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## Spin fluctuations can turn fermions into bosons: superconductivity in strong-coupling paramagnets

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**Abstract.** We study the motion of electrons across atoms which have only two permissible valence states: empty or singly occupied. The model we use is the  $t$ - $J$  model. For the geometry composed of an infinite chain of edge-sharing squares, we show that, at low concentrations of electrons, their spin and charge degrees of freedom 'separate'. Even in the absence of Heisenberg interactions the spin degrees of freedom yield the Heisenberg ground state of the linear chain. The charge degrees of freedom may be modelled by spinless fermions. When two electrons meet in a relative spin singlet, they are locally converted into spinless hard-core bosons. This possibility promotes Heisenberg correlations and simultaneously yields an attraction between the spinless fermions. This physical mechanism is clearly a candidate for an explanation to perovskite superconductivity.

### 1. Introduction

Almost immediately after the discovery of 'high temperature superconductivity' [1], P W Anderson suggested that the natural theoretical model was the Hubbard model on the square lattice in the strong-coupling limit [2]. After a worldwide theoretical effort, the same Hamiltonian is *still* the centre of theoretical research into the phenomenon, although the name seems to have changed to the  $t$ - $J$  model. Despite the clear experimental justification of the model, there is still no theoretical evidence for superconductivity inherent in the model. The failure of the model to exhibit superconductivity has led to various embellishments and even a challenge to the model itself [3]. Although the justification of the model for hole superconductors is dubious [3], this model as a description for electron superconductors seems inescapable. Following on from our treatment of a line of squares connected along their diagonals, in this article we will tackle the more difficult geometry of a line of edge-sharing squares depicted in figure 1. The present geometry has *interconnecting* squares which makes it both an order of magnitude more sophisticated and simultaneously more representative of the two-dimensional square lattice. We will show that charge-carriers moving in the presence of paramagnetic spin correlations are *attracted* to each other.

The physical mechanism which underpins the present analysis is elementary but seems quite general: In paramagnetic systems with short range antiferromagnetic spin correlations, fermions can behave effectively as hard-core spinless bosons. When two fermions meet in a relative spin singlet, exchanging the two particles does *not* yield the expected fermionic minus sign, since the spin singlet antisymmetry contributes a compensating minus sign and the two particles exchange with a bosonic plus sign.

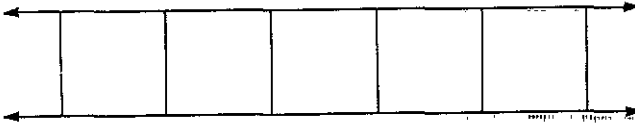


Figure 1. The linear chain of squares geometry. A pair of atoms on a cross bond are called an 'edge bonding pair' in the text.

In order for the mechanism to apply, it must be possible for two particles to be exchanged and so we must study a geometry with topological loops. Triangles cannot be used since two particles behave as one hole, and so the smallest relevant loop is the square.

The second necessary input to the phenomenon is short range paramagnetic spin correlations. It is this second constraint which has hidden the effect in most of the theoretical studies to date. The obvious limit to take is that corresponding to the experimental systems of a few extra holes near half filling. Unfortunately, extra holes in the  $t$ - $J$  model promote short-range *ferromagnetic* spin correlations [4], the opposite physical effect. To stabilize paramagnetism, one either requires strong Heisenberg interactions or sufficient charge-carriers to ensure a high probability of doubly occupied squares. Both of these limits are difficult to tackle theoretically. We should point out that the natural Hamiltonian for the hole superconductors does *not* suffer from this drawback [3], although it is difficult to tackle for other reasons. In this article we will move away from the experimental charge-carrier concentration and study a technically easier limit: low doping of electrons into an otherwise empty lattice. Taking this extreme limit allows paramagnetism to be stabilized by a rather different physical phenomenon; first discovered by Kanomori [5]. In turn, this simplification allows us initially to omit the Heisenberg interaction, which may be required in the experimental limit to stabilize paramagnetism, and to study the charge motion in isolation.

We study the  $t$ -model:

$$H = -t \sum_{\langle ii' \rangle \sigma} (1 - c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}}) c_{i\sigma}^\dagger c_{i'\sigma} (1 - c_{i'\bar{\sigma}}^\dagger c_{i'\bar{\sigma}}) \quad (1)$$

where  $c_{i\sigma}^\dagger$  creates an electron of spin  $\sigma$  (complementary spin  $\bar{\sigma}$ ) on a site  $i$ , and  $\langle ii' \rangle$  denotes nearest neighbour bonds on the 'ladder' geometry of figure 1. The extra bracketed terms are projection operators which ensure that sites can never become doubly occupied. This Hamiltonian simply 'shuffles' or permutes spins about on the lattice by hopping electrons to neighbouring vacant atoms. The geometry is bipartite and so the sign of the hopping matrix element,  $t$ , is irrelevant.

The  $t$ -model is a particularly difficult model to solve. The electrons are free to move about on the lattice yielding charge degrees of freedom, but as they move they carry with them a fixed spin, which can be exchanged with another spin by exchanging the two relevant electrons. The spin and charge degrees of freedom are intimately coupled and, although we can solve non-interacting charge motion and have some understanding of Heisenberg exchange, it is not clear how the interchange between them might behave.

Due to the very simple character of a single particle on our geometry, it is possible to develop a consistent representation for the two-particle interactions. In section 2 we will show how to remodel the system with interacting spinless fermions indicating the sense in which the spin and charge degrees of freedom are decoupled. In section 3

we run through the development of a resulting BCS pairing theory and in section 4 we conclude.

## 2. Interacting spinless fermions

In our modelling we will restrict attention to low concentrations of electrons. The physical content of our approximation is that we will describe up to two electrons in the same square correctly, but we will provide a description for three electrons in a square which has similar characteristics to the original model but does not agree with it. Provided that the concentration of electrons is low, the errors that we make should be irrelevant. Firstly we shall look at the single-particle problem and explain the sense in which its character enables us to successfully describe the two-particle interactions.

### 2.1. The single-particle problem

If we have a single particle on an otherwise empty lattice, then the statistics and spin characteristics are completely irrelevant. The projection operators in equation (1) are irrelevant because an atom can never be doubly occupied with only one electron and the problem reduces to a simple non-interacting Hamiltonian:

$$H = -t \sum_{\langle ii' \rangle} a_i^\dagger a_{i'} \quad (2)$$

where we have omitted the irrelevant spin degree of freedom on the electron which is created by  $a_i^\dagger$  on site  $i$ .

The crucial bonds for the present geometry are the cross bonds which form the connecting edges of the row of squares. We will henceforth call these bonds *edge bonds*. The combinations which diagonalize these bonds also separate the single-particle description into two independent bands. If we denote the bonding combination by  $f_j^\dagger$ , on an edge bond  $j$ , and the anti-bonding combination by  $g_j^\dagger$ , then effectively

$$H = -t \sum_j f_j^\dagger f_j - t \sum_{\langle jj' \rangle} f_j^\dagger f_{j'} + t \sum_j g_j^\dagger g_j - t \sum_{\langle jj' \rangle} g_j^\dagger g_{j'} \quad (3a)$$

which diagonalizes to form

$$H = -t \sum_k f_k^\dagger f_k (1 + 2 \cos k) + t \sum_k g_k^\dagger g_k (1 - 2 \cos k) \quad (3b)$$

with the dispersion depicted in figure 2.

The fact which allows an analytic treatment of this model is that at low energies the *only* excitations are pure edge bonding orbitals. The behaviour of states restricted to pure edge bonding combinations is particularly simple and allows a proper description of the two-particle interactions.

Although we have developed the present analysis for a single particle, the solution simultaneously solves the case of saturated ferromagnetism at the many-particle level. If all the spins are parallel, then the constraint that no atom should be doubly occupied is automatically guaranteed by Pauli exclusion. The problem reduces to the non-interacting spinless fermion description of equation (3), since the spin label is the same

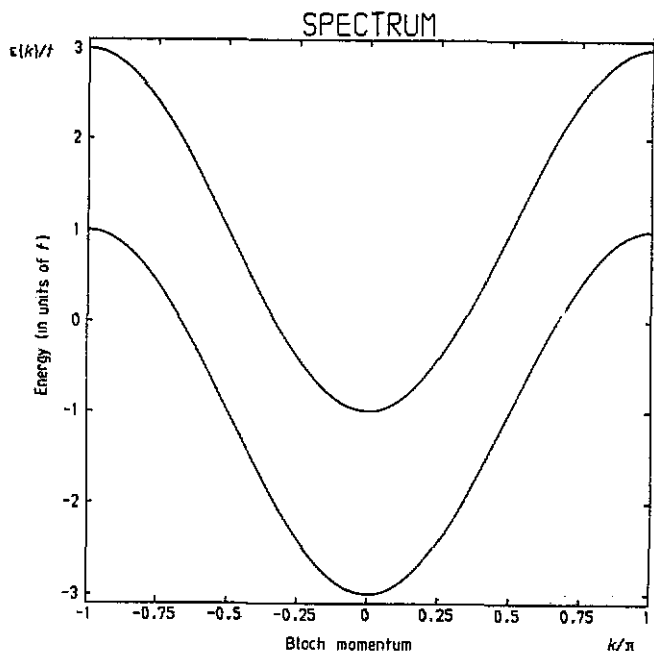


Figure 2. The dispersion for a single particle moving on the linear chain of squares. The lower band involves pure edge bonding states and the upper band involves pure edge anti-bonding states.

for all the particles and hence can be safely omitted. Since electrons are fermions, we must apply anticommutation relations to the many-particle problem, yielding a Fermi surface in the ground state. It is this non-interacting state that we will use as a reference, in order to determine whether the additional interactions are attractive or repulsive.

For electron concentrations up to one per square, the solution comprises only edge bonding combinations. No two electrons ever sit on the same edge bond, and the order of the particles never changes. Each particle may be labelled in sequence *without* modifying the basic description of the problem. It is this fact which enables us to address the situation with arbitrary spin configurations *by comparison* with the non-interacting spinless fermion solution.

For an eigenstate of the Hamiltonian the spin configuration along the chain remains approximately fixed. The particles ordered along the chain can be labelled with a fixed spin configuration which is a linear superposition of many different spin arrangements in the natural basis where all spins are parallel to the  $z$ -axis. There are a collection of spatial configurations that the electrons can get into for which their order does not change, and for which they are only ever found in edge bonding configurations. All these states may be annotated by the spinless fermion description of equation (3). The original Hamiltonian acting on these states has *precisely* the same behaviour as the spinless fermion description. There is one complication that will be addressed in the next subsection: Exchange in the presence of a spin singlet.

2.2. The two-particle problem

In this section we will look at ways to extend the single-particle description of equation (3) to include situations where two electrons meet and *exchange* in a square. We will assume that the spin configuration of the electrons ordered along the chain is *fixed* but that not all the spins are parallel. Our first task is to appreciate the many-particle states that the description of equation (3) can describe. As already explained, the states when all the electrons are separated are properly counted and correctly coupled by this description. The difficulties occur when two particles meet in a square. There are two situations to consider: When the two particles meet in either a relative spin triplet or a relative spin singlet.

The configurations when two particles meet in a relative spin triplet are completely analogous to those found when *all* the spins are parallel, and equation (3) describes all the possibilities precisely. The difficulty is describing the configurations when the two particles meet in a relative singlet.

The spinless fermion description breaks down when two electrons sit in a spin singlet simultaneously on an edge bond. Although the numbers of states are the same, there being a unique state with the edge bond pair in a singlet in the original description corresponding to the state where both spinless fermions are present, the single-particle description does *not* connect them with the correct matrix elements. As an example, when two electrons are in a relative singlet and are also in bonding combinations on neighbouring edge bonds, there are matrix elements allowing the electrons to doubly occupy either edge bond. For the spinless fermion problem this possibility is prohibited by Pauli exclusion. Indeed, it is precisely the use of the spin singlet to avoid Pauli exclusion which constitutes the attraction in our description. Although the edge bonding and edge anti-bonding states are independent at the single-particle level, at the two-particle level they become mixed. In the final section we will interpret this mixing, but now we will proceed to develop the description for situations where there are some singlet correlations in the fixed spin background.

Provided that we restrict attention to electron configurations where each square has either zero, one or two electrons, then we can describe the singlet configurations precisely by the Hamiltonian:

$$\begin{aligned}
 H = & -t \sum_j f_j^\dagger f_j (1 - g_j^\dagger g_j) - t \sum_{(jj')} (1 - P_j g_j^\dagger g_j) f_j^\dagger f_{j'} (1 - P_{j'} g_{j'}^\dagger g_{j'}) \\
 & + t \sum_j g_j^\dagger g_j (1 - f_j^\dagger f_j) - t \sum_{(jj')} (1 - P_j f_j^\dagger f_j) g_j^\dagger g_{j'} (1 - P_{j'} f_{j'}^\dagger f_{j'}) \\
 & - t \sum_{(jj')} (P_j g_j^\dagger f_j^\dagger [f_j f_{j'} - g_j g_{j'}] \alpha_{jj'} + \text{cc}) \tag{4}
 \end{aligned}$$

where  $\alpha_{jj'} = \pm 1$  has the opposite sign for the two contributions connecting the same edge bond and  $P_j$  is an operator which is zero when the two relevant spins are parallel and unity when the two relevant spins are in a relative spin singlet:  $P_j = \frac{1}{4} - \mathbf{S}_1 \cdot \mathbf{S}_2$  in terms of the two relevant spin operators. The two-particle contributions to the edge bonding terms cancel out and are therefore irrelevant. The important term is the final term which promotes the correct behaviour for pairs which meet in relative spin singlets, compensating for the reduced hopping rates in the first terms, which are analogous to the original spinless fermion description.

At this point we should point out the role of the background spin configuration. The operators  $P_j$  behave like Heisenberg operators; they act between nearest-neighbour spins and promote spin correlations which are eigenstates of the nearest-neighbour Heisenberg model. The solutions have translational symmetry and the probability that nearest neighbours are spin singlets are the fixed scaled eigenvalues of the relevant Heisenberg eigenstates. We will not develop the spin excitations any further in this article, although the likely behaviour is straightforward. The more important characteristics for us are the charged excitations.

The effective Hamiltonian is best represented at the two-particle level by

$$H_0 = -t \sum_j f_j^\dagger f_j - t \sum_{\langle jj' \rangle} f_j^\dagger f_{j'} + t \sum_j g_j^\dagger g_j - t \sum_{\langle jj' \rangle} g_j^\dagger g_{j'} \tag{5a}$$

$$H_1 = -t \sum_{\langle jj' \rangle} (P_j g_j^\dagger f_j^\dagger (f_j + \alpha_{jj'} g_j) (\alpha_{jj'} f_{j'} - g_{j'}) + CC) \tag{5b}$$

The pair of electrons which are moved by the final term are on opposite sides of the ladder, as the opposite relative phase of the two operators suggests, and the double occupancy constraint requires. This Hamiltonian transforms into reciprocal space as

$$H_0 = -t \sum_k f_k^\dagger f_k (1 + 2 \cos k) + t \sum_k g_k^\dagger g_k (1 - 2 \cos k) \tag{6a}$$

$$H_1 = \frac{t}{N^2} \sum_j \sum_{kk'} \sum_{qq'} \{ e^{i\psi(k+k'-q-q')} P_j g_k^\dagger f_{k'}^\dagger \times [f_{q'} g_q 2(\cos q' + \cos q) + i(\sin q' - \sin q)(f_{q'} f_q + g_{q'} g_q)] + CC \} \tag{6b}$$

where  $N$  is the number of edge bonds and we have made a particular choice for the phases  $\alpha_{jj'}$ .

We could develop a pairing theory from this description directly, but it is much more transparent if we restrict attention to states composed purely of f-fermions and include the hybridization into the doubly occupied states perturbatively. The effective Hamiltonian is approximately:

$$H = -t \sum_j f_j^\dagger f_j - t \sum_{\langle jj' \rangle} f_j^\dagger f_{j'} - \kappa t \sum_{\langle jj' \rangle} \sum_{\langle jj'' \rangle} P_j \alpha_{jj'} f_{j'}^\dagger f_j^\dagger f_j f_{j''} \alpha_{jj''} \tag{7a}$$

$$\kappa = \frac{1}{2\pi} \int_{k_f}^\pi dx [(1 + 2 \cos k_f - \cos x)^2 - 1]^{-1/2} \tag{7b}$$

where we have chosen the interaction strength to be correct at the Fermi energy. The factor  $\kappa$  is depicted in figure 3 as a function of band filling. The fact that  $\kappa$  is relatively small ensures that we can consider the two-particle interactions as only a weak additional interaction even when the electron concentration becomes quite sizeable. We will develop a BCS pairing theory for this model in the next section, but first we will indicate how this Hamiltonian is derived.

The more precise formulation of the two-particle interaction involves transforming into reciprocal space where second-order perturbation theory yields

$$H_1 = -\frac{t}{N^2} \sum_j \sum_{kk'} \sum_{qq'} P_j e^{ij(k+k'-q-q')} f_k^\dagger f_{k'}^\dagger f_{q'} f_q (\sin k - \sin k')$$

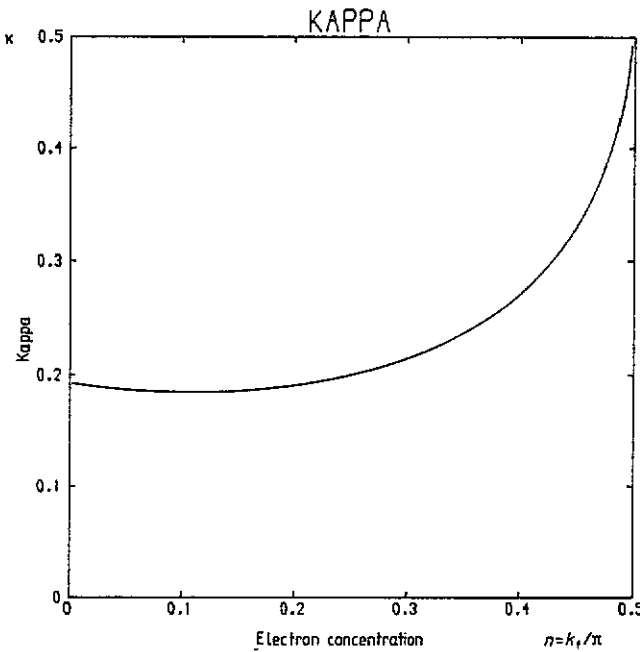


Figure 3. The function  $\kappa$ , which controls the strength of the two-particle interactions, plotted as a function of band filling,  $n = k_f/\pi$ . At half filled, where the g-fermions commence to become occupied and the description breaks down, there is a weak logarithmic divergence.

$$\times (\sin q - \sin q') \frac{1}{2} [B_{kk'} + B_{qq'}] \tag{8a}$$

$$B_{kk'} = \frac{1}{2N^2} \sum_{pp'} \frac{\theta(-t - 2t \cos p - \mu)}{(1 + \cos k + \cos k' - \cos p - \cos p')} \\ = \frac{1}{2\pi} \int_{k_f}^{\pi} dx [(1 + \cos k + \cos k' - \cos x)^2 - 1]^{-1/2} \tag{8b}$$

where  $\mu = -t(1 + 2 \cos k_f)$  is the chemical potential. The interaction strength  $B_{kk'}$  involves virtual excitations including one f-fermion and one g-fermion with momenta  $p$  and  $p'$  respectively. The g-fermion momentum is unconstrained as the g-band is assumed unoccupied, but the f-fermion momentum is restricted to unoccupied states; enforced by the theta function.

If we restrict attention to pairs with zero total momentum then the result reduces to:

$$H_1 = -\frac{t}{N^2} \sum_j \sum_{kk'} \sum_{qq'} P_j f_k^\dagger f_{-k}^\dagger f_{-q} f_q 4 \sin k \sin q \frac{1}{2} [A_k + A_q] \tag{9a}$$

$$A_k = \frac{1}{2\pi} \int_{k_f}^{\pi} dx [(1 + 2 \cos k - \cos x)^2 - 1]^{-1/2} \tag{9b}$$



from which the description of equation (7) naturally follows.

The residual spin interaction is precisely  $P_j = \frac{1}{4} - S_1 \cdot S_2$ , a nearest-neighbour antiferromagnetic exchange interaction. This term induces the Heisenberg ground state for the spin degrees of freedom which in turn leads to a replacement of  $P_j$  by  $P$ ; a  $c$ -number which is the probability of finding nearest neighbours in a relative spin singlet in the Heisenberg ground state. The interaction strength is  $\kappa Pt$ , and the effect of spin excitations is expected to be a weak average decrease in the attraction as the probability that the electrons meet as spin singlets is reduced. There is *not* expected to be any destruction of the charge motion coherence by scattering off low energy spin excitations as might naively be expected.

One complication that spin excitations might contribute is the possibility of non-conservation of momentum in the effective two-particle interactions. This could lead to an increase in the two-particle interaction strength, as the virtual excitations could occur at lower energies. We do not believe that this possibility is actually relevant.

The effective two-particle interaction in our final description is an attraction between pairs of spinless fermions. The spatial symmetry of a pair of spinless fermions is necessarily antisymmetric and so the resulting 'gap' vanishes at the zone centre and grows linearly with wavevector as we shall show in the next section. The other main difference to standard BCS theory is the fact that the attraction is short range in real space, leading to an expectation of a shorter coherence length for a Cooper pair.

It is straightforward to develop a BCS pairing theory for this model, but before we do this we will discuss the approximations and indicate the likely effects of the phenomena omitted.

### 2.3. Approximations

There are several weak points in the present article and we would like to highlight four:

- (i) the spin configuration is assumed to be the Heisenberg ground state;
- (ii) the three-particle interactions have been omitted;
- (iii) we have assumed only virtual excitation of  $g_k^\dagger$  fermions; and
- (iv) the system is one-dimensional and fluctuations are therefore dominant as they are in any interacting system.

(i) For the interacting one-dimensional Hubbard model, the exact solution of Lieb and Wu [6] can be used to show that the spin excitations and charge excitations separate. For the present model we believe that precisely the same separation occurs for the same reasons, although we have not demonstrated the result mathematically. It is conceivable that the translational symmetry could become broken with a type of 'spin Peierls' phase being stable, namely with alternating singlet and uncorrelated bonds in the ground state. It is our belief that this does not happen and that the simple picture of Heisenberg interactions reduced by the necessity for two particles to exchange in a single square is the correct picture.

(ii) When three particles meet in a square, our description ensures that any two in a relative spin singlet can doubly occupy edge bonds, but when a particle hops from one doubly occupied edge bond to another doubly occupied edge bond, the description breaks down. The ground state to three electrons in a square yields ferromagnetic correlations and the equivalent effective repulsion for three particles meeting in a paramagnet is omitted from our description. In order for this effect to become important

we would require a high probability of finding three electrons on a single square and this would only be possible if there was a significant density of g-fermions.

(iii) Our restriction to states composed purely of f-fermions ensures that there are none of the previous problems associated with triply occupied squares, because Pauli exclusion ensures that the f-electrons are separated. The approximation itself however is a more drastic simplification in its own right. A naive estimate of the probability of finding spinless fermions on neighbouring sites and therefore subject to the additional attraction can be found from assuming that the fermions are spatially decorrelated. The probability would then be  $\rho^2$ , where  $\rho$  is the density of spinless fermions. If this were an accurate estimate, then the approximation would soon be very poor. Fortunately, Pauli exclusion ensures that spinless fermions avoid each other as much as possible and this probability is severely reduced. For the present system we find a probability of

$$P = \rho^2 - \left( \frac{\sin \pi \rho}{\pi} \right)^2 \tag{10}$$

that two neighbours are simultaneously occupied, and this is approximately  $(\pi^2/3)\rho^4$  which remains fairly small even up to half filling when the g-fermions start to become directly relevant. Although this contribution is probably the dominant source of error in our calculations, we do not feel that it will be strong enough to affect the picture we present. The relaxation of the approximation will both *severely* complicate the analysis *and* enhance the attraction, by allowing added hybridization into other states when the particles are nearby.

(iv) The anomalous behaviour of quantum fluctuations in one-dimensional systems is so severe, that any long range result that we derive must be viewed as misleading. Fortunately, although the behaviour of phase transitions and such is completely different, the physical phenomenon of an attraction between charge-carriers is a local effect and in two dimensions where the relevant experimental systems are best modelled, the attraction will have a more profound effect. Like many others, we believe that the loss of long range order in one dimension is a bit of a 'red herring'.

### 3. A BCS pairing theory

Developing a BCS pairing theory for the interacting spinless fermion description of equation (7) is elementary. In terms of the following expectation values:

$$F_n = \langle f_j^\dagger f_{j \pm n} \rangle = \frac{2}{N} \sum_{k>0} \langle f_k^\dagger f_k \rangle \cos nk \tag{11a}$$

$$\Delta = (-i) \frac{1}{2} \sum_{j'} \langle f_j^\dagger f_{j'} \rangle \alpha_{jj'} = \frac{2}{N} \sum_{k>0} \langle f_k^\dagger f_{-k}^\dagger \rangle \sin k \tag{11b}$$

we find a mean field description:

$$H = \sum_{k>0} A_k + \sum_{k>0} \begin{bmatrix} f_k^\dagger & f_{-k} \end{bmatrix} \begin{bmatrix} A_k & B_k^* \\ B_k & -A_k \end{bmatrix} \begin{bmatrix} f_k \\ f_{-k}^\dagger \end{bmatrix} + C \tag{12a}$$

in terms of the effective potentials:

$$A_k = -t - 2t \cos k - \mu - tP\kappa[4F_0 - 2F_0 \cos 2k - 2F_2] \quad (12b)$$

$$B_k = 4tP\kappa \sin k\Delta. \quad (12c)$$

The potential  $A_k$  is the renormalized spinless fermion dispersion. The first three terms are the non-interacting dispersion measured with respect to the chemical potential, and the final term describes the additional single-particle hopping resulting from the interaction with a second spinless fermion when it is present. The potential  $B_k$  is the pairing potential and sets the energy scale for the 'gap'. This potential is necessarily antisymmetric in reciprocal space and vanishes linearly with wavevector, although we will see later that, considered as a function of doping, the dependence of  $\Delta$  on the chemical potential is the dominant variation.

The single-particle description of equation (12) can be diagonalized by a Bogoliubov transformation to yield

$$H = \sum_{k>0} (A_k - X_k) + \sum_{k>0} X_k \sum_{\tau} x_{k\tau}^{\dagger} x_{k\tau} + C \quad (13)$$

in terms of two new fermions  $x_{k\tau}^{\dagger}$  with  $\tau = \pm 1$  and an energy of  $X_k = \sqrt{A_k^2 + B_k^2}$ .

The self-consistent 'gap' equation is

$$\Delta = \frac{2}{N} \sum_{k>0} \frac{2tP\kappa \sin^2 k\Delta}{(A_k^2 + 16t^2P^2\kappa^2 \sin^2 k\Delta^2)^{1/2}} \quad (14)$$

which must be solved for the value of  $\Delta$ . If we assume that the gap is small, and linearize the non-interacting bandstructure at the Fermi energy, then the solution for  $\Delta$  is

$$\Delta = \frac{\sqrt{[k_f(\pi - k_f)]}}{P\kappa} \exp\left(-\frac{\pi}{2P\kappa \sin k_f}\right) \quad (15)$$

which yields the weak coupling solution for the gap of  $B_f = 4tP\kappa \sin k_f \Delta$ . Using the favourable values of  $k_f = \pi/2$ ,  $P \sim 3/4$  and  $\kappa \sim 1/5$ , we find a very weak gap of  $B_f \sim t6e^{-10}$ .

The particular values are unimportant, one should only recognize the basic feature that we find a gap on the energy scale of the hopping matrix element which vanishes very quickly at low electron concentrations.

#### 4. Conclusions

Our most important conclusion is that we have found a new physical phenomenon which yields an attraction between charge-carriers.

In standard BCS theory *any* weak attraction imposed on a non-interacting free electron gas yields a pairing solution. The key to the strong-coupling paramagnets is to note that we can compare with a non-interacting *spinless* fermion gas, for which any additional attraction once again yields a pairing solution.

The spinless fermion solution corresponds directly to the behaviour of a saturated ferromagnet. The existence of any low spin correlations behaves as a short range attraction between the spinless fermions. The bulk of this article involves a technical formulation of the many-body aspects of this attraction. Here we will give a simple description of the physical content of the attraction.

When we consider two electrons on an isolated square, hopping via the  $t$ -model, we find that the ground state is a total spin singlet. A careful analysis of the wavefunction shows that it is identical in form to the solution of two spinless hard-core bosons on the same geometry. The natural interpretation is that the spin singlet antisymmetry has converted the pair of fermions into a pair of hard-core bosons. Although one hard-core boson has precisely the same energy as one fermion, two hard-core bosons achieve a lower ground state energy than two fermions on corresponding bipartite geometries. Any description of a hard-core bosonic problem in terms of a spinless fermionic problem necessarily involves an attraction at the two-particle level.

This is the basic physical content of our analysis. The extent to which a pair of electrons meet in a spin singlet is the extent to which the system behaves like a hard-core bosonic system. The system is best considered somewhere between the two pure systems. We have developed our modelling in terms of the spinless fermion system and one might presume that we believe that this is the best description. *This is not the case.* The reason that we have modelled with spinless fermions is simply because spinless fermions yield a non-interacting solution which can be solved exactly. The residual interactions can then be analysed 'perturbatively'. We believe that the spinless hard-core boson description is closer to the truth.

It is not possible for one spin to be simultaneously in a relative spin singlet with two other spins. This fact prohibits the possibility of a fermionic system behaving as a *pure* hard-core boson problem. For the present system the extent to which all relevant nearest neighbours are spin singlet is controlled by the probability  $P$  in our model. For the present case  $P$  is approximately 0.7 and the nearest-neighbour spins meet in a relative spin singlet about 70% of the time. The system is consequently much more hard-core bosonic than fermionic. We would suggest using the model:

$$H = -t \sum_{\langle ii' \rangle} (1 - \bar{P}_j b_i^\dagger b_{\bar{i}}) b_i^\dagger b_{i'} (1 - \bar{P}_j b_{i'}^\dagger b_{\bar{i}'}) \quad (16)$$

where  $b_i^\dagger$  are spinless hard-core boson operators,  $\bar{P}_j = 1 - P_j$  is the operator that tests whether the relevant spin pair is triplet and  $j$  is the edge bond pair composed from the two atoms  $i$  and  $\bar{i}$ . This Hamiltonian describes the motion of electrons in the Heisenberg ground state as a minor modification to the spinless hard-core boson problem. The many-particle contributions involve the probability  $\bar{P}$  which is approximately 0.3 and is a better small parameter than  $P$ . The real complication is that the single-particle spinless hard-core boson system is truly interacting and as yet unsolved. It is our belief that for the two-dimensional systems an analysis based upon a hard-core spinless boson system may prove more fruitful than a corresponding analysis based upon spinless fermions [7]. On a practical level, a description based upon spinless fermions *necessitates* an antisymmetric gap function with nodes and there is no experimental evidence for nodes. A hard-core spinless boson state on the other hand has spherical symmetry.

Although we have restricted attention to the  $t$ -model in this article, an extension to the  $t$ - $J$  model is trivial and simply further stabilizes the pairing. The Heisenberg

interaction becomes:

$$H = -\frac{J}{4} \sum_{\langle ij \rangle} P_j f_j^\dagger f_j^\dagger f_j f_j \quad (17)$$

in our description to the order of our approximations, combined with a minor modification to the pairing potential due to the fact that the virtually excited state involves some Heisenberg energy. The matrix element is reduced by a factor of two since two neighbouring edge bonding states only have a 50% probability of being nearest neighbours. The pairing potential is increased from  $tP\kappa$  to  $tP(\kappa + J/8t)$  where  $J = 4t^2/U$ .

We have developed a pairing theory for our attraction, and at first glance one might be disappointed at the small gap generated by our calculation. Our level of approximation has been unkind to the two particle interactions. The only behaviour allowed by our approximations is a virtual hop from two f-states into a doubly occupied edge bond state, followed by a hop transferring the electrons back into two f-states. It seems clear that a more thorough treatment of the behaviour will strengthen the attraction by allowing the electrons to approach along opposite sides of the ladder to some extent, locally using the g-states. The single-particle spinless hard-core boson model would promote these type of correlations for example.

A more important point is that the experimental systems have features which will strongly enhance the phenomenon we have described. The existence of the intermediate oxygen atoms is the crucial physical consideration. Not only are the hopping matrix elements locally increased by short range Coulomb interactions, but also, the local connectivity topologically frustrates charge motion at the single-particle level. When single-particle motion is frustrated, Pauli exclusion can be partially avoided because one particle can approach a second along a path which is rarely used by the second particle. We believe that this topological consideration is paramount in fostering a large two-particle interaction [7].

The energy scale of the pairing interaction is the hopping matrix element,  $t$ . Room temperature superconductivity is a theoretical possibility.

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