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Topological frustration can lead to superconductivity

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Abstract. We analyse charge motion in geometries composed solely of interconnecting 'diamonds'. Since a diamond is composed of two edge-sharing triangles, these geometries are topologically frustrated. The motion of a single particle across atoms which have restricted valence leads to a type of paramagnetism with only short range correlations in these geometries. When two particles meet in a diamond their behaviour is more bosonic than fermionic, which leads to a form of BCS pairing theory. The attraction can be interpreted as the pair locally unfrustrating the geometrys and a resulting local regaining of lost kinetic energy leads to the attraction.

1. Introduction

The discovery of high temperature superconductivity [1] has led to a theoretical challenge. It is widely believed that phonons cannot be the sole source of the effect, and so the theoretical requirement is a new mechanism which promotes superconductivity. The basic idea of exchanging bosons, which is at the core of the standard explanation for phonon mediated superconductivity, has led to an examination of the exchange of magnons [2] as the cause. The existence of an antiferromagnetic phase in the near vicinity of the superconducting phase is usual in the experimental systems and this has fuelled the theoretical effort. Unfortunately there is still no theoretical evidence that this mechanism is possible, let alone plausible. In this article we will address a completely different possibility: that topological considerations can lead to superconductivity.

The basic idea is elementary, but requires some knowledge of the effects of topology on charge-carrier motion in strong-coupling systems. The first real attempt to study charge motion in strong-coupling systems was performed by Nagaoka [3] who studied the motion of one charge-carrier in an infinitely strong-coupling Hubbard model. In unfrustrated lattices *ferromagnetism* is preferred, since the motion of a particle can be made coherent, with all possible paths that the particle can travel being simultaneously traversed in phase. Motion in a topologically frustrated lattice yields a surprise however. If the hopping matrix elements for charge-carrier motion are negative, then all hops can be chosen in phase, leading again to ferromagnetism, but if the matrix elements are positive, then *not* all hops can be necessarily chosen in phase and the ground state is *not* usually ferromagnetic.

Although it is fairly easy to show that charge motion in frustrated systems does not promote ferromagnetism, it is not so easy to ascertain the magnetic correlations that charge motion does promote. Some simple, but rather contrived, geometries have been solved; the 'sawtooth' geometry [4] and the 'diamond' geometries [4] of interest in this

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article. Interestingly, the phase which is stabilized in these systems is a paramagnetic phase with only very short range spin correlations. Other geometries of interest which have been studied but which have not been solved are the triangular lattice [5] and a limit of the standard two-band model of perovskite superconductivity [6]. Both geometries are readily shown to be frustrated and both models exhibit a short range paramagnetic phase although the triangular lattice ground state is controversial [7].

The point, which is crucial to the present article and which is not immediately obvious, is that in most frustrated systems, even when the system is driven paramagnetic, the charge motion is *still not coherent* for all paths. There are loops around which the particle travels out of phase, leading to a cancelling phase superposition and a corresponding *loss* in kinetic energy. The question being investigated in this article is: although a single particle loses this kinetic energy when alone, is it possible for this energy to be regained when two particles are nearby? The answer appears to be *yes* and this energy gain yields an effective attraction between particles. The simple picture is that when the two particles are brought together, one of the particles *blocks* an incoherent path of the other, and then the first particle can avoid the phase cancellation and recoup its losses. This article is an analysis of a concrete example of this idea.

The picture so far presented is too naive, since *blocking* of motion is clearly repulsive, which is the opposite physical effect to our aim. The resolution to this argument can be found from an understanding of the standard Cooper pairing theory of superconductivity [8]. In BCS theory one starts out with a non-interacting free-electron gas and then one includes a small attraction between the electrons. Electrons are fermions, and fermions repel each other: Pauli exclusion. In order for the theory to apply, we require an additional attraction *given* a hard-core repulsion between particles. In our model, the charge-carriers behave like spinless hard-core bosons or spinless fermions, and the topological effect yields a weak *additional* attraction.

There is a fair amount now known about the strong-coupling limit of the Hubbard model on the diamond geometries central to this article, and we will briefly outline the behaviour. At half filling we find a Mott insulator with a very large gap to charged excitations. Each atom has a localized electron which yields a residual spin $\frac{1}{2}$ degree of freedom. Virtual transitions into charged states lead to a weak antiferromagnetic Heisenberg superexchange interaction. The diamond geometries are some of the few connectivities which yield an exact solution to the quantum mechanical spin $\frac{1}{2}$ Heisenberg model. The solution finds as many diamonds as possible in short range Néel configurations with all the residual atoms, which come in pairs and lie on the short diagonals, pairing up into nearest neighbour singlets [9]. There is no long range magnetic order and in fact all the spin correlations are restricted to lie within the confines of individual diamonds; the correlations between spins on different diamonds vanish. This state is an example of the type of short range paramagnetic state central to the study of topologically frustrated geometries.

When charge is doped into the system and analysed in the t–J model, the resulting behaviour depends on the sign of the relevant hopping matrix element and on the sign of the charge of the carriers. If the hopping matrix element for electrons is negative, then extra electrons prefer the pairs of spins on the short diagonals of diamonds to be in local triplets, whereas extra holes prefer the pairs to be in local singlets. If the hopping matrix elements are positive, then we find the opposite behaviour [4]. Since the Heisenberg interaction promotes a mixture of singlet and triplet pairs, there is always a competition.

In this article we will assume that the electron hopping matrix elements are negative. When electrons are doped into the system, they locally drive some of the Heisenberg singlets into triplet configurations, forming a *spin polaron*. The saturated ferromagnetism to be expected from Nagaoka's theorem [3] is very weak and unlikely to be relevant in anything other than the extreme strong-coupling limit, a rarity in nature. When holes are doped into the system they locally drive some of the Heisenberg triplets into singlet configurations forming a second type of spin polaron. In this article we will be concerned with this limit, and further we will be assuming that the concentration of charge carriers is high enough that all the remnants of the Heisenberg ground state are eradicated and that all the short diagonal spin pairs have been driven into singlets.

We will study small concentrations of holes doped into geometries composed solely of interconnecting diamonds which have strong-coupling spin $\frac{1}{2}$ atoms at their vertices. In section 2 we will develop the basic physical phenomena at work in the system, reminding the reader of the single-particle solution to the relevant limit [4]. In section 3 we will show how to describe the system approximately with spinless hard-core bosons, and then we will show how to describe the system more precisely by spinless fermions. Both descriptions lead to a simple BCS pairing theory. In section 4 we conclude.

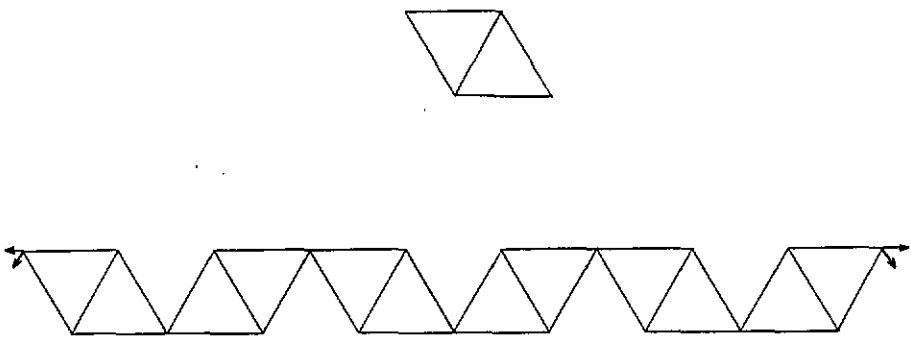

Figure 1. A single diamond and a linear chain of diamonds. All the bonds are assumed to be equal for most of the article. The long diagonal spins are not connected directly.

2. The physical phenomena

In figure 1 we depict a single diamond and a linear chaim of diamonds. In order to understand how many particles behave in our diamond geometries, it is crucial to appreciate the behaviour of various numbers of charge carriers in a single diamond. We will now proceed with a detailed description of the solution to the t-model in one diamond. The t-model is

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

where t is the hopping matrix element, $\langle ii' \rangle$ the nearest neighbours on the chosen geometry and $c^{\dagger}_{i\sigma}$ is an electron creation operator which creates a spin $\frac{1}{2}$ electron on site i with spin σ. This Hamiltonian hops electrons from site to neighbouring site, *provided* that the site which is hopped to is empty.

2.1. One hole in one diamond

We are predominately interested in doping away from half filled, and so the undoped reference state finds each atom with one electron and a spin $\frac{1}{2}$ degree of freedom. A single charge carrier doped into the system is a mobile vacant site, but the spin degrees of freedom on the singly occupied sites are relevant and so even solving for the motion of one charge carrier is a truly many-body problem. One charge carrier on a single diamond corresponds to three electrons in a vacant lattice and so we are simultaneously solving a three-electron problem.

There are three different types of solution: First when the spin background has saturated ferromagnetism, second when the short diagonal is a triplet but the solution has total spin $\frac{1}{2}$ and third when the short diagonal is a singlet and the solution is therefore also total spin $\frac{1}{2}$.

When the spin background has saturated ferromagnetism, the system becomes effectively non-interacting, since the constraint that no atom is doubly occupied is achieved by Pauli exclusion. For this situation we can put the hole into a non-bonding configuration on the short diagonal which yields an energy of $-t$. The hole cannot move from this non-bonding configuration and since there are states at lower energy we will henceforth ignore this possibility. There are three other eigenstates at energies zero and $(1 \pm \sqrt{17})t/2 \simeq 2.5616t$ and $-1.5616t$. The first and most important observation is that these energies are not symmetric when the sign of the hopping matrix element is reversed. The highest energy involves coherent motion with all the paths being traversed in phase, and the hole achieving the maximum permissable kinetic energy. However, the lowest energy finds the particle *losing* energy when it hops from one of the short diagonal sites to the other. Although hopping from one long diagonal site to the other is always in phase, hopping around one of the triangles is out of phase and leads to the observed loss in kinetic energy from the unfrustrated bound. Some of this energy can be recouped by driving the three spins from this spin $\frac{3}{2}$ configuration into a spin $\frac{1}{2}$ configuration.

When the total spin of the system is $\frac{1}{2}$, and the short diagonal pair is in a spin triplet, there are four eigenstates at energies $(1 \pm \sqrt{5})t/2 \sim 1.6180t$ and $-0.6180t$ and $(1 \pm \sqrt{13})t/2 \simeq 2.3028t$ and $-1.3028t$. This configuration clearly does worse than the case of saturated ferromagnetism and corresponds to the standard result of Nagaoka's theorem that ferromagnetism usually yields the ground state. The non-bonding orbital achieves a small quantity of kinetic energy from hybridization with the previous zero energy antisymmetric eigenstate while the previously strongly hybridizing states lose some of their hybridization. For these states motion from one short diagonal atom to the other is still out of phase, but now the motion between long diagonal sites is sometimes also out of phase.

The case of most interest to us is when the short diagonal pair are in a relative spin singlet. Once again there are four states, but now their energies are at $(-1 \mp \sqrt{5})t/2 \simeq -1.6180t$ and $0.6180t$ and $(-1 \mp \sqrt{13})t/2 \simeq -2.3028t$ and $1.3028t$. These results correspond directly to the previous case, but with the one change that motion from one short diagonal site to the other has now become in phase, and so motion around each individual triangle has become coherent. The crucial consideration for the present article is that, although this configuration yields the ground state, the ground state kinetic energy is *not* the unfrustrated bound of $(-1 - \sqrt{17})t/2 \simeq -2.5616t$; some kinetic energy has been intrinsically *lost*. It is important to physically understand this loss.

The motion of the charge carrier on the diamond can be understood by first considering motion around a triangle. Hole motion on a triangle *does* achieve the unfrustrated limit of $-2t$, when the other two spins are in a relative singlet. When the other two spins are in a triplet, however, the best that the hole can achieve is only $-t$. For the triplet case *motion around the triangle involves phase cancellation.* The charge carrier hops between only two atoms gaining the hybridization energy from this single bond.

The ground state for hole motion on the diamond is symmetric. When the hole is on either of the two long diagonal sites, the short diagonal pair is in a relative singlet promoting unfrustrated motion around the triangle on which the hole is situated. When the hole is on a short diagonal site, however, *it is not possible to make both of the pairs of spins which make up the two triangles simultaneously singlet.* The motion around both of the two triangles cannot therefore be simultaneously unfrustrated. The highest simultaneous probability of finding the two bonds singlet is achieved in the ground state to the Heisenberg model for three atoms connected in a line, and this is precisely the state found for the three spins in the ground state. The probability that any one of the two bonds is singlet is three-quarters and when this occurs the particle hops to the relevant long diagonal site in phase. The residual probability of one-quarter that the relevant bond is in a triplet leads to the cancelling superposition and the unavoidable loss in kinetic energy observed in the ground state.

2.2. Two holes in one diamond

There are two basic cases: (1) when the two remaining spins are in a triplet configuration; and (2) when the two remaining spins are in a relative singlet.

The triplet case is straightforward and is once again a completely non-interacting problem, since double occupancy is avoided using Pauli exclusion. There are six eigenstates in all, but if we eliminate the non-bonding state, since the relevant hole is immobile, we are left with three eigenstates. The lowest energy state involves the non-bonding orbital and resides at energy $(-1-\sqrt{13})t/2 \simeq -2.3028t$ whereas the lowest energy state subject to the constraint that both particles are mobile resides at energy $(1-\sqrt{13})t/2 \simeq -1.3028t$. An interesting fact pertaining to this second state, is that it is not possible for both particles to simultaneously sit on the short diagonal. If two particles were to sit on the short diagonal, then both orbitals would have to be used and so one particle would be in the non-bonding orbital and would therefore be immobile. This fact will become very important in our modelling of the next section.

The singlet case is much more interesting and yields the ground state. Again there are six eigenstates, but now the problem is no longer a single-particle problem. Interestingly there is an analogous problem with identical behaviour: that of *spinless hard-core bosons.* The possibility of finding bosonic charge carriers has been suggested before in quantum paramagnetics [14], and our model yields a concrete example of this idea. When the two holes are exchanged, the two spins are necessarily simultaneously interchanged and, since the two spins are in a singlet, the fermionic sign cancels with the sign due to the antisymmetric spin singlet wavefunction leading to a bosonic plus sign. The ground state energy is $(-1-\sqrt{33})t/2 \simeq -3.3723t$ and yields the unfrustrated bound for spinless bosons, very much lower than the unfrustrated bound of $(-1-\sqrt{17})t/2 \simeq -2.5616t$ for spinless fermions. This observation leads to a second possible explanation for superconductivity in this type of strong-coupling system: the charge carriers in these systems are hard-core, since each site can only be singly occupied, but the spin system is not irrelevant and nodes in the spin wavefunction can

conspire with the fermionic antisymmetry of electrons to produce hard-core bosonic charge carriers. We will develop this idea further in the next section, but first we must point out a useful fact which is restricted to the case of diamond geometries which assists a comparison between hard-core bosons and fermions.

One of the major problems met when trying to unravel many-body physics is that the only simple solutions available for comparison are non-interacting solutions. Although we have non-interacting fermions as a solution, the corresponding state for bosons is the non-interacting condensate, and there is no clear solution for the case of hard-core bosons. Although one believes that one achieves a condensate for hard-core bosons, this is by no means a foregone conclusion. Fortunately for the present case of diamond geometries, there is an important fact which allows one to develop a type of weak-coupling BCS-like pairing solution for the case of hard-core bosons. The observation which yields the insight comes from a comparison of the mobile two-fermion solution with the two-boson solution. There is a direct correspondence between the two sets of states which compose the two bases, together with some extra states which are only applicable to the bosonic problem; the states where both charge carriers reside on the short diagonal. Restricted to the states relevant to both problems, *the hopping matrix elements are identical*, and so if the special states are omitted the two descriptions agree. This fact allows us to describe the spinless hard-core bosonic problem as a spinless fermion problem combined with some extra degrees of freedom not present in the fermionic problem. We will develop this idea further in the next section.

2.3. One hole and many diamonds

The main reason for considering the isolated diamond in such detail is because when many diamonds are connected together the behaviour is dominated by the solution to the isolated diamond. If we connect all the diamonds together only at long diagonal sites, then holes can only move from one diamond to another by sitting on the long diagonal site between them. For one hole the ground state of the isolated diamond was achieved by states for which the short diagonal pair were in a singlet when the hole was on a long diagonal site. This fact survives the transition to many diamonds, and the ground state is achieved in the subspace where *all* the diamonds have singlet short diagonal pairs. There are several degrees of freedom which *must* be described at the single-particle level: Each diamond includes two internal degrees of freedom for the spin configurations when the hole resides on one of the short diagonal sites; there are the states when the holes reside on the long diagonal sites; and finally there are the spin correlations between the spins on the long diagonal sites to consider.

The best way to construct the ground state is by applying the Hamiltonian to many different states and finding out which states are connected to which other states. If all the short diagonals are in spin singlets, then we immediately discover that this property is conserved. The spin degeneracy of the long diagonal sites is lifted in *precisely* the same way that it is in the Nagaoka problem. As the hole passes from one long diagonal site to another, so it transfers the extra spin in the relevant diamond in the reverse direction. Nagaoka showed that the degeneracy is broken by loops, and that for bipartite loops ferromagnetism is stabilized. For the present problem the solution is identical, the infinite chain has no loops and so the degeneracy remains. For two- and three-dimensional lattices of diamonds we usually expect the long diagonal sites to yield saturated ferromagnetism.

The internal degrees of freedom may be understood from applications of the Hamiltonian. If the hole starts on a long diagonal site, then it resides in a triangle with a singlet. An application of the Hamiltonian pushes the hole onto a short diagonal site, but it arrives in a bonding orbital and the spin of the triangle remains zero. There are two long diagonal sites in each diamond and the states produced by hopping the hole from each one are distinct and yield the internal degrees of freedom. If the geometry is such that all the long diagonal sites are equivalent, then the ground state is achieved by an equal amplitude superposition of the two states, and this is precisely the three-atom-in-a-line Néel state which yielded the ground state of the isolated diamond. For this case the ground state can be deduced from a subsidiary model without the spin degrees of freedom. If we consider a single charge carrier on a vacant diamond geometry identical in form to the original but with the hopping matrix elements all negative and the elements connecting the long and short diagonals reduced to $-\sqrt{3}t/2$ to take account of the three-quarters probability of hopping, then the ground state energies are the same. The excitations are slightly different, however, since the second internal degree of freedom can come into play.

The single hole motion on a bipartite connectivity of diamonds is soluble in terms of an effective single-particle problem which has the same connectivity as the long diagonal sites together with three degrees of freedom per diamond. We denote short diagonal bonding combinations by j and long diagonal sites by $j\sigma$ where $\sigma = \pm$ labels the two atoms in that diamond. We use operators $a_{j\sigma}^{\dagger}$ for holes on long diagonal sites, $d_j^{\dagger}$ to create the symmetric Néel spin ground state with the hole in the short diagonal bonding combination of the isolated diamond and $e_j^{\dagger}$ to create the lowest lying antisymmetric state with the hole in the short diagonal bonding combination for the isolated diamond. The single-particle solution to *any* geometry of diamonds with all long diagonal spins parallel is then obtained by solving

$$H = -t\sum_j (d_j^{\dagger}d_j + e_j^{\dagger}e_j) - \frac{t}{\sqrt{2}}\sum_{j\sigma}\left[(\sqrt{3}d_j^{\dagger} + \sigma e_j^{\dagger})a_{j\sigma} + a_{j\sigma}^{\dagger}(\sqrt{3}d_j + \sigma e_j)\right] \tag{2}$$

for the relevant diamond geometry where the sum is over the internal bonds in a diamond and σ is positive when hopping from one long diagonal site into the diamond and negative when hopping from the other long diagonal site. The description is overcomplete with the same long diagonal site being described by $a_{j\sigma}^{\dagger}$ for any j connected to the site. All these different operators must be identified.

This result was previously obtained in a different form for the one-dimensional chain of diamonds [4]. The problem being tackled in this article is how to deduce the equivalent model applicable at the two-particle level.

2.4. Two holes many diamonds

It is at this point that we come across some truly new phenomena. In a study of the strong-coupling Hubbard model, the motion of two holes has proven intrinsically very difficult to tackle theoretically. Although Nagaoka's theorem demonstrates that saturated ferromagnetism is stabilized by one hole in a bipartite lattice, the two hole problem is much more difficult. In the near vicinity of the hole there are strong ferromagnetic correlations, but it seems that between the two charge carriers there is a slow spiralling of the spins. This slow spiralling costs each individual charge carrier very little, but enables the two to meet in a relative singlet and this saves energy. A

semi-classical description of this spin spiralling exists in the literature [15] and various quantum mechanical ideas have also been presented [6]. We have nothing further to add on this topic, but will address the rather different problem of two holes on the linear chain of diamonds. The analogous problem for the Hubbard model is dull with the spin degeneracies remaining unbroken, but for the diamond geometries there is a new phenomenon at work, originating from the small probabilities when the two holes are in the same diamond. The degeneracy of the long diagonal spin system is weakly broken and a state very similar to the Heisenberg ground state of the chain is stabilized.

Once again the way to find out the possible phenomena is to apply the Hamiltonian and to find out which states are connected to which other states. Clearly when the particles are not in the same diamond, the single-particle ideas are directly relevant, and so we need only consider the states produced when the holes come together.

Usually when two holes come together they arrive in a diamond where the two remaining spins are in a relative singlet. This singlet is usually the singlet which was on the short diagonal. There is one configuration that can be reached where the configuration is not necessarily a singlet: this is where one hole *follows* the other into the diamond. For the linear chain Hubbard model with nearest-neighbour hopping and infinite Hubbard repulsion, a hole cannot hop to the next site before another hole has left, but for our geometry a hole can hop to a long diagonal site of a diamond while there is a hole on a short diagonal site of the same diamond. When the second hole follows the first hole into the diamond, then the two holes *and* a long diagonal spin are simultaneously in a diamond. These configurations lead to the possibility of finding the two holes in a triplet diamond, but there is a further consideration. If once the second hole has arrived in the diamond the first hole moves onward, then we can reach a spin configuration where *two* long diagonal spins are in the same triangle as the second hole. It is this eventuality which breaks the degeneracy and stabilizes short range singlet correlations amongst the long diagonal spins.

Although this effect constitutes a new and interesting phenomenon, in the present limit it is very weak. The effect *dominates* in the limit of a small concentration of electrons in an otherwise vacant lattice and constitutes the phenomenon which leads to Kanamori paramagnetism in this limit [10].

3. Many-body descriptions

In the previous section we established the states and associated spin correlations which are relevant at low dopings of holes into a half-filled diamond geometry. Although the states relevant to one hole moving around are easy to enumerate, leading to the effective description of equation (2), when two holes or more are present they can produce an alarmingly large number of different possible spin configurations for the spin background. In this section we wish to derive some approximate many-body descriptions for *some* of the states that two holes generate and to show that these descriptions are unstable with respect to fermionic pairing. The basic idea is to select a set of states with *fixed* spin configurations and then to achieve a description where the only relevant degrees of freedom are those of the holes. Equation (2) is an example of such a description since all the original spin labels have gone and we are left with two types of spinless mobile particles. The problem is to extend this type of description to include the two-particle interactions in a way which consistently includes states which

are relevant to the original problem and connects them with the same matrix elements as the original problem.

3.1. Hard-core bosons

In this section we address the problem naively electing to use an approximate representation suggested by the single diamond results. This analysis gives both a simple concrete example of how the many-body aspects might behave and furnishes an interesting way of studying hard-core boson problems.

The first important observation to make is that the holes are truly *hard core*: it is not possible to put two charge carriers on the same atom. Although there are two degrees of freedom corresponding to the internal spin configurations in the single-particle description of equation (2), there is no sense in which these particles may be considered 'non-interacting'. The difficulty associated with deciding the relationship between the two relevant states lead us to consider an approximate description with only one hard-core object.

The states we initially consider correspond to the $d_j^\dagger$ operator. If we break up this operator into two halves corresponding to the two atoms on the short diagonal, then we can consider the model:

$$H = -\frac{\sqrt{3}}{2} t \sum_{l\sigma} (b_l^\dagger b_{j\sigma} + b_{j\sigma}^\dagger b_l) - t \sum_{\langle ll' \rangle} b_l^\dagger b_{l'} \tag{3}$$

where $b_l^\dagger$ creates a hole on one of the short diagonal sites, $b_{j\sigma}^\dagger$ creates a hole on one of the long diagonal sites which are indexed by $\sigma = \pm$ and $\langle ll' \rangle$ correspond to pairs of short diagonal sites. Notice that we are overcomplete in our description, with each long diagonal site having an operator defined for each connected diamond, which must all be identified with each other. A single hole in a lattice where all the long diagonal atoms are equivalent is described by pure $d_j^\dagger$ and $a_{j\sigma}^\dagger$ operators and no $e_j^\dagger$. At low concentrations we might expect this to remain approximately true, and at the single-particle level the $b^\dagger$ constitute an exact description of only these degrees of freedom. The crucial step is deciding on the statistics of the operators and their interactions at the two-particle level.

If we assume that the $b^\dagger$ are *spinless hard-core bosons*, then the description of equation (3) describes fairly well both the single-particle motion restricted to $d_j^\dagger$ particles *and* the states where two holes arrive in the same diamond with a singlet pair of spins. The spin configurations where two holes arrive with a triplet pair of spins are ignored and further, situations with three holes in the same diamond are described erroneously. The surprising fact is that the matrix elements between the relevant states are very similar in the two descriptions; with the small probability that the two holes arrive in a triplet diamond exactly compensating for the loss in kinetic energy from motion around the triplet triangles for a single particle. The only complication is when holes reside on short diagonals on neighbouring diamonds, a situation for which the best local spin configuration is non-trivial and a small quantity of energy is lost in the resulting matrix elements. We will ignore this minor complication and treat the simpler model to start.

The next natural step is to say that since we now have a hard-core boson problem, the ground state will involve a condensate and the system will be superconducting. This argument is not beyond reproach, and the present geometry is simple enough to allow a rather better argument to be employed.

The observation which proves useful is the comparison between fermions and hard-core bosons on an isolated diamond. There is a one-to-one correspondence between the bonding states in the fermionic description resulting from equation (3) and the bosonic states where two bosons are not allowed to simultaneously sit on a short diagonal. Since the particles can only be exchanged within the confines of a single diamond, there is no sign inconsistency in associating the two types of states. This idea then results in a description of the hard-core boson problem in terms of non-interacting fermions together with some hybridization into some other degrees of freedom:

$$H = -\frac{\sqrt{3}}{2}t\sum_{l\sigma}(b_l^\dagger b_{j\sigma} + b_{j\sigma}^\dagger b_l) - t\sum_{\langle ll'\rangle} b_l^\dagger b_{l'} - \frac{\sqrt{3}}{2}t\sum_{l\sigma}\sigma(b_l^\dagger b_{j\sigma}^\dagger f_j + f_j^\dagger b_{j\sigma} b_l) \tag{4}$$

where the $\sigma = \pm$ preserve the bosonic signs, being opposite for hopping to the two distinct long diagonal sites. Now the $b^\dagger$ are fermionic and $f_j^\dagger$ are new operators which create the state where both holes are on the short diagonal sites. This description is an *exact* representation of the corresponding hard-core boson problem.

It is now only a short step to a pairing theory for the fermionic problem. If we assume that the states where two holes are on the same short diagonal are only virtually excited, which is certainly true at low doping, then we can eliminate the $f_j^\dagger$ to leading order producing

$$H = -\frac{\sqrt{3}}{2}t\sum_{l\sigma}(b_l^\dagger b_{j\sigma} + b_{j\sigma}^\dagger b_l) - t\sum_{\langle ll'\rangle} b_l^\dagger b_{l'} + \frac{3}{4}\frac{t^2}{\epsilon}\sum_{ll'\sigma\sigma'}\sigma b_l^\dagger b_{j\sigma}^\dagger \sigma' b_{j\sigma'} b_{l'} \tag{5}$$

where the final term is an *energy-dependent* interaction, depending on the relevant single-particle energy ϵ: $H\Psi = \epsilon\Psi$. For the low energy excitation ϵ is negative; $\epsilon \simeq -3t$ for the linear chain for example. The energy dependence is only truly relevant when the pairs of short diagonal sites become significantly occupied in the ground state. We are only interested in low doping concentrations where $3t^2/4\epsilon$ is negative.

The final term in equation (5) is the expected attraction between fermions resulting from their hybridization into the extra degree of freedom associated with the bosonic state. This final description leads directly to a weak-coupling BCS pairing theory. The fact that the particles are spinless fermions ensures that the pairs must be *antisymmetric* in reciprocal space and that the gap must also be antisymmetric. This antisymmetry is not just a minor quirk of the model but is in fact serious cause for concern. There is no pairing at the zone centre and the gap grows linearly with wavevector. This is physically reasonable since only when the fermionic statistics plays a role, namely when there is a non-trivial Fermi surface, can the bosonic state be used to gain some extra energy. This situation, away from the zone centre, is also precisely where hybridization into the other spin state, the $e_j^\dagger$ state, is allowed. The effects that we have so far excluded in our approximation are equally as large as the effects that we have included. In order to truly justify our assertion that the system superconducts, we must tackle the single-particle energies exactly and show that there is *still* some extra hybridization associated with the two-particle states.

3.2. Weakly interacting fermion description

In this section we treat the description of equation (2) seriously. We impose fermionic statistics on the operators and deduce the form of the two-particle interactions. Although it might seem elementary to deduce the two-particle interactions, in fact it is

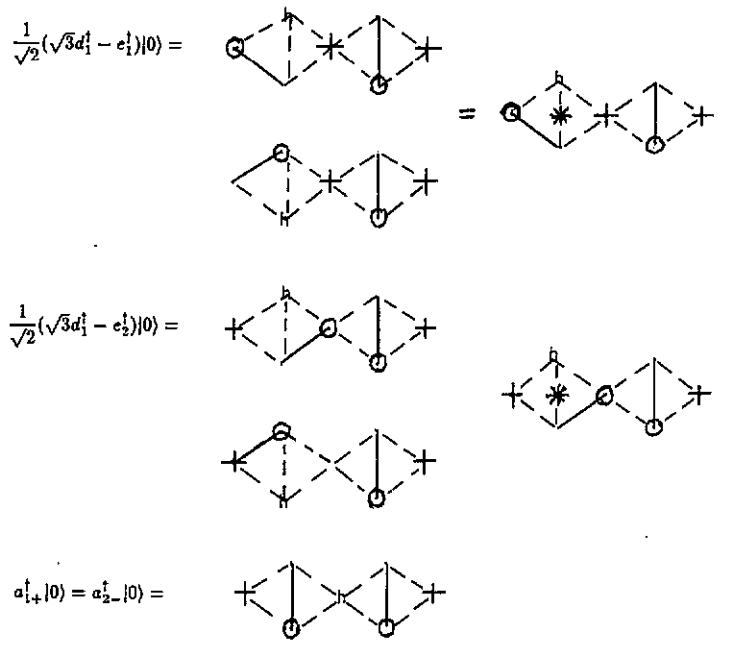

Figure 2. Pictorial representations of the states described by our effective many-body descriptions. The holes are denoted by 'h', extra long diagonal spins are denoted by '+', a singlet pair is denoted by a line with an encircled end and the antisymmetric bonding combination for a hole on a pair of short diagonal atoms is denoted by '*'. (*a*) Single-particle states.

not trivial. In figure 2 we depict a pictorial representation of the states represented by the operators in our analytic description. Not all states described by our new model have concrete representations in the original model, but all such unphysical states are non-bonding in our new model. The non-bonding combination for the model is $\sqrt{3}e_j^\dagger + \sqrt{3}e_{j'}^\dagger + \sigma d_j^\dagger + \sigma' d_{j'}^\dagger$ if we choose σ and σ' for the hops to the long diagonal site connecting the two diamonds labelled by j and j' respectively. If we once again restrict attention to spin configurations where two holes meet in a singlet diamond, then we can use

$$H = 2t\sum_j d_j^\dagger e_j^\dagger e_j d_j - \frac{\sqrt{3}-1}{\sqrt{2}}t\sum_{j\sigma}\left[d_j^\dagger e_j^\dagger a_{j\sigma}(e_j + \sigma d_j) + (e_j^\dagger + \sigma d_j^\dagger)a_{j\sigma}^\dagger e_j d_j\right] \qquad (6)$$

for the two-particle interactions, which in conjunction with equation (2) yield a consistent description for the relevant states. We believe that the effective description is *exact* for the states indicated in figure 2 at the two-particle level. The first term is purely repulsive and corresponds to the loss of motion between the two short diagonal sites when they are both occupied. The second term is the important term and yields the corrections due to the enhanced motion when a pair of holes are in a diamond with a singlet. It is important to realize that we have only included states where the two holes are in a singlet diamond. There are matrix elements promoting triplet diamonds too, but these states are not naturally included into our description although they will lead to further attraction between holes. The two-particle potential that we derive is more repulsive than that for the original system.

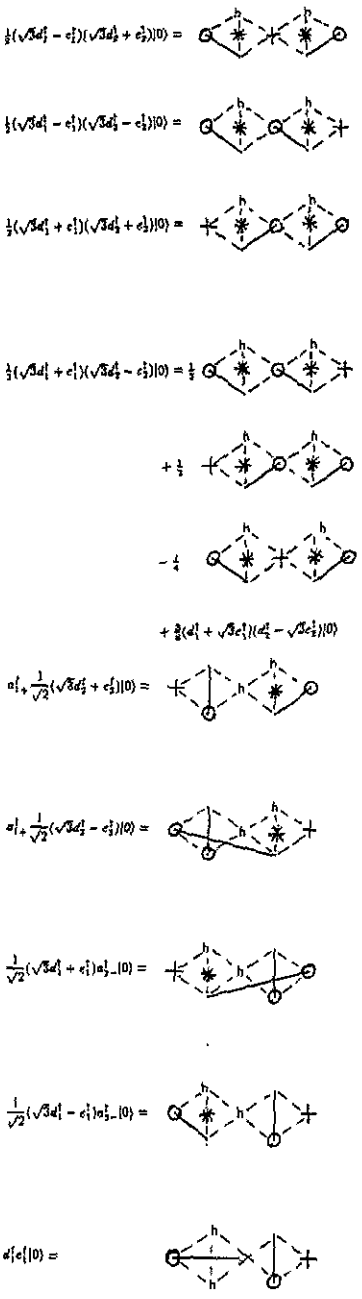

Figure 2. (*b*) Two-particle states. The combination $(d_1^\dagger + \sqrt{3}e_1^\dagger)(d_2^\dagger - \sqrt{3}e_2^\dagger) \mid 0\rangle$ is *non-bonding* in our description and irrelevant to the low energy excitations. There is no obvious spin configuration corresponding to this state.

We now move on to a determination of whether the two-particle interactions are attractive or repulsive. The first step is a diagonalization of the single-particle

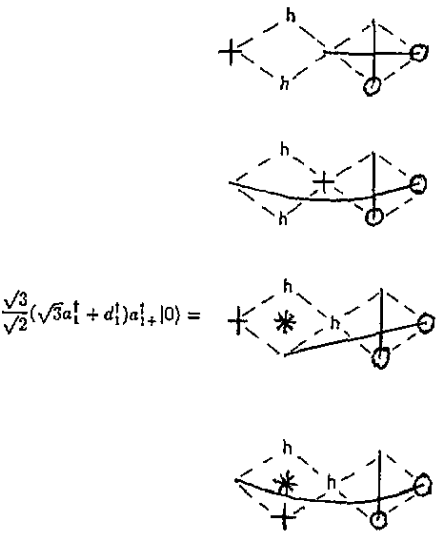

Figure 2. (*c*) The state with a triplet diamond which is omitted from our description, together with the state included in our representation to which the omitted configuration is coupled.

interactions. In reciprocal space

$$H = (-t)\begin{bmatrix} a_k^\dagger & d_k^\dagger & e_k^\dagger \end{bmatrix}\begin{bmatrix} 0 & \sqrt{6}c & \sqrt{2}si \\ \sqrt{6}c & 1 & 0 \\ -\sqrt{2}si & 0 & 1 \end{bmatrix}\begin{bmatrix} a_k \\ d_k \\ e_k \end{bmatrix} \tag{7a}$$

where $c = \cos k/2$ and $s = \sin k/2$, which diagonalizes to yield:

$$H = (-t)\sum_k \tfrac{1}{2}(1 + D_k)g_k^\dagger g_k + t\sum_k \tfrac{1}{2}(D_k - 1)h_k^\dagger h_k - t\sum_k n_k^\dagger n_k \tag{7b}$$

where $D_k = \sqrt{[9 + 16c^2]} = \sqrt{[17 + 8\cos k]}$:

$$a_k^\dagger = \frac{D_k - 1}{\sqrt{2}\sqrt{\{D_k^2 - D_k\}}}g_k^\dagger - \frac{D_k + 1}{\sqrt{2}\sqrt{\{D_k^2 + D_k\}}}h_k^\dagger \tag{7c}$$

$$d_k^\dagger = \frac{2\sqrt{3}c}{\sqrt{\{D_k^2 - D_k\}}}g_k^\dagger + \frac{2\sqrt{3}c}{\sqrt{\{D_k^2 + D_k\}}}h_k^\dagger + \frac{si}{\sqrt{[1 + 2c^2]}}n_k^\dagger \tag{7d}$$

$$e_k^\dagger = \frac{2is}{\sqrt{\{D_k^2 - D_k\}}}g_k^\dagger + \frac{2is}{\sqrt{\{D_k^2 + D_k\}}}h_k^\dagger + \frac{\sqrt{3}c}{\sqrt{[1 + 2c^2]}}n_k^\dagger. \tag{7e}$$

The next step is to find the two-particle potential restricted to the lowest lying branch, by substituting equations (7*c*)–(7*e*) into equation (6).

$$H = \frac{1}{N}\sum_{kk'pp'} g_k^\dagger g_{k'}^\dagger g_{-p'} g_{-p} I(k, k'; p, p')\delta_{k+k'+p+p'} \tag{8a}$$

with

$$I(k, -k, -p, p) = \frac{4t\sin k \sin p}{(D_k^2 - D_k)(D_p^2 - D_p)}\left[6 - (2\sqrt{3} - 3)(D_k + D_p - 2)\right] \tag{8b}$$

where the interaction has been partially symmetrized and we have evaluated the interaction for the most important pairs which have zero total momentum. The requirement that spinless fermion pairs have antisymmetric reciprocal space wavefunctions is manifested in the two factors $\sin k$ and $\sin p$. The interaction vanishes at the zone centre only exhibiting an interaction on states which are affected by Pauli exclusion.

Unfortunately this interaction is *always* repulsive, although it is very small with a large cancellation between the two terms.

Rather than pursue the inclusion of the states omitted from the model, in order to establish the validity of the *phenomenon* we have elected to modify the *model*. By raising and lowering the relative size of the matrix elements we can both weaken the repulsion between the $d_j^\dagger$ and $e_j^\dagger$ fermions and increase the attraction by promoting $a_{j\sigma}^\dagger$ in the ground state.

The obvious extension

$$H_1 = (\Delta - t')\sum_j (d_j^\dagger d_j + e_j^\dagger e_j) - \frac{t}{\sqrt{2}}\sum_{j\sigma}\left[(\sqrt{3}d_j^\dagger + \sigma e_j^\dagger)a_{j\sigma} + a_{j\sigma}^\dagger(\sqrt{3}d_j + \sigma e_j)\right] \quad (9a)$$

$$H_2 = 2t'\sum_j d_j^\dagger e_j^\dagger e_j d_j - \frac{\sqrt{3}-1}{\sqrt{2}}t\sum_{j\sigma}\left[d_j^\dagger e_j^\dagger a_{j\sigma}(e_j + \sigma d_j) + (e_j^\dagger + \sigma d_j^\dagger)a_{j\sigma}^\dagger e_j d_j\right] \quad (9b)$$

simply raises the energy of the short diagonal sites to Δ and reduces the hybridization across the short bonds to t'. There is no intrinsic change in behaviour, and we can readily find the equivalent results for this model:

$$\epsilon_F = \tfrac{1}{2}\left(\Delta + t' - \sqrt{[32t^2 + (\Delta + t')^2]}\right) \quad (10a)$$

for the ferromagnetic ground state energy:

$$\epsilon_S = \tfrac{1}{2}\left(\Delta - t' - \sqrt{[24t^2 + (\Delta - t')^2]}\right) \quad (10b)$$

for the paramagnetic ground state energy which must be relatively stable. If the energies become reversed, then the Nagaoka saturated ferromagnet would be stabilized at the single-particle level.

The analagous calculation for the two-particle interaction potential is straightforward and yields:

$$I(\boldsymbol{k}, -\boldsymbol{k}, -\boldsymbol{p}, \boldsymbol{p}) = \frac{4\sin k \sin p}{(\bar{D}_k^2 - \bar{D}_k)(\bar{D}_p^2 - \bar{D}_p)}\left[6t' - (2\sqrt{3}-3)(t\bar{D}_k + t\bar{D}_p + 2\Delta - 2t')\right] \quad (10c)$$

where

$$\bar{D}_k = \left(8 + 16\cos^2\frac{k}{2} + \frac{(\Delta - t')^2}{t^2}\right)^{1/2} = \left(16 + 8\cos k + \frac{(\Delta - t')^2}{t^2}\right)^{1/2}.$$

It is fairly easy to show that the interaction becomes attractive near empty when the ferromagnetic and paramagnetic phases are near degeneracy.

A simple example is to let $\Delta = 0$ and $t' = t/2$.

Developing the pairing theory from this attractive interaction is no problem, provided that the interaction is attractive at the non-interacting Fermi surface. The characteristic energy scale is the *hopping matrix element* and this clearly allows room temperature superconductivity in principle.

4. Conclusions

In this article we have presented the first analytic attempt to show that charge motion in topologically frustrated systems can involve pairing correlations. For our contrived diamond geometries we have exhibited an attractive interaction between the charge carriers. The interpretation of the effect can follow two lines of reasoning:

The first line points out that when two holes meet in a diamond, they usually meet when the other two spins are singlet. Locally they behave as hard-core spinless bosons in this diamond. Since two such bosons gain more kinetic energy than two equivalent fermions this behaviour constitutes an attraction for the particles, when considered as fermions. Equivalently we can say that nodes in the spin wavefunction can conspire with the fermionic minus sign to convert fermions into bosons and allow the spinless charge carriers in a strong-coupling paramagnet to exhibit bosonic properties. Hard-core bosons condense [11]. We have previously presented just such an explanation for perovskite superconductivity [12].

The second line of reasoning is based solely on an interpretation of the effects of topological frustration on charge motion in strong-coupling systems. First, charge motion drives the system into a strong-coupling paramagnet. Second, even in the paramagnetic phase, the particle motion is usually *still* restricted, with some kinetic energy lost to motion around loops with unhelpful spin configurations. When particles approach each other one particle can locally unfrustrate the connectivity for the other leading to a local gain in kinetic energy. For our particular example the loss in kinetic energy can be traced to the extra spins on the long diagonal sites, which stop particles from always circling triangles with local singlet correlations. Extra charge carriers *replace* these problem spins and when two holes approach each other there are no remaining spins to cause problems, only singlets. We have previously pointed out that the natural strong-coupling limit of the tight binding model of perovskite superconductors is *vigorously* frustrated [13].

These two arguments are not independent and may just be two ways of understanding one phenomenon.

In this article we have studied the t-model and have used topological frustration to stabilize a strong-coupling paramagnet. There is no requirement for this and we could have used the t–J model and allowed the Heisenberg contribution to destabilize the Nagaoka ferromagnetism, but simultaneously kept the Heisenberg interaction weak enough not to stabilize the Heisenberg ground state. This line of argument explains the experimental phase diagram quite well: Néel order is observed in the insulating phase. As holes are doped into the material the antiferromagnetism is lost as the charge motion starts to dominate. The resulting paramagnetic phase still has short range Néel correlations, ensuring only a small loss in Heisenberg energy.

The critical geometric consideration was the *square* and not the triangle. The attraction was caused by enhanced motion in the presence of a singlet, and to get two holes and a singlet we need *four* sites. The triangles are there only to promote strong-coupling paramagnetism. A similar study of the sawtooth geometry [4] yields paramagnetism but no pairing.

We are not claiming that the one-dimensional chain is a superconductor, since it is well known that fluctuations in one dimension are anomalously large. The calculations are a simple pilot for higher dimensional analogues. In practice, provided that the long diagonal spins are all parallel, the description of equation (9) is valid in higher dimensions with fermionic operators. The pairing effect is stronger in higher

dimensions since the probability that the holes reside on the long diagonal sites is increased. Indeed, for the three-dimensional simple cubic arrangement of long diagonal atoms, even the unmodified Hamiltonian yields an attraction between the holes.

We do not believe that all the long diagonal spins will remain parallel in the true ground state in *any* dimension. There is much more energy to be made from paramagnetism around the larger loops which further 'bosonize' the charge carriers.

We believe that the physical mechanism presented in this article can be pressed into service as an explanation for perovskite superconductivity. The two basic requirements of topological frustration and bosonic behaviour of pairs around the smallest loop are certainly true.

Acknowledgments

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