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1989 J. Phys.: Condens. Matter 1 9421

(http://iopscience.iop.org/0953-8984/1/47/012)

J. Phys.: Condens. Matter **1** (1989) 9421–9442. Printed in the UK

Inexact solutions for a single hole in a 'high T_c' model: total spin singlets?

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Received 20 December 1988, in final form 17 April 1989

Abstract. We study the strong-coupling limit of the tight-binding model of 'high-T_c' superconductivity assuming that oxygen hole motion dominates copper spin super-exchange. With charge carriers on oxygen sites, moving via virtual charge fluctuations from stable Cu^{2+} into Cu^{+}, we find behaviour quite unlike the strong-coupling Hubbard model. For the one-dimensional chain of CuO, we prove that ferromagnetism with a mobile oxygen hole, in a local spin singlet configuration with a copper hole, is *not* the ground state. We find a variational state with lower energy. The correlations in this state are locally spin singlet, suggesting a total spin singlet ground state. For the two-dimensional plane of CuO_2, we find a similar picture. Although we cannot prove that the ferromagnet with a mobile oxygen hole, in a local spin singlet configuration, is not the ground state, we can find states with local singlet configurations very close by in energy. Antiferromagnetic fluctuations favour the total spin singlet state, which finds the low-energy charged excitations where the non-interacting Fermi surface lies. This suggests experimental problems in separating strong and weak coupling paramagnets, if one looks at the excitation spectrum. Indeed we suggest this as an explanation for why strong coupling paramagnets such as heavy fermion systems yield agreement between band structure calculations and de Haas–van Alphen experiments.

1. Background

In a recent letter [1], the problem of the motion of a single hole in the natural tight-binding model of 'high T_c' superconductivity [2] was addressed. The terms which were included in that treatment were:

$$\bar{H} = T\sum_{i\sigma} c^{\dagger}_{i\sigma}c_{i\sigma} + U\sum_{i} c^{\dagger}_{i\sigma}c^{\dagger}_{i\bar{\sigma}}c_{i\bar{\sigma}}c_{i\sigma} + E\sum_{j\sigma} p^{\dagger}_{j\sigma}p_{j\sigma} + \sum_{\langle ij\rangle\sigma}(c^{\dagger}_{i\sigma}p_{j\sigma} + p^{\dagger}_{j\sigma}c_{i\sigma}) \tag{1}$$

and in this article we will retain this choice. Nearest-neighbour repulsion is ignored and onsite oxygen repulsion is ignored, but we believe that the basic physical processes can be developed without recourse to these terms *at the one-particle level*. Two distinct limits were analysed in this earlier work, firstly motion by vacating copper sites and secondly motion by doubly occupying copper sites. One limit, the latter, was found to be particularly simple since the ordering of the background spins was ferromagnetic, and as such, unique up to the choice of quantisation direction for the moment. The reason for this simple result was the fact that the motion was unfrustrated and so a direct application

0953-8984/89/479421 + 22 $02.50

of Nagaoka's [3] theorem solved the problem. The first limit, however, turned out to be *'frustrated'* and so Nagaoka's theorem was evaded and the ground state is more difficult to find. Arguments were presented to suggest that the ground state was a total spin singlet or resonating valence bond (RVB) [4] state. Since the space of total spin singlets is not unique in the sense that the space of maximal ferromagnetism was, the actual form of the ground state was side-stepped as being too difficult to find in any other than a vague sense. Since that time, various suggestions for hole motion have been presented in the literature [5, 6] and we feel that some physical insight into how one might decide between these two views is called for. Having previously solved the second limit exactly, we will work almost exclusively with the first limit where holes move by virtual Cu^+ excitations.

One of these two descriptions [5] makes a further assertion that we would like to analyse. There is the suggestion that a single hole added to an oxygen site can be modelled by the Hubbard model on the square lattice in the strong-coupling limit. The hole forms a 'Wannier' orbital centred on a copper site, is in a 'local singlet' configuration with respect to the existing copper hole and moves around the lattice by direct hops to neighbouring 'Wannier' orbitals. The motion of a single hole added to the strong-coupling Hubbard model is to some extent understood and so we can compare the results we obtain on order to test this hypothesis.

The precise limit of interest is that where the hybridisation matrix element t is vanishingly small. In a previous paper [7] the behaviour in this limit was found using a transformation from the original Hamiltonian onto an effective Hamiltonian which is exact to second order in t. Previously we considered the limit where there was one copper hole per site and considered only the dynamics of the oxygen hole:

$$H = E\sum_{j\sigma} p^\dagger_{j\sigma}p_{j\sigma} + (J/2)(1+\alpha)\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}\sum_{\alpha} p^\dagger_{j\sigma}p_{j'\sigma} - J\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}[p^\dagger_{j\sigma}c^\dagger_{i\bar\sigma} - p^\dagger_{j\bar\sigma}c^\dagger_{i\sigma}]\,[c_{i\bar\sigma}p_{j'\sigma} - c_{i\sigma}p_{j'\bar\sigma}] \tag{2}$$

where

$$J = t^2U/(T+U-E)(E-T), \qquad \alpha = (2T+U-2E)/U$$

and we were restricting attention to the case where $-1 < \alpha < 1$ in order that any doped holes go onto oxygen sites. In order to interpret this result a little more, we go back one step and consider the case where only changes of two in copper occupancy are prohibited and we include the on-site contribution to the copper hole energy, which is constant since each site has one copper hole:

$$H = E\sum_{j\sigma} p^\dagger_{j\sigma}p_{j\sigma} - (J/2)(1-\alpha)\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}\sum_{\alpha}[p^\dagger_{j\sigma}c^\dagger_{i\bar\sigma} - p^\dagger_{j\bar\sigma}c^\dagger_{i\sigma}][c_{i\bar\sigma}p_{j'\sigma} - c_{i\sigma}p_{j'\bar\sigma}] + T\sum_{i\sigma} c^\dagger_{i\sigma}c_{i\sigma} - (J/2)(1+\alpha)\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}\sum_{\sigma\sigma'} c^\dagger_{i\sigma}c_{i\sigma'}p_{j'\sigma}p^\dagger_{j\sigma'}. \tag{3}$$

The oxygen hole dynamics is identical to that in equation (2), but we have regrouped the terms in what we feel is a more physically transparent way. The contributions from the two limits have now been segregated. The term with $(1-\alpha)$ corresponds to hopping via double occupancy, while the term with $(1+\alpha)$ corresponds to hopping via a vacant copper site. For motion by doubly occupying a copper site, the intermediate virtually excited state *must* have a singlet spin configuration. This is because both holes occupy the same state on the copper site, which can only happen if they are in a singlet

configuration due to Fermi statistics. For motion by vacating copper sites, the intermediate state usually has two oxygen holes locally and these two holes are only constrained to be in a singlet if they lie on the same oxygen site. The spin labels are seen to be consistent with a picture of a copper hole hopping out onto an oxygen site and then being replaced by another hole sitting on a neighbouring oxygen site. There is a contribution from when the copper hole hops onto a neighbouring oxygen site and then hops back. If this self-energy term is subtracted, leaving just the oxygen hole dynamics (equation (2)), then simple interpretations are complicated because there is a term where the neighbouring spins are parallel and one would naively consider the intermediate virtual state as having both holes on the oxygen site, a situation prohibited by Fermi statistics. One *must* consider the self-energy term in interpretations.

There is an important difference between the contributions from the vacant hopping and double occupancy hopping limits. For double occupancy the contribution vanishes in the absence of oxygen holes, whereas for vacant hopping there is an 'anomalous' contribution even when there are no oxygen holes. The reason for this difference is easy to understand but is very important for interpretations. The creation operators in equations (2) and (3) are *not* the same as those in equation (1). The transformation which takes one from the original description to the description valid to order t^2 hybridises the original states with each other. The operator $c^\dagger_{i\sigma}$ in equations (2) and (3) creates predominantly a copper hole of spin σ on site i, but includes the optimal amount of hybridised oxygen hole. The energy of a transformed c electron therefore includes a contribution from the oxygen component. This is the source of the 'anomalous' contribution. The reason that there is no contribution in the double occupancy limit is because the optimum amount of hybridisation in this limit is none at all and so the transformed operators agree with the original operators in this limit. There is an immediate corollary to this. For the vacant hopping limit, the copper hole in the transformed description has obtained the optimal degree of hybridisation. Any additional holes of the same spin added on neighbouring oxygen atoms can therefore only disrupt this hybridisation gain and lose the system energy. The same is not true for a hole added to a neighbouring oxygen site in a singlet-spin configuration. This situation will correspond to the separate two-particle problem, since the two holes have opposite spin labels and are not constrained by Fermi statistics.

Now let us restrict our attention to the limit $\alpha = 1$, where hopping occurs by virtually vacating copper sites forming Cu^+. We are able to make the local spin character dependence manifest in this vacant hopping limit with a simple rearrangement of terms:

$$H = E\sum_{j\sigma} p^\dagger_{j\sigma}p_{j\sigma} + (T-4J)\sum_{i\sigma} c^\dagger_{i\sigma}c_{i\sigma} + J\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}\sum_{\sigma} p^\dagger_{j\sigma}c^\dagger_{i\sigma}c_{i\sigma}p_{j'\sigma}$$
$$+ (J/2)\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}[p^\dagger_{j\sigma}c^\dagger_{i\bar\sigma} + p^\dagger_{j\bar\sigma}c^\dagger_{i\sigma}][c_{i\bar\sigma}p_{j'\sigma} + c_{i\sigma}p_{j'\bar\sigma}]$$
$$- (J/2)\sum_{\langle ji\rangle}\sum_{\langle ij'\rangle}[p^\dagger_{j\sigma}c^\dagger_{i\bar\sigma} - c^\dagger_{i\sigma}p^\dagger_{i\bar\sigma}][c_{i\bar\sigma}p_{j'\sigma} - c_{i\sigma}p_{j'\bar\sigma}]. \quad (4)$$

The hopping occurs via a single copper site, but the relevant oxygen hole may change site. There *is* a contribution where the oxygen hole remains on the same site, for all the local spin configurations. All hopping involving triplet combinations has a positive matrix element and all hopping involving singlet combinations has a negative matrix element. The remainder of this article will be an attempt to find some of the characteristics to be expected from this completion between enhanced singlet correlations and reduced triplet correlations.

For this Hamiltonian, hole motion is *maximally* frustrated. Furthermore this model seems to be the simplest model with this property, and as such is generic. In the same way that the Hubbard model is often studied as the archetypal many-body Hamiltonian which displays strong-coupling magnetism, the present model should be studied as the archetypal many-body Hamiltonian which displays strong coupling *paramagnetism*. The Hubbard model on frustrated topologies is *not maximally* frustrated.

There are two quite natural questions to ask. Firstly and probably of most interest: what is the ground state for this Hamiltonian? On the assumption that the motion of the added oxygen holes dominates any spin interactions between the copper holes, then the oxygen hole motion will have a preferred spin arrangement for the spins on the copper holes. Determining this spin arrangement constitutes the first problem. The second natural question is about hole motion when the spin interactions between copper holes dominate the hole motion. What is the excitation spectrum of an added hole in a fixed copper spin configuration? The natural spin configuration for the second question is the Néel state, since super-exchange is the dominant interaction between spins, and super-exchange involves antiferromagnetic coupling. In this article we will be concerned with the second question, since the first question is extremely difficult to solve exactly and we have already given the simple arguments which suggest that the ground state is a total spin singlet [1]. We will however obtain some evidence for the true ground state in answering the second question. Local spin correlations around a hole moving through a fixed spin background ought to be similar to the preferred ground state correlations for that mobile hole.

We will base our argument about a difference of opinion which has recently been presented in the literature. On one side is Zhang and Rice [5], who suggest that the motion of an added oxygen hole will be best described by 'Wannier'-like orbitals centred on copper sites [5]. On the other side sit Emery and Reiter [6], who state that Zhang is *wrong* and that the correct definition is in terms of orbitals centred on the oxygen sites. Our own work [1] demonstrates that in the limit of oxygen motion by double occupancy of copper sites, then the basis centred on the oxygen orbitals yeilds the ground state for the motional Hamiltonian. It turns out that Zhang's basis *also* finds the ground state and further predicts the *exact* excitation spectrum for one hole; Emery's does *not*! In the present limit there are complications and the questions are much more difficult to tackle. We will seriously consider two fixed spin arrangements in which to discuss hole motion. Firstly we will analyse ferromagnetism because phase coherence is easier to achieve in this spin arrangement and most of the arguments can be taken further towards a conclusion, and secondly we will consider the Néel state because it can be motivated by a super-exchange argument, and furthermore there is experimental evidence for antiferromagnetism on the phase diagram of the 'high T_c' superconductors.

First of all we must introduce a subtlety which causes most of the conceptual problems. Although the long-range order of the copper hole spins may be perfect, there is the possibility of quite different spin configurations around the vicinity of the mobile oxygen hole. This idea has a long history [8], and this object with its local spin distortion has recently been dubbed a 'spin polaron'. The problem where recent work on this effect has taken place is hole motion in the Néel state of the two-dimensional square lattice Hubbard model in the strong-coupling limit [9]. Here one finds local ferromagnetic spin arrangements which allow the hole to gain kinetic energy locally and regain some of the motional energy that it would achieve from Nagaoka's argument. For our problem the local spin configuration distortions take a quite different form. We find *bound states* with a spin fluctuation bound to the mobile hole. Near the end of this article, however, we

will go as far as considering the polaronic distortion caused by the motion of this *composite* particle.

2. Local singlet correlations

If we consider pure ferromagnetism with the oxygen hole spin parallel to the ferromagnetic background, then as has been previously pointed out [1] the lattice topology for hole motion is frustrated, and this state is not the ground state. Indeed we can determine the spectrum for hole motion and we find

$$\varepsilon = E, \qquad E + 2J(1 + \gamma) \tag{5}$$

where $\gamma = \frac{1}{2}(c_1 + c_2)$ and $c_i = \cos ak_i$. As was previously suggested, the addition of a parallel oxygen hole, only loses the system hybridisation energy and this system is therefore *maximally* frustrated.

There are various ways to group the terms in the Hamiltonian which we will see are related to the descriptions of Zhang and Emery. The first breakdown of the terms relevant to the dymanics of hole motion comes from the representation of equation (3) in the relevant limit where $\alpha = 1$:

$$H_{\text{motion}} = \sum_{\langle ij \rangle} \sum_{\langle ij' \rangle} H^i_{jj'}$$

$$H^i_{jj'} = J \sum_{\sigma\sigma'} c^\dagger_{i\sigma} c_{i\sigma'} p^\dagger_{j\sigma'} p_{j'\sigma}. \tag{6}$$

If we consider H^i_{jj} in isolation, then for a hole on both the copper and oxygen sites, there are two eigenvalues. If the two spins are in a triplet configuration then we find $+J$, while if the two spins are in a singlet configuration then we find $-J$. Obviously states built out of 'local singlets' are energetically favoured. We will describe states which are linear combinations of local singlets for most of this article, relaxing this constraint only near the end.

The second breakdown is that centred of the copper sites, where we group the four bonds surrounding the copper site together:

$$H_{\text{motion}} = \sum_i H_i$$

$$H_i = \sum_{\langle ij \rangle} \sum_{\langle ij' \rangle} H^i_{jj'}. \tag{7}$$

If we consider H_i in isolation, then for the hole on the copper site and one hole on the oxygen site, we find two simple problems. For the triplet spin configurations we find

$$H = \begin{bmatrix} J & J & J & J \\ J & J & J & J \\ J & J & J & J \\ J & J & J & J \end{bmatrix} \tag{8a}$$

in terms of the basis where the oxygen hole is on each of the four surrounding oxygen atoms. There are two eigenvalues, the uniform phase solution is at $+4J$ while there are three solutions at zero energy gain. For the singlet spin configurations we find

$$H = \begin{bmatrix} -J & -J & -J & -J \\ -J & -J & -J & -J \\ -J & -J & -J & -J \\ -J & -J & -J & -J \end{bmatrix} \tag{8b}$$

where we find as expected that singlets move with gain in energy. The two eigenvalues are now zero for the three solutions and $-4J$ for the uniform phase solution. It is this solution which is the 'local singlet' centred on the copper site which we will associate with Zhang's paper [5]. This state is just a sum of four 'local singlets' mentioned in the first breakdown, added with uniform phase. It should be remembered that the states in our description *include* hybridisation with the surrounding oxygen sites and are not therefore simple combinations of the original states as the formalism might suggest.

The third breakdown is that centred on the oxygen sites, where we include two bonds on the same oxygen site:

$$H_{\text{motion}} = \sum_{\langle ij \rangle} \sum_{\langle jj' \rangle} H_{jj'}$$
$$H_{jj'} = \sum_{\langle ij \rangle} \sum_{\langle ij' \rangle} H^{i}_{jj'} \tag{9}$$

and includes terms which connect oxygen sites together. If we restrict attention to H_{jj} then we must consider two copper sites with two holes and an oxygen hole on the central oxygen atom. The local spin configurations are now spin $\frac{3}{2}$ and spin $\frac{1}{2}$. The spin $\frac{3}{2}$ state is unique and resides at energy $+2J$, while there are two spin $\frac{1}{2}$ states which reside at $+J$ and $-J$. If we consider the case with one down spin and two up spins, then there are three states with the down spin on each of the three atoms. In this basis the Hamiltonian is:

$$H = \begin{bmatrix} J & J & 0 \\ J & 0 & J \\ 0 & J & J \end{bmatrix} \tag{10}$$

from which we readily construct the eigenstates mentioned above. If we restrict attention to the ground state at energy $-J$, then this is the state and scheme advocated by Emery [6]. This state is a uniform phase sum of two 'local singlets' defined in the first breakdown.

We are now in a position to find the excitation spectrum of these various choices of 'local singlets' in a chosen copper hole spin background. First let us consider ferromagnetism. If we allow all singlet combinations of pairs of holes on neighbouring copper and oxygen atoms, which corresponds to the first breakdown, then we find that we may use the square copper lattice to describe the periodicity, but there are four states per unit cell corresponding to the singlet being with the four neighbouring oxygen atoms. This choice is *not* orthogonal, since there is overlap between singlets with the same oxygen atom but associated with different copper atoms. The orthogonality matrix is

$$O_{\alpha\alpha'} = \begin{bmatrix} 1 & x/2 & 0 & 0 \\ x^*/2 & 1 & 0 & 0 \\ 0 & 0 & 1 & y/2 \\ 0 & 0 & y^*/2 & 1 \end{bmatrix} \tag{11}$$

where

$$x = \exp(iak_x) \qquad y = \exp(iak_y).$$

The Hamiltonian in this basis may be written

$$H_{\alpha\alpha'} = -\frac{J}{2}\begin{bmatrix} 1+x^*+x & 2+2x & 2+y^*+x & 2+y+x \\ 2+2x^* & 1+x+x^* & 2+y^*+x^* & 2+y+x^* \\ 2+x^*+y & 2+x+y & 1+y^*+y & 2+2y \\ 2+x^*+y^* & 2+x+y^* & 2+2y^* & 1+y+y^* \end{bmatrix} \tag{12}$$

which is readily solved by observing that

$$H_{\alpha\alpha'} = (J/2)\,\mathbf{1} - 2J[2\boldsymbol{aa}^{*\mathrm{T}} + \boldsymbol{ba}^{*\mathrm{T}} + \boldsymbol{ab}^{*\mathrm{T}}] \tag{13}$$

in terms of the natural basis

$$\boldsymbol{a} = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \qquad \boldsymbol{b} = \frac{1}{2}\begin{bmatrix} x \\ x^* \\ y \\ y^* \end{bmatrix} \qquad \boldsymbol{c} = \frac{1}{2}\begin{bmatrix} x \\ y \\ -y \\ -x \end{bmatrix} \qquad \boldsymbol{d} = \frac{1}{2}\begin{bmatrix} xy \\ 1 \\ -xy \\ 1 \end{bmatrix}. \tag{14}$$

The $\boldsymbol{c}$ and $\boldsymbol{d}$ vectors decouple and yield the spectrum defined by

$$\begin{bmatrix} 1+\gamma/2 & \gamma+1/2 \\ \gamma+1/2 & 1+\gamma/2 \end{bmatrix}\varepsilon = \frac{J}{2}\begin{bmatrix} 1 & \gamma \\ \gamma & 1 \end{bmatrix} \tag{15}$$

in terms of the structure factor $\gamma = \boldsymbol{a}^{*\mathrm{T}}\boldsymbol{b} = \boldsymbol{c}^{*\mathrm{T}}\boldsymbol{d} = \frac{1}{4}(x + x^* + y + y^*) = \frac{1}{2}(c_1 + c_2)$. This diagonalises to form two dispersionless bands at $J/3$ and J.

The $\boldsymbol{a}$ and $\boldsymbol{b}$ vectors also decouple and yield the spectrum defined by:

$$\begin{bmatrix} 1+\gamma/2 & \gamma+1/2 \\ \gamma+1/2 & 1+\gamma/2 \end{bmatrix}\varepsilon = (-2J)\begin{bmatrix} 2+2\gamma & (1+\gamma)^2 \\ (1+\gamma)^2 & 2\gamma+2\gamma^2 \end{bmatrix} \tag{16}$$

which in turn diagonalises to form

$$\varepsilon = -\tfrac{2}{3}(1+2\gamma)J \pm \tfrac{1}{3}[73 + 40\gamma - 32\gamma^2]^{1/2}J. \tag{17}$$

These dispersions are plotted in figure 1.

The second calculation we perform is that corresponding to the Zhang basis on a ferromagnetic background. The periodicity is again that of the square lattice and we have only one state per unit cell. Again we find that the basis is not orthogonal, but this presents no problems and we find the simple dispersion

$$\varepsilon = \left[-\frac{(7+8\gamma)}{(2+\gamma)}\right]J. \tag{18}$$

This is also plotted in figure 1.

The third calculation we perform is based on the Emery basis on a ferromagnetic background. The periodicity is again the square lattice, but now we find that there are two states per unit cell corresponding to the two oxygen atoms. Since the states

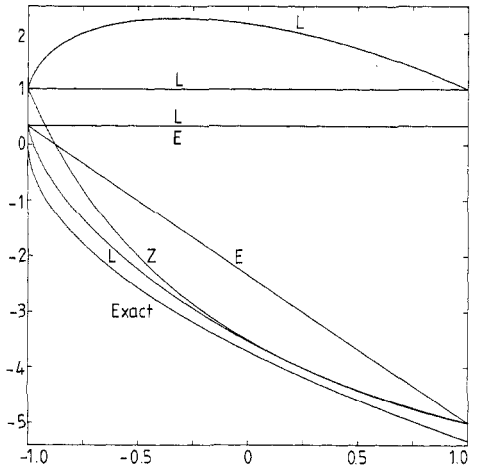


Figure 1. The dispersions for the three local singlet calculations in the ferromagnetic background spin configuration. The wavevector dependence of the hole momentum is always a function of the structure factor γ_k. The line labelled L is the calculation for all local singlet variations; the line labelled Z is the calculation for Zhang's basis centred on the copper sites and the line labelled E is the calculation for Emergy's basis centred on the oxygen sites. All three calculations agree at $\boldsymbol{k} = \mathbf{0}$ ($\gamma_k = 1$).

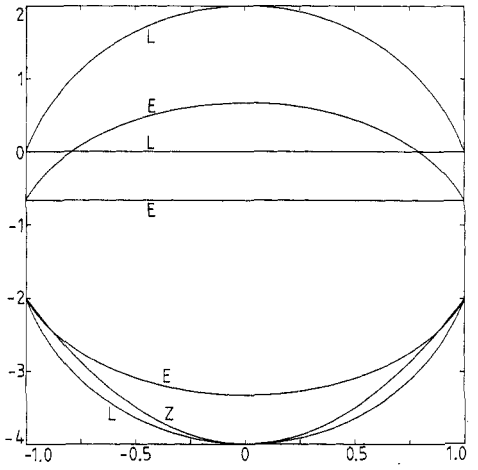


Figure 2. The dispersions for the three local singlet calculations in the Néel state background spin configuration. The notation is identical to that for figure 1. The ground state is found at $\gamma_k = 0$, which is the non-interacting Fermi surface in reciprocal space. The zone centre $\gamma_k = 1$ and the Néel zone boundary $\gamma_k = -1$ are seen to be degenerate.

correspond to different oxygen atoms, they are all orthogonal and we find the simple Hamiltonian matrix

$$H_{\alpha\alpha'} = \frac{J}{3}\begin{bmatrix} 1 - 8\bar{c}_1^2 & -8\bar{c}_1\bar{c}_2 \\ -8\bar{c}_1\bar{c}_2 & 1 - 8\bar{c}_2^2 \end{bmatrix} \tag{19}$$

with $\bar{c} = \cos ak_i/2$, which diagonalises to give

$$\varepsilon = J/3, -(J/3)(7 + 8\gamma). \tag{20}$$

The first important result to emerge from this analysis is the fact that if all that is desired is the lowest-energy hole state, then *all three* calculations yield the same state. This is the uniform phase superposition of 'local singlets' on all possible lattice positions. Since the local states for both the Zhang and Emery bases were uniform phase, we can build the state in question. The second observation is that the Emery basis gives a slightly worse description of the lower lying excitation branch than the Zhang basis. Considering that there are twice as many degrees of freedom in Emery's basis, Zhang does surprisingly well.

We now move on to the more interesting physical case of hole motion on the Néel antiferromagnetic background. We perform the same three calculations as before.

First let us consider the four state per unit cell basis of unrestricted 'local singlets', which corresponds to the first breakdown. We immediately discover an important difference between the Néel state and the ferromagnetic state. Since a 'local singlet' replaces a background spin with a singlet configuration, the states associated with the singlet on the two different sublattices correspond to different values of the z component of total

spin. Only singlets associated with the same sublattice are coupled by the Hamiltonian. We immediately find a degeneracy and can associate the two classes of states with the spin of the added particle. If we now restrict attention to one sublattice, then we find that the basis is orthogonal and using the same notation as before we find the Hamiltonian matrix

$$H_{\alpha\alpha'} = -\frac{J}{2}\begin{bmatrix} 1 & 2-x^2 & 2-xy^* & 2-xy \\ 2-(x^*)^2 & 1 & 2-x^*y^* & 2-x^*y \\ 2-yx^* & 2-yx & 1 & 2-y^2 \\ 2-y^*x^* & 2-y^*x & 2-(y^*)^2 & 1 \end{bmatrix} \tag{21}$$

which becomes

$$H_{\alpha\alpha'} = (-2J)[2\boldsymbol{aa}^{*\mathrm{T}} - \boldsymbol{bb}^{*\mathrm{T}}] \tag{22}$$

in terms of the 'natural basis'.

The $\boldsymbol{c}$ and $\boldsymbol{d}$ vectors decouple again, but now they correspond to degenerate states which gain no energy whatsoever. The $\boldsymbol{a}$ and $\boldsymbol{b}$ vectors decouple to yield the spectrum defined by

$$\begin{bmatrix} 1 & \gamma \\ \gamma & 1 \end{bmatrix}\varepsilon = J\begin{bmatrix} 2\gamma^2-4 & -2\gamma \\ -2\gamma & 2-4\gamma^2 \end{bmatrix} \tag{23}$$

which in turn diagonalises to form

$$\varepsilon = -J \pm [9-8\gamma^2]^{1/2}J. \tag{24}$$

These dispersions are plotted in figure 2.

The second calculation involves the Zhang basis. The hole hops only to next-nearest neighbours and, restricting attention to the up sublattice, we find one state per unit cell (which is now larger) which has dispersion

$$\varepsilon = -2J(2-\gamma^2). \tag{25}$$

This dispersion is only plotted in figure 2.

The third calculation is for the Emery basis. By associating the states with oxygen atoms, we include 'local singlets' which are associated with *both* sublattices. The separation of states into two degenerate classes remains and is associated with the spin of the Emery eigenstate, the up eigenstates being associated with the up lattice. We associate oxygen atoms with their nearest-neighbour copper atom with the consistent spin, which yields four states per antiferromagnetic unit cell. The states are orthogonal as before, and we find the Hamiltonian matrix

$$H_{\alpha\alpha'} = \frac{J}{3}\begin{bmatrix} -3 & 1-2x^2 & 1-2xy^* & 1-2xy \\ 1-2(x^*)^2 & -3 & 1-2x^*y^* & 1-2x^*y \\ 1-2x^*y & 1-2xy & -3 & 1-2y^2 \\ 1-2x^*y^* & 1-2xy^* & 1-2(y^*)^2 & -3 \end{bmatrix} \tag{26}$$

which in terms of the 'natural basis' becomes

$$H_{\alpha\alpha'} = -(2J/3)\,\mathbf{1} + (4J/3)\boldsymbol{aa}^{*\mathrm{T}} - (8J/3)\boldsymbol{bb}^{*\mathrm{T}}. \tag{27}$$

The $\boldsymbol{c}$ and $\boldsymbol{d}$ contributions are dispersionless at energy $(-2J)/3$, while the spectrum for the $\boldsymbol{a}$ and $\boldsymbol{b}$ vectors satisfies

$$\begin{bmatrix} 1 & \gamma \\ \gamma & 1 \end{bmatrix} \left(\varepsilon + \frac{2J}{3}\right) = \frac{4J}{3} \begin{bmatrix} 1-2\gamma^2 & -\gamma \\ -\gamma & \gamma^2 - 2 \end{bmatrix} \tag{28}$$

which in turn diagonalises to give

$$\varepsilon = (4J/3) \pm (2J/3)[9 - 8\gamma^2]^{1/2}. \tag{29}$$

This dispersion is also plotted in figure 2.

We arrive at the second result of this article. The basis of Zhang does a good job of describing the motion of the oxygen hole in a Néel background, but the Emery basis does not. The reason for this is the fact that the holes have an associated spin and hence a natural sublattice. The Zhang basis is localised around its relevant spin, but the Emery basis has to extend onto an unfavourable lattice site.

We are now in a position to discuss the relevance of our results to the two existing pictures in the literature. If one is interested in well separated holes on a ferromagnetic background at low temperatures, then both of the pictures give quite similar results. We find a uniform phase (viz $\boldsymbol{k} = \boldsymbol{0}$ and $\gamma_0 = 1$) ground state with a local dispersion which looks very similar to the dispersion for the non-interacting square lattice near empty.

Why would anyone be interested in a ferromagnetic background when modelling the real experimental situation? One quite reasonable answer is that if the kinetic energy of the oxygen hole *locally* dominates the copper hole spin coherence energy, then we might expect to form large spin polarons with quite different local spin configurations. In the Hubbard model for the square lattice, the hole motion in the absence of spin interactions drives the background spins ferromagnetic, and so studying the energy gain from hole motion in a ferromagnetic background and comparing it with hole motion in the ground state, suggested by the spin coherence, gives the energy scale on which the hole motion disrupts the spin coherence. If we try to follow this line of argument for the present system, then we run into some severe difficulties. Firstly we do *not* have any proof that the ground state spin coherence is ferromagnetic. Indeed even if we accept that the hole will bind a 'spin flip', avoiding the 'frustration', we can still not invoke Nagaoka's theorem because the Hamiltonian connects states with quite different local spin configurations and local spin singlets are particularly preferred, suggesting a total spin singlet ground state. If the ground state is RVB, then we would expect holes to form spin polarons with RVB correlations and *not*, as the Hubbard model might suggest, ferromagnetic correlations. Secondly for the Hubbard model on the square lattice, the motion of an added hole *automatically* disrupts the antiferromagnetism. In the simplest picture one finds a 'trail' of broken 'bonds' behind the hole. Antiferromagnetism is therefore a particularly bad state for hole motion and large amounts of energy are obtainable from ferromagnetic spin polarons. In our calculations, there is only a minor difference between the energy gain from the motion of a hole on ferromagnetic background, $-5J$, and the energy gain from the motion of a hole in the Néel state, $-4J$. The foundations for the spin polaron argument are not as well founded in our calculations as for the square lattice Hubbard model.

If we move on to the question of whether the motion of the oxygen hole can be modelled by the square lattice Hubbard model, then our work *suggests* but does not prove that it probably cannot be so modelled. If the ground state for the motion of the added hole were RVB as we believe, then there is just no comparison. Even if this is not the case, then the disparity between the hole motion in ferromagnetic and antiferromagnetic

spin arrangements ought to convince one that the two systems behave in importantly different ways.

3. Polaronic effects

Now let us move on to the final type of calculations which take us away from the idea of 'local singlet' and suggest the form of both the ground state and the spin polaronic behaviour of the present model. Variational calculations are the most direct method of trying to determine the ground state of most spin Hamiltonians and so we will present a simple variational approach for finding the ground state energy of a single hole moving in a given spin background. As well as determining local spin polaronic distortions, these calculations should also convince the reader that the 'local singlet' description is far from exact and really rather crude.

Firstly let us look at the linear chain. The questions that we are asking on the square lattice are equally valid for the linear chain, where it is not clear what copper spin arrangement the motion of an oxygen hole would prefer. The calculations for the phase coherence of 'local singlets' on the linear chain, corresponding to the previous square lattice calculations of § 2, are straightforward. We find an energy gain of $-\frac{7}{3}J$ for motion on a ferromagnetic background and $-2J$ for the Néel state. Similar to the results for the square lattice, we find that the minimum energy for the ferromagnetic spin arrangement occurs at the zone centre, while for the Néel state, we find the minimum energy at neither the zone centre *nor the zone boundary* but strangely half way to the zone boundary. The 'local singlet' configurations are *very* short-range polaronic effects. The motion of the hole is hugely enhanced by turning over a neighbouring copper spin. How much better can we do by extending the range of the polaron and allowing more distant spins to turn over in sympathy with the hole motion? It is to this question that we address ourselves next.

The basic idea is variational. We decide a basic spin arrangement, which will be either ferromagnetic or antiferromagnetic, and then delocalise a hole on the oxygen sites with the phase coherence suggested by the 'local singlet' calculations. We then include states which the Hamiltonian connects to this chosen state as a variational basis. We include states which are energetically preferred and this is the only subtle aspect to the calculation.

First we consider the hole bound to one spin flip on a ferromagnetic background. We assume that there is a uniform phase coherence for the hole, as was suggested by our pilot calculations. The residual freedom in the description is the distance between the hole and the spin flip. Using the *normalised* basis corresponding to the states described in figure 3(*a*), we find the Hamiltonian matrix

$$H = \begin{bmatrix} -\varepsilon & 2\sqrt{2} & 0 & 0 & 0 & . \\ 2\sqrt{2} & 1-\varepsilon & 1 & 0 & 0 & . \\ 0 & 1 & 2-\varepsilon & 1 & 0 & . \\ 0 & 0 & 1 & 2-\varepsilon & 1 & . \\ 0 & 0 & 0 & 1 & 2-\varepsilon & . \\ . & . & . & . & . & . \end{bmatrix}. \tag{30}$$

Truncating this matrix in ascending order, we can determine a sequence of approximations to the ground state energy. We find

$$0J, -2.372J, -2.467J, -2.472J, -2.472J, \ldots.$$

This solution has converged, showing that the hole is tightly bound to the spin flip, and furthermore that the 'local singlet' calculation is only qualitative.

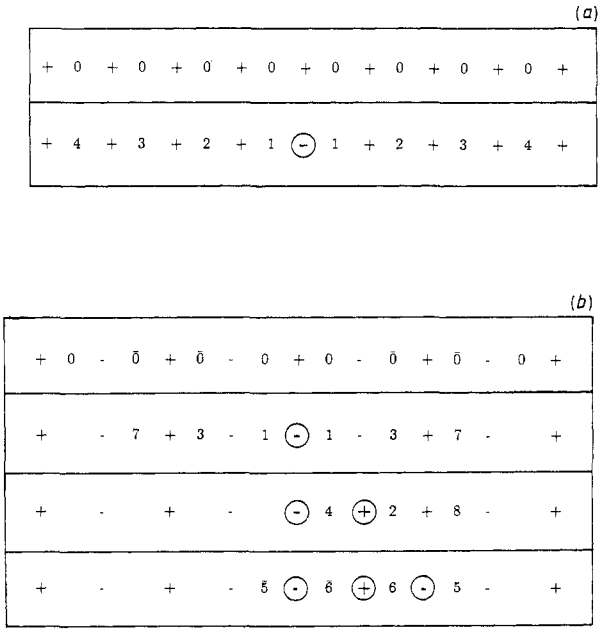


Figure 3. The chosen basis of states for our polaronic calculations on the one-dimensional chain. (*a*) ferromagnetism with one spin flip; (*b*) Néel ordering. The symbols +/− relate to the copper site, meaning up and down spins respectively. The numbers relate to the positions of the hole on the oxygen sites. The different numerical values correspond to the order in which the particular variation is included. When a number has a 'bar', then this contribution has an extra phase from the other contributions, arising from the fact that the Bloch wavevector of the hole has been assumed on the non-interacting Fermi surface.

Now let us perform the corresponding calculation for the Néel state. The Néel state is a mixture of components with different values of total spin. There is a component with maximal total spin corresponding to ferromagnetism in the x–y plane and there are components with zero total spin. Unlike the ferromagnetic example, the local polaron in the Néel state can form local arrangements with either high or low total spin. By analysing the local correlations in the vicinity of the polaron, we should be able to deduce the total spin that the hole prefers. Using the normalised basis outlined in figure 3(*b*) (where we have assumed that phase coherence suggested by the pilot calculation of § 2),

we find the Hamiltonian matrix

$$H = \begin{bmatrix} -\varepsilon & 2 & 0 & 0 & 0 & . \\ 2 & -\varepsilon & 1 & 0 & 1 & . \\ 0 & 1 & -\varepsilon & 1 & 0 & . \\ 0 & 0 & 1 & 1-\varepsilon & 1 & . \\ 0 & 1 & 0 & 1 & 1-\varepsilon & . \\ . & . & . & . & . & . \end{bmatrix}. \tag{31}$$

Truncating this matrix in ascending order yields

$$0J, -2.000J, -2.236J, -2.271J, -2.477J, -2.533J, -2.603J, -2.614J, -2.657J, \ldots.$$

The energy even at this low level of approximation is lower than the ferromagnet with one bound spin flip. The ground state is *not* a single spin flip on a ferromagnetic background, as naive Hubbard model arguments might suggest.

Let us consider the local correlations in our polaron. If we compare the phase of the first component and the third component, then we can find the local correlations left behind by the hole once it has passed. If the relative phase is negative, then the spin pair is predominantly triplet and the ground state preferred should be ferromagnetic. If the relative phase is positive, then the spin pair is predominately singlet and the ground state preferred should be a total spin singlet. *This argument predicts a total spin singlet* for the linear chain, as expected from our previous arguments [1]. In fact, almost all the local correlations between pairs of copper spins, *once the hole has passed by*, are singlet. Remember that the two copper spins on either side of an oxygen hole tend to be parallel. This is a strong argument for a total spin singlet ground state for the linear chain in this limit.

Another simple calculation can be performed, which tests the internal structure and consistency of our approximation scheme. If we look for a uniform phase solution for a mobile oxygen hole in the Néel state, we can find out whether the ferromagnetic solution is relatively stable at that Bloch vector. If we use the same basis states as for the spin singlet variations, then there are only minor modifications because for some states the previous pase cancellations now reinforce. The corresponding eigenvalues of the truncated matrix are

$$2J, 0J, -1.236J, -1.681J, -1.770J, -2.076J, -2.190J, -2.259J, -2.280J, -2.333J, \ldots.$$

When we analyse the local spin character of copper hole pairs, once the hole has passed, we now find strong triplet correlations. This suggests that the ferromagnetic ground state is indeed stable at this Bloch vector and the ground state energy should be tending towards the previously calculated value of $-2.472J$. Even with our fairly extensive basis, we have still got a fair way to go before the polaron achieves the true ground state energy. We might therefore expect to need large variational bases in order to achieve reliable ground state energies. The ground state energy for the mobile oxygen hole on a background of copper spins is lower than $-2.657J$, but may be quite a lot lower.

Now let us move on to the two-dimensional copper oxide plane. There are some new physical phenomena to consider in two dimensions which were not present in one dimension. The oxygen hole may now move around non-trivial topological closed loops.

In the analysis of the Hubbard model, it was this effect which led to ferromagnetism being stable at the one-hole level. Phase coherence is easier to maintain in a pure ferromagnetic phase. As long as the hole carries a bound spin flip, one might try to resurrect this argument to justify the Hubbard model picture of ferromagnetic polarons drifting about on a Néel background. Competing with this phenomenon is the phenomenon that we have found in the one-dimensional calculations: holes prefer the copper spins on the path that they trace out to be in local singlet configurations. Which physical effect dominates? Let us perform our polaronic calculations to try to answer this question.

We start out with the uniform phase ferromagnetic calculation where the hole has one bound spin flip. The states we employ are detailed in figure 4(*a*) and the corresponding Hamiltonian matrix is

$$H = \begin{bmatrix} -\varepsilon & 4\sqrt{2} & 0 & 0 & 0 & . \\ 4\sqrt{2} & 1-\varepsilon & \sqrt{2} & 1 & 0 & . \\ 0 & \sqrt{2} & 4-\varepsilon & \sqrt{2} & 2 & . \\ 0 & 1 & \sqrt{2} & 2-\varepsilon & 0 & . \\ 0 & 0 & 2 & 0 & 3-\varepsilon & . \\ . & . & . & . & . & . \end{bmatrix}. \tag{32}$$

The eigenvalues of the truncated matrix are

$$0J, -5.179J, -5.278J, -5.318J, -5.323J, -5.324J, -5.324J, \ldots.$$

Again we find that the spin flip is tightly bound to the hole and the ground state solution has been achieved with this small basis of states.

We can extend this calculation by allowing the Bloch wavevector dependence of the hole to vary. The hole only moves to neighbouring sites when it carries the spin flip with it. This only occurs when the hybridisation between the states '0' and '1' is considered. Replacing the matrix element $4\sqrt{2}$ by $4\sqrt{(1+\gamma)}$ in equation (32) is the only change and the resulting essentially exact calculation is plotted in figure 1.

Next we consider the motion of the hole in the Néel state. We now come across a difficulty. In one dimension, the Bloch vector for the added hole was uniquely determined by the 'pilot' calculation, where attention was restricted to nearest-neighbour singlets, to be half-way to the zone boundary. For our two-dimensional pilot calculation we find that the lowest energy state has a large reciprocal space degeneracy. Indeed we find the minimum when $\gamma_k = 0$ and this condition defines *the square Fermi surface for the non-interacting problem*. We expect the best total spin singlet Bloch vector to be somewhere on this Fermi surface, but where? We are unable to answer this question, but suggest that it is likely that the degeneracy remains. We have tried calculating at the $\boldsymbol{k} = (\pi/a)(1, 0)$, $\boldsymbol{k} = (\pi/(2a))\,(1, 1)$ and $\boldsymbol{k} = (\pi/(2a))(1, -1)$ points and get very similar results.

If we restrict attention to the $\boldsymbol{k} = (\pi/(2a))(1, 1)$ point, then using the basis of states detailed in figure 4(*b*) (overleaf), we find the Hamiltonian matrix

$$H = \begin{bmatrix} -\varepsilon & 4 & 0 & 0 & 0 & . \\ 4 & -\varepsilon & 1 & \sqrt{2} & 1 & . \\ 0 & 1 & -\varepsilon & 0 & 0 & . \\ 0 & \sqrt{2} & 0 & -\varepsilon & 0 & . \\ 0 & 1 & 0 & 0 & 1-\varepsilon & . \\ . & . & . & . & . & . \end{bmatrix}. \tag{33}$$

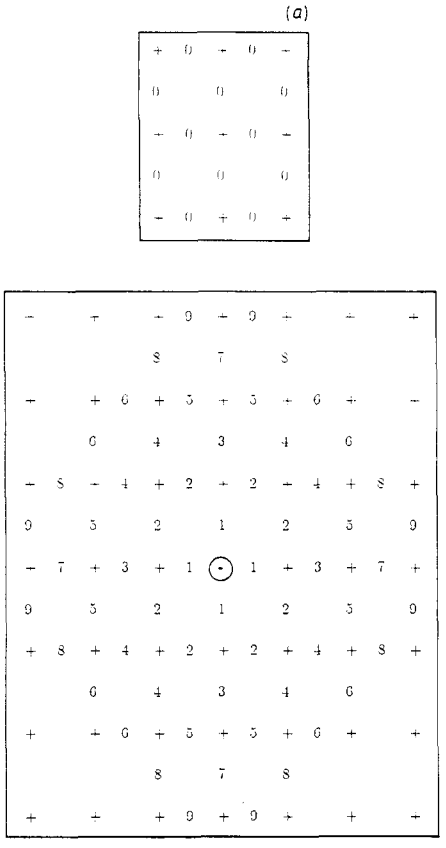
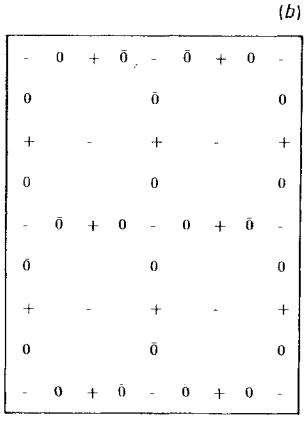
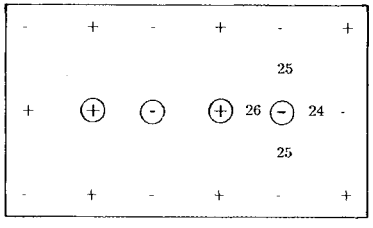
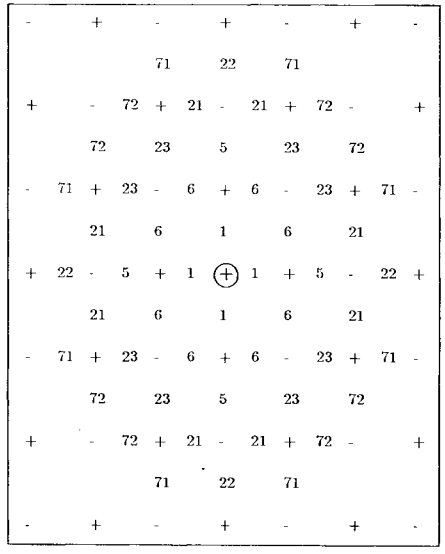


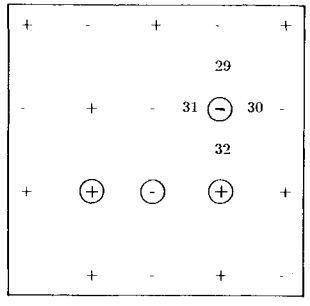
Figure 4. The chosen basis of states for the polaronic calculations on the two-dimensional plane. (*a*) Ferromagnetism with one spin flip; **overleaf** (*b*) Néel ordering; (*c*) chequer-board ordering. The notation is identical to that of figure 3. The assumed Bloch wavevector for the oxygen hole is $(\pi/(2a))(1, \pm 1)$ for (*b*) and $(\pi/(2a))(1, 0)$ for (*c*). The first point lies on the non-interacting fermi surface, but the second point does not.

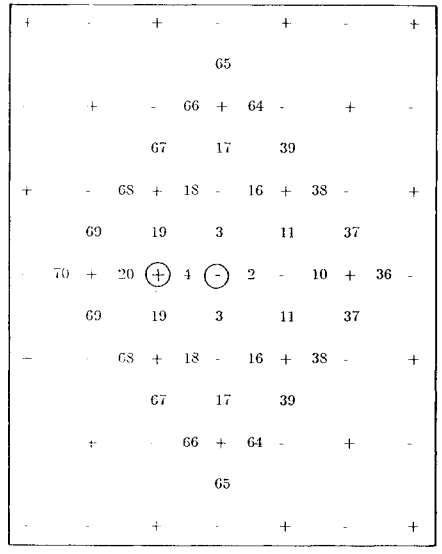
Figure 4(b)











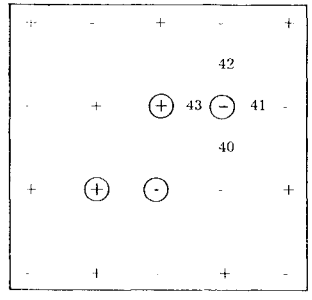
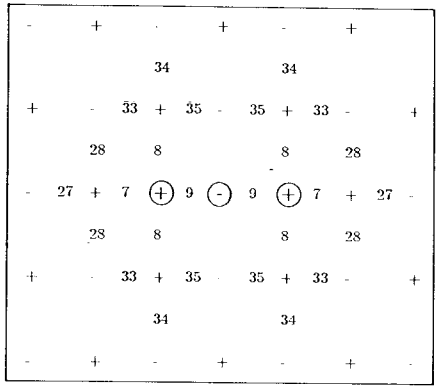
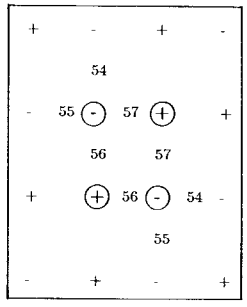
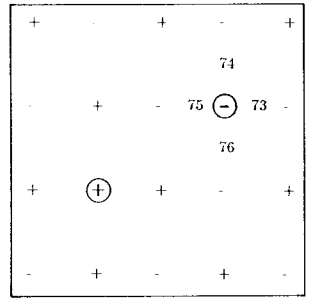
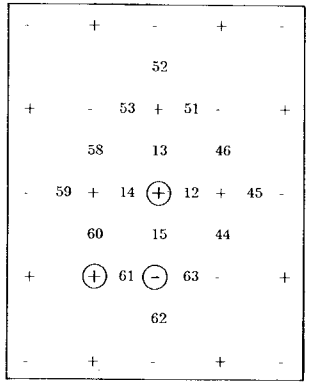


Figure 4(b) (*continued*)









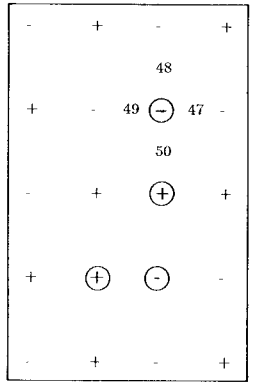
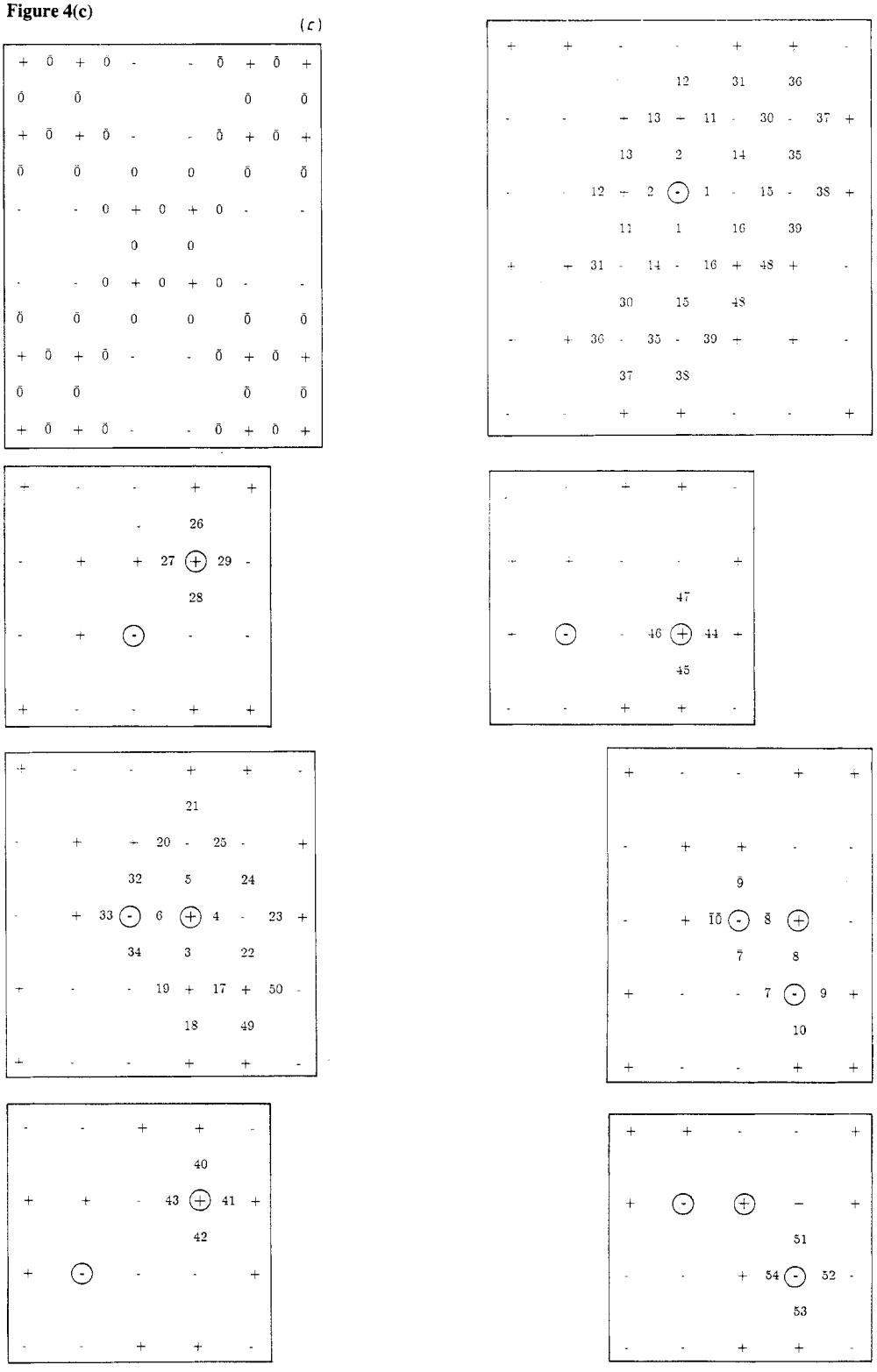


Figure 4(c)



The truncated matrix yields the eigenvalues

$0J, -4J, -4.123J, -4.359J, -4.452J, -4.528J, -4.713J, -4.724J, -4.750J, -4.765J,$
$-4.776J, -4.820J, -4.840J, -4.862J, -4.886J, -4.908J, -4.915J, -4.935J, -4.966J,$
$-4.980J, -4.983J, -4.991J, -4.994J, -5.021J, -5.023J, -5.026J, -5.028J, -5.030J,$
$-5.035J, -5.039J, -5.043J, -5.048J, -5.053J, -5.055J, -5.060J, -5.069J, -5.071J,$
$-5.073J, -5.078J, -5.082J, -5.085J, -5.088J, -5.091J, -5.094J, -5.096J, -5.099J,$
$-5.103J, -5.106J, -5.109J, -5.113J, -5.116J, -5.118J, -5.121J, -5.125J, -5.129J,$
$-5.132J, -5.135J, -5.138J, -5.139J, -5.141J, -5.146J, -5.148J, -5.149J, -5.151J,$
$-5.153J, -5.154J, -5.156J, -5.156J, -5.157J, -5.157J, -5.157J, -5.157J, -5.157J,$
$-5.159J, -5.161J, -5.164J, -5.169J \ldots$.

We have not yet reached the energy obtained for the ferromagnetic state, but the energy is dropping continuously with each new variation as the polaron spreads out. Our belief is that the limit for the energy determined in this calculation is lower than the ferromagnetic solution and that the ground state is not the local singlet moving around in a ferromagnetic background. Finding out the local correlations amongst the copper spins once the oxygen hole has passed is now more involved, because the oxygen hole can move along various paths from each copper site. We find, as expected, that the local correlations are singlet in character. If we consider the ferromagnetic calculation at this wavevector, then the energy from that hole state is quite a lot higher than that for the present calculation, which further suggests that there is a new local spin order.

The corresponding calculation at the Bloch wavevector $\boldsymbol{k} = (\pi/a)(1, 0)$ is straightforward and we find minor changes due to the different phase coherence and choice of relavant states. The energy we find from similar variations is also $\sim -5.1J$ and the local spin correlations are predominantly singlet. Interestingly, for this Bloch vector there are lines of CuO parallel to the x and y directions with uniform phase, and if we analyse the local spin character of the hole motion along these lines we find local triplet character. The triplet character is much weaker than the singlet character and we treat this as a residual effect due to the rather small scale of our polaron.

Our next calculation is for an oxygen hole with uniform phase coherence in the Néel state, in order to find out whether the ferromagnetic solution is locally stable at $\boldsymbol{k} = 0$. Again the modifications to our variations are minor, corresponding to phase cancelling becoming phase reinforcing as in the one-dimensional case. We reach an energy of $-4.927J$ with strong local triplet correlations, suggesting that the ferromagnetic state is indeed stable. It should be borne in mind that this energy is to be compared with $-5.324J$, which is the true ground state energy for the ferromagnet with one bound spin flip. There is a huge discrepancy and if this discrepancy were the same for the total spin singlet calculation, then the total spin singlet would be the ground state by quite an appreciable energy.

Our next calculation was in a quite different state. We elected to use the spin arrangement with rows of ups alternating with rows of downs. This state, like the Néel state, has both total spin singlet components and fully ferromagnetic components. We found a variational energy of ~ -5.15J with a choice of wavevector $\boldsymbol{k} = (\pi/2a))(0, 1)$ and about 25 variations. The local correlations were triplet parallel to the lines of spins and singlet perpendicular to the spins. The ferromagnetic calculation has a similar energy at this wavevector and the existence of local singlet correlations in our trial wavefunction strongly suggests that the total spin singlet state is close in energy, if not lower in energy at this wavevector.

Our final calculation is our best evidence for the ground state of this Hamiltonian being a total spin singlet. Guessing that the best reciprocal space phase coherence for the hole lies on the non-interacting Fermi surface, we tried to choose a spin state which has ferromagnetic and total spin zero components and *simultaneously* is associated with magnetic coherence at a reciprocal space wavevector which lies on the Fermi surface. Our choice was the 'chequer board' state, where four parallel spins in a small square are used as the building block for the Néel state with twice the lattice period. Using the basis suggested in figure 4(*c*), we obtained an energy of $\sim -5.22J$ at the reciprocal lattice point $\boldsymbol{k} = (\pi/(2a))(1, 0)$ for the hole phase coherence, which has components quite close to the non-interacting Fermi surface but not actually on it. This was achieved with a basis of approximately 50 states and is now very close to the ferromagnetic solution of $\sim -5.324J$. The local correlations are again dominantly singlet in spin character for the copper spin background.

4. Conclusions

Desire for a Hubbard model description of 'high T_c' superconductivity focused attention on 'local singlet' combinations of oxygen and copper holes, which would correspond to filled or empty sites in the Hubbard model description [5]. We suggest another interpretation for a 'local singlet' as a small polaronic distortion of paramagnetic fluctuations around the charge carrier. The natural extension of this idea suggests that if the motion of the oxygen holes dominates the super-exchange interaction between copper holes, then the strong-coupling ground state is a paramagnetic total spin singlet state or RVB state.

In our calculations the super-exchange energy has been assumed negligible. The natural way to include this contribution is to include an energy penalty proportional to the number of ferromagnetically aligned bonds in each variational state. The energy penalty then reduces the size of the polaronic distortion and makes our 'pilot' local singlet description more relevant. Considering this pilot calculation in the Néel state as the 'super-exchange limit', we find that charge carriers have lowest energy at $\gamma_k = 0$, viz at the *non-interacting Fermi surface*. Considering our polaronic calculations as a perturbation about this limit, we would predict that the charge carriers lower their energy by forming local *singlet* fluctuations and *not* ferromagnetic fluctuations as the Hubbard model would suggest. The basic reason for this is that at $\gamma_k = 0$ the ferromagnetic local singlet calculation yields an energy of $\sim -3.5J$, which is higher than the local singlet calculation in the Néel state at $-4J$. Ferromagnetic fluctuations would therefore *lose* the hole kinetic energy, unless they were simultaneously associated with a change in Bloch wavevector.

One very important result to emerge is that the charge carriers have lowest energy on the non-interacting Fermi surface. Experimentally this causes a difficulty in distinguishing strong and weak coupling paramagnetism by looking at the excitation spectrum of the charge carriers in reciprocal space. The natural probes of photoemission, positron annihilation and de Haas–van Alphen would all be expected to yield similar results in both limits. This possibility has already been encountered in the study of heavy-fermion systems. In these materials the role of the copper atom is taken by either cerium or uranium. The reduction in size for the f shell over the d shell in copper ensures that the f electrons are strong coupling, displaying only two possible charge states. When de Haas–van Alphen is used to probe the low lying charged excitations, however,

remarkable agreement is obtained between the experimental results and *weak*-coupling band theory [10]. This has always been rather a surprise, with only the Luttinger theorem to soften the blow. Our calculations would suggest that this result is quite *natural* for stong-coupling paramagnetism.

The natural tight-binding Hamiltonian for heavy fermion systems is the Anderson lattice [11], and to tighten the connection between our results and those for heavy fermions we should point out that the 'high T_c' model can be mapped onto the Anderson lattice by making an *exact* transformation [12].

The strong-coupling picture is seen to diverge from the weak-coupling picture experimentally, when the effective mass of the charge carriers is measured. Strong-coupling paramagnetic charge carriers are found to be very heavy, hence the name heavy fermions. Does our calculation predict that the oxygen holes should be very heavy? The energy scale of the oxygen hole dispersion is J, whereas a weak-coupling calculation will renormalise the copper band to the Fermi surface and predict an energy scale t. We do therefore predict an enhanced effective mass and the two types of system appear quite analogous. There is a second effect which increases the effective mass of the quasiparticles. The quasiparticles we are constructing are polarons, and as such they carry around local spin configurations. This local spin distortion gives a contribution to the effective mass. Although we have not calculated this effect, an inspection of our pilot calculation dispersions, e.g. equation (18), should convince the reader that these objects are slower than the corresponding free dispersion would suggest by a factor of 2 or so.

A final point to bear in mind is that, in our two-dimensional calculations, for all the different Bloch wavevectors that we have given the hole, there is a sympathetic local spin configuration yielding a ground state energy of less than $-5J$. The associated spread in the hole energy, if we *include* the local spin rearrangement, is very small as the Bloch wavevector varies. It is not clear whether this is a real effect or just a statement about our variational technique, but it might suggest further 'heaviness' for the hole.

In conclusion, for the motion of an oxygen hole in the limit of motion by virtual excitation of Cu^+, we have shown that simple ferromagnetic solutions for the background spins can be easily beaten by states with local spin singlet correlations in one dimension. We believe that the same situation occurs in the two-dimensional plane, but we have much weaker evidence for this. The super-exchange interaction between neighbouring copper holes strongly favours the state with local singlet correlations.

One would like to tackle the problem of *pairs* of charge carriers in this system to answer the superconductivity questions, but much more work is needed at this elementary single-particle level before such questions can even be considered in this limit.

Acknowledgments

The author wishes to acknowledge useful discussions with J M F Gunn, W Barford, D Bullett and D Bird.

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