PHYSICA A

Effective Hamiltonian for the motion of holes in the Hubbard–Anderson model

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The motion of (interacting) holes in the Hubbard–Anderson model for high-T_c superconductivity is translated into the motion of (coupled) spinless fermions. The entities responsible for the coupling are localized spin excitations and are described by bosons. The new description shows resemblance with the BCS description of electrons and phonons of the "classical" superconductors.

1. Introduction

Strongly correlated electron systems in a two-dimensional space have been the subject of numerous theoretical papers in recent times. This theoretical work has the ultimate aim to explain the behaviour of the recently discovered high-T_c superconducting copper oxides [1].

One of the models that has been studied intensively is the Hubbard–Anderson (HA) model [2, 5–7, 10, 11]. It has the essential features of a strongly correlated electron gas that shows an antiferromagnetic (AF) (short-range) order at sufficiently low temperatures. It seems to be essential for the phenomenon of superconductivity in the copper oxides that they have a nearly half-filled band of one-electron states.

According to the present understanding of the behaviour of the new superconductors charge transport takes place in the Cu–O planes, in which the electrons move from one site to a neighbouring site on a square lattice. This motion is described adequately in the Hubbard model [8] and for large on-site Coulomb repulsion repulsion between electrons by the HA model. Whereas the Hubbard model accounts for the fermion character of the electrons, which excludes double occupation of a site by electrons of the same spin, the HA model also excludes the occupation of a site by two electrons of opposite spin.

In the latter model, the possibility of *virtual* double occupations results in an AF coupling between electrons on neighbouring sites.

In the HA model half filling corresponds with one electron per site. The system is an AF Heisenberg system in which no charge transport is possible, because there are no empty sites.

Near half filling means that there are holes, i.e. empty sites, in the system. Now the system contains two types of "particles":

– holes,
– excitations of the AF system of electrons.

If an electron moves to an empty neighbouring site, it displaces the hole in the opposite direction. In this process the moving electron conserves its spin direction and may therefore lead to an excitation of the AF system. So the motion of a hole is coupled with an excitation of the AF system.

It is the aim of this paper to describe the HA model with a small number of holes with an effective Hamiltonian that contains two types of variables:

– fermion variables representing the holes,
– boson variables representing the excitations of the AF system.

The analysis resulting in this approximative description of the HA model leans heavily on the so-called Marshall rule for AF systems [9]. This rule can be generalized readily for the HA model [10]. It defines optimal phases for the components of the ground-state (GS) wave function for an appropriate restricted basis.

Section 2 is devoted to the "Marshall" states for the HA model, in particular for systems with two holes. The Marshall states for two holes describe the free motion of the holes. This has already been studied in detail in refs. [10, 11]. In section 3 we also discuss the effects of perturbations, corresponding to those parts of the HA Hamiltonian that were left out in defining the Marshall states.

In section 3 we make a translation of the Marshall states in terms of the free motion of spinless fermions in a field theory. The complete Hamiltonian for this field theory contains three terms:

– a free-fermion term, representing an unperturbed motion of the holes over a restricted part of the lattice,
– a free-boson term for the dynamics of the excitations of the AF system for fixed positions of the holes,
– a term representing the coupling between the two types of particles.

The second term originates from the AF Heisenberg term of the HA Hamiltonian, whereas the third term corresponds with the part describing the motion of a hole to a neighbouring site. The Hamiltonian for the two coupled fields shows a resemblance with the BCS Hamiltonian for "classical" superconductors [12]. The excitations with a boson character replace the phonons of the BCS theory, whereas the holes replace the electrons.

In section 4 remarks are made about a generalization of the approach of section 3 to systems with more holes.

The appendix deals with the orthogonality of states with a localized excitation of the AF system and with the dynamics of such an excitation.

2. The Hubbard–Anderson model

In this paper we use the HA model on a two-dimensional square lattice with the Hamiltonian [3–5]

$$H_{HA} = H_1 + H_2 + H_3 , \tag{1}$$

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

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

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

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 $\langle i, j, k \rangle$. Before and after the action of H_{HA} we project onto the subspace without doubly occupied sites. This results in states in which 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 the following subsections we introduce a number of states that can be described by this model.

2.1. The pseudo-vacuum state

The pseudo-vacuum is the GS of the half-filled system, which is equivalent to a Heisenberg antiferromagnet with an interaction between neighbours given by H_2. The parts H_1 and H_3 of H_{HA} are ineffective, because no holes are available. The part H_2 can be written in the form [3, 5]

$$H_2 = J \sum_{\langle i,j \rangle} (S_i \cdot S_j - \tfrac{1}{4}) , \qquad J = 4 \frac{t^2}{U} , \tag{5}$$

$$S_{iz} = \tfrac{1}{2}(c_{i+}^\dagger c_{i+} - c_{i-}^\dagger c_{i-}) , \tag{6}$$

$$S_{i+} = S_{ix} + iS_{iy} = c_{i+}^{\dagger}c_{i-} \; , \qquad S_{i-} = S_{ix} - iS_{iy} = c_{i-}^{\dagger}c_{i+} \; . \tag{7}$$

The GS has been the subject of numerous studies. Although no complete solution has been found so far, some exact properties are known. Marshall has shown that the GS has total spin $S = 0$ [9]. Furthermore he derived a rule for the relative phases of the components of the GS. These components are Ising configurations, i.e. the eigenstates of the z-components of all the individual spin operators. In the GS all Ising configurations with $M = 0$, M being the S_z eigenvalue, have nonzero coefficients. On these grounds and the orthogonality of the eigenstates of H_2 one sees that the GS is unique. There are strong suggestions that there is an unstable long-range order at zero temperature. See for example refs. [13, 14], in which the GS is studied within the resonating-valence-bond method. At finite temperatures there is no long-range order according to the theorem of Mermin and Wagner [15].

The lattice we will use throughout this paper is a rectangular part of the square lattice with periodic boundary conditions, consisting of $4M \times 4N$ sites. The fourfold for both directions is chosen to give a relatively simple form for the GS of the system with 0, 1 or 2 holes. We will indicate the two sublattices by A and B. The pseudo-vacuum is denoted by $|0\rangle$. All other states discussed in this section are constructed with help of the proper operators acting on the pseudo-vacuum.

2.2. States with one hole

States with one hole are constructed by operating with an annihilation operator on $|0\rangle$:

$$c_{i\sigma}|0\rangle \quad (i \text{ on } A) \, , \qquad c_{j\sigma}|0\rangle \quad (j \text{ on } B) \, . \tag{8}$$

These states are also Marshall states in the sense that interchange of an up and a down spin on the same sublattice results in an Ising configuration with the same sign as the initial Ising configuration. Both Ising configurations are components of one and the same state. This operation for spins on different sublattices gives a change of sign.

Now we discuss the effect of the different parts of H_{HA} on states with one hole. The part H_1 interchanges an electron and a hole on neighbouring sites with conservation of the electron's spin direction. This process results in a phase mismatch for the Ising components of the state, i.e. Marshall's rule is broken locally. The resulting state is characterized by a local spin excitation (SE). The SE will be discussed in more detail when we consider the states with two holes.

The one-hole states in eq. (8) are approximate eigenstates of H_2 with a slightly higher energy than $|0\rangle$, because four bonds in the AF state are broken.

The part H_3 displaces the hole over one of the following vectors (taking the lattice constant equal to unity):

$$\boldsymbol{\delta}_0 = (\pm 2, 0), (0, \pm 2) \qquad (H_{3,0}), \tag{9}$$

$$\boldsymbol{\delta}_1 = (1, \pm 1), (-1, \pm 1) \qquad (H_{3,1}). \tag{10}$$

In this way the displacements are subdivided in two classes, defining two distinct parts of H_3:

$$H_3 = H_{3,0} + H_{3,1}. \tag{11}$$

Essential in these displacements is that the hole stays on the same sublattice and that all the relative Marshall phases are conserved. As an illustration we consider the displacement of a hole on site i (on A) to site i' (on A) by a term in $H_{3,0}$ or $H_{3,1}$ corresponding to the index set (i, j, i'). The index j represents a site on B that is a neighbour of both i and i'. The relevant matrix element is

$$-\frac{t^2}{U} \langle 0|c_{i'+}^\dagger \sum_\sigma (c_{i\sigma}^\dagger c_{j\sigma} c_{j-\sigma}^\dagger c_{i'-\sigma} + c_{i\sigma}^\dagger n_{j-\sigma} c_{i'\sigma})c_{i+}|0\rangle$$

$$= -\frac{t^2}{U} \langle 0|n_{i+} S_{j-} S_{i'+} - n_{i'+} n_{j-} n_{i+} + S_{i-} S_{j+} n_{i'+} - S_{i-} n_{j+} S_{i'+}|0\rangle. \tag{12}$$

From Marshall's rule it follows that all four contributions in the second line of eq. (12) are positive. The uniform sign of all the matrix elements of this type makes it possible to define a Marshall state for the one-hole system, so that the hole can occupy all positions of a restricted set of sites. For $H_{3,0}$ this set is a quarter lattice, i.e. the set of sites connected by the vectors $\boldsymbol{\delta}_0$. In this way four equivalent Marshall states can be defined [10]. They represent the fourfold-degenerate GS of the zeroth-order Hamiltonian $H_2 + H_{3,0}$. For $H_{3,1}$ the restricted set is a sublattice, resulting in two equivalent Marshall states: the twofold-degenerate GS of the zeroth-order Hamiltonian $H_2 + H_{3,1}$. The Marshall states describe the free zeroth-order motion of a hole. In ref. [10] we showed that an elementary triangle of three positions of a hole results in frustration (see fig. 2 of [10]). As a consequence, the combination of both parts of H_3 must be excluded to achieve an optimal zeroth-order motion. Calculations on the 4×4 open-ended system with two holes – in which elementary triangles can occur for both holes – affirm this [11].

There exists an ambiguity in the definition of the state $|0\rangle$. On the one hand one can define it as the GS of the half-filled system. On the other hand one can

consider a variational state $|0\rangle$ that minimizes the ground-state energy of the zeroth-order Hamiltonian for the restricted set of one-hole states. In general, one can state that a proper definition of $|0\rangle$ depends on the number of holes of the system, which is a constant of motion, and on the zeroth-order Hamiltonian one considers. In all cases we will restrict ourselves to a singlet state for the pseudo-vacuum obeying Marshall's rule.

2.3. States with two holes

For two holes one can also define a number of zeroth-order states (i.e. Marshall states) along the same lines as for one hole. Again $H_2 + H_{3,0}$ or $H_2 + H_{3,1}$ can be chosen as the zeroth-order Hamiltonian. In the $H_2 + H_{3,0}$ GS the holes occupy sites on different quarter lattices and their motion is quasi-free: Only if the holes are very near to each other their motion will be different from that of one hole. All matrix elements of the zeroth-order Hamiltonian are nonnegative. The GS is degenerate and these degenerate stationary two-hole states can be combined into states belonging to an irreducible representation of the translation group. They are given in eqs. (4.15)–(4.17) of ref. [10]. They are built up from two-hole states, which are constructed by acting with one of the following operators on $|0\rangle$:

$$c_{j-}c_{i+} - c_{j+}c_{i-} \qquad (i \text{ on A}, j \text{ on B}), \tag{13}$$

$$c_{i'-}c_{i+} + c_{i'+}c_{i-} \qquad (i \text{ and } i' \text{ on A}),$$
$$c_{j'-}c_{j+} + c_{j'+}c_{j-} \qquad (j \text{ and } j' \text{ on B}), \tag{14}$$

and summing over the sites of two different quarter lattices with proper coefficients. In choosing the "creation operator for a hole pair" according to eqs. (13) or (14), one assures that the state is also an eigenstate of the total spin: $S = 0$ for eq. (13) and $S = 1$ for eq. (14). Eq. (13) corresponds to a fourfold-degenerate GS and eq. (14) to a twofold one.

In the nondegenerate $H_2 + H_{3,1}$ GS, the holes are neighbours and form a bound pair that can move over the lattice via $H_{3,1}$. Again all the matrix elements are nonnegative. The state has Bloch vector $k = (0, 0)$ and total spin $S = 0$. It is built up from two-hole states constructed by acting on $|0\rangle$ with the operator of eq. (13) and summing over all possible pairs of neighbouring sites with proper coefficients. For details, see the section on zeroth-order states of ref. [11].

As to the effects of H_1 we enter the domain of systems in which two types of pseudo-particles play a role: the holes and the localized excitations of the AF background. There is an intricate problem as to the definition of an ortho-

gonalized set of states with fixed hole positions and with a localized excitation that will be discussed later on in this section.

First, we give an example of the creation, motion and absorption of a localized excitation. The different stadia considered in this example are shown in fig. 1.

The first two pictures correspond to the action of H_1 on a two-hole state that shifts one of the holes to a neighbouring site:
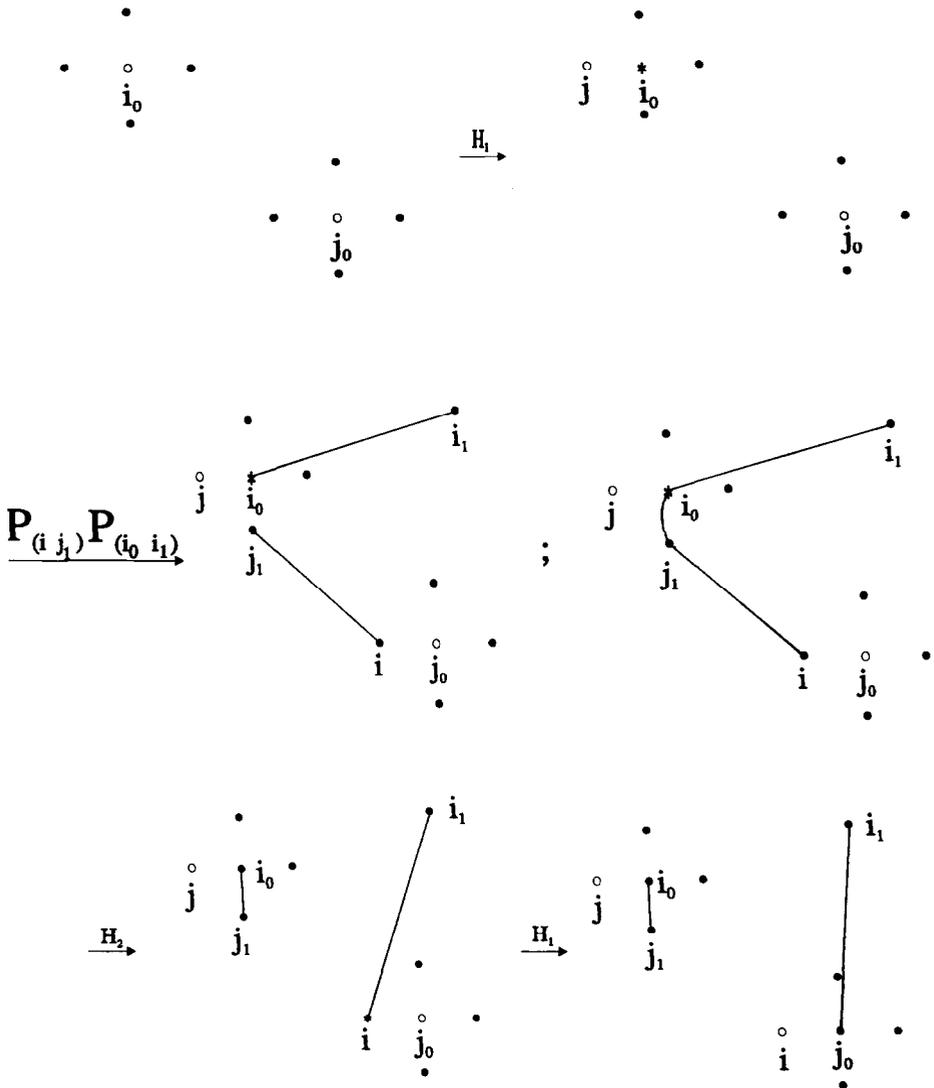

Fig. 1. The creation, motion and absorption of an SE.

$$-t \sum_{\sigma} c^{\dagger}_{i_0 \sigma} c_{j \sigma} (c_{j_0 -} c_{i_0 +} - c_{j_0 +} c_{i_0 -}) |0\rangle \, , \tag{15}$$

so that the final result is a state with holes on j_0 and j. The sites j and i_0 are neighbours. The effect of H_1 is, apart from shifting the hole, the creation of a phase mismatch on site i_0, because the relative phases of the Ising components are such that the electron on i_0 still behaves as if it pertains to sublattice B. The phase mismatch is a local excitation of the AF Heisenberg system and hereafter it will be called a spin excitation (SE). We intend to describe the SE as a boson and to find the proper operators. The first step is to analyze the effect of H_2, which generally gives a shift of the SE over its sublattice. Consider the shift of the SE to a neighbouring site of j_0. On that site it can be annihilated by a reverse process in the sense that the shift of the hole on j_0 to this neighbouring site restores all Marshall phases. In order to realize this process we project the state of eq. (15) on a state with a singlet for the "wrong" pair (i_0, i_1) and also for the "right" pair (i, j_1), with the restriction that the pairs (i_0, j_1) and (i, j_0) are neighbours. The position of i_1 is arbitrary apart from the condition that it belongs to sublattice A. For the projection operator on the singlet for a pair (i, j) we use

$$P_{(ij)} = \tfrac{1}{4} - S_i \cdot S_j \, . \tag{16}$$

The curved line in the fourth picture of fig. 1 indicates the Heisenberg interaction for the spins on the neighbouring sites i_0 and j_1. This interaction results in a transformation of the state with singlets for (i_0, i_1) and (i, j_1) into one with singlets for (i_0, j_1) and (i, i_1), as follows from

$$4 \frac{t^2}{U} (S_{i_0} \cdot S_{j_1} - \tfrac{1}{4})(\tfrac{1}{4} - S_{i_0} \cdot S_{i_1})(\tfrac{1}{4} - S_i \cdot S_{j_1})$$

$$= -4 \frac{t^2}{U} (\tfrac{1}{4} - S_{i_0} \cdot S_{j_1})(\tfrac{1}{4} - S_{i_1} \cdot S_i)(\tfrac{1}{4} - S_{i_0} \cdot S_{i_1})(\tfrac{1}{4} - S_i \cdot S_{j_1}) \, . \tag{17}$$

This operator has only one matrix element unequal to zero, corresponding with the transition between the two states mentioned just before eq. (17). For fixed i and all possible i_1 (on A) and j_1 with the restriction that j_1 represents a neighbour of i_0, the total expression for the matrix element that gives a transition of the SE from i_0 to i is given by

$$\langle 0 | (c^{\dagger}_{i+} c^{\dagger}_{j-} - c^{\dagger}_{i-} c^{\dagger}_{j+})(c^{\dagger}_{j_0 +} c_{i+} + c^{\dagger}_{j_0 -} c_{i-})$$

$$\times 4 \frac{t^2}{U} (S_{i_0} \cdot S_{j_1} - \tfrac{1}{4})(\tfrac{1}{4} - S_{i_0} \cdot S_{i_1})(\tfrac{1}{4} - S_i \cdot S_{j_1})$$

$$\times (c^{\dagger}_{i_0 +} c_{j+} + c^{\dagger}_{i_0 -} c_{j-})(c_{j_0 -} c_{i_0 +} - c_{j_0 +} c_{i_0 -}) |0\rangle \, . \tag{18}$$

Summarizing the meaning of the different factors in this expression we have:

– The third line, which represents the initial state after a shift of one of the original holes on positions (i_0, j_0) to the neighbouring position j, resulting in the hole pair (j, j_0) and an SE on i_0.

– The second line, which represents the exchange interaction for the neighbour pair of sites (i_0, j_1) under the condition that the pairs (i_0, i_1) and (i, j_1) are in a singlet state. This interaction shifts the SE from i_0 to i.

– The first line, which gives a shift of the second hole from j_0 to i which includes the annihilation of the SE on i. The last picture of fig. 1 corresponds to a part of the state $(c_{j-}c_{i+} - c_{j+}c_{i-})|0\rangle$.

The initial and final states are not properly normalized, but to determine the exact normalization factors one has to know a spin correlation function for $|0\rangle$, which cannot be determined for the limit of large systems we are interested in. However, one knows for sure that these factors are of order one. The phase factors of the initial and the final state are as given in expression (18).

One finds that all contributions to expression (18), i.e. for all substates of $|0\rangle$ with their proper Marshall sign, are positive. So the shift of the SE from i_0 to i is characterized by a positive matrix element in our convention for the phases of the initial and final states.

Now we make the following hypothesis as to the existence of states with a local excitation:

Hypothesis. There exists an orthonormal set of singlet states with two holes on one sublattice and an SE on the other. By the action of H_2 the SE moves over its sublattice.

Calculations supporting the hypothesis are described in the appendix. There, the dynamics of a localized phase mismatch and the orthogonality of the corresponding states are studied for half-filled rings with four spins $\frac{1}{2}$ and six spins $\frac{1}{2}$.

NB. 1. In expression (18) only the transition of an SE to a neighbouring site of the second hole is taken into account. This is not a relevant restriction, because the motion of holes (by H_3) and that of the SE (by H_2) can be treated as independent processes in our approximation.

NB. 2. The number of independent singlet states for fixed hole positions and a spin background with $2N$ spins $\frac{1}{2}$ is

$$NR_{s=0} = \binom{2N}{N} - \binom{2N}{N-1}. \tag{19}$$

The number of independent states with an SE for fixed hole positions (also

singlet states) is smaller, because of the phase conditions imposed by the SE. The number $NR_{S=0}$ grows much faster than the number of sites of a sublattice with increasing system size. We expect that this gives enough freedom to find a set of independent singlet states which obey the conditions of an SE. Furthermore, we expect that such a set can be found that obeys the hypothesis, at least in good approximation.

Summarizing, we can distinguish two types of elementary "particles" in the system:

– holes, for which the free motion is determined by $H_{3,i}$, $i = 0$ *or* $i = 1$,
– spin excitations, that can move over their sublattices by H_2.

The part H_1 gives a motion of a hole together with the creation or annihilation of an SE. One may also take into consideration processes in which two excitations are generated by the same hole by two consecutive shifts to a neighbouring site. These processes can also be described by the effective Hamiltonian we will give in the next section.

3. The effective Hamiltonian

The construction of an effective Hamiltonian can be performed for a fixed number of holes. For any fixed number one has to choose spin quantum numbers for the lattice of occupied sites. This is realized by letting the (combination of) creation operators for holes like in eqs. (8), (13) and (14) correspond with a given representation of the rotation group of the total spin. The state $|0\rangle$ is always a Marshall singlet state.

In this section we give a complete description of the representation of the motion of two holes in terms of spinless fermions in interaction with a boson field, corresponding to the excitations of the AF background. The fact that double occupation of a site by holes is not possible in the HA model is included in the fermion representation of the holes. It seems natural to choose boson variables to describe the SE: The creation of an SE in a Marshall state corresponds with an appropriate summation over bilinear terms in fermion variables. See eqs. (6) and (A.3)–(A.5).

The case we analyze in detail is represented in its unperturbed motion by eq. (13) with the zeroth-order Hamiltonian $H_2 + H_{3,0}$ *or* $H_2 + H_{3,1}$. The GSs of both Hamiltonians are singlet states. The unperturbed motion is expressed in terms of states with two spinless fermions, one on either sublattice:

$$\alpha_i^\dagger \beta_j^\dagger \|0\rangle\!\rangle \qquad (i \text{ on A}, j \text{ on B}) . \tag{20}$$

The pseudo-vacuum is indicated by $\|0\rangle\!\rangle$. It is the AF state without holes with

the absolute values of the coefficients of the different Ising components still free to be chosen, in order to minimize the ground-state energy for two holes with interaction. The normalization of the states in eq. (20) is still not determined, but we only use this representation to find a corresponding one for the different parts of the effective Hamiltonian, which will be found apart from the absolute values of its coefficients. It is the form of this Hamiltonian that matters in this paper and not the precise values of its coefficients.

The first term of the Hamiltonian that we consider in its new form is H_3. The essence of ref. [10] is that the total effect of this term can be described by a bilinear expression in terms of the fermion variables α_i and β_j. The two types of holes can move over their sublattice A respectively B, making transitions to nearest- or next-nearest-neighbour sites on their sublattices. We expect the two classes of transitions to have different coefficients in the effective Hamiltonian. In its new form H_3 reads

$$H_3' = \nu_1 \sum_{|i-i_1|=\sqrt{2}} \alpha_{i_1}^\dagger \alpha_i + \nu_2 \sum_{|i-i_2|=2} \alpha_{i_2}^\dagger \alpha_i$$
$$+ \nu_1 \sum_{|j-j_1|=\sqrt{2}} \beta_{j_1}^\dagger \beta_j + \nu_2 \sum_{|j-j_2|=2} \beta_{j_2}^\dagger \beta_j \ . \tag{21}$$

The coefficients ν_1 and ν_2 are positive as follows from the discussions in relation to eq. (12) and the explicit form of the GSs of $H_2 + H_{3,0}$ and $H_2 + H_{3,1}$ for the two-hole system [10, 11]. The term H_3' must be considered to be a projection of H_3 on a space of singlet states with two holes. For every position of the holes one has to consider one singlet state chosen in such a way that it results in the lowest possible energy of the eigenvalue problem at hand. The GSs of the restricted problem defined by $H_2 + H_{3,0}$ or $H_2 + H_{3,1}$ are Marshall states. In this paper we make the hypothesis that also for the perturbed systems, with a Hamiltonian that contains the projection of all parts of H_{HA}, the two-hole states with one hole on either sublattice have a spin background that obeys Marshall's rule.

The next term we discuss is H_1. It shifts a hole to a neighbouring site and creates or annihilates an SE. If the creation and the annihilation of an SE are described by the boson operators

$$e_i^\dagger, e_i \quad (i \text{ on } A) , \qquad d_j^\dagger, d_j \quad (j \text{ on } B) , \tag{22}$$

then the translation of H_1 reads

$$H_1' = -t' \sum_{\langle i,j \rangle} [\beta_j^\dagger \alpha_i (e_i^\dagger + d_j) + \alpha_i^\dagger \beta_j (e_i + d_j^\dagger)] \ . \tag{23}$$

The parameter t' is positive. The term H_1' resembles the interaction of an individual electron in the BCS theory with a phonon mode, which in second order leads to an effective interaction between electrons [16].

The term H_2 gives effectively a transport of an SE over its sublattice. Its new form is a sum of bilinear terms in the creation and annihilation operators of the SE. The starting point to determine the new form is expression (18), which is translated into

$$
\begin{aligned}
&\langle\!\langle 0 \| \beta_j \alpha_i \alpha_i^\dagger \beta_{j_0} e_i \\
&\times (-\nu_{ii_0}) e_i^\dagger e_{i_0} \\
&\times e_{i_0}^\dagger \beta_j^\dagger \alpha_{i_0} \alpha_{i_0}^\dagger \beta_{j_0}^\dagger \| 0 \rangle\!\rangle \, .
\end{aligned}
\tag{24}
$$

In this matrix element the third line represents the initial state with holes on j and j_0 and an SE on i_0. In the second line the SE is shifted from site i_0 to i. The first line corresponds with the final state. The negative coefficient $-\nu_{ii_0}$ is introduced to give the matrix element a positive value, in accordance with expression (18). The actual determination of the coefficients is quite difficult, but for our present purpose it suffices that the ν_{ii_0} are positive. It is likely that they are a function of the distance $|i - i_0|$: Presumably, ν_{ii_0} decreases with increasing distance $|i - i_0|$, because the chance that the SE, made by a hole, moves to a neighbouring site of the other hole and is absorbed by it, decreases with increasing distance between the holes.

Of course, H_2 must also be able to describe the motion of an SE on sublattice B (with indices j). Therefore, the new form of H_2 is

$$
H_2' = - \sum_{\langle i_1, i_2 \rangle} \nu_{i_1 i_2} (e_{i_1}^\dagger e_{i_2} + e_{i_2}^\dagger e_{i_1}) - \sum_{\langle j_1, j_2 \rangle} \nu_{j_1 j_2} (d_{j_1}^\dagger d_{j_2} + d_{j_2}^\dagger d_{j_1}) \, .
\tag{25}
$$

The index pairs $\langle i_1, i_2 \rangle$ and $\langle j_1, j_2 \rangle$ denote all possible pairs on both sublattices.

Summarizing, the effective Hamiltonian for a suitable space of singlet states with two holes is

$$
H' = H_1' + H_2' + H_3' \, .
\tag{26}
$$

4. Summary and remarks about a generalization

In the foregoing sections we have developed a model for the interaction of two holes in the HA model. The analogy with the BCS mechanism for the coupling of two electrons becomes clear by means of the isomorphism

electrons with spin up (down) ↔ holes on sublattice A (B) .

phonons   ↔ localized spin excitations .

It must be remarked that we restricted ourselves to singlet states.

The creation operators for a pair of holes and the pseudo-vacuum play an important role in the determination of the zeroth-order motion of the pseudo-particles, which are considered to be free in their motion over a restricted set of lattice sites. The central question in the problem of generalization of this picture for more holes is: What could be the free motion of e.g. four holes in such a system? Could that correspond to a set of states that is generated by acting with two operators of the type of expression (13) on the pseudo-vacuum?

In the case that the effective Hamiltonian of eq. (26) results in a bound state for a single pair of holes, i.e. a state in which the two holes have a finite average distance, one could imagine that two pairs do not interfere if they do not come too close. In other words: Within a bound pair an SE is exchanged and is restricted in its freedom to move. At a sufficient distance the AF ordering of the spin background will not be disturbed, so giving the possibility for a second bound pair to move independently of the first one. Along these lines of thought one may come to the idea that these bound pairs form a boson condensate, which is responsible for the superconducting current. This boson condensation has the feature that the interaction between two holes results in a bound state in direct space and not a pairing in k-space as is the case for electrons in the BCS theory.

Appendix A

In this appendix we want to make the hypothesis acceptable that an orthonormal set of singlet states with two holes on one sublattice and an SE on the other sublattice exists and that the dynamics of the SE over its sublattice is well defined.

First we remark that two states $|A\rangle$ and $|B\rangle$ are orthogonal if the positions of the holes of $|A\rangle$ are different from those of $|B\rangle$. So we only have to consider the orthogonality of states with fixed hole positions (holes on one sublattice) and an SE (on the other sublattice) and see if a proper dynamics for the SE can be defined. In subsection 2.3 we gave a mechanism for the motion of an SE over its sublattice. This mechanism originates from an RVB description of the pseudo-vacuum and the two-hole states that is used in ref. [11].

Effectively, the free motion of an SE in the HA model is the motion of a localized spin excitation in an AF spin-$\frac{1}{2}$ system. The GS and the low-lying

excited states of the AF-$\frac{1}{2}$ Heisenberg system for a small number of spins are well known. That is the reason why we will work with the Heisenberg system instead of the HA system with holes. We assume that if orthogonal states, with a localized spin excitation that moves over a sublattice, can be found in the Heisenberg system, such orthogonal states can also be found in the HA system with holes. As examples we consider rings with four and six spins $\frac{1}{2}$.

The GS of a ring with $2N$ spins $\frac{1}{2}$ for the AF Heisenberg Hamiltonian

$$H = \sum_{n=1}^{2N} (S_n \cdot S_{n+1} - \tfrac{1}{4}) \tag{A.1}$$

is the pseudo-vacuum $|0\rangle$. It has total spin $S = 0$ and obeys Marshall's rule. We introduce a state with a localized spin excitation on site $2n + 1$ by the action of the operator $2s_{2n+1,z}$ on $|0\rangle$ (for the even-numbered sublattice an analogous line of reasoning is possible). The new state has a phase mismatch on site $2n + 1$ in the sense that an interchange of spins of opposite direction between site $2n + 1$ and a neighbouring site does not correspond to opposite phases of the Ising configurations in contrast to the situation for the GS. This feature holds for interchanges between site $2n + 1$ and *both* neighbouring sites. The state

$$2s_{2n+1,z}|0\rangle \tag{A.2}$$

has total spin $S = 1$ according to the Wigner–Eckart theorem [17]. However, the set of states of this type which correspond to different sites of the odd sublattice is not orthogonal. By means of Fourier summations of these states we get a set of orthogonal states, each of which transforms according to a representation of the translation group characterized by a k-value:

$$|k\rangle = \sum_{n=0}^{N-1} e^{-ikn} 2s_{2n+1,z}|0\rangle , \qquad k = 0, \frac{2\pi}{N}, \ldots, \frac{2\pi}{N}(N-1) . \tag{A.3}$$

After normalizing each Bloch state,

$$c_k^2 \langle k | k \rangle = 1 , \tag{A.4}$$

we perform the inverse Fourier transformation

$$\|n\rangle\rangle = \sum_k e^{ikn} c_k |k\rangle , \qquad n = 0, 1, \ldots, N-1 . \tag{A.5}$$

The set $V = \{(1/\sqrt{N})\|n\rangle\rangle ; n = 0, 1, \ldots, N-1\}$ is an orthonormal set of states. Due to the fact that in general the c_k are unequal for different k, one has to

check explicitly whether the state $\|n = 0\rangle\!\rangle$ has a localized phase mismatch on site 1. If this is the case, each state $\|n\rangle\!\rangle$, $n = 0, 1, \ldots, N-1$, has a localized phase mismatch on site $2n + 1$. Such a localized phase mismatch will be called an SE too, despite the fact that the states $\|n\rangle\!\rangle$ have $S = 1$ in contrast to the states with an SE in the HA model, which have $S = 0$. If the Bloch states of eq. (A.3) are H eigenstates, the dynamics of the SE over its sublattice can be defined properly.

First we consider the ring with four spins $\frac{1}{2}$. Its GS is

$$|0\rangle = \frac{1}{2\sqrt{3}} [2(|+-+-\rangle + |-+-+\rangle)$$
$$- (|++--\rangle + |+---+\rangle + |--++\rangle + |-++-\rangle)] . \qquad (A.6)$$

The Bloch states of eq. (A.3) correspond to $k = 0$ and $k = \pi$. One finds an orthonormal set of states with an SE on site 1 respectively site 3, given by

$$\|n = 0\rangle\!\rangle = \frac{1}{2\sqrt{2}} [\sqrt{2}(|+-+-\rangle - |-+-+\rangle)$$
$$- (|++--\rangle + |+---+\rangle - |--++\rangle - |-++-\rangle)] ,$$
$$\|n = 1\rangle\!\rangle = \frac{1}{2\sqrt{2}} [\sqrt{2}(|+-+-\rangle - |-+-+\rangle)$$
$$+ (|++--\rangle + |+---+\rangle - |--++\rangle - |-++-\rangle)] .$$

The states $|k = 0\rangle$ and $|k = \pi\rangle$ have H eigenvalues $E_0 = -2$ respectively $E_\pi = -1$. For the dynamics of the SE we introduce the factor $\exp(-iE_k t)$, so that

$$H(\exp(-iE_k t)c_k|k\rangle) = i\frac{\partial}{\partial t}(\exp(-iE_k t)c_k|k\rangle)$$
$$= E_k(\exp(-iE_k t)c_k|k\rangle) . \qquad (A.7)$$

Only the relative phases between the states $|k, t\rangle$ are relevant, so one is allowed to divide a linear combination of them by $\exp(-iE_0 t)$. Furthermore, if the SE resides on site 1 at $t = 0$, the moving SE obeys

$$c_0|k = 0\rangle + e^{-it}c_\pi|k = \pi\rangle = A\{c_0|k = 0\rangle + c_\pi|k = \pi\rangle\}$$
$$+ B\{c_0|k = 0\rangle - c_\pi|k = \pi\rangle\} . \qquad (A.8)$$

The solutions for A and B are

$$A = \tfrac{1}{2}(1 + e^{-it}) \quad \text{and} \quad B = \tfrac{1}{2}(1 - e^{-it}) . \qquad (A.9)$$

So the chance to find the SE on site 1 respectively site 3 at time t is

$$P(1, t) = \tfrac{1}{2}(1 + \cos t) \quad \text{and} \quad P(3, t) = \tfrac{1}{2}(1 - \cos t) \, . \tag{A.10}$$

For $t = 2m\pi$, m being a nonnegative integer, the SE resides on site 1. For $t = (2m + 1)\pi$ the SE resides on site 3.

So for the four-ring, the SE moves over its sublattice and is well described by an orthonormal set of states.

The second example is the ring with six spins $\tfrac{1}{2}$. The GS is a singlet state and obeys Marshall's rule. The operator for the translation over one lattice spacing has eigenvalue -1 if it acts on the GS. For shortness we do not give the explicit expressions of the states occurring in this example.

Along the lines of eqs. (A.3)–(A.5) one can derive three orthonormal states with an SE on site 1, respectively 3 and 5. Because the states $|k\rangle$, $k = 0$, $\tfrac{2}{3}\pi$ and $\tfrac{4}{3}\pi$ of eq. (A.3) are not H eigenstates, in contrast to the case of the four-ring, the dynamics of the SE is not properly defined. This is equivalent with the statement that if H acts on a state of set V, it produces more than only a linear combination of the states $\|n\rangle\rangle$, because H also contains nonlinear terms. We restrict ourselves to the linear terms in the supposition that they form the dominant contribution. The energy expectation values of the states $|k\rangle$ and $\|n\rangle\rangle$ are given in table I. Treating the states $|k\rangle$ as H eigenstates, the equation describing the dynamics of the SE reads

$$c_0|k = 0\rangle + \mathrm{e}^{-\mathrm{i}\omega t}c_{2\pi/3}(|k = \tfrac{2}{3}\pi\rangle + |k = \tfrac{4}{3}\pi\rangle)$$
$$= A\|0\rangle\rangle + B\|1\rangle\rangle + C\|2\rangle\rangle \, . \tag{A.11}$$

The states $|k = \tfrac{2}{3}\pi\rangle$ and $|k = \tfrac{4}{3}\pi\rangle$ are each others complex conjugates. The value of ω is positive, because it is the energy expectation value of $|k = \tfrac{2}{3}\pi\rangle$ minus the one of $|k = 0\rangle$. At $t = 0$ the SE resides on site 1. The solution of eq. (37) results into the following chances to find the SE on site 1, 3 or 5 at time t:

$$P(1, t) = \tfrac{1}{9}(5 + 4\cos \omega t) \quad \text{and} \quad P(3, t) = P(5, t) = \tfrac{2}{9}(1 - \cos \omega t) \, . \tag{A.12}$$

Table I
Energy expectation values.

State	EEV
$|k = 0\rangle$	$-10(1 + \tfrac{1}{9}\sqrt{13})$
$|k = \tfrac{2}{3}\pi\rangle$	$-\tfrac{8}{9}(8 + \sqrt{13})$
$|k = \tfrac{4}{3}\pi\rangle$	$-\tfrac{8}{9}(8 + \sqrt{13})$
$\|n = 0, 1, 2\rangle\rangle$	-11.56

So under the assumption that the projection onto the linear vector space, spanned by V, is a good approximation, the SE in the six-ring moves over a sublattice and is described by an orthonormal set of states.

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