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The two-hole ground state of the Hubbard–Anderson model, approximated by a variational RVB-type wave function

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In this paper the Hubbard–Anderson model on a square lattice with two holes is studied. The ground state (GS) is approximated by a variational RVB-type wave function. The holes interact by exchange of a localized spin excitation (SE), which is created or absorbed if a hole moves to a nearest-neighbour site. An SE can move over the sublattice on which it is created. A variational calculation of the GS and the GS-energy is performed for an open-ended 4×4 lattice with two holes with the restriction that the SE is neighbouring both holes and does not move over its sublattice. It is found that the two holes prefer a bound state in which their mutual distance is 1 or $\sqrt{2}$ (with lattice spacing 1).

1. Introduction

Since the discovery of high-T_c superconducting oxides there has been a growing interest in strongly correlated electron systems. Anderson [1] has suggested that the physics of these oxides is contained in the two-dimensional (2D), large-U, single-band Hubbard model. In this model doubly occupied sites are prohibited and the Hubbard Hamiltonian can be transformed into an effective Hamiltonian, called the Hubbard–Anderson (H–A) Hamiltonian [2],

$$H_{\mathrm{H-A}} = H_1 + H_2 + H_3 \,, \tag{1}$$

$$H_1 = -t \sum_{\langle i,j \rangle} \sum_{\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{H.c.}) \,, \tag{2}$$

$$H_2 = 2\frac{t^2}{U} \sum_{\langle i,j \rangle} \sum_{\sigma} (c^{\dagger}_{i\sigma} c_{i-\sigma} c^{\dagger}_{j-\sigma} c_{j\sigma} - n_{i\sigma} n_{j-\sigma}) \,, \tag{3}$$

$$H_3 = -\frac{t^2}{U} \sum_{\langle i,j,k \rangle} \sum_{\sigma} [(c^{\dagger}_{i\sigma} c_{j\sigma} c^{\dagger}_{j-\sigma} c_{k-\sigma} + c^{\dagger}_{i\sigma} n_{j-\sigma} c_{k\sigma}) + \text{H.c.}] . \tag{4}$$

We consider a positive hopping parameter t and a large on-site Coulomb repulsion U, so that $0 < t \ll U$. A pair of nearest-neighbour sites is denoted by $\langle i,j \rangle$, a triple for which i and k are different nearest neighbours of j by $\langle i,j,k \rangle$. A site is either occupied by an electron with z-component of its spin $\frac{1}{2}\sigma$, $\sigma = \pm 1$ ($\hbar = 1$), or empty, i.e. occupied by a hole.

In this paper we study the two-hole ground state (GS) of the H–A model on a $4M \times 4N$ square lattice with periodic boundary conditions. In section 2 the system without holes is considered. Its GS, the pseudo vacuum, is approximated by an RVB-type wave function. Two holes are made by an operator acting on the pseudo vacuum. In sections 3 and 4 the zeroth- and first-order GS of the two-hole system are described. A numerical study of the 4×4 open-ended system is discussed in section 5.

2. The system without holes

At half filling, i.e. all sites occupied by one electron, the H–A model is equivalent to a spin-$\frac{1}{2}$ antiferromagnetic (AF) Heisenberg model. Disregarding an additive constant, $H_{\text{H-A}}$ reduces to

$$H_{\text{Heis}} = J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j , \qquad J = 4\frac{t^2}{U} , \tag{5}$$

with $\langle i,j \rangle$ denoting nearest-neighbour sites on the square lattice.

Liang, Doucot and Anderson proposed a variational RVB-type wave function for the GS of this model [3]. It is a singlet state and it obeys the sign rule for the GS of a spin-$\frac{1}{2}$ AF Heisenberg model on a bipartite lattice, derived by Marshall [4]. We rewrite the GS wave function (eq. 2 of [3]) in the form of a determinant with creation operators and denote it by $|0\rangle$, the pseudo vacuum. It is convenient to divide the square lattice into an odd and an even numbered sublattice. See fig. 1.

Then,

$$|0\rangle = \begin{vmatrix} (1\,2) & (1\,4) & \cdots & (1\,16MN) \\ (3\,2) & (3\,4) & \cdots & (3\,16MN) \\ \vdots & & & \\ (16MN-1\,2) & (16MN-1\,4) & \cdots & (16MN-1\,16MN) \end{vmatrix} | \, \rangle . \tag{6}$$

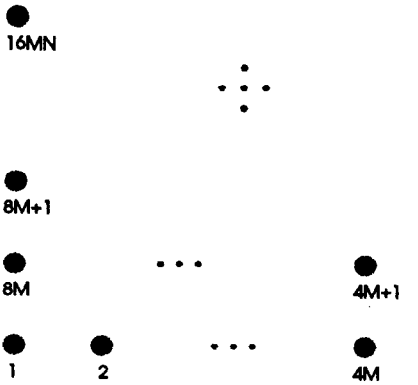

Fig. 1. Numbering of lattice, convenient for determinant notation.

The symbol $(i\ j)$ denotes the product of a positive parameter h_{ij} and a combination of electron creation operators representing a singlet bond on sites i and j, i.e.

$$(i\ j) = h_{ij}(c^{\dagger}_{i+}c^{\dagger}_{j-} - c^{\dagger}_{i-}c^{\dagger}_{j+})\,.$$

Such a bond only connects sites of different sublattices. The parameter h_{ij} can be interpreted as a weight factor for a bond as a function of its length. The real vacuum is denoted by $|\ \rangle$. Note that $(i\ j)$ and $(k\ l)$ commute for distinct i, j, k and l, so that the determinant obeys the usual determinant calculation rules. As [3] mentions, the strong but tenable assumption is made that the amplitude of each bond covering in $|0\rangle$ can be factorized into a product of bond amplitudes. In [3] the values of the bond amplitudes h_{ij} which lead to the lowest GS-energy of a 32×32 lattice are variationally determined. The tendency is that the bond amplitude h_{ij} decays fast with increasing bond length.

3. Zeroth-order states of the two-hole system

In [5] the zeroth-order GS for the one-hole and two-hole system are discussed in terms of Ising configurations [6]. It turns out that in zeroth order the holes move over their quarter lattices (QL), i.e. they make steps over *two* lattice spacings in the x and y direction. With zeroth-order GS is meant the GS of the dominant part of $H_{\mathrm{H-A}}$, called H_0. This GS is characterized by the fact that it is non-frustrated [5]. The first-order GS is the GS of $H_{\mathrm{H-A}}$, for which $H_{\mathrm{H-A}} - H_0$ is used to add frustrated components to the zeroth-order GS in an optimal way. I.e. those frustrated components are added that couple to the

zeroth-order components in the energetically most favourable way. The frustrated components form "bridges" between the zeroth-order components.

In this paper we study the GS of the two-hole system in the RVB language. Therefore, consider a creation operator for a singlet pair of holes on sites i_0 on the odd sublattice and j_0 on the even sublattice: $c_{j_0-}c_{i_0+} - c_{j_0+}c_{i_0-}$. Then

$$(c_{j_0-}c_{i_0+} - c_{j_0+}c_{i_0-})|0\rangle \tag{7}$$

has the same phases for all Ising configurations and the same total spin ($S = 0$) as

$$|(i_0\, j_0)\rangle = (-1)^{(i_0+j_0-3)/2} \times \begin{vmatrix} (1\,2) & \cdots & (1\,j_0-2) & (1\,j_0+2) & \cdots & (1\,16MN) \\ \vdots & & & & & \\ (i_0-2\,2) & \cdots & (i_0-2\,j_0-2) & (i_0-2\,j_0+2) & \cdots & (i_0-2\,16MN) \\ (i_0+2\,2) & \cdots & (i_0+2\,j_0-2) & (i_0+2\,j_0+2) & \cdots & (i_0+2\,16MN) \\ \vdots & & & & & \\ (16MN-1\,2) & \cdots & (16MN-1\,j_0-2) & (16MN-1\,j_0+2) & \cdots & (16MN-1\,16MN) \end{vmatrix} |\,\rangle\,. \tag{8}$$

The parameters h_{ij} may differ from those in $|0\rangle$. They are expected to stay positive, because for positive h_{ij} the spin background obeys Marshall's sign rule and therefore has optimal H_2-energy. This corresponds to the experimental fact that the copperoxide-planes of high-T_c superconductors have an AF spin ordering.

Throughout sections 3 and 4 we concentrate on the correct treatment of the phase factors, which are $+1$ or -1, because we deal with real states and expressions. Doing this, we keep in mind that all parameters are determined variationally when at last we minimize the energy-expectation value of the GS-approximation.

The zeroth-order GS is built up from two-hole configurations like in eq. (8). Its structure is given in [5] and can be found by splitting $H_{\mathrm{H-A}}$ into

$$H_0 = H_2 + H_{3,0} \quad \text{and} \quad H' = H_1 + H_{3,1}\,. \tag{9}$$

The H_0-GS with $S = 0$ is fourfold degenerate:

$$|(1,2)\rangle\,, \quad |(3,4)\rangle\,, \quad |(1,4)\rangle \quad \text{and} \quad |(2,3)\rangle\,. \tag{10}$$

The numbers indicate the quarter lattices (QL) on which the holes move around due to $H_{3,0}$. These H_0-GSs can be linearly combined into Bloch states [5]:

$$|\boldsymbol{k}\rangle = |(1,2)\rangle \pm |(3,4)\rangle\ , \quad \boldsymbol{k} = \begin{cases}(\pi,0)\\(\pi,\pi)\end{cases}, \tag{11}$$

$$|\boldsymbol{k}\rangle = |(1,4)\rangle \pm |(2,3)\rangle\ , \quad \boldsymbol{k} = \begin{cases}(0,\pi)\\(\pi,\pi)\end{cases}. \tag{12}$$

To give $|(1,2)\rangle$, etc., explicitly, we number the sites and the QL (1–4) as in fig. 2. A site on QL 1,2,3,4 has coordinates $(2m,2n)$, $(2m-1,2n)$, $(2m-1,2n-1)$, $(2m,2n-1)$. Then $|(1,2)\rangle$ reads

$$|(1,2)\rangle = \sum_{m,n,p,q} (-1)^{m+n+p+q}\alpha_{mnpq} \\ (c_{2p-1,2q;-}c_{2m,2n;+} - c_{2p-1,2q;+}c_{2m,2n;-})|0\rangle\ , \tag{13}$$

in which the summation is over the integers m, n, p and q, so that it corresponds to all combinations of site indices of QL 1 and 2. The phase factor is such that each $H_{3,0}$-matrix element is zero or negative for positive coefficients α_{mnpq} [5]. The coefficients depend on the distance between the holes and must be determined variationally. In the calculations we work with real coefficients to allow them to be rendered negative by the minimalization procedure. The expression $(c_{2p-1,2q;-}c_{2m,2n;+} - c_{2p-1,2q;+}c_{2m,2n;-})|0\rangle$, shorthand $(c_{j_0-}c_{i_0+} - c_{j_0+}c_{i_0-})|0\rangle$, is (disregarding amplitudes) equal to $|(i_0\ j_0)\rangle$ in eq. (8). For the phase factor, it is convenient to number the sites as described before eq. (13). For the determinant expression, however, it is better to use the numbering corresponding with eq. (8). The other three H_0-GSs are described analogously.

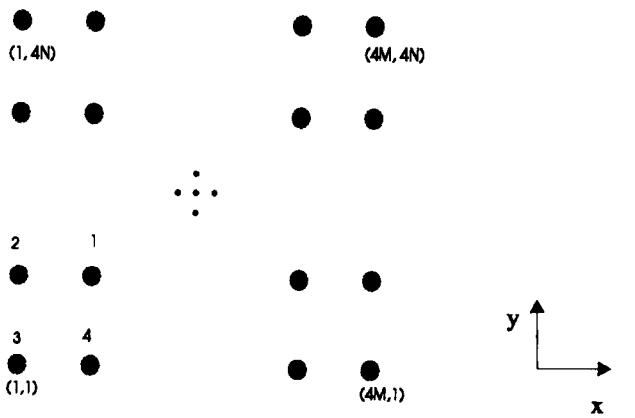

Fig. 2. Numbering of lattice as an xy-coordinate frame and numbering of QL.

Besides the states in eq. (10), one can construct a "bound" state. It corresponds to a different choice for H_0:

$$H_0 = H_2 + H_{3,1} \quad \text{and} \quad H' = H_1 + H_{3,0} . \tag{14}$$

In the zeroth-order bound GS the holes are always nearest neighbours. Other positions of the holes lead to frustration if one considers the expectation value of the total $H_{\mathrm{H-A}}$ (eq. (2.10) of [5]). Frustration is likely to raise the energy and therefore should be avoided, if possible. The bound GS is a Bloch state with $\boldsymbol{k} = (0,0)$ and $S = 0$. In zeroth order it reads (1–4 denote QL)

$$|(0,0)\rangle = |(1,2)\rangle' + |(3,4)\rangle' + |(1,4)\rangle' + |(2,3)\rangle' , \tag{15}$$

with

$$|(i,j)\rangle' = \sum_{i_0,j_0} (-1)^{\mu} (c_{j_0-} c_{i_0+} - c_{j_0+} c_{i_0-})|0\rangle . \tag{16}$$

The summation is over all sites i_0 of Ql i and j_0 of QL j with the restriction that i_0 and j_0 are nearest neighbours. The optimal $H_{3,1}$-phases are expressed by $(-1)^{\mu}$, with

$$\mu = \begin{cases} 0 & \text{for a pair of neighbour holes in the } x\text{-direction} , \\ 1 & \text{for a pair of neighbour holes in the } y\text{-direction} . \end{cases}$$

The expression $(c_{j_0-} c_{i_0+} - c_{j_0+} c_{i_0-})|0\rangle$ is (disregarding amplitudes) equal to $|(i_0\, j_0)\rangle$ in eq. (8).

4. First-order states of the two-hole system

The largest unfrustrated sets of two-hole configurations with $S = 0$ are the zeroth-order states in eqs. (11), (12) and (15). We expand the sets by introducing the first-order two-hole configurations that result if H_1 acts on the zeroth-order configurations. The most important first-order term is H_1, because its amplitude t is much larger than the amplitude of H_3, which is t^2/U. Both terms give an order-one contribution, because they act on a hole. This in contrast to H_2, which is of the order of the number of electrons on the lattice.

The term H_1 displaces a hole to a neighbouring site, leaving behind a spin excitation (SE). Excitation, because the spin on that site has ferromagnetic phase relations with its neighbors. This is energetically unfavourable due to H_2. The SE created by a hole can be absorbed by the same hole via the inverse

H_1-process. But an SE can also give rise to a hole–hole interaction if it is absorbed by the second hole via H_1. If the second hole is not initially a neighbour of the first hole, the SE can move over its sublattice towards a neighbour site of the second hole via H_2. Then it may be absorbed by the second hole via H_1. We found phase relations coupling the first-order configurations optimally to the zeroth-order configurations.

For example, consider the configuration in eq. (8) and let j_1, on the even sublattice, be a neighbour site of i_0. The configuration is depicted in fig. 3a for a 4×4 lattice. By one term of H_1 the hole on i_0 is displaced to j_1, leaving behind an SE on i_0 (fig. 3b). Disregarding amplitudes, one gets

$$
\begin{aligned}
&-(H_1)_{i_0,j_1}|(i_0\ j_0)\rangle = (-1)^{(i_0+j_0-3)/2} \\
&\times \begin{vmatrix}
(1\,2) & \cdots & (j_1-2) & (i_0) & (j_1+2) & \cdots & (j_0-2) & (j_0+2) & \cdots & (16MN) \\
\vdots & & & & & & & & & \\
(i_0-2\,2) & \cdots & (j_1-2) & (i_0) & (j_1+2) & \cdots & (j_0-2) & (j_0+2) & \cdots & (16MN) \\
(i_0+2\,2) & \cdots & (j_1-2) & (i_0) & (j_1+2) & \cdots & (j_0-2) & (j_0+2) & \cdots & (16MN) \\
\vdots & & & & & & & & & \\
(16MN-1\,2) & \cdots & (j_1-2) & (i_0) & (j_1+2) & \cdots & (j_0-2) & (j_0+2) & \cdots & (16MN)
\end{vmatrix} | \rangle \\
&= |(j_1\ j_0); i_0\rangle \,. \qquad (17)
\end{aligned}
$$

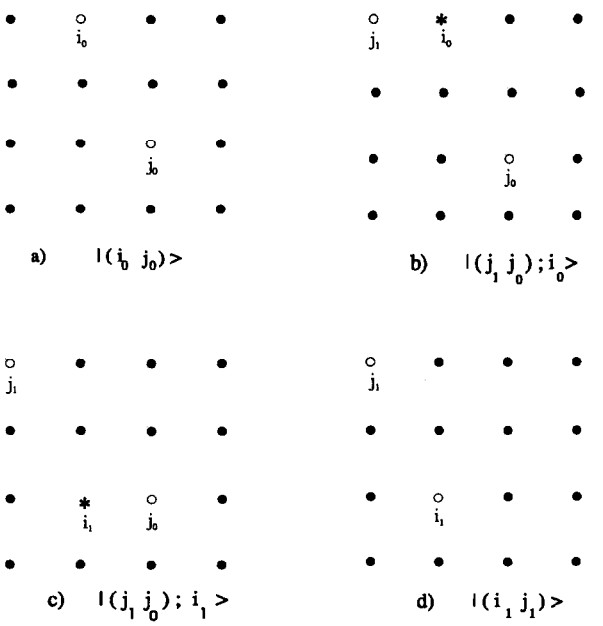

Fig. 3. Interaction of two holes by exchange of an SE.

Note that in eq. (17) the row labeled i_0 and the column labeled j_0 are gone. For convenience all columns after the first one are labeled with the second site of the singlet bond. The first site of the singlet bond is the row index. The column formerly labeled j_1 now has label i_0: all its entries are singlets connecting sites of the odd sublattice to i_0, which is also on the odd sublattice.

We use $-H_1$ to derive a first-order configuration with an optimal connection to the zeroth-order configuration $|(i_0\ j_0)\rangle$, i.e.

$$\langle (j_1\ j_0); i_0|(H_1)_{i_0,j_1}|(i_0\ j_0)\rangle < 0\,. \tag{18}$$

One can show that the SE can move over its sublattice via H_2. Each position of the SE corresponds with a state of the same form as eq. (17) (figs. 3b and 3c). One can derive the following two rules:

Rule 1. If the SE, created by a hole, reaches a neighbour site of the other hole, it can be absorbed by that hole via H_1 if and only if the final two-hole configuration has a minus sign relative to the initial two-hole configuration. The initial and final configuration belong to the zeroth-order GS.

For example, the initial configuration $|(i_0\ j_0)\rangle$ occurs in the GS as

$$(-1)^{\varphi}|(i_0\ j_0)\rangle = (-1)^{\varphi}(c_{j_0-}c_{i_0+} - c_{j_0+}c_{i_0-})|0\rangle\,,$$

and the final configuration $|(i_1\ j_1)\rangle$ (fig. 3d) occurs in the GS as

$$(-1)^{\varphi\pm1}|(i_1\ j_1)\rangle = (-1)^{\varphi\pm1}(c_{j_1-}c_{i_1+} - c_{j_1+}c_{i_1-})|0\rangle\,.$$

The phases $(-1)^{\varphi}$ and $(-1)^{\varphi\pm1}$ are determined by

- H_0; does one consider the GS-approximation with $(-1)^{m+n+p+q}$ or $(-1)^{\mu}$?
- which Bloch state one considers.

Rule 2. A hole can absorb the SE it created if and only if the final two-hole configuration has the same sign as the initial two-hole configuration. The initial and final configuration belong to the zeroth-order GS.

Both rules result in a reduction of the number of neighbour sites of a hole on which the SE can be absorbed.

5. Numerical study of the 4 × 4 open-ended system

To see which state, the one based on $H_2 + H_{3,0}$ or the one based on $H_2 + H_{3,1}$, is energetically most favourable, we performed an exact variational calculation of the zeroth-order and first-order energies and states for the 4×4 open-ended system. Open-ended, to study the dependence of the energies and the coefficients α_{mnpq} (see eq. (13)) on the distance between the holes within a tractable size of the calculations.

Because of the system being open-ended one has to work with the states $|(1,2)\rangle$ etc. of eq. (10) and $|(1,2)\rangle'$ etc. of eq. (15) instead of the Bloch states. The states are linearly combined in such a way that they transform according to irreducible representations of the point group of the square lattice, C_{4v} [7]. The coefficients α_{mnpq} now depend on the distance between the holes and the position of the hole pair on the 4×4 lattice. In eq. (15) one has to add a position dependent coefficient $\alpha_{i_0 j_0}$,

$$|(i\ j)\rangle' = \sum_{i_0, j_0} (-1)^{\mu} \alpha_{i_0 j_0} (c_{j_0-} c_{i_0+} - c_{j_0+} c_{i_0-}) |0\rangle \ . \tag{19}$$

Furthermore, in the first-order two-hole configurations the coefficients also depend on the position of the SE. The two-hole configurations that transform into one another by operators of C_{4v} have the same coefficient.

In the calculations we use the bond amplitudes (h_{ij} of eq. (6)) of the best GS-approximation of the pseudo vacuum of [3] and interpolated values for the amplitudes of singlet bonds of lengths 2, 4 and 6. The bond amplitudes are kept fixed. See table I. The coefficients α are the only variational parameters in our calculations.

First, consider the states of eq. (10). Define

$$|(1,2)\rangle = e_1 \ , \quad |(3,4)\rangle = e_2 \ , \quad |(1,4)\rangle = e_3 \quad \text{and} \quad |(2,3)\rangle = e_4 \ .$$

These four $(H_2 + H_{3,0})$-GSs are linearly combined into four orthogonal states, transforming according to irreducible representations of C_{4v} [7]:

Table I
Bond amplitudes of singlet bonds.

Manhattan length of singlet bond	Bond amplitude
1	1.00000
2	0.30000
3	0.12500
4	0.07000
5	0.03125
6	0.01000

$|1\rangle = e_1 + e_2 + e_3 + e_4$ transforms according to the 1D irreducible representation A_1.

$|2\rangle = e_1 + e_2 - e_3 - e_4$ transforms according to the 1D irreducible representation B_1.

$|K_1\rangle = e_1 - e_2 - e_3 + e_4$ and $|K_2\rangle = e_1 - e_2 + e_3 - e_4$ transform according to the 2D irreducible representation E.

The number of zeroth-order configurations and first-order configurations – with an SE – are denoted in column two and three of table II. Both rules of section 4 were used to derive optimal first-order configurations. Forced by the size of the computational problem, we only considered first-order configurations with the holes on Manhattan distance two and a non-moving SE neighbouring both holes. For states $|1\rangle$ and $|2\rangle$ the first-order configurations are given in figs. 4 and 5. The configurations of fig. 4 are only optimal on the 2×2 squares, hereafter denoted by $\ominus$. Optimal means that the coupling of the first-order configurations (always with an SE) to the zeroth-order configurations (always without an SE) obeys eq. (18). So, in an $\ominus$ each configuration of fig. 4 is optimally coupled with two zeroth-order configurations. On the 2×2

Table II
Results of the 4×4 open-ended system

$t/U = 0.10$	#0th order confs.	#SE confs.	$\langle H_2 + H_{3,0} \rangle$	$\langle H_2 + H_{3,1} \rangle$	$\langle H_2 + H_3 \rangle$	$\langle H_{H-A} \rangle$
$\|1\rangle$	64	32	−5.43	–	−5.35*	−7.42
$\|2\rangle$	64	36	−5.43	−5.77***	−5.60	−7.85
$\|K_1\rangle$	64	34	−5.43	–	−5.43	−6.89*
$\|K_2\rangle$	64	34	−5.43	–	−5.43	−6.89*
$\|(0,0)\rangle$	24	36	–	−5.37**	−5.37**	−8.17**

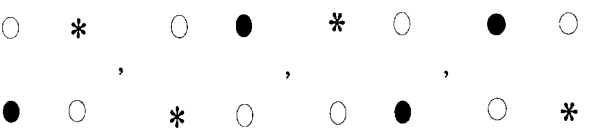

Fig. 4. "Diagonal" first-order configurations.

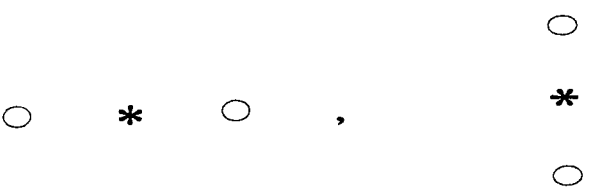

Fig. 5. "Stretched" first-order configurations.

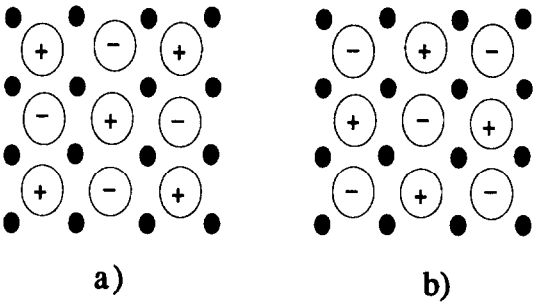

Fig. 6. Pattern of optimal and non-optimal squares for (a) state $|1\rangle$ and (b) state $|2\rangle$.

squares, hereafter denoted by $\oplus$, the couplings are not optimal and we do not add any of the corresponding diagonal first-order configurations to the linear combination that approximates the GS. Fig. 6a shows the pattern of optimal squares ($\ominus$) and non-optimal squares ($\oplus$) for state $|1\rangle$. Fig. 6b does the same for $|2\rangle$.

The configurations of fig. 5 are optimal on the whole 4×4 lattice and therefore all of them are added. For $|K_1\rangle$ the first-order configurations are given in fig. 7. They are optimal on the whole 4×4 lattice. Analogously for $|K_2\rangle$: see fig. 8.

Now, consider the bound state. It transforms according to B_1 of C_{4v}. We keep calling the bound state $|(0,0)\rangle$, although it is not a Bloch state anymore. The first-order configurations are of the type depicted in fig. 4. They are optimal on the whole 4×4 lattice.

Table II gives the results of the variational calculations for the commonly used values $t = 1$ and $U = 10$.

- The entry $\langle j|H_i|j\rangle$ of table II means that $\langle j|H_i|j\rangle / \langle j|j\rangle$ is minimalized with respect to the coefficients α. We will denote this minimalized energy by $\langle\!\langle j|H_i|j\rangle\!\rangle$. The number of the coefficients α ranges from 4 to 18.
- In columns four, five and six we worked with a linear combination only

Fig. 7. First-order configurations of $|K_1\rangle$.

Fig. 8. First-order configurations of $|K_2\rangle$.

containing the appropriate zeroth-order two-hole configurations. In column seven the appropriate first-order configurations were included as well.

- With $*$ is meant that the optimal $H_{3,0}$-phases, which are taken as starting point, are unstable. I.e. the minimilization of the energy renders some of the coefficients α negative, whereas the optimal $H_{3,0}$-phases correspond with positive α-values.
- With $**$ is meant that the optimal $H_{3,1}$-phases, starting point for the bound state, are stable.
- With $***$ is meant that the coefficients α are rendered with such values that all configurations have optimal $H_{3,1}$-phases.
- The other energies correspond to optimal $H_{3,0}$-phases.

5.1. *Comments on the results*

5.1.1. *Zeroth-order states*

- The energy $\langle H_2 + H_{3,0} \rangle$ is the same for $|1\rangle - |K_2\rangle$, because they are linear combinations of $\{e_i, i = 1\text{–}4\}$, which is the fourfold degenerate $(H_2 + H_{3,0})$-GS.
- The equality $\langle\langle (0,0)|H_2 + H_{3,1}|(0,0)\rangle\rangle = \langle\langle (0,0)|H_2 + H_3|(0,0)\rangle\rangle$ holds, because all $H_{3,0}$-matrix elements for the zeroth-order state $|(0,0)\rangle$ are zero.
- The states $|K_1\rangle$ and $|K_2\rangle$ transform according to the 2D irreducible representation E of C_{4v} and are orthogonal. All their energy-expectation values are exactly the same (in zeroth and first order), because C_{4v} is also the symmetry group of H_1, H_2, $H_{3,0}$ and $H_{3,1}$, separately.
- For the zeroth-order states we have

$$\langle\langle 2|H_2 + H_{3,1}|2\rangle\rangle < \langle\langle j|H_2 + H_{3,0}|j\rangle\rangle < \langle\langle (0,0)|H_2 + H_{3,1}|(0,0)\rangle\rangle ,$$

with j one of the set $\{1,2,K_1,K_2\}$.
Note that $|2\rangle$ in $\langle\langle 2|H_2 + H_{3,1}|2\rangle\rangle$ is an extension of $|(0,0)\rangle$ in $\langle\langle (0,0)|H_2 + H_{3,1}|(0,0)\rangle\rangle$, because in $|2\rangle$ the holes can also be at Manhattan distance three or five.

- The line with label $|2\rangle$ shows that for the zeroth-order state $|2\rangle$ frustration in an elementary triangle results in a preference of $H_{3,0}$-phases above $H_{3,1}$-phases: in $\langle\langle 2|H_2 + H_3|2\rangle\rangle$ all two-hole configurations have optimal $H_{3,0}$-phases. The underlying idea is explained in section 2 of [5]. There it is shown that $H_{3,1}$-phases lead to frustration in first order, whereas $H_{3,0}$-phases lead to frustration in second order.
The energy $\langle\langle 2|H_2 + H_3|2\rangle\rangle$ is lower than $\langle\langle (0,0)|H_2 + H_3|(0,0)\rangle\rangle$. So, if one only considers $H_2 + H_3$, there is a preference for $H_{3,0}$-phases.
There is an additional cause for the system to prefer $H_{3,0}$-phases above $H_{3,1}$-phases as shown by $\langle H_2 + H_3 \rangle$ for $|1\rangle - |K_2\rangle$. The coefficients α suggest

two tendencies: holes prefer to sit on the edge of the 4×4 lattice with many optimal $H_{3,0}$-couplings and holes prefer to sit on the edge of the $\ominus$ squares. The disturbance by holes on the edge of the open-ended lattice of the resonance of short singlet bonds is smaller than by holes in the interior of the lattice. That is why the position on the edge benefits the H_2-energy.
In the 2×2 squares denoted by $\ominus$, the two-hole configurations with the holes on Manhattan distance one are optimally coupled via $H_{3,1}$. In $\oplus$ the $H_{3,1}$-couplings are non-optimal.
In the 2×2 squares of $|K_1\rangle$ and $|K_2\rangle$ – both do not have $\oplus$ or $\ominus$ squares – there are as many optimal as non-optimal $H_{3,1}$-couplings. In $|1\rangle$ there are four $\ominus$ squares versus five $\oplus$ squares and in $|2\rangle$ there are five $\ominus$ squares versus four $\oplus$ squares.
With these arguments, one can understand the order of $\langle H_2 + H_3 \rangle$ for $|1\rangle$–$|K_2\rangle$. State $|1\rangle$ has $\ominus$ squares lying more in the interior of the lattice, causing a mixture of $H_{3,0-}$ and $H_{3,1}$-phases. States $|K_1\rangle$ and $|K_2\rangle$ do not have the restriction of $\ominus$ and $\oplus$ squares. State $|2\rangle$ has the advantages of both tendencies.

5.1.2. First-order states

The influence of H_1 is visible in the column of table II with label $\langle H_{\mathrm{H-A}} \rangle$. As mentioned earlier, the optimal first-order two-hole configurations represent an interaction between the holes. In $\ominus$ squares there are four optimal first-order configurations. In $\oplus$ squares the first-order configurations are not optimal and thus not added to the linear combination approximating the GS. The coefficients α and $\langle H_{\mathrm{H-A}} \rangle$ for $|1\rangle$–$|K_2\rangle$ make clear that the state is more favourable if it has more $\ominus$ squares which are optimally coupled by $H_{3,0}$. The state $|(0,0)\rangle$ has nine $\ominus$ squares, which are optimally coupled by $H_{3,1}$. From table II we conclude that the overall GS for the 4×4 lattice in this approximation is the bound state $|(0,0)\rangle$.

It is an open question whether the bound state is still the GS if one includes more first-order states. Namely those with the SE not neighbouring both holes or even one of the holes (via H_2 an SE can move over its sublattice). Furthermore, the calculations show the following tendencies:

- An SE prefers to have as little as possible nearest- and next-nearest-neighbour spins. This is due to the H_2-expectation value.
- For the states $|1\rangle$–$|K_2\rangle$ the absolute values of the coefficients of the two-hole configurations become smaller if the distance between the holes increases. See fig. 9.

The last tendency is due to two effects. The optimal H_1-couplings stimulate the holes to be neighbours. Note that the amplitude of $H_1(t)$ is larger than the amplitude of H_3 (t^2/U). The optimal $H_{3,0}$-couplings to the configurations with

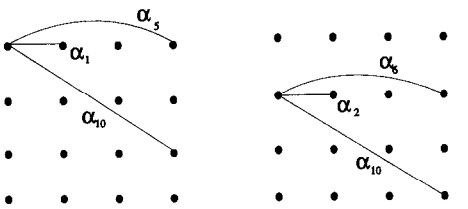

Fig. 9. Coefficients of some two-hole configurations.

two neighbouring holes explains the order of the coefficients α_5 and α_{10} in $|2\rangle$ and α_6 and α_{10} in $|1\rangle$. See fig. 9. The question is how far the decrease of the coefficients goes for macroscopical systems. If $\lim_{r\to\infty}|\alpha| = c$ with $c > 0$, then the best approximation of the GS based on optimal $H_{3,0}$-phases has a large entropy advantage in comparison with the bound state $|(0,0)\rangle$. If $c = 0$, then the two holes are bound too, but not as drastically as in $|(0,0)\rangle$.

In view of the size of the calculations, it is necessary to use a different calculation method for larger systems. An alternative may be to derive an effective Hamiltonian, describing the holes and the SE as quasi-particles. Such a Hamiltonian can possibly cope with a larger number of holes and SE. Furthermore, it can be more manageable than the H–A Hamiltonian.

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