{\sqrt{2}} (P_{26,31} - P_{26,32}) + \frac{1}{\sqrt{2}} P_{31,4} + \frac{1}{\sqrt{2}} P_{32,4}, \]

\[ c_{1,\downarrow} = \frac{1}{\sqrt{2}} (P_{0,13} + P_{0,14}) + \frac{1}{\sqrt{2}} P_{13,26} - \frac{1}{\sqrt{2}} P_{14,26} \]
\[ + \frac{1}{2} (P_{11,21} - P_{11,22}) - \frac{1}{\sqrt{2}} (bP_{11,23} + aP_{11,24}) \]
\[ + \frac{1}{2} (P_{12,21} + P_{12,22}) - \frac{1}{\sqrt{2}} (aP_{12,23} - bP_{12,24}) \]
\[ + \frac{1}{2} (P_{21,31} - P_{21,32}) - \frac{1}{2} (P_{22,31} + P_{22,32}) \]
\[ + \frac{1}{\sqrt{2}} (aP_{23,31} + bP_{23,32}) - \frac{1}{\sqrt{2}} (bP_{24,31} - aP_{24,32}) \]
\[ - \frac{1}{\sqrt{2}} (P_{25,33} - P_{25,34}) - \frac{1}{\sqrt{2}} P_{33,4} - \frac{1}{\sqrt{2}} P_{34,4}, \]

\[ c_{2,\uparrow} = \frac{1}{\sqrt{2}} (P_{0,11} - P_{0,12}) - \frac{1}{\sqrt{2}} P_{11,25} - \frac{1}{\sqrt{2}} P_{12,25} \]
\[ - \frac{1}{2} (P_{13,21} + P_{13,22}) + \frac{1}{\sqrt{2}} (bP_{13,23} + aP_{13,24}) \]
\[ - \frac{1}{2} (P_{14,21} - P_{14,22}) - \frac{1}{\sqrt{2}} (aP_{14,23} - bP_{14,24}) \]
\[ - \frac{1}{2} (P_{21,33} + P_{21,34}) + \frac{1}{2} (P_{22,33} - P_{22,34}) \]
\[ + \frac{1}{\sqrt{2}} (aP_{23,33} - bP_{23,34}) - \frac{1}{\sqrt{2}} (bP_{24,33} + aP_{24,34}) \]
\[ - \frac{1}{\sqrt{2}} (P_{26,31} + P_{26,32}) + \frac{1}{\sqrt{2}} P_{31,4} - \frac{1}{\sqrt{2}} P_{32,4}, \]

\[ c_{2,\downarrow} = \frac{1}{\sqrt{2}} (P_{0,13} - P_{0,14}) - \frac{1}{\sqrt{2}} P_{13,26} - \frac{1}{\sqrt{2}} P_{14,26} \]
\[ - \frac{1}{2} (P_{11,21} - P_{11,22}) - \frac{1}{\sqrt{2}} (bP_{11,23} + aP_{11,24}) \]
\[ + \frac{1}{2} (P_{12,21} + P_{12,22}) + \frac{1}{\sqrt{2}} (aP_{12,23} - bP_{12,24}) \]
\[ + \frac{1}{2} (P_{21,31} + P_{21,32}) + \frac{1}{2} (P_{22,31} - P_{22,32}) \]
\[ + \frac{1}{\sqrt{2}} (aP_{23,31} - bP_{23,32}) - \frac{1}{\sqrt{2}} (bP_{24,31} + aP_{24,32}) \]
\[ + \frac{1}{\sqrt{2}} (P_{25,33} + P_{25,34}) - \frac{1}{\sqrt{2}} P_{33,4} + \frac{1}{\sqrt{2}} P_{34,4}, \]
where

$$P_{\alpha,\beta} = |E_\alpha\rangle\langle E_\beta|$$  \hspace{1cm} (B.5)

and

$$a = a_1 + a_2$$  \hspace{1cm} (B.6)
$$b = a_1 - a_2.$$

To obtain the annihilation operators of the $I-$th dimer, the index $I$ should be added ($c_{1(2),\sigma} \rightarrow c_{I,1(2),\sigma}$, $P_{\alpha,\beta} \rightarrow P_{\alpha,\beta}^{(I)}$) in (B.1)-(B.4).
Appendix C

To present the Hamiltonian $\overline{\mathcal{H}}$ in a compact form we first introduce the following operators ($\mu, \nu = 1, 2$):

\[
\begin{align*}
  s^+_{I,\mu;J,\nu} & = a^+_{I,\mu;\uparrow} a_{J,\nu;\downarrow}, \\
  s^-_{I,\mu;J,\nu} & = a^+_{J,\nu;\downarrow} a_{I,\mu;\uparrow}, \\
  n_{I,\mu;J,\nu;\sigma} & = a^+_{I,\mu;\sigma} a_{J,\nu;\sigma}, \\
  n_{I,\mu;J,\nu} & = \sum_{\sigma} n_{I,\mu;J,\nu;\sigma}, \\
  s^z_{I,\mu;J,\nu} & = \frac{1}{2} \left( n_{I,\mu;J,\nu;\uparrow} - n_{I,\mu;J,\nu;\downarrow} \right); \\
  s^+_{I,\mu;J,\nu} & = a^+_{I,\mu;\uparrow} a_{J,\nu;\downarrow}, \\
  s^-_{I,\mu;J,\nu} & = a^+_{J,\nu;\downarrow} a_{I,\mu;\uparrow}, \\
  n_{I,\mu;J,\nu;\sigma} & = a^+_{I,\mu;\sigma} a_{J,\nu;\sigma}, \\
  n_{I,\mu;J,\nu} & = \sum_{\sigma} n_{I,\mu;J,\nu;\sigma}, \\
  s^z_{I,\mu;J,\nu} & = \frac{1}{2} \left( n_{I,\mu;J,\nu;\uparrow} - n_{I,\mu;J,\nu;\downarrow} \right).
\end{align*}
\]
The operators $s^\pm_{I,\mu; J,\nu}$, $\tilde{s}^\pm_{I,\mu; J,\nu}$, $\tilde{s}^\pm_{I,\mu; J,\nu}$, are not strictly the spin operators, they, however, show some similarities to the true spin operators (as e.g. (11)-(13)) and therefore they can be called "hopping spin operators". Moreover, the following abbreviations have to be used:

$$Q(I, \mu; J, \nu) = \vec{S}_{I,\mu} \cdot \left( \vec{s}_{I,\mu; J,\nu} + \vec{s}_{I,\mu; J,\nu} \right), \quad (C.2)$$

$$R(I, \mu; J, \nu) = \vec{S}_{I,\mu} \cdot \vec{S}_{J,\nu} n_{I,\mu; J,\nu}, \quad (C.3)$$

$$R^{z,\pm}(I, \mu; J, \nu) = (S^z_{I,\mu} S^\pm_{J,\nu} - S^\pm_{I,\mu} S^z_{J,\nu}) s^\mp_{I,\mu; J,\nu}, \quad (C.4)$$

$$R^{-,+}(I, \mu; J, \nu) = (S^-_{I,\mu} S^+_{J,\nu} - S^+_{I,\mu} S^-_{J,\nu}) s^\mp_{I,\mu; J,\nu}. \quad (C.5)$$

The Hamiltonian $\overline{H}$ (cf (24)) with the use of (C.1) - (C.5) takes on the form

$$\overline{H} = \sum_I \overline{H}_I - t \sum_{I,\sigma} \left[ a^+_I a_{I+1,\sigma} + a^+_I a_{I+1,\sigma} + a^+_I a_{I+1,\sigma} a_{I+1,\sigma} \right]$$

$$-2t\beta \sum_I [Q(I, 1; I + 1, 1) + Q(I + 1, 2; I, 2)]$$

$$+2t\delta \sum_I [Q(I, 2; I + 1, 1) + Q(I + 1, 1; I, 2)]$$

$$-t\beta^2 \sum_I [R(I, 1; I + 1, 2) + R^{z,-}(I, 1; I + 1, 2)$$

$$+R^{z,+}(I, 1; I + 1, 2) + R^{-,+}(I, 1; I + 1, 2)$$

$$+R(I + 1, 2; I, 1) + R^{z,-}(I + 1, 2; I, 1)$$

$$+R^{z,+}(I + 1, 2; I, 1) + R^{-,+}(I + 1, 2; I, 1)]$$
\[-t \delta^2 \sum_I \left[ R(I, 2; I + 1, 1) + R^{z-} (I, 2; I + 1, 1) \right. \]

\[ + R^{z+} (I, 2; I + 1, 1) + R^{-+} (I, 2; I + 1, 1) \]

\[ + R(I + 1, 1; I, 2) + R^{z-} (I + 1, 1; I, 2) \]

\[ + R^{z+} (I + 1, 1; I, 2) + R^{-+} (I + 1, 1; I, 2) \left] \right. \]

\[ + t \beta \delta \sum_I \sum_{\mu=1}^2 \left[ R(I, \mu; I + 1, \mu) + R^{z-} (I, \mu; I + 1, \mu) \right. \]

\[ + R^{z+} (I, \mu; I + 1, \mu) + R^{-+} (I, \mu; I + 1, \mu) \]

\[ \left. + R(I + 1, \mu; I, \mu) + R^{z-} (I + 1, \mu; I, \mu) \right. \]

\[ + R^{z+} (I + 1, \mu; I, \mu) + R^{-+} (I + 1, \mu; I, \mu) \right] \]

\[-t \sum_{I \neq J, \mu} \sum_{\mu=1}^2 a^+_{I, \mu, \sigma} a_{J, \mu, \sigma} \]

\[-2t \beta \sum_{I \neq J} \sum_{\mu=1}^2 Q(I, \mu; J, \overline{\mu}) + 2t \delta \sum_{I \neq J} \sum_{\mu=1}^2 Q(I, \mu; J, \mu) \]

\[-t (\beta^2 + \delta^2) \sum_{I \neq J} \sum_{\mu=1}^2 \left[ R(I, \mu; J, \mu) + R^{z-} (I, \mu; J, \mu) \right. \]

\[ + R^{z+} (I, \mu; J, \mu) + R^{-+} (I, \mu; J, \mu) \left. \right] \]

\[ + 2t \beta \delta \sum_{I \neq J} \sum_{\mu=1}^2 \left[ R(I, \mu; J, \mu) + R^{z-} (I, \mu; J, \mu) \right. \]

\[ + R^{z+} (I, \mu; J, \mu) + R^{-+} (I, \mu; J, \mu) \left. \right] \]

where $H^d_I$ is given by (14). It should also be noted that the operators $a^+_{l, \alpha, \sigma}$ ($a_{l, \alpha, \sigma}$), entering in (C.1) and (C.2), are in fact, dependent on $\beta$ and $\delta$ (see (29)). The decomposition of the Hamiltonian $H$ (C.6) according to the terms
proportional to $\beta$, $\delta$, $\beta^2$, $\delta^2$ and $\beta\delta$ has thus only a formal character in order to keep the presentation of the Hamiltonian $\overline{H}$ in a compact form.

The formula (C.6) is the complete expression.

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