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## Two particles in the Hubbard model: topology versus Pauli exclusion

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**Abstract.** We solve the Hubbard model for the case of two particles on an arbitrary Bravais lattice exactly. Although the ground state is almost always a spin singlet, agreeing with the work of Kanamori, for topologically frustrated lattices with positive hopping matrix elements, we find that the ground state is a spin triplet. This topological effect is shown to be rather weak, and does not always survive the jump to finite densities in the thermodynamic limit, where Pauli exclusion strongly stabilises a low spin state. For the two-dimensional triangular lattice and the three-dimensional face-centred cubic lattice, the competition is fiercer and it is not clear whether the ferromagnetism survives.

### 1. Introduction

The Hubbard model is used to describe a variety of physical systems [1]. The reasoning is straightforward: it is probably the *simplest* model which purports to describe the competition between chemical bonding and short-range Coulomb interactions between particles. When chemical bonding dominates, the particles become effectively independent and may be described using a ‘single-particle’ description. The interest emerges in the opposite limit, when the short-range Coulomb interactions dominate. For this limit the particles may not be thought of as independent, and perform ‘correlated’ motion; namely doing rather different things in the absence of other particles than they would do when other particles are nearby. The basic character of a strongly correlated system can be very different to its weak-coupling counterpart, and the Hubbard model may be used to try to understand the physical explanations for these differences. This is our main motivation for studying the model.

The Hubbard model is conceptually very simple, having basically only two ‘parameters’; a dimensionless ratio, corresponding to the relative magnitudes of the energy scales of the bonding and the short-range Coulomb repulsion, and the number of electrons in the system. There is a second important consideration, however, and that is the topological connectivity of the atoms in the system. The effects of the connectivity will play a dominant role in the conclusions of our study.

The Hubbard model is very difficult to solve in general, but there are a few tractable limits. Weak coupling, when the bonding dominates, leads to a non-interacting electron gas and is therefore fairly well understood. Even for weak coupling, however, there are some surprises. For a bipartite lattice at half-filling, an

infinitesimal short-range Coulomb repulsion drives the system through a metal-insulator transition [2], a result which is not contained in the free electron description. Apart from this result and its analogues for non-bipartite connectivities, one should be fairly content with a nearly free electron description for the model. Strong-coupling, in comparison, is hardly understood at all. At half-filling, the model maps onto an insulating spin-half Heisenberg model [2], which is now believed to exhibit long range Neel order for most bipartite systems, even for the two-dimensional square lattice of current interest [3]. If the density is varied away from half-filling, the behaviour remains a mystery. For infinitely strong-coupling, when one hole is added to an otherwise half-filled system, Nagaoka demonstrated that, for bipartite systems, ferromagnetism is to be expected [4]. Whether or not this result survives the thermodynamic limit into a finite density of holes is still an open question [5]. The physical phenomena and interpretational problems encountered in the study of the Nagaoka problem are *precisely* analogous to those found in the limit of this article and so we will now spell out the basic ideas.

Firstly, topology plays an important role in Nagaoka's analysis and, for the case of antiferromagnetically frustrated topologies with positive hopping (namely bonding) matrix elements, ferromagnetism is *not* the ground state. We will show an analogous result for our limit, with frustrated topologies showing special behaviour. Secondly, in attempting to extend Nagaoka's result to finite densities, one encounters the effects of Fermi statistics and in particular Pauli exclusion. Electrons are fermions and this means that no two electrons can sit in the same quantum mechanical state. This fact then leads to the observation that two electrons with the same quantum numbers cannot get too close together and therefore suffer some form of 'effective repulsion'. For the Hubbard model, where it is assumed that there is only one state per atom, this effective repulsion corresponds to a restriction of at most one electron of each spin being allowed on any one atom at any one time. The Hubbard model involves an additional repulsion; the short-range Coulomb repulsion acting between pairs of electrons of opposite spins on the same atom. In the strong-coupling limit, it might naively be argued that since the content of both effects is to prohibit double occupancy of atoms, then the physical effects would be expected to be similar. This is in fact not true, and the Fermi statistics assumption involves the stronger constraint that the wavefunction should be antisymmetric under exchange of the two particles, which in turn leads to a 'stronger' repulsion in two and higher dimensions. This difference in behaviour, comparing the repulsions between parallel and antiparallel spins, will lead to the dominant complication in attempting to go to the thermodynamic limit in our analysis.

The limit that we tackle in this article is of two electrons in an otherwise empty Bravais lattice. We solve this problem for all relative strengths of the bonding and repulsion. Although the solution to this problem is unambiguous, we go on to show that taking the thermodynamic limit is probably an insurmountable problem and so in a very similar way to the Nagaoka result, it is not clear as to the meaning of our result.

The low-density limit of the Hubbard model has been previously studied by Kanamori [6], who used an approximate technique to deduce that paramagnetism is to be expected. There was no topological influence on his analysis and he found it difficult to predict ferromagnetism for Nickel, a system which, incidentally, has an antiferromagnetically frustrated structure; the face-centred cubic (FCC) lattice.

The Hubbard model has some innate symmetries, which can be used to deduce

the corresponding results for two holes in an otherwise full system. Mapping particles onto holes and vice versa is equivalent to changing the sign of the hopping matrix element, and so the behaviour of two holes can be deduced by studying two electrons in the system with the opposite sign matrix element. For bipartite lattices, there is a further symmetry, where the relative sign of the orbitals on the two natural sublattices is reversed, and this also changes the sign of hopping matrix element. Therefore the behaviour of two holes in an otherwise full bipartite system is identical to the behaviour of two electrons in an otherwise empty bipartite system.

In section 2 we solve the two-particle problem exactly and in section 3 we analyse a few small triangular lattice clusters, in order to try to deduce whether the solution extends to larger numbers of holes. In section 4 we look at an analytic ‘Gutzwiller’ approximation and show that the approximation ‘predicts’ the conjecture of this article. In section 5 we draw conclusions.

## 2. Two particles in an otherwise empty lattice

In this section we exactly solve the problem of the Hubbard model with two and only two electrons in an arbitrary Bravais lattice topology. Our motivation is twofold: firstly we would like to use the result in order to deduce the likely phase diagram of the Hubbard model when near empty, and secondly, for the strong-coupling limit, we would like to obtain a physical understanding of the topological phenomena which break the spin symmetry and stabilise the resulting coherence.

This problem has been tackled before, for finite but vanishingly small electron densities, with various techniques [6], but we believe that the natural dependence of the result on topology has been missed in these previous analyses. The reader is directed towards the book by Daniel Mattis [6] which is relevant and provides context for the present article. We will solve the simpler problem of two electrons in an otherwise empty lattice and leave the non-trivial problem of extending the result to finite densities to a later date.

The Hubbard model may be written down in real space as

$$H = - \sum_{ii'\sigma} t_{ii'} c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i c_{i\sigma}^\dagger c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}} c_{i\sigma} \quad (2.1)$$

where  $c_{i\sigma}^\dagger$  creates a particle of spin  $\sigma$  on site  $i$ , the short-range Coulomb repulsion is assumed to be onsite with strength  $U$ , and the hopping is often assumed to be between nearest-neighbours with strength  $t$ . The most interesting limit to this problem is the strong-coupling limit, where  $U \gg t$ , and we will pay particular attention to this limit by analysing the residual phenomena as  $U \mapsto \infty$ .

Although we expect the basic physical phenomena to be in real space, it transpires that the problem is more amenable to reciprocal space analysis, mainly due to the existence of Bloch’s theorem. In reciprocal space the Hubbard Hamiltonian may be rewritten as

$$H = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\mathbf{p}\mathbf{p}'} \sum_{\mathbf{G}} \delta_{\mathbf{k}+\mathbf{k}'-\mathbf{p}-\mathbf{p}'-\mathbf{G}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\bar{\sigma}}^\dagger c_{\mathbf{p}\bar{\sigma}} c_{\mathbf{p}'\sigma} \quad (2.2)$$

where  $c_{\mathbf{k}\sigma}^\dagger$  creates an electron in a Bloch orbital,  $N$  is the number of atoms, and  $\epsilon(\mathbf{k})$  is the single-particle spectrum, containing all the information about the hybridisation

connectivity. We are assuming one atom per unit cell in a periodic Bravais lattice. It is crucial to appreciate the dependence of our analysis on our choice of *periodic boundary conditions*. In the absence of periodicity, the corresponding loss of Bloch's theorem leads to technical complications of little interest to the physics. We will also assume a discrete set of points in reciprocal space in order to avoid problems with the 'thermodynamic limit'.

The analysis is *variational* in nature, but we include *all* possible variations and hence deduce the exact ground state. The most general two particle wavefunction with  $S_z = 0$  is

$$|\phi\rangle = \sum_{\mathbf{k}\mathbf{k}'} A_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow}^\dagger |0\rangle \quad (2.3)$$

where  $A_{\mathbf{k}\mathbf{k}'}$  is symmetric for singlet solutions and antisymmetric for triplet solutions. The  $A_{\mathbf{k}\mathbf{k}'}$  are complex parameters which we will determine variationally.

The variational energy is simply

$$\begin{aligned} E &= \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} \\ &= \left( \sum_{\mathbf{k}\mathbf{k}'} (\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}')) |A_{\mathbf{k}\mathbf{k}'}|^2 + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\mathbf{p}\mathbf{p}'} \sum_{\mathbf{G}} A_{\mathbf{k}\mathbf{k}'}^* \delta_{\mathbf{k}+\mathbf{k}'-\mathbf{p}-\mathbf{p}'-\mathbf{G}} A_{\mathbf{p}\mathbf{p}'} \right) \\ &\quad \times \left( \sum_{\mathbf{k}\mathbf{k}'} |A_{\mathbf{k}\mathbf{k}'}|^2 \right)^{-1} \end{aligned} \quad (2.4)$$

which is made stationary by the solutions to the Schrödinger equation

$$(\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}')) A_{\mathbf{k}\mathbf{k}'} + \frac{U}{N} \sum_{\mathbf{p}\mathbf{p}'} \sum_{\mathbf{G}} \delta_{\mathbf{k}+\mathbf{k}'-\mathbf{p}-\mathbf{p}'-\mathbf{G}} A_{\mathbf{p}\mathbf{p}'} = E A_{\mathbf{k}\mathbf{k}'}. \quad (2.5)$$

The triplet solutions to equation (2.5) do not involve  $U$ , due to Pauli exclusion and satisfy

$$E_T = \epsilon(\mathbf{k}) + \epsilon(\mathbf{k}') \quad (2.6)$$

where  $\mathbf{k} \neq \mathbf{k}'$ , whereas the singlet solutions are more sophisticated and for the non-vanishing combination

$$A(\mathbf{q}) = \sum_{\mathbf{p}\mathbf{p}'} \sum_{\mathbf{G}} \delta_{\mathbf{q}-\mathbf{p}-\mathbf{p}'-\mathbf{G}} A_{\mathbf{p}\mathbf{p}'} \quad (2.7)$$

the spectrum satisfies

$$1 = \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\mathbf{G}} \delta_{\mathbf{q}-\mathbf{k}-\mathbf{k}'-\mathbf{G}} [E_S - \epsilon(\mathbf{k}) - \epsilon(\mathbf{k}')]^{-1}. \quad (2.8)$$

The remainder of the problem is simply to deduce whether the ground state energy is contained in the solutions of equations (2.8) or (2.6).

In order to investigate this formalism, we solve the square and triangular loops with nearest-neighbour hopping in the next two subsections, before moving on to deduce the lattice result.

### 2.1. The square loop

The square loop with periodic boundary conditions has four  $\mathbf{k}$ -points, with single-particle energies;  $-2t, 0, 2t, 0$ . The two-particle triplet states are sums of single-particle energies and take the values;  $-2t, 0, 2t$ , since from Pauli exclusion, each state may only be singly occupied. The lowest energy state is therefore at  $-2t$ .

For the singlet states, we find the lowest energy at  $\mathbf{q} = 0$ , for which equation (2.8) reduces to

$$1 = \frac{U}{4} \left( \frac{1}{E_S + 4t} + \frac{1}{E_S - 4t} + \frac{2}{E_S} \right) = \frac{U(E_S^2 - 8t^2)}{E_S(E_S^2 - 16t^2)}. \quad (2.9)$$

This equation always contains the ground state, which ranges from  $E_S \mapsto -4t + U/4$  in the weak-coupling limit to  $E_S \mapsto -2\sqrt{2}t - 4t^2/U$  in the strong-coupling limit. Solving the two-particle problem directly shows that these results are correct.

Particle-hole symmetry, applied to the Hubbard model, ensures that the similar problem of two holes in an otherwise full system can be modelled by changing the sign of the hopping matrix element,  $t$ . For the square, the topology is bipartite, and this ensures that the physics is identical for either sign of the hopping matrix element. Considered together, these two symmetries show that two holes in an otherwise full system behave in an identical fashion to two particles in an otherwise empty bipartite lattice.

One quite crucial observation is that even in the limit  $U \mapsto \infty$ , the singlet is the ground state by a huge energy margin. Naively one might suppose that kinetic exchange [7] would be the dominant physical effect in this limit, stabilising the singlet on a  $t^2/U$  energy scale. This turns out to be a very weak effect, being dominated by a topological contribution on the  $t$  energy scale. We will return to this point in subsection 2.6.

### 2.2. The triangular loop

The triangular loop with periodic boundary conditions has three  $\mathbf{k}$ -points, with single-particle energies;  $-2t, t, t$ . The two-particle triplet states are sums of single-particle energies and take the values;  $-t, 2t$ . The lowest energy state is at  $-t$ .

For the singlet states, once again the lowest energy resides at  $\mathbf{q} = 0$ , where

$$1 = \frac{U}{3} \left( \frac{1}{E_S + 4t} + \frac{2}{E_S - 2t} \right) = \frac{U(E_S + 2t)}{(E_S + 4t)(E_S - 2t)}. \quad (2.10)$$

This equation always contains the ground state, which ranges from  $E_S \mapsto -4t + U/3$  in weak coupling to  $E_S \mapsto -2t - 8t^2/U$  in strong-coupling. These results are easily directly proved to be correct.

For the triangle, although the particle-hole symmetry is still relevant, the topology is *not* bipartite. This introduces a complication which *reverses* the result found near empty. If we change the sign of the hopping matrix element, using  $-t \mapsto s > 0$ , then the best triplet solution resides at  $-2s$ . The best paramagnetic solution now has a non-zero Bloch momentum and satisfies

$$1 = \frac{U}{3} \left( \frac{2}{E_S - s} + \frac{1}{E_S + 2s} \right) = \frac{U(E_S + s)}{(E_S - s)(E_S + 2s)}. \quad (2.11)$$

The lowest energy solution ranges over  $E_S = -2s + U/3$  in weak coupling to  $E_S = -s - 2s^2/U$  in strong-coupling. The ground state is a triplet.

Once again, it is instructive to observe that even in the limit  $U \mapsto \infty$ , the ground states are strongly stabilised by purely topological effects.

### 2.3. The lattice

In this section we consider the problem for the lattice and show the result that: for a lattice whose single-particle ground state has only spin degeneracy, the interacting two-particle ground state is necessarily singlet, whereas for a lattice whose single-particle ground state has non-trivial degeneracy, the interacting two-particle ground state is necessarily triplet. This result picks out topologically frustrated lattices for special treatment. Frustrated lattices with positive hopping matrix elements are expected to have triplet ground states, while all other lattices are expected to have singlet ground states.

To prove this result, we observe that the lowest energy singlet to equation (2.8) is likely to have zero total Bloch momentum, and so we define the function

$$F(E) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E - 2\epsilon(\mathbf{k})} \quad (2.12)$$

which comes from equation (2.8) evaluated at  $\mathbf{q} = 0$ , and we have used the fact that the Bravais lattice has inversion symmetry. The singlet spectrum is found when  $F(E) = 1/U$ . The position of the energy of the lowest energy solution may be deduced by thinking about the analytic structure of this function. For the case where the single-particle ground state has only spin degeneracy, there is a unique minimum single-particle energy,  $\epsilon(\mathbf{k}_0)$  say. If we call the next lowest single-particle energy  $\epsilon(\mathbf{k}_1)$ , then the lowest triplet state is at energy  $E_T = \epsilon(\mathbf{k}_0) + \epsilon(\mathbf{k}_1)$ . For  $E < 2\epsilon(\mathbf{k}_0)$  the function  $F(E)$  is negative and for the repulsive Hubbard model there can be no solution to  $F(E) = 1/U$ . For  $2\epsilon(\mathbf{k}_0) < E < 2\epsilon(\mathbf{k}_1)$ , the function  $F(E)$  ranges continuously over all real values, starting at  $+\infty$  and ending at  $-\infty$ . There is clearly a singlet solution somewhere in this region. Let us now consider the value of

$$F(E_T) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\epsilon(\mathbf{k}_0) + \epsilon(\mathbf{k}_1) - 2\epsilon(\mathbf{k})}. \quad (2.13)$$

The first term in this sum is positive and all the subsequent terms are negative. The crucial observation is that the positive term which occurs at  $\mathbf{k}_0$  is *exactly* cancelled by the term which occurs at  $\mathbf{k}_1$ , and so  $F(E_T) < 0$ . This in turn implies that the singlet solution must have occurred at a lower energy, and is consequently relatively stable. The ground state for this case is therefore necessarily a singlet.

Conversely, for the case where there is a non-trivial degeneracy to the ground state of the single particle spectrum, at  $\mathbf{p}_0$  and  $\mathbf{p}_1$  say, then the lowest energy triplet state is  $E_T = \epsilon(\mathbf{p}_0) + \epsilon(\mathbf{p}_1) = 2\epsilon(\mathbf{p}_0)$ . If we reconsider  $F(E)$  for this case, then it remains true that for  $E < 2\epsilon(\mathbf{p}_0)$ , then  $F(E) < 0$ . For this case we must also consider non-zero momenta, but again there are no singlet solutions below  $E_T$ , since  $\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}') > 2\epsilon(\mathbf{p}_0) = E_T$  for all  $\mathbf{k}$  and  $\mathbf{k}'$ . Therefore, there is certainly no singlet solution at a lower energy than the triplet solution. If the function  $F(E)$  is analytic, then it is also clear that there must be a finite energy gap between the triplet ground state and the lowest energy singlet state when  $F(E) = 1/U$ , provided that the repulsion  $U$  is non-vanishing.

The theorem is therefore ‘if and only if’, with only pathological exceptions.

### 2.4. Possible consequences

In this subsection we consider the likely consequences of our result for the Hubbard model on various simple lattices. For bipartite lattices we predict, along with

Kanamori [6], that the phase diagram should yield paramagnetism at low concentrations for *all* values of  $t/U$ . This result is then applicable to the square lattice model of current interest in the study of the perovskite superconductors.

For frustrated lattices, such as the triangular lattice or FCC lattice, one might expect ferromagnetism at low concentrations, when the hopping matrix element has the relevant sign (namely usually for low concentrations of holes). This is a possible explanation for Kanamori's inability to understand ferromagnetic Nickel, because his model predicted paramagnetism whatever the lattice structure, and Nickel crystallizes with a FCC structure which is topologically frustrated. Unfortunately, the extension of our results across the thermodynamic limit is non-trivial as we shall show in the next subsection.

### 2.5. Dimensionality and the thermodynamic limit

In this subsection we consider the energy scale on which the Hubbard repulsion modifies the total energy, and in particular the dependence on dimensionality. We will restrict attention to the singlet ground state and approximately solve equation (2.8).

If we rewrite the two-particle energy as  $E_S = 2\epsilon(0)[1 - \Delta]$ , where  $\Delta$  is the dimensionless correction to the non-interacting problem, then equation (2.8) becomes

$$\Delta = \frac{1}{N} \left( -\frac{2\epsilon(0)}{U} + \frac{1}{N} \sum_{\mathbf{k} \neq 0} \frac{1}{1 - \Delta - \gamma_{\mathbf{k}}} \right)^{-1} \quad (2.14)$$

where  $\gamma_{\mathbf{k}} = \epsilon(\mathbf{k})/\epsilon(0)$  is the structure factor of the lattice which has been normalized to unity.

The problem has then been reduced to deducing the characteristics of the quantity

$$G(N) = \frac{1}{N} \sum_{\mathbf{k} \neq 0} \frac{1}{1 - \Delta - \gamma_{\mathbf{k}}} \quad (2.15)$$

as a function of system size. If we assume that the contribution from  $\Delta$  is vanishingly small, and take the continuum limit with a 'cut off' corresponding to  $\mathbf{k} \neq 0$ , then

$$G(N) \mapsto \int_{\text{BZ}} \frac{d^d \mathbf{k}}{V(\text{BZ})} \frac{1}{1 - \gamma_{\mathbf{k}}} \sim \text{constant} \times \int_{\alpha N^{-1/d}}^{\beta} \frac{k^{d-1} dk}{k^2} \quad (2.16)$$

and so in three dimensions  $G(N)$  becomes constant while in two dimensions  $G(N)$  diverges logarithmically

$$\Delta = \frac{\alpha_3}{N} \quad \text{for } d = 3 \quad (2.17a)$$

$$\Delta = \frac{\alpha_2}{N \ln N} \quad \text{for } d = 2 \quad (2.17b)$$

It is now clear that the assumption that the contribution from  $\Delta$  in evaluating  $G(N)$  should be vanishingly small is confirmed.

The most important consequence of these results, is that as the system size is scaled up, the energy loss induced by the repulsion is quite different for a singlet pair in comparison to a triplet pair. The corresponding result for a triplet pair is  $\Delta \sim \alpha N^{-2/d}$ , which arises from the form of  $\gamma_{\mathbf{k}}$  at small  $\mathbf{k}$ . For both two and three



dimensions, the loss in energy for the singlet becomes vanishingly small in comparison to the loss in energy for the triplet as the system size diverges. This type of result is the main reason for suggesting that the two-particle result may not survive the thermodynamic limit.

Further insight into this problem may be obtained by considering finite numbers of particles in a system with diverging system size. Treating the non-interacting singlet solution as the starting point and employing a Gutzwiller variational *ansatz* [9], leads immediately to the result that the energy density correction to the non-interacting energy is of order  $1/N$  and decays as the inverse system volume. Since the corresponding difference in the non-interacting energy density versus ferromagnetic energy density is of order  $1/N^{2/d}$ , for three dimensions the low spin solution must win. For two dimensions the argument is inconclusive, although this may merely suggest that a Gutzwiller *ansatz* is an overestimate of the energy loss, as it is for the two-particle case where the logarithmic dependence is lost. We have a brief look at triangular clusters in section 3, in order to try to discover whether the two-particle result extends to three particles in two dimensions. We also employ an analytic Gutzwiller *ansatz* for all electron densities in section 4, which gives further evidence for the likely phase diagram.

As well as the two-dimensional triangular lattice, the result for the FCC lattice is also inconclusive. This is because the density of states for the FCC lattice shows low-dimensional behaviour, since the relevant states may be restricted to lie in one  $xy$  plane with no corresponding loss in hopping energy. Although the observation that the relevant ground state degeneracy is one-dimensional suggests that the behaviour should mimic two dimensions, in fact the reciprocal-space points corresponding to type I antiferromagnetism, namely  $(2\pi/a)(1, 0, 0)$ ,  $(2\pi/a)(0, 1, 0)$  and  $(2\pi/a)(0, 0, 1)$ , lead to special van Hove singularities yielding a square root divergence and pseudo-one-dimensional behaviour. The topological effects are immensely strong for the FCC lattice.

For the two antiferromagnetically frustrated lattices of most physical interest, the strength of the topological contribution is comparable with that of the Pauli exclusion contribution.

### 2.6. A simple explanation

We conclude this section with a simple explanation for why non-frustrated systems might be expected to have singlet ground states. Similar conceptual pictures appear in the work of Shastry *et al* [5].

For nearest-neighbour hopping, the kinetic energy may be thought of as analogous to the Laplacian in the continuum, for which the ground state has uniform phase. Even considering the two-particle problem as a one-particle problem in a higher-dimensional space, this analogy still holds. In this larger representation, the Hubbard interaction acts as a potential barrier along the 'leading diagonal'. The stability of the singlet state may be considered to correspond to the fact that 'nodes cost kinetic energy'. The ground state is expected to maintain uniform phase in real space and, therefore, to correspond to the singlet spin configuration.

For frustrated lattices this argument breaks down. Instead of minimising the Laplacian one is maximising the Laplacian. In terms of 'nodes', one is attempting to introduce as many as possible into the wavefunction. There is no guarantee that all these nodes should be restricted to real space, and introducing some 'nodes' into the

spin wavefunction in conjunction with the spatial wave function cannot be ruled out. Our triplet ground states are a concrete manifestation of this effect.

The strong-coupling limit with  $U = \infty$  deserves special consideration. There is still a very strong stabilising effect, which arises purely from the relationship between Fermi statistics and topology. Only when the two particles are nearby can the Hubbard interaction be felt, and so we would quite naturally expect to find a local manifestation of the phenomenon. Indeed, the single-loop analyses of subsections 2.3 and 2.4 contain the effect, and may be used to motivate an understanding of the mechanism. When  $U = \infty$ , the only residual ‘interaction’ between the particles, is the interference between the different phases when the particles are interchanged. The behaviour of two particles on small loops directly leads to this interference between motion and statistics. The lowest order interchange occurs when a particle is taken once around a loop on which the second particle sits. When we allow the hopping phase to be optimised, then the resulting superposition of the states with or without interchange interferes constructively for the ground state spin symmetry and destructively for the other spin state. This might then be expected to be the dominant process in the strong-coupling limit. The results of subsections 2.3 and 2.4 are perfectly consistent with the predictions for the two-dimensional square and triangular lattices respectively, and may be used, in a convoluted fashion, to give a prediction for the energy scale on which the magnetic coherence is stabilised, in terms of the probability of finding pairs of delocalised particles on the same loop.

### 3. The triangular lattice

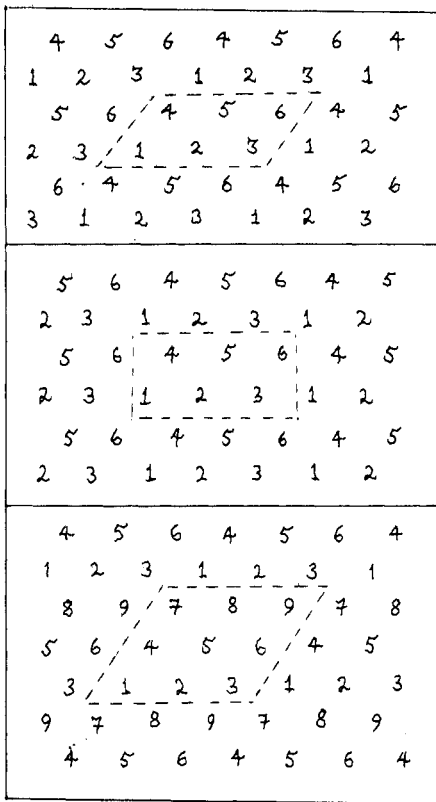
Perhaps the simplest antiferromagnetically frustrated topology is the two-dimensional triangular lattice with positive nearest-neighbour hopping matrix elements. The result of the last section suggests that the ground state for two electrons hopping around in an otherwise empty triangular lattice would be a spin-triplet state. The ground state for this particular lattice is in fact unique and can be written down in both real and reciprocal space

$$c_{\mathbf{Q}\uparrow}^\dagger c_{-\mathbf{Q}\uparrow}^\dagger |0\rangle = \frac{i\sqrt{3}}{N} \left( \sum_{i_1 i_2} c_{i_1\uparrow}^\dagger c_{i_2\uparrow}^\dagger + \sum_{i_2 i_3} c_{i_2\uparrow}^\dagger c_{i_3\uparrow}^\dagger + \sum_{i_3 i_1} c_{i_3\uparrow}^\dagger c_{i_1\uparrow}^\dagger \right) |0\rangle \quad (3.1)$$

where  $i_1$ ,  $i_2$  and  $i_3$  are labels which run over the three natural real-space sublattices respectively, and where  $\pm\mathbf{Q}$  correspond to the two degenerate minima of the single-particle non-interacting excitation spectrum. The ground state energy is  $-6t$ , which can be readily understood from the real-space representation. In each real-space configuration, both particles take full advantage of the hops onto the unique unoccupied sublattice, with all other hops cancelling out. This then constitutes an idea applicable to smaller clusters, which may also be split up into three sublattices. In practice, we have always found this state (with zero probability of finding both particles on the same sublattice and with unique ‘chirality’ but appropriate real-space weighting) constitutes the triplet ground state of clusters with free boundary conditions.

The main motivation for studying small clusters of atoms, is to try to find counter-examples opposing an attempt at extending the two-particle theorem to a three-particle theorem. In the non-interacting limit, there is no hope of extending the theorem to higher densities, since the ground state is paramagnetic. However, for

the strong-coupling limit, the Nagaoka problem near half-filling also predicts ferromagnetism and so it is quite natural to conjecture that ferromagnetism persists all the way from two particles in an otherwise empty lattice to one hole in an otherwise half-filled lattice.



**Figure 1.** The chosen clusters for our exact diagonalisation calculations. The numbers denote the sublattice on which the relevant atom lies, and the unit cells have been marked. The ground state energies for the second two choices are presented in table 1.

Since we have a theorem for two particles and a theorem for  $N - 1$  particles, the first non-trivial test cluster involves at least *five* atoms. Five atoms is particularly unappealing for triangular connectivity, and so we have elected to calculate with the two six-atom periodic clusters depicted in figure 1. The single-particle spectrum of the first cluster is very degenerate, with one state at  $6t$ , two states at zero energy and the other three states are all degenerate at  $-2t$ . For this case it is immediate that ferromagnetism is the ground state for three electrons, since all three electrons may be included with the unfrustrated bound. For the second cluster the situation is less clear, since the single-particle spectrum now is one state at  $6t$ , two states at  $t$ , one state at  $-2t$  and two degenerate ground states at  $-3t$ . Although the first two electrons will necessarily be in a relative triplet, the third electron does not achieve the unfrustrated bound, and loses a full hop due to the effects of Pauli exclusion. In fact, an exact solution of the strong-coupling three-particle problem demonstrates that the ground state is indeed ferromagnetic, with a gap of  $0.6974t$  to the lowest-lying total spin-half

state. At this rather small size of cluster, the ferromagnetism seems to remain stable, supporting the conjecture that ferromagnetism remains at all doping concentrations up to half-filling. Moving on to four particles produces a surprise. Even though all other concentrations below half band-filling yield a ferromagnetic ground state, four particles have a total spin-singlet ground state, and further there is a spin-1 excitation below the lowest ferromagnetic solution. Cluster calculations are clearly not enough to deduce any general trends at this order.

**Table 1.** The results from our exact diagonalisation of the clusters depicted in figure 1. The results marked (†) agree with our conjecture and those marked (\*) disagree with our conjecture.

Six-particle cluster (positive matrix elements)					
Particle number	Total spin	Lowest energy	Second lowest energy	Second highest energy	Highest energy
1	1/2	-3.0000	-2.0000	1.0000	6.0000
2	1	-6.0000(†)	-5.0000	4.0000	7.0000
2	0	-4.9018	-4.7791	3.6056	9.8036(†)
3	3/2	-8.0000(†)	-5.0000	5.0000	8.0000
3	1/2	-7.3026	-6.1200	6.8941	8.9227(†)
4	2	-7.0000	-4.0000	5.0000	6.0000
4	1	-7.6146	-6.8133	6.1849	7.5202(*)
4	0	-8.1693(*)	-5.7856	6.6559	7.0891
5	5/2	-6.0000(†)	-1.0000	2.0000	3.0000
5	3/2	-5.3324	-5.0000	4.0000	4.5616
5	1/2	-4.6814	-4.6765	3.8173	4.7030(†)
Nine-atom cluster (positive matrix elements)					
1	1/2	-3.0000	+0.0000	0.0000	6.0000
2	1	-6.0000(†)	-3.0000	3.0000	6.0000
2	0	-5.2749	-4.5498	4.3723	10.5498(†)
3	3/2	-6.0000	-3.0000	3.0000	6.0000
3	1/2	-7.5747(*)	-5.5027	7.2468	9.7163(†)

For the present investigation, there is a competition between a topological effect which prefers ferromagnetic order and Pauli exclusion which naively prefers a total spin singlet. If we consider the infinitely strong-coupling triangular lattice Hubbard model with the opposite sign of matrix element, then the two effects should be in accord rather than in conflict. Analysis of the second six-atom cluster of figure 1, supports this idea, although once again the four-particle problem yields an unexpected spin-1 ground state. The relevant ground state energies are detailed in table 1.

The two six-atom clusters yield a ferromagnetic ground state at the three particle level. This fact suggests that there might be a general result at the three-particle level for periodic boundary conditions. The nine-atom cluster of figure 1 immediately eliminates any hope of this. Although the two-particle problem yields ferromagnetism, an additional particle involves a loss of  $3t$  from the non-interacting bound, and this Pauli-induced loss is much greater than the best low-spin result, which is the three-particle ground state by a full  $1.5747t$ . The only hope of demonstrating the conjecture

that the infinitely strong-coupling triangular lattice is ferromagnetic for all fillings below half-filling and paramagnetic for all dopings above half-filling, seems to reside in ‘finite-size scaling’ simulations and even then seems beyond present-day computers.

Another question one can address with these small cluster calculations is whether or not the boundary conditions are important. In order to tackle this question, we have studied the seven-site cluster of a ring of six atoms and one central atom, with free boundary conditions. This cluster has been analysed previously [8]; it shows varied behaviour. Although the two theorems are found to be true at strong-coupling, the two-electron system exhibits a low-spin ground state as the Hubbard repulsion is reduced. The reason is simple, the free boundary conditions break the single-particle degeneracy of the ground state, and so the theorem applies but the frustration is lost. Extending the strong-coupling problem to three particles produces a further surprise, because the three-particle ground state is found to be low spin at  $-4.9262t$  in comparison with the best high-spin energy of  $-4.6458t$ . We believe that only periodic boundary conditions should be studied, because the ‘chiral’ degeneracy remains, and this is the crucial manifestation of topological frustration.

#### 4. An analytic Gutzwiller treatment

Although some quite special limits of the Hubbard model are amenable to exact analysis, *most are not*. The present article treats two particles in an otherwise empty lattice, and the case of one charge carrier in an otherwise half-filled *strong-coupling* Hubbard model constitutes the Nagaoka problem [4]. Even the Nagaoka problem is only soluble on a restricted class of topologies. Although a little is now known about the physical phenomena that are present in these special situations, attempts to extend the ideas to finite concentrations of holes have been unsuccessful. In this section, we will look at one technique that does allow general concentrations of electrons.

One technique which yields an estimate for the total energy for all electron densities in the strong-coupling limit, is the ‘Gutzwiller approximation’ [9]. Although magnetic correlations are ignored, the dominant contribution from the restriction of single occupancy to each site is achieved, in principle. In our limit, the Gutzwiller *ansatz* involves projecting out all states with doubly occupied atoms from the non-interacting solution. As described, the *ansatz* would yield a variational estimate for a paramagnetic state, which could then be used to prove that a competitive state is unstable. In practice, however, an application of the *ansatz* is analytically too difficult and most calculations involve uncontrolled approximations which go under the name ‘cluster approximations’. We will perform such a ‘cluster approximation’ and thereby give up hope of any rigorous conclusions. Our calculation should simply be considered as indicative. When the ‘cluster approximations’ are compared directly with exact results, the calculated energies are found to be within 20% and as such yield a viable indication of relative stability of different phases in clear-cut situations. Some numerical results employing the real Gutzwiller wavefunction may be found in the work of Schiba [9].

We employ the simple scheme of Razafimandimby [9] in the limit where the Hubbard constant diverges, namely  $U \mapsto \infty$ , and the doubly occupied sites are assumed to be absent. The Gutzwiller approximation to the total energy is simply

$$E_G = -2Ztn_1(1 - 2n_0)(1 - n_0) \frac{[(1 - n_0)^2 - n_1^2]}{[(1 - n_0)^4 + n_1^4]} \quad (4.1)$$

where  $Z$  is the coordination number of the lattice and

$$n_0 = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle_n = \frac{1}{N} \sum_{\epsilon(\mathbf{k}) < \epsilon(\mathbf{k}_n)} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle_n \quad (4.2a)$$

$$n_1 = \langle c_{i\sigma}^\dagger c_{i'\sigma} \rangle_n = \frac{1}{N} \sum_{\epsilon(\mathbf{k}) < \epsilon(\mathbf{k}_n)} \exp[i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_{i'})] \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle_n \quad (4.2b)$$

are the on-site and nearest-neighbour single-particle correlation functions evaluated in the non-interacting paramagnetic ground state.

We compare this Gutzwiller energy with the energy of the saturated ferromagnet

$$E_F = -Ztn_2 \quad (4.3)$$

where

$$n_2 = \sum_{\sigma} \langle c_{i\sigma}^\dagger c_{i'\sigma} \rangle_F = \frac{1}{N} \sum_{\epsilon(\mathbf{k}) < \epsilon(\mathbf{k}_F)} \exp[i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_{i'})] \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle_F \quad (4.4)$$

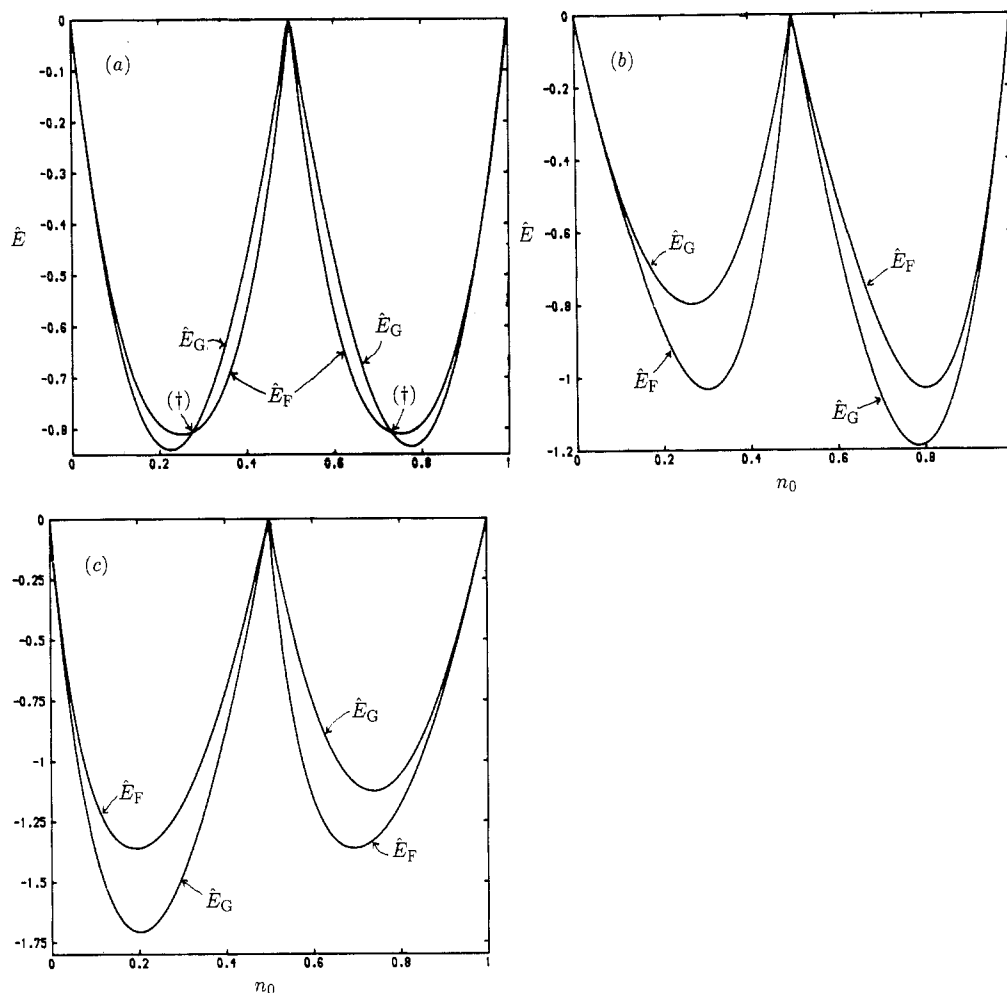
is the nearest-neighbour single-particle correlation function evaluated in the ferromagnetic state with the same particle density as in the paramagnetic state but with a different Fermi surface, surrounding twice as many particles.

In figure 2 we compare the Gutzwiller energy with the energy of the saturated ferromagnet for the square, the triangular and the FCC lattices.

The result is in perfect agreement with our strong-coupling conjectures. The square lattice shows Kanamori paramagnetism near empty, transiting at about  $n_0 = 0.275$  to Nagaoka ferromagnetism, which is relatively stable up to half-filling. For concentrations above half-filling, particle-hole symmetry implies a corresponding transition near  $n_0 = 0.725$ . The triangular lattice shows ferromagnetism below half-filling and paramagnetism above half-filling for our choice of a positive hopping matrix element. The FCC lattice shows paramagnetism below half-filling and ferromagnetism above half filling for our choice of a negative hopping matrix element.

More 'accurate' determinations of the paramagnetic to ferromagnetic phase transitions have been published [9], but this is always accepting that such behaviour is real [5].

The dimensional dependence alluded to in section 2, is predicted by this technique. In the low-density limit, there is a dull contribution to both calculations coming from the fact that  $\epsilon(0) \neq 0$ . This leads to a contribution  $\hat{E} = -2Ztn_0$ , together with degeneracy breaking corrections of higher order. There are two types of corrections: firstly a term coming from the low-energy dispersion of the energy bands, which contributes to both states in different ways, and secondly the Gutzwiller correction to the non-interacting paramagnetic energy. The first contribution can be directly attributed to Pauli exclusion and therefore always favours the paramagnetic state. If the low-energy Bloch dependence is quadratic, then this contribution scales as  $n_0^{(d+2)/d}$ . The second contribution is only applicable for the paramagnetic phase and corresponds to the effects of the Hubbard repulsion and therefore favours the ferromagnetic state. Expanding (4.1) shows that this contribution scales as  $n_0^2$ . For three dimensions the Pauli exclusion argument clearly dominates, whereas for two dimensions we have the limiting case. The two contributions are comparable and their relative sizes must be studied for each case independently, as we have done in this section. The FCC lattice corresponds to one pseudo-dimension and ferromagnetism always wins in one dimension, although this result should be viewed as a breakdown of the Gutzwiller approximation for the true one-dimensional chain.



**Figure 2.** A comparison between our analytic Gutzwiller energy, denoted  $\hat{E}_G$ , and the energy of the saturated ferromagnet, denoted  $\hat{E}_F$ . The energies have been normalized 'per atom' and are calculated as a function of electron density per spin. (a) The square lattice. The points denoted  $(\dagger)$  mark the position where a phase transition would be expected. The ferromagnetic state is predicted to be relatively stable near half-filling and the paramagnetic state is predicted to be stable near empty and full. (b) The triangular lattice where the hopping matrix element is assumed to be positive. The ferromagnetic state is predicted to be relatively stable below half-filling and the paramagnetic state is predicted to be stable above half-filling. (c) The FCC lattice, where the hopping matrix element is assumed to be negative. The ferromagnetic state is predicted to be relatively stable above half-filling and the paramagnetic state is predicted to be stable below half filling.

## 5. Conclusions

For two holes moving around under the action of the Hubbard model in an otherwise empty lattice, the total spin of the ground state depends on the topological connectivity. For systems with a non-degenerate single-particle ground state, the pair is in a relative singlet and for systems with a degenerate single-particle ground state, the

pair is in a relative triplet. This result suggests that antiferromagnetically frustrated systems with positive hopping matrix elements should exhibit special behaviour, in an analogous way to that found for the Nagaoka problem.

The thermodynamic limit poses severe technical difficulties, and this casts severe doubts upon the relevance of our result for real systems. For three-dimensional systems with only discrete single-particle degeneracy, ferromagnetism is not to be expected for a finite number of holes greater than the ground state degeneracy. For two-dimensional systems and for three-dimensional systems with a one-dimensional single-particle ground state degeneracy, the result may be relevant, but more work needs to be performed to justify its use.

We conjecture that the strong-coupling ground state to the triangular lattice Hubbard model with a positive hopping matrix element, is ferromagnetic for concentrations less than half-filled and paramagnetic for concentrations greater than half-filled. This result is consistent with Nagaoka's theorem, the theorem in this article and most of the cluster calculations performed with periodic boundary conditions. It is also 'predicted' by our analytic Gutzwiller calculations.

We believe that the infinitely strong-coupling limit at *all* concentrations of particles may be understood by considering the smallest loop in the structure. For the Nagaoka problem this readily predicts the lattice result, and the results of this article are also predicted by the smallest loop. If we take the triangular lattice as an example, then the triangle is the smallest loop. There is only one relevant state, and this predicts ferromagnetism below half-filling and paramagnetism above half filling. Moving on to the square lattice, we find two relevant states to the square. With two particles we find a singlet ground state, whereas for three particles we find a ferromagnetic ground state. This suggests paramagnetism at low band-filling with a transition to ferromagnetism near half band-filling. At infinitely strong-coupling, we believe that the dominant effect comes from Fermi statistics and may be thought of in real space as 'swapping' over two particles by taking one of the two around a loop. This is the motivation behind our assertion.

Although we have not achieved a demonstration that long-range magnetic phase coherence results in the infinitely strong-coupling Hubbard model, there is a second level on which our result can be considered. For the Nagaoka result, the thermodynamic limit has also proved difficult, but a certain degree of understanding has arisen from the idea of a 'spin polaron' [10]. Since the topological effects are local in character, one expects that the coherence in the vicinity of the hole may well be ferromagnetic, even though there is no long-range order. The same idea may be applied to the result of the present paper. Even if there is no long-range order, at the two-particle level, one would still expect strong triplet correlations to be present as the particles are brought together.

Finally, we would like to point out that ferromagnetic Nickel crystallizes into a FCC structure, and this is a topologically frustrated structure with a one-dimensional single-particle ground state degeneracy. The frustration for the FCC lattice appears to be the strongest topological effect considered in this article, and so geometry may well play a role in stabilising the ferromagnetism of Nickel.

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## References

- [1] Hubbard J 1965 *Proc. R. Soc. A* **285** 542  
Anderson P W 1987 *Science* **235** 1196
- [2] Lieb E H 1989 *Phys. Rev. Lett.* **62** 1201  
Hirsch J E 1985 *Phys. Rev. Lett.* **54** 1317
- [3] Fischer M A and Young P have produced independent contributions with collaborators.
- [4] Nagaoka Y 1966 *Phys. Rev.* **147** 392
- [5] e.g. Shastry B S, Krishnamurthy H R and Anderson P W 1990 Instability of the Nagaoka ferromagnetic state of the  $U = \infty$  Hubbard model *Preprint*.  
There have been some recent attempts to extend Nagaoka's result to two holes. All such calculations *with periodic boundary conditions* seem to suggest that ferromagnetism is not the ground state. It is then suggested that Nagaoka's result does not survive the thermodynamic limit. The preprints that we have recieved to date, are not sufficiently relevant to the present article, because insufficient thought has been directed to the boundary conditions, but we consider it to be worth pointing out that some people believe that there is a problem here.
- [6] Kanamori J 1963 *Prog. Theor. Phys.* **30** 275  
Mattis D C 1981 *The Theory of Magnetism* (Berlin: Springer)
- [7] Anderson P W 1959 *Phys. Rev.* **115** 2
- [8] Callaway J 1987 *Phys. Rev. B* **35** 8723
- [9] Gutzwiller M C 1965 *Phys. Rev.* **137** A1726  
Razafimandimby H A 1982 *Z. Phys. B* **49** 33  
Goryachev E G and Kuzmin F V 1988 *Phys. Lett.* **131A** 481; 1989 *Phys. Lett.* **137A** 423  
Ogata M and Shiba H 1989 *J. Phys. Soc. Japan* **58** 2836  
More recent work by Shiba H
- [10] de Gennes P G 1960 *Phys. Rev.* **118** 141