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An exactly soluble one-dimensional quantum mechanical Heisenberg and Nagaoka *t–J* model

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Abstract. For a quasi-one-dimensional 'sawtooth' topology we show that the quantum mechanical ground state of the Heisenberg Hamiltonian has only nearest neighbour singlet correlations. The ground state is multiply degenerate with precisely as many ground states as atoms in the system. In fact we can associate each ground state with a special site that has a fixed spin. Allowing this special site to become a hole, in a frustrated *t–J* description, allows us to deduce the ground state for the motion of one hole in the *presence* of the Heisenberg interactions. When the hopping is unfrustrated we look at the competition between t and J and find a reasonable description for a 'polaron'. The polaron maintains low spin.

1. Introduction

A central theme of solid state physics is the electronic properties of matter. The fundamental physical phenomena at work are: Pauli exclusion because electrons are fermions and Coulomb repulsion because electrons are charged, which try to keep electrons apart, competing with chemical bonding which comes from the attraction to the positive nuclei in the relevant configuration and the kinetic energy of the electronic motion. When chemical bonding dominates, the electronic properties are well modelled by band theory, but when Coulomb repulsion dominates, modelling is more difficult. In this article, we are interested in the limit of strong Coulomb repulsion, which has become known as the strong coupling limit.

Perhaps the simplest model which displays the basic phenomena is the Hubbard model [1]:

$$H = -t \sum_{\langle ii' \rangle \sigma} c^{\dagger}_{i\sigma} c_{i'\sigma} + U \sum_{i} c^{\dagger}_{i\sigma} c^{\dagger}_{i\bar{\sigma}} c_{i\bar{\sigma}} c_{i\sigma} \tag{1.1}$$

which is a single orbital tight binding model. The $c^{\dagger}_{i\sigma}$ create electrons of spin σ (complementary spin $\bar{\sigma}$) on the ith atom and obey anticommutation relations. The first term corresponds to chemical bonding and is assumed to contribute only to the nearest neighbour atoms, denoted by $\langle ii' \rangle$, and the second term corresponds to short range Coulomb repulsion and is assumed to contribute only when the two electrons are on the same atom. This model was designed to represent the narrow band electrons found in transition metals and we also have this physical picture in mind.

When the chemical bonding or 'hopping' dominates, viz $t \gg U$ where t is assumed positive, we find a free electron picture with a well defined band structure. The effects

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of the Coulomb repulsion may be included using the Hartree–Fock approximation, but this does not alter the basic physical picture until the advent of itinerant magnetism at the Stoner criterion [2]. The description is valid for all densities of electrons and suggests very similar behaviour at all densities until magnetism with its various spatial symmetries intercedes [3].

When the Coulomb repulsion dominates, viz $U \gg t$, we find descriptions which depend strongly on the density of electrons. To leading order the Coulomb repulsion prohibits double occupancy of sites and we find:

$$H_0 = -t \sum_{\langle ii' \rangle \sigma} (1 - c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}}) c^\dagger_{i\sigma} c_{i'\sigma} (1 - c^\dagger_{i'\bar{\sigma}} c_{i'\bar{\sigma}}) \tag{1.2}$$

where the additional projection operators restrict hops from singly occupied atoms to neighbouring vacant atoms. Since only one electron can sit on any one atom at any one time, there is a spin degeneracy while the electron is on the atom. The manner in which the degeneracy is lifted, *if* it is lifted, is the basic physical question. In general this question is very difficult to answer, but there are two limits which are amenable to analysis. Before we move on to an analysis of these two limits, we point out the role of *topology* in this problem, since the two cases treated in this article have 'special' topologies.

Most simple lattices are bipartite, which means that the lattice splits quite naturally into two sublattices for which all nearest neighbours of one sublattice are on the other sublattice. Changing the relative sign of the states on these two sublattices leads to invariance when the sign of the hopping matrix element is reversed. Combining this symmetry with mapping particles onto holes then leads to particle-hole symmetry for the Hubbard model. There is a special class of topologies, including the two cases studied in the present article, which do not exhibit particle–hole symmetry. In this paper we will assume that the hopping matrix element, t, is positive and we will show that holes and particles exhibit quite different behaviour.

Returning to the two tractable cases, the first is when there are only two electrons in the system, then the spin symmetry is either singlet, suggesting paramagnetism in the low density limit, or triplet, suggesting ferromagnetism in the low density limit. It turns out that the *connectivity* of the lattice decides this question with a singlet being the usual ground state [4] and the triplet is only found when the two particles are holes and the lattice connectivity is antiferromagnetically frustrated [5]. The lattice connectivities that we consider in this article are all frustrated and this was one of our motivations in commencing this study.

The second amenable limit is when all sites except one have one electron and the final atom has either no electrons or two electrons and has the only mobile charge carrier. The magnetic coherence predicted in this limit constitutes the Nagaoka problem and was shown to be usually ferromagnetic by Nagaoka [6]. The only case where ferromagnetism is *not* predicted is when the charge carrier is a hole and again the lattice connectivity is antiferromagnetically frustrated. It is not known what type of magnetic coherence results for the case of frustrated topologies and in this article we exactly solve the Nagaoka problem for two very simple non-trivial one-dimensional frustrated topologies, showing that the ground state is a total spin singlet with short range singlet bonds in both cases.

Although the Nagaoka problem gives an indication of the magnetic coherence preferred by a charge carrier in a strong coupling system, there is an important proviso. Although the motion of the charge carrier breaks the spin degeneracy at order t, there

is only *one* charge carrier and so there is no macroscopic contribution to the total energy until the density of charge carriers is finite. The correction to the Nagaoka Hamiltonian in this limit *does* give a macroscopic contribution and so should have a region of dominance. This conflict of interests is the major area of concern in this article.

The leading correction to the Nagaoka Hamiltonian is [7]:

$$H_1 = \frac{J}{2} \sum_{\langle ii' \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i'} \tag{1.3}$$

the Heisenberg Hamiltonian [8] where the antiferromagnetic coupling is $J = 4t^2/U$, the spin operators are $\boldsymbol{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} c^\dagger_{i\sigma} \hat{\boldsymbol{\sigma}}_{\sigma\sigma'} c_{i\sigma'}$, $\hat{\boldsymbol{\sigma}}$ are Pauli matrices and we are including each bond with a single J.

When there is precisely one electron per site, then none of the electrons can move and we find a Mott insulator [9]. The Heisenberg Hamiltonian is the leading order interaction between the localised spins. The Heisenberg Hamiltonian is of interest in its own right as a model for localised magnetism when the hopping is frozen out.

Although the classical limit of the Heisenberg model, when the total spin is large, is soluble, the quantum mechanical model has proven very difficult to solve in general and even the solution to the one dimensional chain required the Bethe *ansatz* [10]. It is generally believed that long range Néel antiferromagnetism with a reduced moment is the ground state of non-frustrated topologies, where long range order is allowed, but in frustrated systems there is controversy and the triangular lattice Heisenberg model was the original system for which the resonating valence bond state was proposed [11]. In this article we present a non-trivial exactly soluble quantum mechanical ground state to a Heisenberg model on a one-dimensional frustrated topology.

There has been a recent resurgence of interest in the competition between Heisenberg and Nagaoka interactions due to high temperature superconductivity. In these materials there is a Mott insulating parent compound which exhibits Néel order. Upon doping the Néel order is lost and replaced by superconductivity. This behaviour is being modelled by the strong coupling t–J model of (1.2) combined with (1.3). The parent compound corresponds to the half filled Heisenberg antiferromagnet and superconductivity is associated with the added charge carriers moving around using the Nagaoka Hamiltonian in the presence of the Heisenberg interactions [12]. The topology of the spins is the unfrustrated square lattice of copper atoms, but if the charge resides as holes on oxygen sites then there are limits where the hole motion is both frustrated and unfrustrated [13].

The biggest problem in analysing the t–J model is that *the Heisenberg ground state of the relevant topology is unknown* and the natural analysis involves treating the Heisenberg ground state as a reference and then including a charge carrier moving by Nagaoka hops 'perturbatively'. There have been two basic approaches: firstly the spins can be treated as classical and then the ground state is soluble and the charge motion can be properly handled [14] and secondly simultaneous approximations can be made in treating both interactions [15]. Neither of these two approaches is particularly satisfying as it is unclear as to the source of the effects found in any treatment. In this article we have an exact quantum mechanical ground state and so we need only treat one of the two terms perturbatively. The basic physical picture proposed for this model is 'spin polarons' [16]. The Nagaoka interactions drive a small region around the charge carrier from Heisenberg correlations into Nagaoka correlations and the composite object drifts slowly about the lattice. For the square lattice, these ideas suggest ferromagnetic

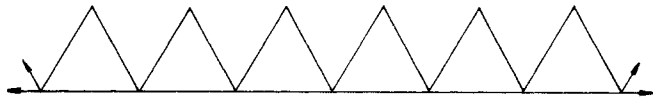

Figure 1. The 'sawtooth' topology. Each bond is assumed identical.

correlations around the charge, which are *not* observed in exact cluster calculations [17]. We will look for analytic polarons in our model in order to test these ideas.

In this article we have forsaken the physical topology in favour of a topology which allows an exact analysis. This allows us to make unequivocal statements about our particular connectivity and hence make some of the physical ideas concrete, but the connection to the experimental systems is rather tenuous.

In section 2 we present the exact ground states on our chosen topologies and in section 3 we analyse the competition between the Heisenberg and Nagaoka contributions and the validity of the polaronic ideas.

2. Exact solutions

2.1. The 'sawtooth' geometry

The 'sawtooth' connectivity considered in this article is depicted in figure 1. Each bond is assumed identical and we find two distinct types of sites. 'Backbone' sites are connected to two other backbone sites and two 'vertex' sites, whereas vertex sites are only connected to two backbone sites. The best way to picture this topology is as a string of equilateral triangles connected in a chain.

The Heisenberg Hamiltonian on this topology can be rewritten as:

$$H_1 = \frac{J}{2}\sum_T (|\boldsymbol{S}_1 + \boldsymbol{S}_2 + \boldsymbol{S}_3|^2 - \tfrac{9}{4}) \tag{2.1}$$

where the sum is over all triangles, denoted by T, and the spins $\boldsymbol{S}_1$, $\boldsymbol{S}_2$ and $\boldsymbol{S}_3$ lie on the vertices of the triangles. It is clear that each triangle must have the lowest possible total spin simultaneously allowable in the ground state. The simple observation that allows a solution to this problem is that, due to the fact that there are *two* distinct spin half states for the triangle, we can simultaneously make *all* triangles have total spin 1/2, the minimum possible. The energy of this state is $E_0 = -(3/4)JN_T$ where N_T is the number of triangles. We use this energy scale to define our Heisenberg vacuum for the rest of this article.

In this article we use *valence bond* representations for our spin configurations. Low spin states are achieved by pairing up electrons into singlet configurations or valence bonds. Any remaining electrons are all assumed to have parallel spins. This choice of basis ensures that the states used are eigenstates of the total spin with a total spin corresponding to the spin of the unpaired electrons. There is one major subtlety in employing this type of basis: *non-orthogonality*. Although the total spin of the states is known, the different basis states have non-trivial overlaps with each other and if all possible pairings are included then the basis is *overcomplete*. As well as being an eigenstate of the total spin, a valence bond state is also an eigenstate of some *restricted* total spin operators. The total spin of any two paired electrons is zero and further the

Figure 2. A ground state for the Heisenberg Hamiltonian on the 'sawtooth' geometry. The lines with 'encircled' ends denote singlet bonds.

total spin of any set of electrons all of which are paired is also zero. The fact which leads us to the solution of our Heisenberg model is that the total spin of a set of electrons all bar one of which are paired is total spin *half*. For the 'sawtooth' topology each triangle has total spin half if it includes a valence bond and there are various ways to lay down valence bonds and ensure this.

One of the degenerate ground states is depicted in figure 2. The 'special' site with the 'bare' spin can be chosen anywhere on the lattice and serves to label the ground state degeneracy. This is the first situation where non-orthogonality causes confusion. As the 'bare' spin is moved around, the resulting basis is *overcomplete*. If we choose the special site to be each vertex of a particular triangle in turn, then the three corresponding ground states are *linearly dependent*. In fact a complete basis of 'up' ground states can be obtained by restricting the special site to the backbone and the same goes for 'down' sites. Although there are as many ground states as atoms in the lattice, they split into two because the total spin of the state has been chosen to be a half.

This analysis can also be applied to the linear chain connectivity and although we may arrive at the decoupling into distinct bonds of (2.1), it is not possible to simultaneously choose all bonds to be total spin zero which is where the two problems part company.

Our choice of *free* boundary conditions plays an active role in the present analysis. If we were to assume periodic boundary conditions, then there would be only *two* ground states and no special site from which the Nagaoka ground state could be deduced. As the system size diverges, the results should not depend critically on boundary conditions and so we chose the boundary conditions most suitable to our requirements.

The next natural question to ask is about excitations. The enormous degeneracy of the ground state confuses the issue, but it turns out to be possible to construct a hierarchy of local excitations which are all eigenstates of the Heisenberg Hamiltonian and include all the possible local spin configurations. The basic idea is to observe that if we cut the chain at the special site and include some extra triangles, whatever spin configuration we choose for the additional triangles, the Heisenberg interactions can never alter the spin arrangement in the original lattice. The valence bond state of figure 2 is therefore *locally* an eigenstate. A second way to consider the excitations, corresponds to breaking bonds in the vicinity of the special site. The justification is the same, but this second idea is the natural way to consider excitations in *finite* systems where the number of atoms is constant. We depict a few of these excitations in figure 3, including all the possibilities when either one or two new triangles are included. Analysis of larger clusters yields the belief that the excitation spectrum is gapless. At the three triangle level there is a spin three-halves state at energy $E_0 + 0.3654J$ for example. Clearly as the size of the inclusion diverges so we can describe all the possible spin configurations. The only source of concern is that this local description of excitations is over complete and non-orthogonal.

Now let us move on to the Nagaoka problem and consider the motion of a charge carrier in the system. The single-particle excitation spectrum can be deduced from the two atom per unit cell basis:

Figure 3. Local excitations of the Heisenberg Hamiltonian acting on the 'sawtooth' topology. The lines with 'encircled' ends denote singlet bonds.

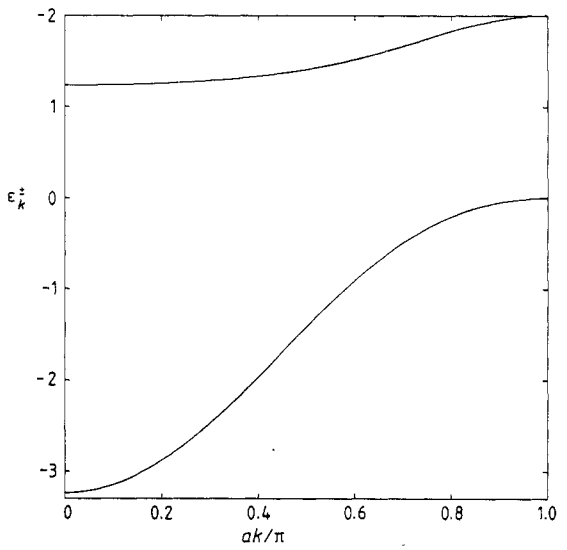

Figure 4. The band structure of non-interacting electrons in the 'sawtooth' geometry.

$$H_0 = (-t)\begin{bmatrix} 0 & 2\cos(ak/2) \\ 2\cos(ak/2) & 4\cos^2(ak/2) - 2 \end{bmatrix} \tag{2.2}$$

which diagonalises to yield the band structure:

$$\varepsilon_k^{\mp} = (-t)[2\cos^2(ak/2) - 1 \pm \sqrt{(1 + 4\cos^4(ak/2))}] \tag{2.3}$$

which is depicted in figure 4. It is clear that the topology is antiferromagnetically *frustrated* as there are triangles in the connectivity. Another way to observe the frustration, which also yields a measure of the effect, is to look at the band structure. Although the lowest energy is $-3.2361t$, which is the unfrustrated limit, the highest

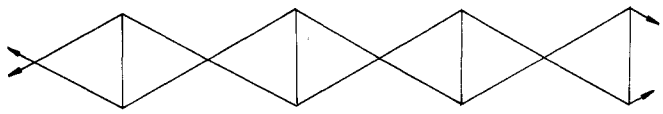

Figure 5. The 'diamond' topology. Each bond is assumed identical.

energy is only $2.0t$. The difference between these two values is a fair measure of the extent to which the lattice is frustrated.

In the Nagaoka problem, one hole is doped into an otherwise half filled lattice, subject to the constraint that at most one electron can sit on any one site at any one time. If the band were purely ferromagnetic, then the best one could do would be to take the electron from the highest state in the band structure of figure 4. The question is, is it possible to choose the spin arrangement of the half filled state in such a way that the electron can be extracted from a state of higher energy?

Let us consider the state depicted in figure 2, where the bare spin is replaced by the added hole. As the hopping Hamiltonian moves the hole around, we find that we connect together all the states which made up the ground state manifold of the Heisenberg Hamiltonian. In this context the orthonormality is not a problem and we find precisely the same number of states as atoms in the lattice. With a careful choice of signs, we discover that in the two-atom basis the hopping Hamiltonian for a delocalised *hole* becomes identical to (2.2). The nearest neighbour spin configuration *unfrustrates* the hole motion completely and in this state the hole energy achieves its theoretical bound and we find the Nagaoka ground state. An added hole drives the spin background into a short range singlet state.

Now let us consider the full *t–J* model in the presence of the added charge carrier. It turns out that the bare spin gains *zero* energy from its bonds since it has a quarter probability of being in a singlet and three quarters probability of being in two of the three triplet states. It therefore follows that *cutting* the bonds by replacing the bare spin by a hole does not change the Heisenberg energy at all. In the presence of the charge carrier, the state is an eigenstate of the Heisenberg Hamiltonian and further is the ground state. The quantum mechanical Heisenberg model and strong coupling Hubbard model are simultaneously soluble when there is one hole in an otherwise half filled 'sawtooth' connectivity. The topology is effectively unfrustrated by the spin state and we obtain the lowest conceivable ground state energy of $E_0 - 3.2361t$.

So far we have considered the case of frustrated hopping. If the hopping matrix element t were negative or alternatively if we consider the addition of one extra electron rather than a hole, then the topology does *not* frustrate hole motion and Nagaoka's theorem implies that the ground state of the hopping Hamiltonian would be ferromagnetic. Unfortunately the competition between the low spin Heisenberg ground state and the high spin hopping interactions is not as tractable as the previous limits and so we leave this problem to the approximate analysis of the next section.

2.2. The 'diamond' connectivity

Our second consideration is the topology depicted in figure 5. Once again there are two types of sites, 'central' sites which are connected to four 'edge' sites and edge sites which are connected to two central sites and one other edge site. For this case we consider the

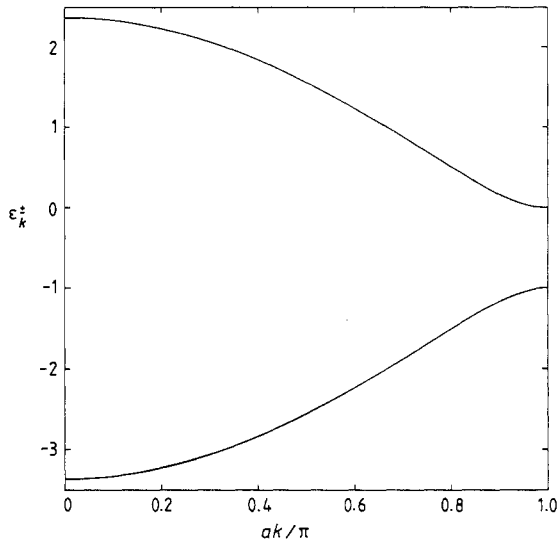

Figure 6. The band structure of bonding non-interacting electrons in the 'diamond' geometry.

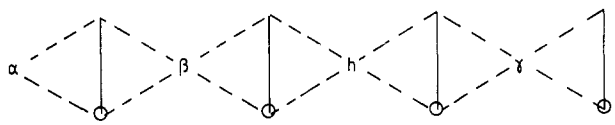

Figure 7. A state from which the ground state of the Nagaoka problem on the 'diamond' topology can be constructed. The labels α, β, γ denote arbitrary but fixed spins. The lines with 'encircled' ends denote singlet bonds.

Nagaoka problem first. There are now three atoms in a unit cell, but it is clear that taking anti-phase combinations of two neighbouring edge atoms yields a non-bonding combination. The single-particle excitation spectrum can again be deduced from the two relevant atoms per unit cell basis:

$$H_0 = (-t)\begin{bmatrix} 0 & 2\sqrt{2}\cos(ak/2) \\ 2\sqrt{2}\cos(ak/2) & 1 \end{bmatrix} \tag{2.4}$$

which diagonalises to yield the band structure:

$$\varepsilon_k^{\pm} = (-t/2)[1 \pm \sqrt{(1 + 32\cos^2(ak/2))}] \tag{2.5}$$

which is depicted in figure 6. It is clear that this topology is also frustrated, and comparing the unfrustrated lower bound in figure 6 of $-3.3723t$ with the highest lying excitation of $2.3723t$, we find that the effect is strong but seemingly not as strong as the previous case.

The Nagaoka problem for the frustrated limit of this lattice is also exactly soluble. A state which can be used to generate one of the multiply degenerate ground states is depicted in figure 7, where all the pairs of electrons on neighbouring edge atoms form spin singlets. Indeed the spins α, β and γ all along the chain can take any values and still generate a ground state. These values serve to label the ground states and this situation

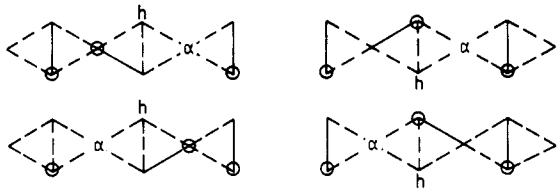

Figure 8. The states which go together with the state in figure 7 to yield the Nagaoka ground state. The hole is in the non-bonding orbital. The lines with 'encircled' ends denote singlet bonds.

is perfectly analogous to the strong coupling chain where the degeneracy is 2^N in contrast to the previous degeneracy of N. When the hopping Hamiltonian acts on this state it produces states like those depicted in figure 8. Taking these states as a basis, the operation of the hopping Hamiltonian is closed. This fact is not trivial and depends on the fact that the two states in figure 8 are non-orthogonal. Using delocalised combinations of these three states as a basis, we find:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} E = (-t) \begin{bmatrix} 0 & 3\cos\frac{ak}{2} - i\sin\frac{ak}{2} & 3\cos\frac{ak}{2} + i\sin\frac{ak}{2} \\ 3\cos\frac{ak}{2} + i\sin\frac{ak}{2} & 2 & 1 \\ 3\cos\frac{ak}{2} - i\sin\frac{ak}{2} & 1 & 2 \end{bmatrix} \tag{2.6}$$

which diagonalises to yield the bandstructure:

$$\varepsilon_k^{\pm} = (-t/2)[1 \pm \sqrt{(9 + 16\cos^2(ak/2))}] \qquad \varepsilon_k^0 = (-t) \tag{2.7}$$

which is depicted 'upside down' in figure 9 as a particle spectrum for comparison with figure 6.

The three states do *not* correspond to the three atoms per unit cell, but are restricted to the non-bonding combinations. The third state corresponds to an internal *spin* degree of freedom. In fact there is a 'reciprocal relationship' between the total spin of pairs of neighbouring edge atoms and the bonding symmetry of the hole when it lies on the bond. If the total spin is zero then the hole resides in the non-bonding combination and if the total spin is unity then the hole resides in the bonding combination. The total spin of each bond may be used to label the excitation spectrum of the Nagaoka problem.

Comparing the single-particle spectrum in figure 6 with the excitation spectrum in figure 9, we find that there is an energy saving of $0.6277t$ in using the Nagaoka ground state rather than the perfect ferromagnet. Also of interest is the fact that the ground state spin configuration does *not* completely unfrustrate the topology and the optimum value of $3.0t$ leaves a residual $0.3723t$ of unobtainable energy, when compared with the unfrustrated bound.

Now let us move on the Heisenberg Hamiltonian considered on the topology of figure 5. We may write:

$$H_1 = \frac{J}{2}\sum_T (|S_1 + S_2 + S_3|^2 - \tfrac{9}{4}) - \frac{J}{2}\sum_B (|S_4 + S_5|^2 - \tfrac{3}{2}) \tag{2.8}$$

where the first sum is over triangles, T, as before, but the bonds between neighbouring

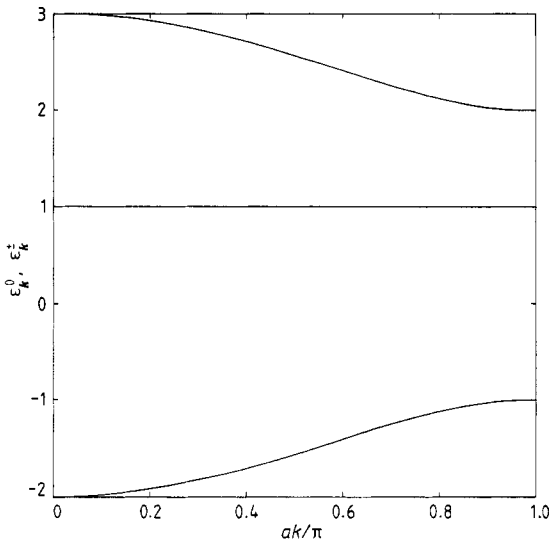

Figure 9. The band structure of the subspace defined by figures 7 and 8, which yields the Nagaoka ground state.

edge sites, B, are double counted in the first sum and compensated for by the second sum where S_4 and S_5 are two neighbouring edge sites making the bond B. The minimisation of this Hamiltonian is more sophisticated than before. Although it is clear that low spin is best for each triangle, a simultaneous choice of high spin for all bonds, B, is desirable. Unfortunately such a simultaneous choice is impossible in general and some triangles have high spin in the ground state.

There is a second way to write the Heisenberg Hamiltonian on this topology which allows a separation of degrees of freedom in an analogous way to the non-bonding separation for the hopping Hamiltonian. If we use 'j' to index the centre atoms and 'I' to index the nearest neighbour *pairs* of edge atoms then:

$$H_1 = \frac{J}{2}\sum_{\langle jI\rangle} \boldsymbol{S}_j \cdot \boldsymbol{S}_I + \frac{J}{2}\sum_I (\boldsymbol{S}_I \cdot \boldsymbol{S}_I - \tfrac{3}{2}) \tag{2.9}$$

where $\boldsymbol{S}_I = \boldsymbol{S}_4 + \boldsymbol{S}_5$ is the sum of the spins on the two relevant edge atoms. In this representation it is clear that $\boldsymbol{S}_I \cdot \boldsymbol{S}_I$ the total spin of *any* bond commutes with the Hamiltonian and as such is a conserved quantity and all such total spins can be used to label the excitation spectrum.

Singlet bond-spins effectively 'cut' the chain, and so the problem reduces to solving finite lengths of Heisenberg coupled spin chain with alternating spin magnitudes of one and a half. As the previous representation suggests, the Heisenberg energy is minimised with the edge bonds being spin one and so the ground state resides in the space where *all* edge bond spins are one. Unfortunately any linear chain of Heisenberg coupled spins is immensely difficult to solve, requiring the Bethe *ansatz*. The ground state is difficult to describe and involves *long range singlets* unlike any of the states so far considered.

Our final consideration in this section is the behaviour of the full t–J Hamiltonian in the presence of one free charge carrier on the topology of figure 5. For this case there are *three* relevant states to consider: the total spin singlet ground state to the Heisenberg

Hamiltonian with long range singlet correlations, the short range singlet state which is the ground state to the frustrated Nagaoka problem and the perfect ferromagnet which is the ground state to the non-frustrated Nagaoka problem. There are two competitions to consider and neither are exactly soluble. Firstly we have the competition between low spin states where the Heisenberg interactions prefer triplet edge bonds and the frustrated hopping prefers singlet edge bonds. Secondly we have the competition between the Heisenberg triplet edge-bond state and perfect ferromagnetism. Both of these problems are severely complicated by the fact that the Heisenberg ground state is difficult to describe. Although we have found the excitation spectrum of a hole in the two Nagaoka ground states, depicted in figures 6 and 9, we are unable to deduce the corresponding excitation spectrum for the Heisenberg ground state. These competitions will be considered approximately in the next section.

3. Polarons

3.1. The 'sawtooth' geometry

In this section we consider the full *t–J* model with one added charge carrier in an otherwise singly occupied 'sawtooth' topology. The frustrated case finds the short range singlet state of the last section for all values of t and J and we are considering the case of unfrustrated hopping in this section. Maintaining the positivity of our hopping matrix element, t, the frustrated hopping corresponds to an extra *hole* and the unfrustrated case, that we are moving onto, corresponds to an extra *particle*.

When J dominates, we expect the particle to be in the zone boundary state of the previous section at energy $E_0 + U - 2.0t$. This state has lost $1.2361t$ from the Nagaoka bound and clearly when t dominates J much of this hopping energy can be regained locally by converting Heisenberg correlations into Nagaoka correlations in the vicinity of the hole. Our task is to try to model the changeover and to find a reasonable description for the ground state when t starts to dominate.

In the absence of J, when t dominates, Nagaoka showed that ferromagnetism yields the ground state energy. In most topologies ferromagnetism is non-degenerate, but in our sawtooth topology the fact that neighbouring triangles are linked by a unique atom means that the non-frustrated Nagaoka ground state is multiply degenerate. If we consider figure 2 where the special spin is replaced by the hole, then the space of Nagaoka ground states finds all the depicted bonds as triplets. The hole always finds 'triplet triangles' and so sees ferromagnetism around *all* the closed loops in the topology. This satisfies the coherence restrictions of Nagaoka which only apply around closed loops. All the triplets can be chosen independently and so the degeneracy is huge, including states with all possible total spins, including total spin zero.

The Heisenberg interactions prefer a low total spin and in all our calculations we find that total spin zero always yields the ground state.

If we restrict attention to total spin zero then the first problem is to find a useful basis with which to describe the spin configurations. The separation into bonds depicted in figure 2 leads to a rather useful representation. We may label the states according to the total spin of each of these bonds. This splits the space into orthogonal subspaces and the size of each subspace is simply the number of total spin zero combinations which can be made out of the triplet bonds. If there are only a few triplet bonds then we find a 'degeneracy' of 1,0,1,1,3,6 states for 0,1,2,3,4,5 triplet bonds respectively. We will

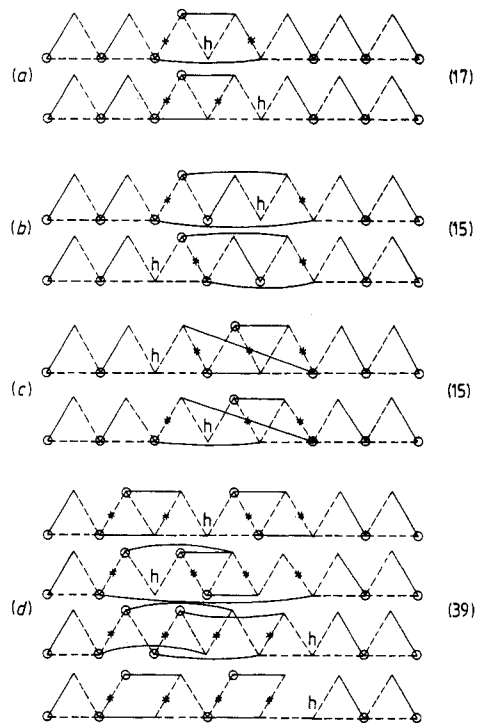

Figure 10. Representatives from the states which form our polaronic basis. The number of similar states included is given in parentheses and the labels (a–d) are used in figures 11 and 12. The character * on a bond denotes that the bond is triplet. This can be forced by taking the average of the two states with the relevant atoms interchanged. The lines with 'encircled' ends denote singlet bonds.

assume that only a few singlet bonds become triplet in our calculations and moreover that the triplet bonds are localised in the vicinity of the hole. Clearly these assumptions become unjustifiable when $t \gg J$ and the polaron becomes large, but the assumptions also break down when $J \gg t$ because we know that the Heisenberg excitations are fairly long range distortions.

When we allow the full t–J Hamiltonian to act on this basis then we find two disconnected subspaces. The subspace where all bonds are singlet is disconnected and yields the eigenstates of the previous section. Although the Nagaoka contribution respects the total spin of the bonds, the Heisenberg interactions do not and we find that the Hamiltonian connects all our other basis states to each other. This allows the possibility of *smooth* transitions where the average number of triplet bonds grows smoothly as J/t reduces and this is what we find with the one exception of the initial first order transition out of the subspace outlined in the previous section.

Our calculation is variational and we use a basis based on the states depicted in figure 10. The states depicted in figure 10 all have total spin zero and so are composed of linear sums of valence bond configurations. The total spin of any particular bond may be deduced by 'swapping' the two relevant particles over. Spin singlet bonds are anti-symmetric under interchange, whereas triplet bonds are symmetric under interchange. Bonds can be forced into local triplet configurations by taking the average of the initial

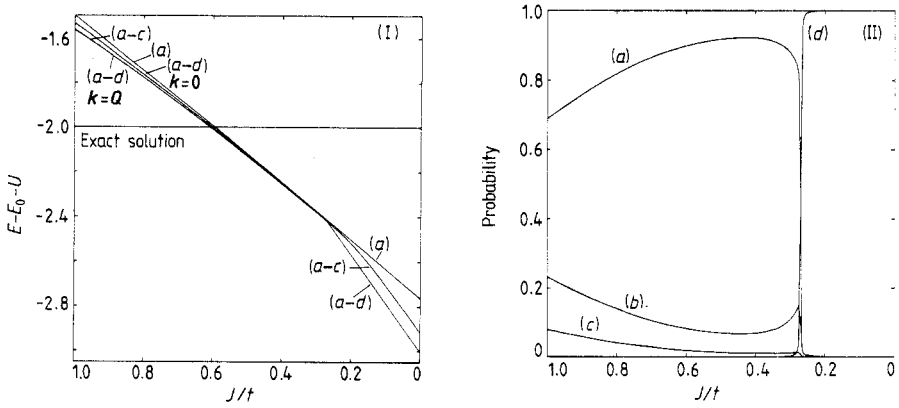

Figure 11. (I) The energies of some of our variational calculations. The basis states included in the calculation are denoted by the labels of figure 10. (II) The wavefunction distribution for the lowest energy state we have found. The curves denote the probability of finding the hole in the subspaces indicated in figure 10.

state together with the state where the relevant electrons making the bond are 'swapped' over. In figure 10, bonds which have been labelled * are to be considered symmetrised and therefore *triplet* bonds. The 'polaron' is delocalised with a chosen Bloch momentum and the *t–J* Hamiltonian projected into this subspace is diagonalised. The results are shown in figure 11.

Figure 11(I) shows the energies of the lowest lying states, for various sizes of basis. We also present calculations at the zone centre ($k = 0$) and antiferromagnetic zone boundary ($k = Q$) for the largest variational basis of eighty-six states. The zone boundary state is always lower in energy than the zone centre, as it is in the Heisenberg ground state. The ferromagnetic ground state requires uniform zone centre phase coherence but this behaviour is restricted to the *internal* symmetry of the polaron. The bandwidth of the lowest lying excitation can be deduced from the gap between the two relevant curves, and we find that the bandwidth is minute suggesting both that there is a spin configuration sympathetic to each different Bloch momentum and secondly that the polarons are very 'heavy'. A further way to understand the small bandwidths is to observe that the polarons are effectively localised, being tied to a sophisticated spin configuration in real space which only has a minor overlap with its neighbouring counterpart.

The predicted behaviour is straightforward. For $J > 0.6t$ we find that the Heisenberg ground state is relatively stable. As J is reduced below this value we predict a sharp transition into a polaron which is predominantly composed of the two-triplet states of figure 10(a). As J is further reduced, the polaron becomes *better* represented by the states of figure 10(a) as the Nagaoka contribution becomes more important. When J is reduced to about $0.4t$, the three triplet bond states of figure 10(b) start to become important and the hole starts to use these states to gain more hopping energy. Before these states take over, however, there is a fairly sharp transition into a larger polaron with *four* triplet bonds, at $J \sim 0.27t$. Studying the energies of figure 11(I) shows that if the variational states are restricted to the two and three triplet bond subspace, then the polaron would become three bonds wide only at the reduced energy of $J \sim 0.2t$. Closer inspection of the larger polaron shows that it is predominantly made out of states which

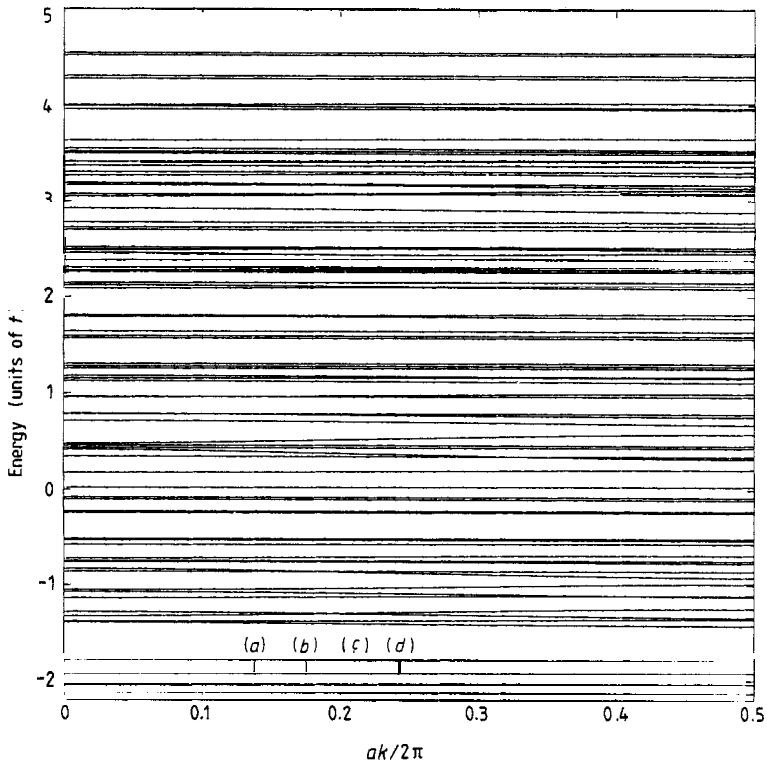

Figure 12. The bandstructure of our variational ground state at $J = 0.5t$. The dispersions are clearly narrower than either energy scale, since $t = 1$ and $J = 0.5$.

are connected by hopping to the first state in figure 10(d). These states are only very weakly connected to the states in the smaller polaron by the Heisenberg Hamiltonian, which explains the rather sharp transition.

In figure 11(II) we give a breakdown of the spin character of the polarons we find. The change in character between the two triplet bond polaron to the four triplet bond polaron is the striking feature.

Clearly our basis becomes an inadequate description for very small values of J/t, but it seems plausible that the polaron will grow in length in a rather 'jerky' way, being centred on states which firstly optimise the Heisenberg energy for a fixed number of triplet bonds and which secondly have a minute overlap with the corresponding states with less triplet bonds.

For the cases we have considered we find that *even* numbers of triplet bonds are preferred over odd numbers. One triplet bond involves a change of total spin, but it is not clear why three triplet bonds should be stepped over. We consider this a mystery and wonder whether five triplet bonds are ever stable.

Finally we present in figure 12(a) a 'band structure' for our calculation when $J = 0.5t$. The higher lying states are not particularly important but a careful analysis of the lowest four states shows them to have the character of the four states depicted in figure 10. The lowest lying branch is predominantly the two-triplet state. The next lowest lying branch is predominantly the *three* triplet state and the four-triplet state involved in the transition

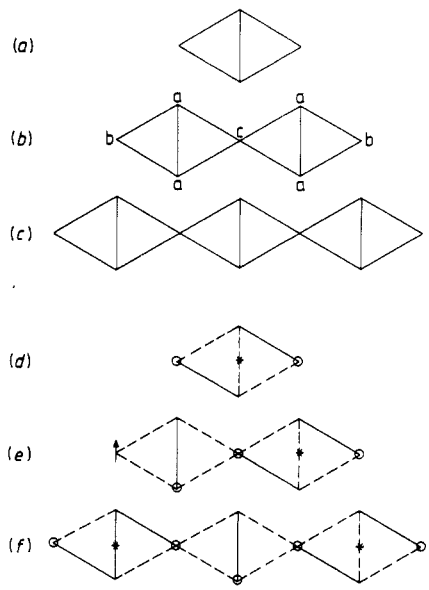

Figure 13. The clusters of 'diamonds' that we have performed calculations on. The atoms in figure 13(*b*) are annotated with labels used in figures 15 and 16. The lines with 'encircled' ends denote singlet bonds.

is only third lowest. The fourth lowest branch corresponds to the states where two triplets are separated by a singlet bond. The bandwidth of the excitations is related to neither the hopping nor the Heisenberg energy scales.

3.2. 'Diamond' geometry

The basic difficulty in studying this limit is the fact that the Heisenberg Hamiltonian is not exactly soluble. We therefore have to resort to cluster calculations and try to deduce the behaviour of the infinite chain as a limit.

Our first task is to analyse the ground state to the Heisenberg Hamiltonian. This will set the energy scale which the Nagaoka interactions need to dominate. We study the clusters depicted in figure 13. The smallest cluster is of interest since it achieves the lower bound suggested by (2.8) (viz $E_1 = (-7J/4)N_B$ since $N_T = 2N_B$) of $(-7J/4)$ with the state depicted in figure 13(*d*). The larger clusters yield energies of $-2.8815J$ and $-4.0692J$ respectively, which are quite far away from the lower bound. A comparison is achieved by measuring energies *per diamond* and we find contributions of $-1.75J$, $-1.4407J$ and $-1.3564J$ for the clusters of figure 13(*a–c*) respectively. This indicates that the probability of finding a high spin triangle is not negligible in the ground state. The situations where triangles have high spin *require* long singlet bonds and so we find a distribution of singlet bond lengths in this case unlike the previous cases where the ground states were describable in terms of nearest neighbour singlets. In fact states composed solely of nearest neighbour singlets are not far away in energy. The states depicted in figure 13(*d–f*) have energies $-1.75J$, $-2.5J$ and $-4.25J$ respectively, yielding $-1.75J$, $-1.25J$ and $-1.4167J$ *per diamond* respectively. Although at this small cluster level the state in figure 13(*f*) is actually the ground state, the infinite cluster limit yields $-1.25J$ per diamond which is easily beaten by the chain of high edge-bond spins. The fact that these local distortions are quite near in energy is an important consideration in interpreting our polaron results.

In contrast to the Heisenberg ground state we have the Nagaoka ground states. For the frustrated case we find the states where all the edge-bonds are singlets, as depicted in figure 7. This state is simultaneously an eigenstate of the Heisenberg Hamiltonian with energy $(-3J/4)N_B$. Each diamond loses about J when compared to the lower bound and about $0.6J$ when compared to the limit of the cluster calculations which we take to be the true ground state of the Heisenberg Hamiltonian. This then sets the energy scale for the frustrated competition, with bonds being turned from triplet into singlet if the gain in hopping energy is larger than $0.6J$.

The unfrustrated Nagaoka problem is once again quite subtle. Since each diamond is connected to its neighbours by a unique atom, again we find that Nagaoka ferromagnetism is degenerate. The ground states find one of the two triangles in each diamond with its maximum spin of three-halves; in fact the triangle furthest from the hole. With this choice the hole finds ferromagnetic diamonds and hence has Nagaoka phase coherence around *all* the closed topological loops, ensuring the ground state energy. The ground state degeneracy is the same as that found in a chain of independent spins of magnitude three-halves and chain length N_B. This includes states of very low spin and we find the state which is sympathetic to the Heisenberg interactions in the subspace with minimum total spin. Employing the representation of (2.8) yields a lower bound on the Heisenberg energy of $E_1 = (-J/4)N_B$, on the assumption that all the remaining triangles have the minimum possible spin. Although this bound is unobtainable in general, it does give a measure of the energy scale for the unfrustrated competition. The Nagaoka contribution from a diamond will turn the relevant triangle from low spin to high spin if the gain in hopping energy is larger than about $1.0J$.

So far we have considered the spin correlations well away from the hole, now we consider the hole itself. For the previous case of the sawtooth topology, although there were two distinct types of sites, even when $J \gg t$ the hole delocalised across all sites on an energy scale of t. This occurs because the Heisenberg contribution is equal on *all* sites on the sawtooth geometry. This is *not* true for the diamond geometry. When $J \gg t$ the Heisenberg energy on the diamond topology is maximised when the hole sits on the *bond* sites. The hole can still delocalise on the two atoms which constitute the bond, yielding a gain of t. For the frustrated case we find the hole in the non-bonding combination of orbitals whereas for the unfrustrated case the hole resides in the bonding combination. The 'reciprocal relationship' then ensures that if the hole moves on, the bond is left in a singlet or triplet respectively. For the frustrated case the hole *remains* localised in the vicinity of the singlet bond, which is a constant of the motion, but for the non-frustrated case the hole can freely delocalise.

We now move on to calculations involving the competition between Nagaoka and Heisenberg correlations. We perform ground state calculations for the full t–J Hamiltonian acting on a single charge carrier which is restricted to move in one of the finite clusters of figure 13(a, b).

The smallest cluster is particularly useful since it demonstrates the variety of possible spin correlations with a host of phase transitions. The frustrated case is straightforward and involves the two states depicted in figure 14(a). When $J \gg t$ the hole resides on the edge sites in the state $|1\rangle$ with the hole in the non-bonding orbital at energy $-J-t$. As the hopping is increased, the only effect is that the hole hybridises onto the central sites into the state $|2\rangle$, yielding an energy of $-2.3028t - 0.9097J$, a huge gain in hybridisation energy for a very modest loss of Heisenberg energy. The unfrustrated limit involves *two* phase transitions. When $J > 1.1t$, we find the hole in the state predominantly composed of $|\bar{1}\rangle$ with a small admixture of $|\bar{2}\rangle$, as depicted in figure 14(b). These states are completely

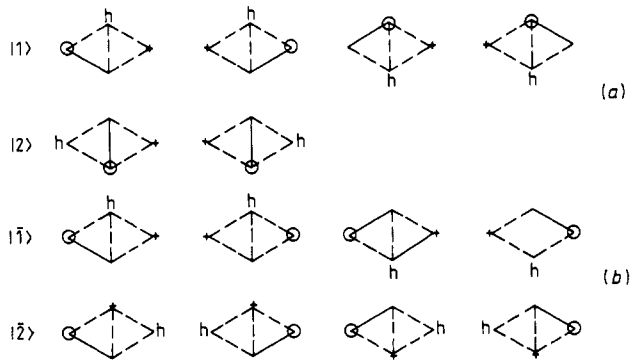

Figure 14. States which make up some of the ground states of the cluster of figure 13(*a*). The lines with 'encircled' ends denote singlet bonds.

analogous to the frustrated case, but with the bonding combination of orbitals. In the states $|1\rangle$ and $|\bar{1}\rangle$ the two bonds on the opposite side of the diamond from the hole have the highest probability of being singlet, being *three-quarters* each. This is perfect for the frustrated case but disastrous for the unfrustrated case. When $J < 1.1t$, the unfrustrated case evolves a new ground state which remains total spin half but finds the bonds opposite the hole with the lowest probability of being singlet, being *one quarter* each. When $J < 0.173t$ there is a final transition to the high spin state of Nagaoka.

The second cluster of figure 13 exhibits the basic physics to be expected in the frustrated limit. There are now two bonds and even in the limit $J \gg t$ one of the two bonds is implicitly singlet due to the reciprocal relationship. As J is reduced there is a sharp transition as the second bond is driven singlet. This transition occurs when $J = 0.48t$. We study the wavefunction in figure 15, giving the probabilities for the hole to sit on each of the possible atoms. When $J \gg t$ the tendency to sit on edge sites is observed and even quite close to the first order transition the hole still avoids the triplet bond. The transition can be associated with the hole 'spreading out' into the triplet region. The basic solution that is found for the frustrated limit is that the hole tends to move around in the region of the lattice with singlet edge bonds gaining optimum hybridisation in that region with minor loss in Heisenberg energy and simultaneously avoiding any region of triplet bonds where the Heisenberg energy is optimised until the energy gain is large enough to turn a bond from high to low total spin.

The unfrustrated limit for this cluster does not show the phase transitions of the smallest cluster although the changes in wavefunction are very similar. In figure 16 we picture the wavefunction, giving the probabilities for the hole to sit on each of the atoms, together with a breakdown of the spin correlations whilst the hole is restricted to lie on the edge bonds. When $J \gg t$ the hole sits on an edge bond on one of the diamonds while the other diamond is predominantly in the state depicted in figure 13(*d*). The hole cannot hybridise onto a '*b*-site' because the probability of leaving the edge-bond triplet is negligible. As the hopping is increased, firstly the diamond on which the hole sits becomes higher spin, marked by the possibility for the hole to visit the '*b*-sites', and the drop in probability for the state depicted in figure 13(*d*) to be found (curve marked (*a*1)). Finally at $J \simeq 0.1t$ both diamonds become high spin in a smooth but rapid transition. The whole system remains a total spin singlet. This is the basic physics of the unfrustrated

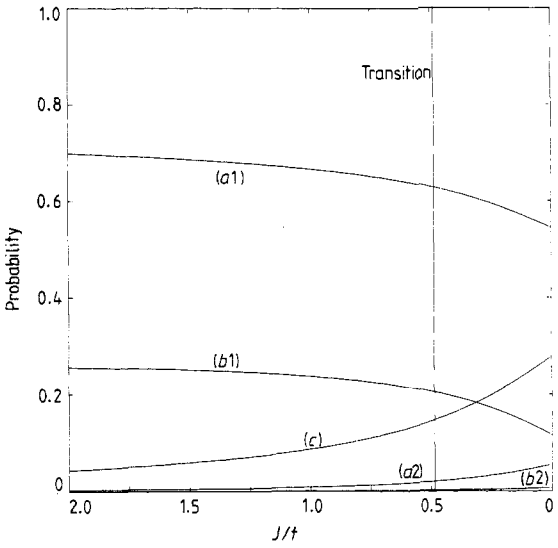

Figure 15. The wavefunction decomposition of the frustrated ground state to the cluster depicted in figure 13(*b*), when the ground state has one singlet and one triplet edge-bond. The labels denote the atoms, with '1' indicating the atoms by the singlet edge-bond and '2' indicating the atoms by the triplet edge-bond. The state is the ground state only to the left of the line labelled 'transition'.

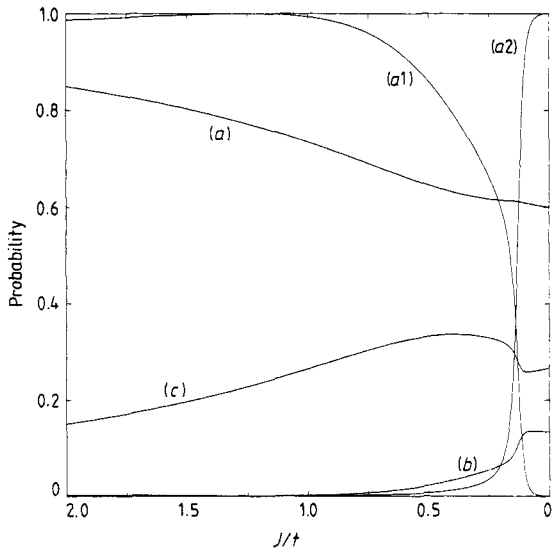

Figure 16. The wavefunction decomposition of the unfrustrated ground state to the cluster depicted in figure 13(*b*). The labels denote the atoms and the two curves marked (*a*1) and (*a*2) denote the probabilities that: (*a*1) the 'diamond' without the hole is in the state of figure 13(*d*); and (*a*2) the total spin of the triangle furthest from the hole is three halves *both given that the hole is on an edge-bond.*

limit. The hole turns neighbouring diamonds from low spin to high spin states, within the total spin zero subspace.

4. Conclusions

The major achievement in this article has been the construction of exact ground states to quantum mechanical Hamiltonians of interest in solid state physics.

We have studied two topologies; the 'sawtooth' and 'diamond' topologies. The ground state to the Heisenberg Hamiltonian has been found for the 'sawtooth' lattice whereas the 'diamond' topology has been shown to have the same ground state as an infinite chain of spins of alternating lengths one and one half, although this subsidiary problem has not been solved. The Nagaoka problem, where one charge moves around in an otherwise half filled infinitely strong coupling lattice, has been solved for both topologies. The 'sawtooth' lattice is completely unfrustrated by the state composed of nearest neighbour singlets and the 'diamond' lattice remains weakly frustrated in the ground state where all edge-bonds are nearest neighbour singlets.

We have also studied the full *t–J* model with the intention of constructing analytic 'spin polarons'. We have obtained variational states which we believe exhibit the basic physics, although our polaronic calculations are in no sense rigorous.

For the 'sawtooth' geometry we find that the Heisenberg and Nagaoka models are *simultaneously* soluble in the frustrated limit, but that there is a competition between low spin Heisenberg correlations and high spin Nagaoka correlations in the unfrustrated limit. We predict a sequence of changes in behaviour as a spin polaron forms and changes size. The hole destroys *pairs* of singlet bonds, replacing them with triplet bonds. Although locally we find high spin *loops*, the total spin remains low. The first transition is first order but the second transition is smooth but rapid.

For the 'diamond' geometry we find *two* distinct types of competition. In the frustrated limit we find a polaron which increases in size by discrete jumps. The lattice can be split into two regions; a region where the edge-bonds are singlet and the hole wanders around at will, and a region where the edge-bonds are triplet and the hole is very rarely found. There are a sequence of first order transitions as the hole extends the size of its domain by turning edge-bonds from triplet to singlet. In the unfrustrated limit we find a competition within the subspace where *all* edge-bonds are triplet. The Heisenberg interactions want low spin 'diamonds' and the Nagaoka interactions prefer high spin 'diamonds'. Once again we find polarons with smooth but rapid transitions between different behaviours. The hole turns neighbouring 'diamonds' from low to high spin in a sequence of smooth transitions.

We have found *concrete* examples of 'spin polarons'. The polarons are *very* heavy being essentially localised around their spin distortions. Transitions between polarons of different sizes are *very* rapid. The total spin of the system is a very poor measure of the characteristics of the polaron since the total spin remains zero while dramatic changes in behaviour occur. A careful study of local spin correlations is *required* if an understanding of the polaron is to be achieved.

What relevance do our results have to real materials and in particular to more reasonable topologies? The basic difference between the present geometries and higher dimensional examples are the number and variety of *loops*. The basic reason that the present cases are soluble is that the loops are all disconnected from each other and the correlations can be solved locally. In higher dimensions interpenetrating loops soon

destroy any hope of exact analysis, but what effects will they include? We believe that it is only necessary to consider small loops because in real materials the probability that a hole circuits a large loop *without* a Heisenberg-like interaction intervening is small. The larger loops can be expected to smooth out any changes in polaronic behaviour, but not to change the basic picture.

Polarons seem to be a useful concept for the study of the strong coupling Hubbard model.

Note added in proof. The competition between the two types of low energy state for the Heisenberg model on the diamond connectivity is not adequately resolved by our small cluster calculations and will be reexamined at a later date.

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