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Nagaoka ferromagnetism versus long-range hopping in the one-dimensional Hubbard model

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Abstract. The infinite-U one-dimensional Hubbard model is 'solvable' in the limit that the nearest-neighbour hopping is dominant and infinitesimal longer-range hopping lifts the one-dimensional spin degeneracy. In this limit the Hubbard model maps onto an effective spin interaction: cyclic or ring exchange with a variety of lengths and strengths. For bipartite geometries we find a region of stable ferromagnetism, which originates from the mechanism intrinsic to Nagaoka's ferromagnetism. We look at connectivities that limit exactly to the square-lattice connectivity as the *range* of the infinitesimal hopping diverges. When we extend this hopping range, we find that the stable region of ferromagnetism shrinks, eventually vanishing as the infinitesimal hopping range diverges and we limit to the square-lattice geometry. Since the calculation involves a non-trivial density of particles in the thermodynamic limit, it suggests how the proposed region of ferromagnetism may become lost for the case of the two-dimensional square lattice, as numerical simulations predict.

1. Introduction

The advent of perovskite superconductivity has induced fresh and protracted study of the phase diagram of the Hubbard model [1]. Although the model is quite simple, the physical limit suggested by the experiments involves the electronic motion being dominated by the Coulombic repulsion, the so-called strong-coupling limit, which is extremely difficult to understand. Although in the real materials there is clearly a strong antiferromagnetic interaction, it can be argued that as the doping is increased the effect of the antiferromagnetic interaction becomes less relevant, and by the time that the system is metallic the physics is being controlled by the hole motion [2]. This is by no means an accepted fact, with the competition between antiferromagnetic exchange and hole motion being the most heavily studied model [3], but the physics introduced by the hole motion is definitely an important area to investigate. We will restrict our attention to the extreme limit of $U = \infty$ where the antiferromagnetic interactions are completely eliminated and the spin physics is controlled by the charge motion. For this limit the model becomes marginally simpler, reducing to the *single-parameter* model, the t-model:

$$H = -t_1 \sum_{\langle ii' \rangle \sigma} (1 - c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}}) c^\dagger_{i\sigma} c_{i'\sigma} (1 - c^\dagger_{i'\bar{\sigma}} c_{i'\bar{\sigma}}) \tag{1.1}$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron of spin σ (complementary spin $\bar{\sigma}$) on an atom i. The model hops electrons between nearest-neighbour atoms, denoted by $\langle ii' \rangle$, and the factors $(1 - c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}})$ ensure that sites can never become doubly occupied, hence enforcing the constraint that one charge state for each atom is eliminated: that with two electrons on

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the atom. This model yields a single line on the Hubbard model phase diagram, and need only be solved as a function of band filling.

This particular limit has been studied previously, with two basic results surfacing: firstly, for the low-density limit one expects Kanamori paramagnetism [4], and secondly, for the high-density limit (near half filling), one might expect Nagaoka ferromagnetism [5]. The most interesting phase is clearly the paramagnetic phase, which would be expected to correspond to the limit found in perovskite superconductors, under the caveat that the hole motion is the dominant physical interaction. We will not be concerned with this paramagnet here, but rather we will be looking at the less interesting phase of Nagaoka ferromagnetism.

Nagaoka ferromagnetism is controversial. The initial work, performed by Nagaoka, involved the study of a single hole in an otherwise pure bipartite geometry [5]. It is fairly straightforward to *rigorously* prove that the ground state to this problem is ferromagnetic, although the energy involved in the degeneracy breaking is incredibly small. Taking this result at face value, one would then like to deduce that when a low density of holes is introduced, they will each induce a region of ferromagnetic polarization around themselves, all of which can align to yield a long-range ferromagnet. So desirable is it to make these statements, that it has even been suggested that a *pair* of holes will feel an attractive force, since each hole can make use of the other hole's ferromagnetic region, gaining additional room to move in and consequently lowering kinetic energy [6]. Unfortunately, the numerical simulations do *not* agree with this picture, and indeed, usually one finds a low-spin ground state in contradiction with this picture. Even for the lowest doping of two holes, where one might naively expect maximum benefit from the interaction, one finds a total-spin singlet ground state. There is a variety of calculations in the literature, both analytic and numerical, that show evidence for [7] and against [8] Nagaoka ferromagnetism.

It is crucial to reach the thermodynamic limit with a *finite* hole density in addressing this issue. In this article we will look at models for which there is a region of Nagaoka ferromagnetism in the thermodynamic limit, and we will study the stability of this phase. It is the issue of how this phase is destroyed in the thermodynamic limit that is of major concern in an attempt to understand how the ferromagnetism might become lost in the two-dimensional square lattice.

The major flaw in the argument supporting Nagaoka ferromagnetism in the thermodynamic limit is that the most violent force between the particles has been omitted in the discussion: fermionic statistics. A single hole moving around has no statistics, because it has no other holes to exchange with. However, two particles moving around in a ferromagnetic region repel each other much more strongly than a pointwise repulsion, since antisymmetrization of the pair wavefunction restricts each electron to only effectively *half* the region, since there exists a direction parallel to which the electrons *never* exchange. It has been previously suggested [9], that by a judicious choice of spin wavefunction, the motion of the holes can cease to be controlled by Fermi statistics and can become similar to that of hard-core bosons, with the holes freely able to orbit each other with consequently more room to move in and more kinetic energy available. The problem is the choosing of this spin wavefunction, which has proved amazingly subtle to think about.

Although we have made little progress with the two-dimensional model of most interest, we have found a class of models that are tractable, and are not too far removed from the two-dimensional systems. Recently, the present authors have shown how to map one-dimensional systems with dominant nearest-neighbour hopping and infinitesimal longer-range hopping onto effective spin models [10]. The fundamental idea is that the spin and charge degrees of freedom separate for these models. The charge degrees of freedom remain identical to the spinless Fermi gas at the level analysed, but the one-dimensional

spin degeneracy is lifted by the longer-range hopping, and exhibits a variety of possible characteristics. We were able to find the phase diagram for very short-range hopping, and found a finite region of stable Nagaoka ferromagnetism [10]. In this article we introduce a sequence of models that have hopping increasingly similar to the square-lattice model, and find bounds on the region of stable Nagaoka ferromagnetism. The basic result is that as the range of hopping is increased, so the region of stable ferromagnetism shrinks, eventually vanishing in the limit of infinite-range hopping.

In section 2 we briefly review the mathematical method of solving the models. In section 3 we evaluate bounds on the region of stable ferromagnetism and in section 4 we perform some numerical simulations to show that some of the calculations are probably exactly correct. In section 5 we conclude.

2. Mapping to a spin Hamiltonian

The fundamental reason that we can solve our class of models is that the spin and charge degrees of freedom become completely independent. In general, even when we have spin–charge separation, this independence is lost, and is only reestablished in the low-energy limit.

In order to successfully describe the behaviour of the one-dimensional Hubbard model, we need to use a representation for which the charges can move while the spin order along the chain remains frozen. To this end we have introduced a representation for which the spins and charges are separated:

$$c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} \ldots c^\dagger_{i_n\sigma_n} \mid 0\rangle \equiv f^\dagger_{i_1} f^\dagger_{i_2} \ldots f^\dagger_{i_n} \mid \sigma_1\sigma_2\ldots\sigma_n\rangle \tag{2.1}$$

where the $f^\dagger_i$ operators are assumed fermionic and control the motion of the charges alone, and the spins are ordered along the chain and are controlled directly with spin operators, $\hat{S}_\alpha$. In terms of this representation, the original hopping becomes

$$\begin{aligned} c^\dagger_{i\sigma} c_{i+n\sigma} = f^\dagger_i f_{i+n} \sum_{\chi_i=0}^{1} \sum_{\chi_{i+1}=0}^{1} \cdots \sum_{\chi_{i+n-1}=0}^{1} \prod_{m=1}^{n-1} \left[f^\dagger_{i+m} f_{i+m} \right]^{\chi_{i+m}} \\ \times \left[1 - f^\dagger_{i+m} f_{i+m} \right]^{1-\chi_{i+m}} \frac{1}{2} \left[1 + \sigma \hat{S}^z_{\alpha_i} \right] \hat{R}_{\alpha_i, \alpha_{i+n}-1} \end{aligned} \tag{2.2}$$

where the χ_l measure whether or not an electron is on a particular site i, and in terms of which the $\alpha_l = \sum_{m=1}^{l} \chi_m$ count how many electrons come before a particular site, making a useful spin label. The first two f operators move the charge. The summations over the χ variables break the states down into all possible charge configurations between the two end points of the charge transfer. The operator involving the z-component of spin ensures that the electron moved has the correct spin, and the final spin arrangement conserving the spin order along the chain is effected by

$$\hat{R}_{\alpha,\alpha+n} = \prod_{\beta=\alpha}^{\alpha+n-1} \left[\frac{1}{2} + 2\hat{S}_\beta \cdot \hat{S}_{\beta+1} \right] \tag{2.3}$$

which involves a string of spin operators, which shuffle the spins along conserving their order along the chain. Each term

$$\left[\frac{1}{2} + 2\hat{S}_\alpha \cdot \hat{S}_{\alpha+1} \right]$$

provides an elementary permutation of the two spins involved, and so the product is just a simple cyclic permutation of the relevant spin variables. Due to the central role that these cyclic permutations hold in our analysis, we have introduced a notation for such a permutation, $\hat{R}_{\alpha,\alpha+n}$, and we are using the letter R to represent the idea of 'ring exchange', which is often how this concept has been labelled in the literature.

The inclusion of longer-range hopping is accomplished by

$$H_1 = -\sum_n t_{1+2n} \sum_{i\sigma} (1 - c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}}) c^\dagger_{i\sigma} c_{i+1+2n\sigma} (1 - c^\dagger_{i+1+2n\bar{\sigma}} c_{i+1+2n\bar{\sigma}}) \tag{2.4}$$

where the t_{1+2n} are infinitesimal matrix elements of variable *relative* magnitudes. We have presumed that the lattice is bipartite, and so we have restricted attention to hops *between* the two natural sublattices. The details of our transformation and how to apply it can be found elsewhere [10, 11], and we will only briefly explain the results of direct relevance to the current phase boundary argument here. We can perform degenerate perturbation theory immediately using (2.2), yielding:

$$H_{\text{deg}} = K_0 + \sum_n K_n \sum_\alpha \left[\hat{R}_{\alpha,\alpha+n} + \text{cc} \right] \tag{2.5}$$

where the matrix elements, K_n, can be deduced from

$$K_n = -\sum_{r=n+1}^{\infty} t_r \left\langle f_0^\dagger f_r \sum_{\chi_1=0}^{1} \cdots \sum_{\chi_{r-1}=0}^{1} \delta \left(\sum_{s=1}^{r-1} \chi_s - n \right) \prod_{m=1}^{r-1} \left[f_m^\dagger f_m \right]^{\chi_m} \left[1 - f_m^\dagger f_m \right]^{1-\chi_m} \right\rangle \tag{2.6}$$

where the δ-function ensures that exactly the correct number of electrons are involved in the exchange, the periodicity inherent in the charge-motion ground state ensures that we may consider a particular site to measure correlations from, and we must evaluate these correlation functions for the spinless fermion ground-state wavefunction. The form of this result is quite easy to understand: when an electron is hopped across $r - 1$ atoms, it passes a variable number of intermediate electrons, n say. The spin wavefunction incurs a cyclic permutation, involving the spin on the hopping electron and the spins on the n electrons passed over. Obviously, the maximum number of spins occurs when the chain is completely filled between the two ends of the hop, and so $n < r$, explaining the restriction in our summation. The strength of the resulting interaction is controlled by the motion of the fermions in our charge ground state: the free-fermion gas. To contribute to a specific cyclic permutation, we must have precisely n electrons between the ends of the hop, *and* contributions to the charge ground state from situations where both the initial and final charge configurations occur. The correlation functions in equation (2.6) measure precisely these likelihoods.

The effective spin interaction for our model is therefore just a superposition of ring exchanges over all ranges up to the maximum hopping range. The matrix elements for these interactions are controlled by the probabilities of finding the relevant spatial configurations of fermions in the spinless fermion ground state. We can rerepresent the spinless-fermion correlation functions as determinants and then evaluate them [11], either analytically for small systems or numerically for large systems.

3. Phase boundaries

In this section we will develop some analytic bounds on where the phase boundary between saturated ferromagnetism and a second phase might be. We will consider some *classical* states and deduce when the ferromagnetic ground state becomes unstable with respect to them. Although these calculations only provide a lower bound, we believe that sometimes these calculations yield the true phase boundary. Numerical evidence for this assertion will be presented in the next section. Unfortunately, due to the variational nature of our calculations, we cannot rule out another type of instability, which occurs prior to ours, allowing the system to transit into a phase with less interesting physics. For example, one could conceive of a weird form of ferrimagnetism, with only a minor distortion away from ferromagnetism. We cannot discount this possibility, although we do not believe in it.

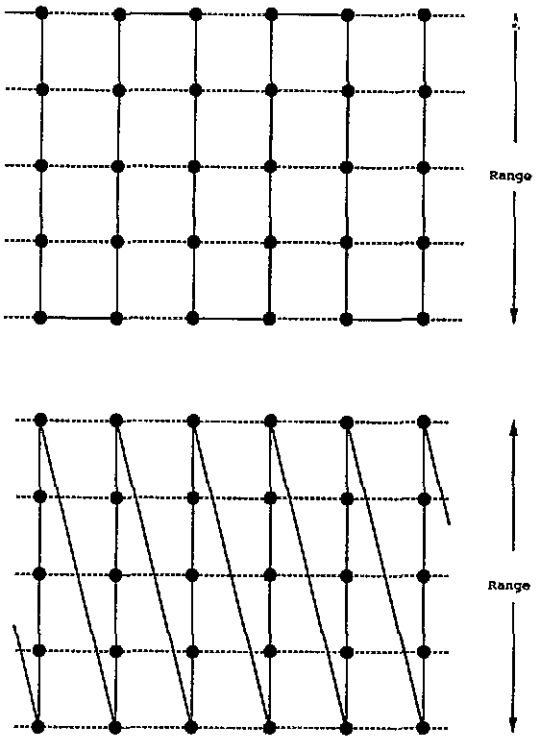

Figure 1. The two geometries under current investigation. The bold lines denote the strong one-dimensional hopping, and the dashed lines denote the infinitesimal additions. Black circles correspond to atoms.

We will consider two distinct geometries, both of which can be chosen to limit to the two-dimensional square lattice, although in rather different ways. We depict the two geometries in figure 1: the first geometry breaks translational symmetry, and involves a distribution of bonds of different ranges, whereas the second geometry retains translational symmetry and includes only equal bonds. We can limit to the square lattice in a two-stage process: firstly we can allow the range of the hopping to diverge, and secondly we can increase the strength of the bonds until all the bonds are of equal strength. In this article we will deal with the first process, yielding infinite-range bonds in the limit, but we have

been unable to make significant progress in increasing the strength of the bonds above infinitesimal.

The first classical state that we consider is that where we force the two natural sublattices to be saturated, but allow them to rotate in opposite directions and pick up an angle θ. Since the overlap between any two classical states with two spin-$\frac{1}{2}$ atoms at relative angle θ is $\cos^2(\theta/2)$, we can evaluate the overlap between any configuration that occurs from our ring-exchange interactions and the original state. The calculation is just a direct evaluation of (2.2), where the charge Hamiltonian is the spinless Fermi gas, and we have to evaluate the ring-exchange correlation functions for our classical spin state. We look at each range of hopping in turn, evaluating a spread of ranges by summing the results. It proves useful to define the function

$$f_n(x) = \left\langle f_i^\dagger f_{i+1+2n} \prod_{r=1}^{2n} \left[1 - f_{i+r}^\dagger f_{i+r} + x f_{i+r}^\dagger f_{i+r}\right]\right\rangle \tag{3.1}$$

in terms of which the energy of our classical state is

$$E_n(\theta) = -t_{1+2n}\left[\frac{1+\cos(\theta/2)}{2} f_n(\cos(\theta/2)) + \frac{1-\cos(\theta/2)}{2} f_n(-\cos(\theta/2))\right] \tag{3.2}$$

which follows directly from resumming (2.2), using the result that:

$$\langle \hat{R}_{0,2n}\rangle = \langle \hat{R}_{0,2n-1}\rangle = \cos^{2n}(\theta/2). \tag{3.3}$$

It has previously been shown [11] that

$$f_n(x) = (1-x)^{2n} \begin{bmatrix} n_1 & n_0 - \frac{1}{1-x} & n_1 & \dots & n_{2n-2} & n_{2n-1} \\ n_2 & n_1 & n_0 - \frac{1}{1-x} & \dots & n_{2n-3} & n_{2n-2} \\ n_3 & n_2 & n_1 & \dots & n_{2n-4} & n_{2n-3} \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ n_{2n} & n_{2n-1} & n_{2n-2} & \dots & n_1 & n_0 - \frac{1}{1-x} \\ n_{2n+1} & n_{2n} & n_{2n-1} & \dots & n_2 & n_1 \end{bmatrix} \tag{3.4}$$

from which we can immediately deduce the energy, $E_n(\theta)$, in terms of the single-particle correlations of the free-fermion gas

$$n_r = \langle f_{i+r}^\dagger f_{i+r}\rangle = \frac{\sin n_0 \pi r}{\pi r} \tag{3.5}$$

where n_0 is the original electron density.

The function $f_n(x)$ is quite easy to differentiate, yielding a sum over $2n$ determinants, each of which is identical to $f_n(x)/(x-1)$ with the exception that one out of the $2n$ terms $1/(1-x)$ is missing. Given this result it is relatively easy to hunt out the characteristics of the function $E_n(\theta)$.

Close to ferromagnetism, viz. $\theta = 0$, the behaviour is much simplified. As should be expected, the determinant collapses down to one term

$$E_n(0) = -t_{1+2n} n_{1+2n} \tag{3.6a}$$

and the derivative simplifies to

$$\frac{\mathrm{d}E_n}{\mathrm{d}\theta}(0) = 2n n_0 n_{1+2n} - 2\sum_{m=1}^{n} n_m n_{1+2n-m} + \tfrac{1}{2}\left[n_{1+2n} - f_n(-1)\right] \tag{3.6b}$$

which can be evaluated with a single determinant. If the instability were towards an infinitesimal angle, θ, then the phase boundary would correspond to a zero in this derivative, marking the degeneracy between ferromagnetism and the ferrimagnet. Direct numerical calculations at non-zero θ have shown that the first instability does indeed occur towards infinitesimal rotations, and we have evaluated the predicted phase boundary for our two geometries as a function of inverse range in figures 2 and 3 for the spread of ranges and a single range respectively. One feature seems immediately clear: as the range of hopping diverges, so the phase boundary converges towards unity.

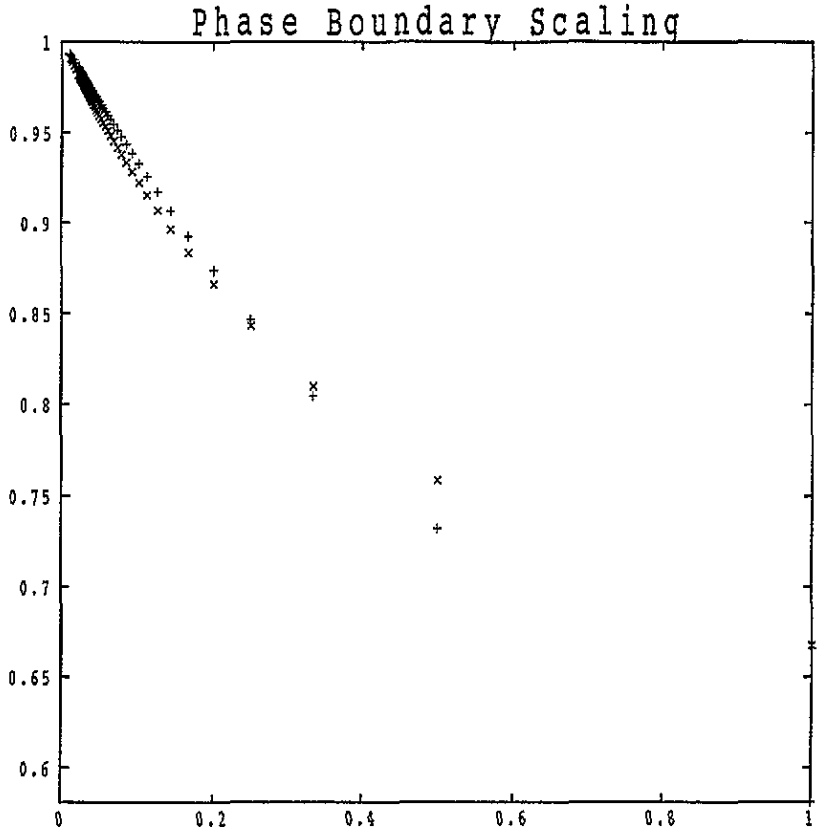

Figure 2. The phase boundaries between ferromagnetism and the classical spin states explained in the text, for the geometry with a spread of bond ranges. We plot the phase boundary as a function of inverse range $(1/n)$ for the infinitesimal bonds where the bond length is $1 + 2n$. Crosses correspond to an infinitesimal ferrimagnetic distortion and plus signs correspond to an infinitesimal spiral distortion.

Although this ferrimagnetic instability appears to dominate at short-range hopping, at longer range we have found that a classical spiral appears to become favourable. We will now introduce this second classical state. The development is very similar to the previous case, with the two-sublattice ferrimagnet being replaced by a classical uniform spiral, rotating through an angle ϕ from spin to spin.

It is straightforward to evaluate the the ring-exchange correlations for the spiral, and we find

$$\langle \hat{R}_{0,r} \rangle = \cos^r(\phi/2)\cos(r\phi/2) \tag{3.7}$$

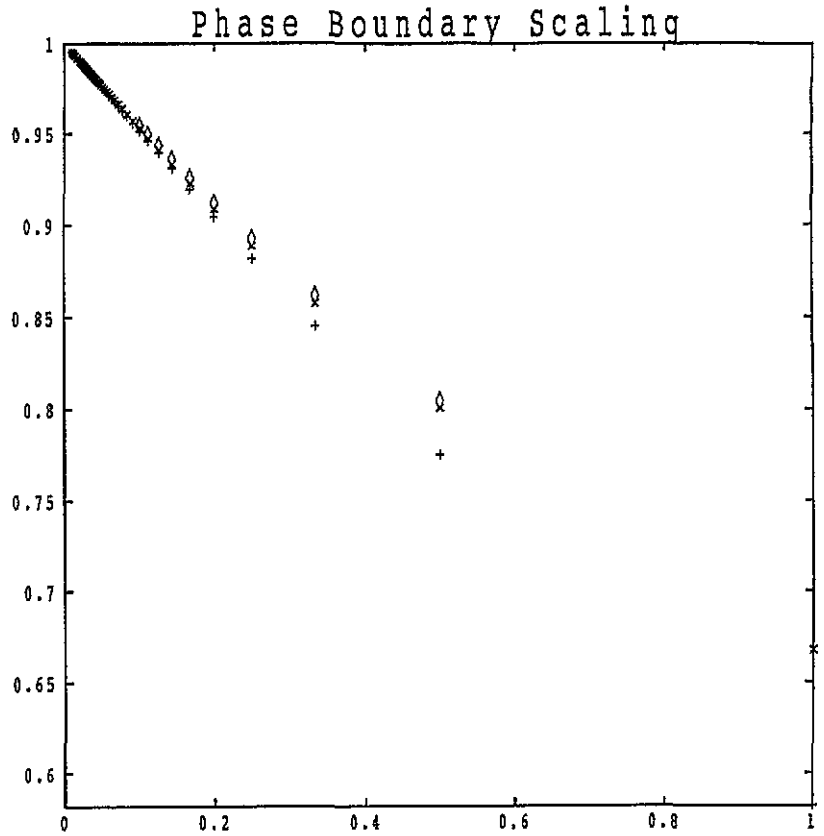

Figure 3. The phase boundaries between ferromagnetism and the classical spin states explained in the text, for the geometry with a single bond range. We plot the phase boundary as a function of inverse range $(1/n)$ for the infinitesimal bonds where the bond length is $1 + 2n$. Crosses correspond to an infinitesimal ferrimagnetic distortion, plus signs correspond to an infinitesimal spiral distortion and diamonds correspond to a finite pitch spiral chosen with the optimum pitch.

where the large rotation originates from the spin that has moved over the long distance. The geometric nature of this result leads immediately to the result

$$F_n(\phi) = \frac{1}{2}\left[f_n(\cos(\phi/2)e^{(i\phi/2)}) + f_n(\cos(\phi/2)e^{(-i\phi/2)})\right]$$
$$= \mathrm{Re}\left[f_n(\cos(\phi/2)e^{(i\phi/2)})\right] \tag{3.8}$$

for the energy of the state $F_n(\phi)$.

The behaviour close to ferromagnetism is rather more difficult to derive, due to the slightly more sophisticated dependence on ϕ, but one can soon show that

$$\frac{d^2F_n}{d\phi^2}(0) = \frac{(-1)}{2}f^{(1)}(1) + \frac{(-1)}{4}f^{(2)}(1)$$
$$= (1 + 2(n - \tfrac{1}{2})n_0)\sum_{r=1}^{n} n_r n_{1+2n-r} - nn_0n_{1+2n} - n(n - \tfrac{1}{2})n_0^2 n_{1+2n}$$

$$+ n_{1+2n} \sum_{m=1}^{2n-1} (n - m/2) n_m^2 - \frac{1}{2} \sum_{r \neq s}^{2n} n_{|r-s|} n_s n_{1+2n-r} \tag{3.9}$$

a rather simpler result for the phase boundary. We have plotted the resulting phase boundaries for this classical state in figures 2 and 3, and once again we can see that as the range of hopping diverges so the phase boundary to this type of instability converges to unity.

Unfortunately, there is a complication to these simple results: the instability is not necessarily towards an infinitesimal angle. Although for the case of a spread of ranges we find that the strongest instability is towards an infinitesimal spiral, for the single-range case we find that the infinitesimal spiral is less potent than the ferrimagnetic instability, but that the strongest instability of all is to a classical spiral with a *finite* pitch. The pitch of the best spiral is tuned to the electron density, with a rough guide that the spiral turns through 2π between holes along the chain, with the instability occuring when the holes are on average about the same distance apart as the range of the additional infinitesimal bond $(2n + 1)$.

Instabilities to infinitesimal classical distortions will yield precise phase boundaries even for the quantum case, whereas finite-pitch spirals will necessitate quantum fluctuations, which will play a role in the energetics. Although we would expect a phase transition exactly where the analytical calculation predicts for the case of a spread of ranges, we would expect that the analytical calculation would only predict a lower bound for the case of the single-range geometry. We give numerical evidence supporting these assertions in the next section.

The physics anticipated from the two instabilities that we have considered is very different. For the two-sublattice ferrimagnet, we would still expect the behaviour to be dominated by the huge ferromagnetic moment, whereas the spiral phase is expected to be a low-spin magnet with subtle properties. The reader should bear in mind that the solutions predicted are spin–charge separated, and so the spin-state magnetism is convoluted with the metallic charge state yielding only minor, if any, residual spin correlations observable with normal experimental probes [11]. For both cases we find a spiral solution is ultimately the predicted spin state, making a connection with previous proposals for such a possibility [12].

4. Exact diagonalization studies

The analytical calculations for the phase boundaries described in the previous section were all lower bounds to the actual phase boundary. Although we can say that the ferromagnetism will be unstable with respect to some secondary phase, we cannot say with certainty what this second phase is, nor can we tell the particular moment at which the transition will occur. In order to investigate whether or not our predictions are overshadowed by some as yet unconsidered physics, we have performed some finite-size scaling studies of some exact-diagonalization calculations on the effective ring-exchange spin models.

By the horrendously numerically intensive procedure of evaluating each of the $\sim 2^n$ determinants in equation (2.6), we can calculate the coefficients, K_n, in the effective ring-exchange spin model, for any chosen electron density and hopping range. These coefficients can then be inserted, as bond strengths, into a Lanczos exact-diagonalization calculation for the spin wavefunction of a finite system. Obviously, the type of model that we can analyse is severely restricted by the very small system size necessitated by this technique. Since we can only handle around twenty-four spins, we are restricted to hopping ranges of at most

$n = 4$, and even for this case the chains of up to eight yield 'inconsistent' interactions and cannot be included.

Due to the fact that we are looking for phase transitions, we have elected to present only a small selection of total-energy calculations. We have chosen to plot $\epsilon(N)/N$, an intensive energy, in order that different states will converge to finite values. This choice leads to complications, since as the system size increases, so the density of excitations increases and the low-lying excitations collapse down onto the ground state, complicating the picture. One must be aware of this when attempting interpretation, and must focus on the relative *order* of energies and not their absolute values.

In order to assist in interpretation there are a few fundamental ideas that should be born in mind. Firstly, a ferrimagnetic solution can be identified by a steady precession of ground states with increasing total spin. Since the ratio of magnetic moment to maximum moment, m/M say, converges to a finite fraction, the magnetic moment must steadily increase. Secondly, a spiralling solution will involve a type of 'beating', as the length scale from the spiralling 'interferes' with the length of the chain. We would expect a sequence of total-spin singlets to yield the ground state, with one additional spiral in each subsequent state, and the period between such states defining the 'pitch' of the spiral. Thirdly, the difference between first-order and second-order transitions should also be immediately apparent. For a second-order transition there is a 'continuous' sequence of excitations that carries us from one type of ground state to the other, and when there is a phase transition this sequence of excitations should *invert*. For a first-order transition there should be no direct relationship between the two phases and the excitations of each phase should remain above the ground state, viz. two independent superimposed spectra should simply 'slide' past each other.

We will deal with the case of a spread of bonds first, because the analytic prediction is straightforward: for all possibilities we predict a *classical* instability to an infinitesimal distortion. For the cases of the range, $1 + 2n$, being $n = 1, 2$ or 3, we expect an instability to a two-sublattice ferrimagnet, while for ranges of $n > 3$ we anticipate an instability to a total-spin singlet spiral state.

In figure 4 we have finite-size scaled the total energy per spin against inverse system size for two concentrations of electrons and the case when there are two available hopping ranges. The transitions occur at $n_{c1} = 0.731\,92$ for the spiral and $n_{c2} = 0.758\,47$ for the ferrimagnet. The first density should find both states stable, whereas the second should find only the ferrimagnet stable. We have scaled states of two varieties: solid lines denote states whose difference from the maximum spin is fixed and usually small, whereas dotted lines denote states whose absolute spin is fixed and small. For both systems, the character of the ground state changes in such a way as to suggest that there is a preferred ferrimagnetic moment (as the system size increases, the expected value of total spin rises in such a way as to keep the ratio approximately constant). The calculations are in good agreement with the analytical predictions from the last section, that the ratio of the magnetic moment to its saturated value should be $m/M = 0.548\,033$ for $n_0 = 0.7$ and $m/M = 0.896\,133$ for $n_0 = 0.75$. The low-spin states do not scale very smoothly, which may indicate that there is no 'metastable' spiral phase. There is no new state observable that could overturn our classical predictions.

In figure 5 we have finite-size scaled the total energy per spin against inverse system size for two concentrations of electrons and the case when there are four available hopping ranges. The transitions occur at $n_{c1} = 0.846\,48$ for the spiral and $n_{c2} = 0.843\,08$ for the ferrimagnet. The first density should find both phases stable and the second density should find neither phase stable. The results are in good agreement with this picture, with the low-spin state clearly being preferred in the first case. The results clearly depend strongly

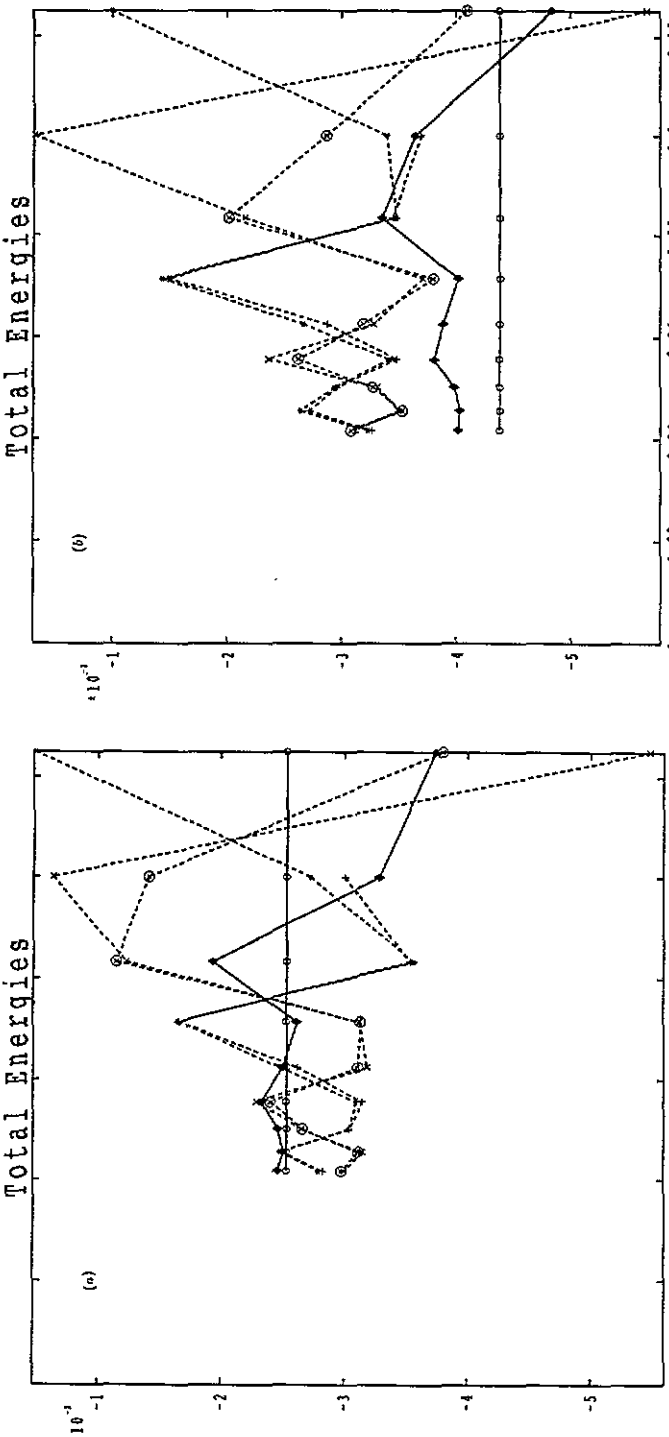

Figure 4. A finite-size scaling analysis for the low-energy excitations at $k = 0$ and $k = Q$, for the effective ring-exchange model corresponding to the $U = \infty$ Hubbard model with a spread of hopping ranges up to $n = 2$. We have calculated for the two cases of electron densities (a) $n_0 = 0.70$ and (b) $n_0 = 0.75$. Solid lines correspond to states scaled with a fixed value for $S_{max} - S$, and dashed lines correspond to states scaled with a fixed value for S, the total spin of the state. In both figures the solid lines connect similar states but the dashed lines do not necessarily. For the first case the ground state is clearly ferrimagnetic with a sizable moment as predicted, while for the second case the ground state is clearly ferrimagnetic with a very large moment.

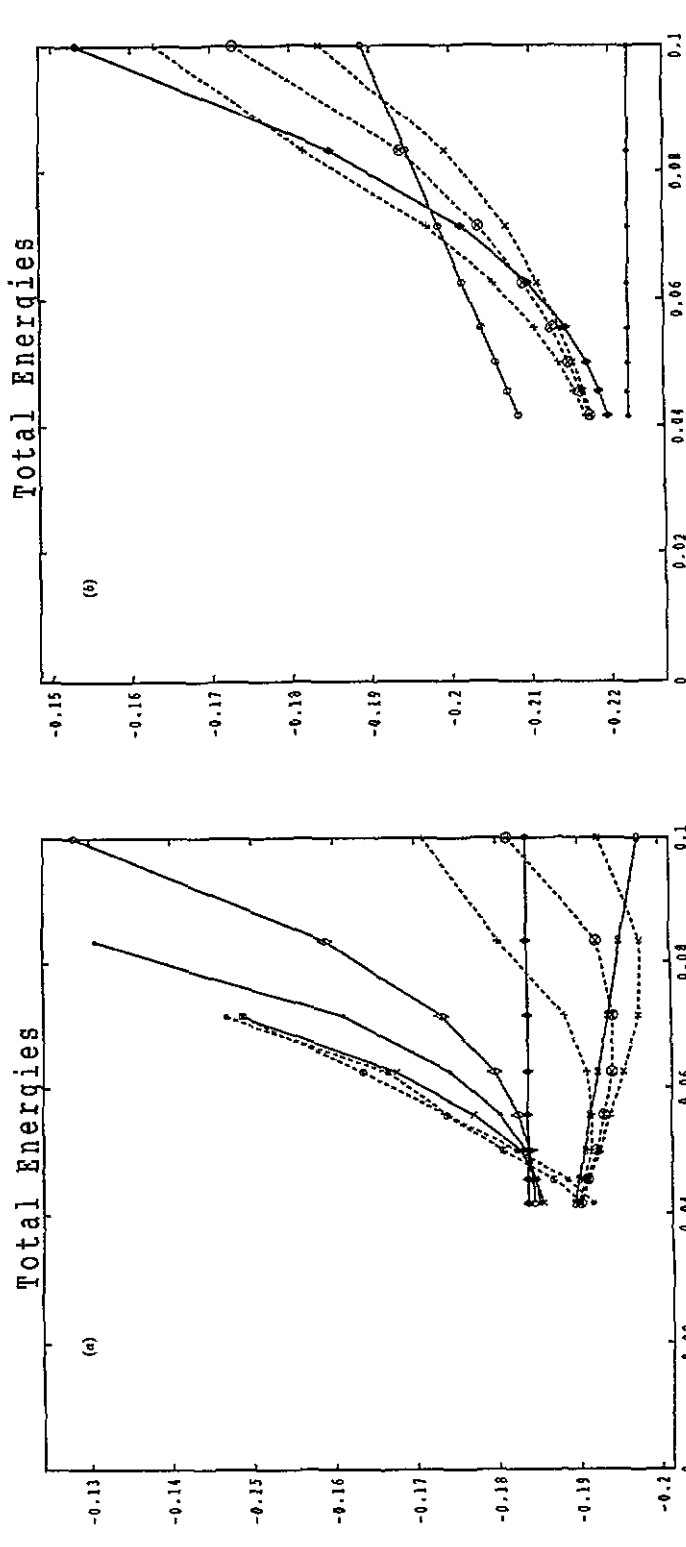

Figure 5. A finite-size scaling analysis for the low-energy excitations at $k = 0$ and $k = Q$, for the effective ring-exchange model corresponding to the $U = \infty$ Hubbard model with a spread of hopping ranges up to $n = 4$. We have calculated for the two cases of electron densities (a) $n_0 = 0.84$ and (b) $n_0 = 0.85$. Solid lines correspond to states scaled with a fixed value for $S_{max} - S$, and dashed lines correspond to states scaled with a fixed value for S, the total spin of the state. In both figures the lines connect similar states. For example (a), the earliest ground states correspond to the zone boundary and involve a 'half twist', while the incoming ground state for the largest sytem corresponds to the zone centre and involves a full twist. Clearly the ground state for case (a) is a form of spiral with a repeat distance of about thirty or so spins, rather longer range than is predicted by the classical calculations. For case (b) the ground state is the saturated ferromagnet as predicted by our analytical calculations.

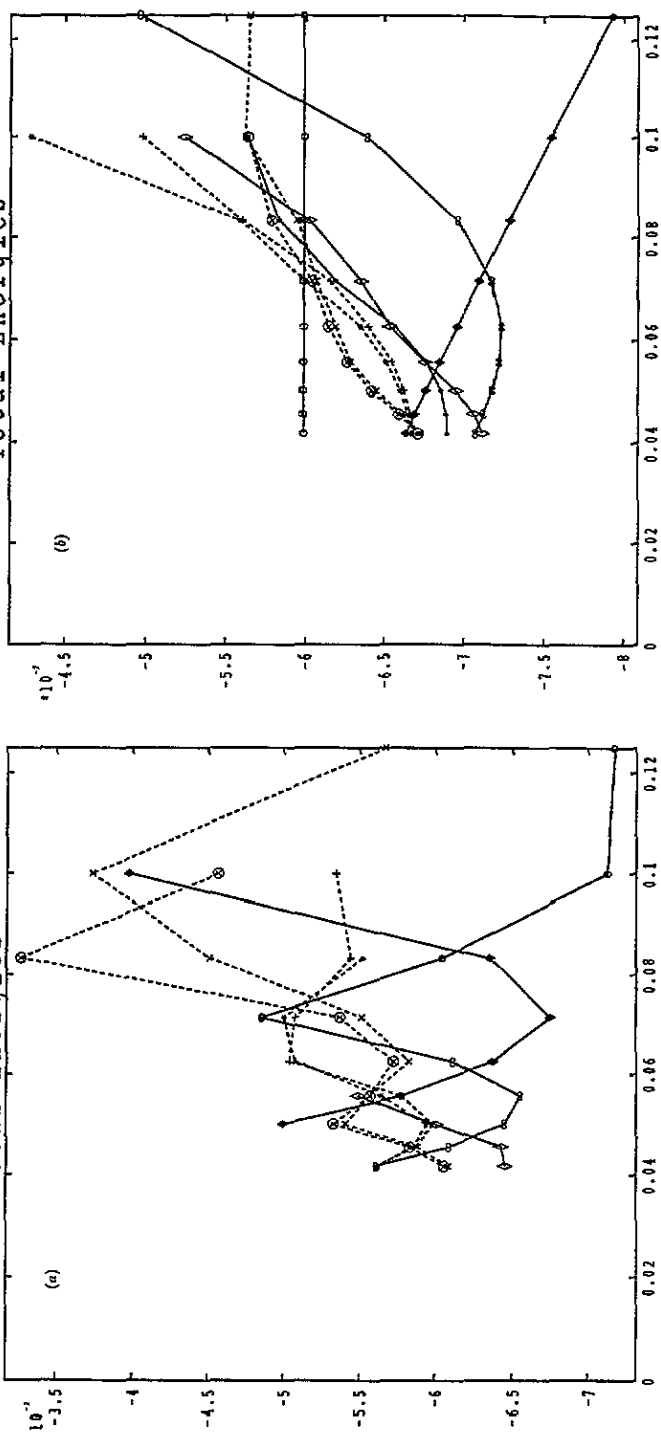

Figure 6. A finite-size scaling analysis for the low-energy excitations at $k = 0$ and $k = Q$, for the effective ring-exchange model corresponding to the $U = \infty$ Hubbard model with a single hopping range of $n = 3$. We have calculated for the two cases of electron densities (a) $n_0 = 0.87$ and (b) $n_0 = 0.88$. Solid lines correspond to states scaled with a fixed value for $S_{max} - S$, and dashed lines correspond to states scaled with a fixed value for S, the total spin of the state. In both figures the lines connect similar states. For both examples there is clearly a singlet state commensurate with the chain length every eight spins or so, leading to an interpretation of a spin spiral with a pitch of about $\pi/4$. This spiral 'tightens' as the electron density increases, which is the *opposite* behaviour to the classical predictions. Example (a) finds this singlet state relatively stable, whereas example (b) finds saturated ferromagnetism relatively stable.

on range, although the predicted angle, $\phi = 0.118\,921\pi$, does not appear to agree well with with the spiral picked out by our choice of periodic boundary conditions. The tiny loss of moment $m/M = 0.981\,585$ also for the first case is clearly unobtainable for our small systems. The strange 'crossover' behaviour comes from the spiral phase at $k = 0$ becoming relatively stable against saturated ferromagnetism under the action of the weakening effect of the periodic boundary conditions. This indicates that the phase transition is probably second order. Once again, there is no signature of a new piece of physics that is likely to overwhelm the picture of a classical instability.

These results, together with various other unmentioned calculations, give us confidence that, for the system with a spread of hopping ranges, the ferromagnetic state is unstable with respect to a classical instability involving either ferrimagnetism for short-range hopping or infinitesimal spirals for longer-range hopping.

We now turn our attention to the single-range hopping model, for which the classical predictions are more involved. In figure 6 we have finite-size scaled the total energy per spin against system size for two concentrations of electrons and the case where we hop only to the third possible range. The second-order transitions occur when $n_{c1} = 0.845\,24$ for the spiral and $n_{c2} = 0.857\,36$ for the ferrimagnet. For this case, however, the lowest classical instability that we found was at $n_{c3} = 0.8618$, and the instability was to a *finite* spiral of pitch 0.4629π. Neither of our chosen densities should yield a classical instability, although it is clear from the calculation that our first choice has a low-spin ground state and our second choice does not. As expected, quantum fluctuations are relevant for this case and further stabilize the classical spiral with finite pitch. The additional stabilization is quite weak however, amounting to a concentration of only about 1%. There is a clear length scale in the singlet ground state, which can be picked out as the 'beating' with the length of the chain, and this length scale is similar to the predicted classical spiral pitch. Also there is no continuous branch of excitations connecting the two types of ground state, and so we presume that this is a first-order transition, as expected.

Once again, the classical predictions are born out by the numerical calculations, although now the classical results are only good to about 1%. The results for the single-range hopping model suggest a first-order instability to a *quantum-mechanical* spiral state with finite pitch.

5. Conclusions

For the two very particular models presented, we have shown that long-range hopping weakens Nagaoka ferromagnetism, eventually eradicating it in the limit that the range of hopping diverges. The phase that replaces the ferromagnetism has been predicted to be a spiral phase, although the quantum mechanics of the spins almost certainly tempers this result.

We attribute this result to the spin–charge separation, with the judiciously chosen spiral including phases that compensate the statistical Fermi phases from exchange, allowing the holes to hop over each other with a more hard-core-boson-like character. The very best single-particle state we believe to be the Nagaoka ferromagnet, and so we would promote any lack of Nagaoka ferromagnetism in the square-lattice Hubbard model as being evidence that the system favours a more collective ground state.

The instability predicted in our analysis is fairly easy to understand: when there is a single hole, Nagaoka's theorem enforces ferromagnetism. The physical cause of the ferromagnetism is the hole circling around closed loops. For a bipartite geometry, a complete path around a loop involves a cyclic permutation of an *odd* number of fermions.

This in turn ensures a *positive* statistical phase. Phase coherence is therefore guaranteed by ferromagnetism. The problems occur when holes circle loops in which other holes are present. The first example of this occurs when the inverse of the density of holes, viz. their average separation, becomes equal to the length of a *relevant* loop. For this case, on average, there become *two* holes in a loop, and circulation occurs via exchange. Since there is now an *even* number of fermions involved, there is a *negative* statistical phase and we would obtain phase cancellation in a ferromagnet. If we include a slow spiral into the spin wavefunction, then we can compensate the statistical phase with a phase in the spin wavefunction, reinstating phase coherence for the hole motion. We would require a single additional phase per relevant loop length, and hence the pitch should be controlled by this loop length.

The key physical idea controlling this effect is that of a *relevant* loop. The probability of an isolated hole cycling around short loops is clearly usually higher than the probability of cycling around large loops. One would therefore quite naturally presume that the smallest loop controls the physics, and to some extent it does. There is, however, a caveat: the smallest loops control the physics on their own length scale. For low densities of holes we want ferromagnetism around short loops: an infinitesimal spiral ensures ferromagnetism on short length scales. For the longer loops, where there is a sizable probabilty of exchange of a pair of holes, phases can be introduced into the wavefunction that do *not* compromise the more important small loop motion.

The path towards a two-dimensional calculation has been designated a two-stage process in this article, with an initial jump to infinite-range hopping, and then a second step to a competition between the finite- and infinite-range hops. We have successfully overcome the first step, and have seen that there is new physics encountered. We have not tackled the second step, which could easily completely reverse all our phenomena and replace them with something completely dull. The truth is that we only have faith to support our belief that these calculations might be relevant to two dimensions.

The key to our solutions is the fact that we can control the changes in the spin wavefunction. When the charges hop over each other, the spin wavefunction changes in such a way that the old spin order along the chain is reintroduced for the new ordering with the spin on the charge that moved being repositioned into its new site along the ordered chain of spins. This change in spin wavefunction constitutes a loss in possible kinetic energy, as the original hopping-matrix element is reduced by this change. However, the change is energetically favourable, because of the reduction in statistical phase cancellation that results. It is this competition, when altering the spin wavefunction, between losing kinetic energy directly and gaining from enhanced collective phase coherence, that decides whether spin–charge separation will be favourable.

It is instructive to consider what might be expected in two dimensions, at least in simple terms. The first main result from increasing the strength of the longer-range hops is that the Nagaoka ferromagnetic correlations spread out perpendicular to the one-dimensional chain into the second dimension. These correlations become associated with two dimensions, and our labelling by order along the one-dimensional chain ceases to be very efficient. This is the start of the fundamental difficulty of trying to set up a spin–charge-separated description in two dimensions: we might still anticipate that the charged excitations would be collective 'slopping about', but now we would need to slop a two-dimensional 'patch', and it is very difficult to invent a labelling scheme that maintains such short-range connectivity between the *electrons* in two dimensions and not the atoms: we still need to keep our labels on the electrons, but we need to set up a spin wavefunction that correlates electrons close together but allows collective motion with the *relative* spin correlations held fixed. Although we do

not know how to set up such a description, it does not mean that the physics of the model is not controlled by such behaviour. In one dimension we can use the order along the chain to 'rationalize' the mathematics and this is the reason for the 'success' of our analysis. As well as our labelling scheme becoming less useful, the way in which the spin wavefunction changes becomes much more subtle. The desire to pick up phases when circling loops changes dramatically as particles come close to other particles. The spin wavefunction becomes a fairly strong function of the local charge configuration. This effect has two results: firstly it becomes much more difficult to model the spin wavefunction and secondly it becomes much more difficult to tell whether the system is spin–charge separated, because in a free Fermi system the spin wavefunction changes wildly as the electrons move about.

One can still ask whether or not the effects causing the spin–charge separation are strengthened or weakened in limiting towards two dimensions: the enhanced probability for exchange means that the forces driving the state paramagnetic are stronger, but the resulting degree of low-spin correlations attainable is severely reduced, since there are more competing neighbours to try to correlate with. It is non-trivial to try to compare the energy attainable from collective motion with that from independent motion, and we are unable to make progress in two dimensions.

It would not be surprising if Nagaoka's theorem did not survive the thermodynamic limit.

References

[1] Hubbard J 1963 *Proc. R. Soc.* A **276** 238
Long M W 1991 *Int. J. Mod. Phys.* B 5 865
Anderson P W 1987 *Science* **235** 1196
[2] Long M W 1989 *J. Phys. Condens. Matter* **1** 9421
[3] Zhang F C and Rice T M 1988 *Phys. Rev.* B **37** 3759
Emery V J and Reiter G 1988 *Phys. Rev.* B **38** 4547
[4] Kanamori J 1963 *Prog. Theor. Phys.* **30** 275
[5] Nagaoka Y 1966 *Phys. Rev.* **147** 393
[6] Nagaev E L 1974 *Phys. Status Solidi* b **65** 11
[7] von der Linden W and Edwards D M 1991 *J. Phys. Condens. Matter* **3** 4917
[8] Putikka W O, Luchini M U and Ogata M 1992 *Phys. Rev. Lett.* **69** 2288
Barbieri A, Riera J A and Young A P 1990 *Phys. Rev.* B **41** 11 697
Trugman S A 1990 *Phys. Rev.* B **42** 6612
[9] Long M W and Zotos X 1993 *Phys. Rev.* B 48 317
[10] Long M W, Castleton C M W and Hayward C A 1994 *J. Phys. Condens. Matter* **6** 481
[11] Long M W, Castleton C M W and Hayward C A 1994 *J. Phys. Condens. Matter* **6** submitted
[12] Shraiman B I and Siggia E D 1988 *Phys. Rev. Lett.* **61** 465