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Ring exchange and the Heisenberg and Hubbard models

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Abstract. We study ring-exchange or cyclic-permutation correlations in one-dimensional quantum spin-half systems. For the Heisenberg model we show numerically that these correlations decay as $\hat{\mathsf{R}}_n \sim 1/\sqrt{n}$, although we can deduce nothing about any possible important logarithmic corrections. As such, ring-exchange correlations are much longer range than the more commonly considered spin–spin correlation functions. By considering the relationship between solitonic excitations and cyclic permutations, we suggest a way to predict the value of J_2/J_1 at which the phase transition between a gapped and gapless phase occurs in the next-nearest-neighbour Heisenberg model, suggesting $J_2 = 4J_1$ as the exact transition point. For the Hubbard model with a spin–charge-separated solution, we show that the occupation number, n_k, is a 'convolution' of the cyclic-permutation correlations of the spin ground state with the *anyonic* occupation number of the charge ground state, with the integration being over statistical phase. We deduce the one-eighth singularity previously found for the $U = \infty$ Hubbard model using this new route.

We show that for the limit where nearest-neighbour hopping dominates longer-range hopping in the $U = \infty$ Hubbard model, the single-particle correlation function, n_k, for an infinitesimal concentration of holes in a half-filled system, is identical to the Fourier transform of the cyclic-exchange correlations of the corresponding spin wavefunction. For the elementary t_1–t_2 model, we show a relationship between the singularity which occurs at the Fermi surface, the so-called Luttinger-liquid singularity, and the long-range Heisenberg-model cyclic-permutation correlations.

1. Introduction

The role of quantum mechanics in spin physics has entertained the last generation of many-body theorists. The one-dimensional Heisenberg model has been solved using the Bethe *ansatz* [1], and the low-temperature physics of the model has been successfully understood by a combination of field-theoretic [2] and conformal-invariance [3] ideas. Even provided with these results, it is still not easy to interpret the 'behaviour' of the Heisenberg model. There is certainly a divergence in the sublattice magnetization, since the spin–spin correlations decay as $\boldsymbol{S}_n \cdot \boldsymbol{S}_{i+n} \sim (-1)^n (\ln n)^{1/2}/n$, and there are low-energy 'spin-wave'-like excitations, and so one might like to interpret the behaviour using classical ideas. Alternatively, there are also solitonic spin-half excitations [4], and one might like to try to interpret the behaviour using this 'spinon' route. Which description is more relevant?

Due to the enormous degree of attention devoted to classical magnetism, the natural methods of interpretation are well known, to the extent that they are even taught in undergraduate physics. The same cannot be said for the solitonic description, which remains a mystery to all but many-body theorists. We would like to suggest that the central 'tool' for studying solitons in quantum spin systems is the *cyclic permutation*, which plays the analogous role to the spin–spin correlation function in classical magnetism.

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Cyclic permutations or ring exchanges involve sliding a contiguous set of spins either one atom to the right or one atom to the left. The 'displaced' spin, which would be 'overwritten' by the move is replaced in the gap left at the other end. If one thinks about total-spin conservation, then one is led to believe that this is the *simplest* operation which allows 'sliding' motion of the spins subject to a total-spin-conservation constraint.

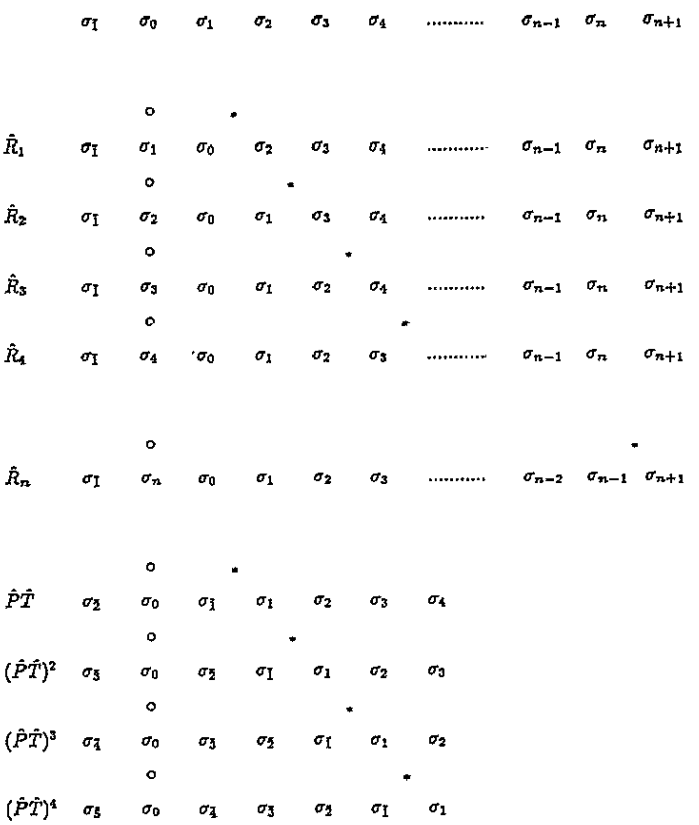

Figure 1. The action of the cyclic permutation and related operators on an arbitrary spin state, as a function of range. The domain walls created are marked by $*$ and $\circ$.

The action of cyclic-exchange permutations is depicted in figure 1. An extraneous spin (marked by $\circ$) is extracted and moved, leaving a pair of spins originally at second neighbour now at nearest neighbour (denoted by $*$). As the *range* of the cyclic permutation is increased, so these two distortions are separated. A related operation is depicted below, for which the same pair of second neighbours is sequentially separated, although now the extraneous spin is placed between variable partners. The Fourier transform of the *range* of cyclic-permutation correlations should give information about the motion of these defects.

If we consider the saturated Néel state, then we are immediately led to some interpretation: although the spin–spin correlations are long range, the cyclic-permutation correlations all *vanish* identically. The action of the cyclic-permutation operators is to insert a finite region of Néel state with the sublattices reversed, states automatically orthogonal to the original. Together with this region are necessarily the two phase boundaries between

the two different Néel orderings. These 'domain walls' play the role of the solitons in the classical limit, and our cyclic permutations create these 'excitations' in pairs. As the range of the cyclic permutation diverges, so the domain walls are pushed further apart, and so we might expect information about the solitons from the long-range behaviour of the cyclic permutations.

If we consider the totally quantum-mechanical dimer state [5], then we are led to complementary intuition: the spin–spin correlations vanish identically once we go beyond nearest neighbours, whereas the cyclic permutations decay much more slowely although still exponentially. Since each spin is correlated only with one of its nearest neighbours, it is easy to understand the lack of spin–spin correlations. The cyclic permutations, however, once again insert a finite region of the second phase into the ground state, creating a pair of domain walls. At first sight, one might have expected the cyclic-permutation correlations to vanish for the same reason as for the Néel state, but the two ground states are not *locally* orthogonal and so we still obtain some correlations. We will interpret the cyclic-permutation correlations as 'creation' operators for domain walls, and so we will expect them to measure the number of domain walls in the ground state. Since there is a finite gap to excitations in the dimer Hamiltonian, we would expect a finite number of domain walls, but if the gap were to close we would expect the domain walls to proliferate. We will exhibit a lot of numerical evidence for this picture.

The spin–spin correlations and cyclic-permutation correlations measure complementary properties: when there is order in the system and the excitations are local 'spin-wave'-like excitations then the spin–spin correlations are long range and the cyclic-permutation correlations vanish. When the 'order' in the system is lost, we believe that it is caused by a proliferation of solitonic excitations, and so the spin–spin correlations become short range while the cyclic-permutation correlations become dominant. Of course, things are not quite as straightforward as this, since there is always a sublattice magnetization divergence in the gapless phase, and it is really only the amplitude that vanishes when the order is lost. Similarly, as we shall see, the long-range aspects of the cyclic-permutation correlations are also always singular in the gapless phase, although their amplitude becomes *larger* as the magnetization vanishes. Once a gap appears, we would expect *both* types of correlation to exponentially decay, since the excitations are somehow related to this behaviour [6].

The picture we wish to paint is that of spin–spin correlations measuring the number of spin-wave-like excitations in the system while cyclic-permutation correlations measure the number of solitonic excitations, both in a rather loose sense. If the system has a phase transition associated with a softening of the solitonic excitations, then this shows up in the long-range characteristics of the cyclic-permutation correlations, whereas if the system has a phase transition associated with a softening of the spin waves, then this shows up in the long-range characteristics of the spin–spin correlations. We will look at the phase transition in the J_1–J_2 model with just this interpretation in mind.

Together with this rather pure interpretation of one-dimensional quantum spin physics, we will also make a connection to quantum-charge physics, and in particular the infinite-U Hubbard model. When electrons move around in quasi-one-dimensional systems, longer-range hopping involves an electron passing over a variable number of intermediate electrons in its motion. If we consider a spin–charge-separated description, where we describe the spin wavefunction along some chosen ordering independently from the position of the 'holes' in the system, then a longer-range hop involves the spin on the electron that is being bodily-moved changing its position down the spin wavefunction combined with a shunt of all the intermediate spins by one electron position to compensate: this process is just a cyclic permutation of the spin system. As far as the spin system is concerned, $\sum_\sigma \langle c^\dagger_{i\sigma} c_{i'\sigma} \rangle$ is

composed of cyclic permutations on the spin system combined with probabilities of the number of spins involved which come from the charge motion; that is a sort of convolution of the ring-exchange correlations over the charge correlations [7]. The quantity n_k, the single-particle occupation number, is the Fourier transform of these hopping correlations and as such is directly related to the Fourier transform of the cyclic-permutation correlations.

If we consider a single hole in an otherwise half-filled system, then presuming that there is no spatial symmetry breaking, that is the hole is equally likely to be found anywhere, then the charge wavefunction is *uniform*. Under this restriction n_k is almost exactly the Fourier transform of the cyclic-permutation correlations, as we shall show. The Luttinger-liquid singularity at the Fermi surface, which is found in spin–charge separated systems [8], is therefore directly related to the cyclic-permutation correlations found in the spin wavefunction. We will try to elucidate this relationship.

In section 2 we will look at cyclic permutations in quantum-spin physics, using the J_1–J_2 Heisenberg model as a concrete example. In section 3 we will look at cyclic permutations in spin–charge-separated systems, using the t_1–t_2 infinite-U Hubbard model as a concrete example. In section 4 we will conclude.

2. Quantum spin systems

2.1. Numerical approximations

This article involves numerical attempts to find power laws. For the free-fermion gas, we have accurate calculations for ranges over hundreds of atoms, and we give convincing evidence. For other situations we use the Lanczos algorithm on small (26-site) clusters and are not very convincing. We employ various elementary fitting procedures which are all relatively stable, but which do *not* yield accurate results. *If* the quantity has a power-law behaviour, then it is likely that we will pick up the exponent with an error of order 10% . We do not go to long range in real space, and so any long-range phenomena are *not* predicted well. Do not believe all you read!

2.2. Some mathematical ideas

Although we could start out with some calculations, indicating the type of result we desire to 'establish', instead we will start out with some relatively obscure mathematical relationships which we believe to be relevant.

Our first task is to select some relevant objects to work with: we have chosen the translation operator, $\hat{\mathbf{T}}$ say, and the transposition operator which permutes the two spins on atom zero and atom one, $\hat{\mathbf{P}} \equiv \frac{1}{2} + 2\hat{S}_0 \cdot \hat{S}_1$ say. We will be concerned with periodic translationally invariant systems, and so we will assume $[\hat{\mathbf{H}}, \hat{\mathbf{T}}] = 0$, that is that we can work with eigenstates of the translation operator which from Bloch's theorem can be chosen to have eigenvalues the phase e^{iQ}, and that $\hat{\mathbf{T}}^N = 1$, where N is the number of atoms in the system. In terms of these objects and assumptions it is quite straightforward to define the quantities of interest to us.

The cyclic-permutation operators, $\hat{\mathbf{R}}_n$ say, can readily be found in terms of $\hat{\mathbf{T}}$ and $\hat{\mathbf{P}}$. The operators which transpose the spins on atoms n and $n+1$ are just $\hat{\mathbf{P}}_n \equiv \frac{1}{2} + 2\hat{S}_n \cdot \hat{S}_{n+1} = \hat{\mathbf{T}}^n \hat{\mathbf{P}} \hat{\mathbf{T}}^{-n}$, and in terms of these the cyclic-permutation operators are, $\hat{\mathbf{R}}_n = \hat{\mathbf{P}}_0 \hat{\mathbf{P}}_1 \cdots \hat{\mathbf{P}}_{n-2} \hat{\mathbf{P}}_{n-1}$, where the spin on the nth atom is carried sequentially along the

chain to the origin. Writing the product down yields

$$\hat{\mathbf{R}}_n = \left[\hat{\mathbf{P}}\hat{\mathbf{T}}\right]^n \hat{\mathbf{T}}^{-n}. \tag{2.1}$$

There is a 'strange' sort of quasiperiodicity inherent to the cyclic-permutation opertors, since $\hat{\mathbf{R}}_{N-1} = \hat{\mathbf{T}}$, and so $\left[\hat{\mathbf{P}}\hat{\mathbf{T}}\right]^{N-1} = 1$. Sensible choices of Bloch phase involve $e^{i(N-1)k} = \pm 1$, quite different to the eigenvalues of $\hat{\mathbf{T}}$.

The first quantity of interest to us is the Fourier transform of the spin–spin correlation functions. This can be found directly from the state obtained by applying the spin operator from the atom at the origin to the ground state:

$$S_k \equiv \sum_{n=1}^{N} e^{ink} \langle Q|\hat{S}_0 \cdot \hat{S}_n|Q\rangle = \langle Q|\hat{S}_0 \left[\sum_{n=1}^{N} e^{in(k-Q)}\hat{\mathbf{T}}^n\right] \hat{S}_0|Q\rangle. \tag{2.2}$$

The second quantity of interest to us is the Fourier transform of the cyclic-permutation correlation functions. Once again we can obtain this quantity directly:

$$R_k \equiv \sum_{n=1}^{N-1} e^{ink} \langle Q|\hat{\mathbf{R}}_n|Q\rangle = \langle Q| \left[\sum_{n=1}^{N-1} e^{in(k-Q)} \left[\hat{\mathbf{P}}\hat{\mathbf{T}}\right]^n\right] |Q\rangle. \tag{2.3}$$

Although at first sight these two results look similar, there are some important differences. Firstly, the periodicity is different. Secondly, the spin–spin correlations involve 'fixing' a spin on a special site and then comparing it with other sites, whereas the cyclic-permutaion correlations are quite direct.

We have reached the point of our mathematical digression: both Fourier transforms can be written down in terms of a geometric sum of *unitary* operators, and divergences in these quantities must involve 'significant' components of either $\hat{S}_0|Q\rangle$ being an eigenstate of $\hat{\mathbf{T}}$, or $|Q\rangle$ being an eigenstate of $\hat{\mathbf{P}}\hat{\mathbf{T}}$.

2.3. The x–y model

Although this model is peripheral, the 'simplicity' of the solution has led us into devoting much energy to its analysis. The model is

$$H = J \sum_n \hat{S}_n^{\perp} \cdot \hat{S}_{n+1}^{\perp} = \frac{J}{2} \sum_n \left[b_n^{\dagger} b_{n+1} + b_{n+1}^{\dagger} b_n\right] \tag{2.4}$$

in terms of the spin perpendicular to the z-direction, $\hat{S}_n^{\perp}$, and hard-core boson operators $b_n^{\dagger}$. Unlike the Heisenberg model, the sign of J is irrelevant and the model simultaneously describes in-plane ferromagnetism or antiferromagnetism. Since the particles cannot exchange, we can use either type of statistics. The hard-core constraint leads to an immediate exact solution if fermionic statistics [9] are used. Since the exact solution is the non-interacting free-electron gas, we can evaluate all correlation functions, in principle, in terms of single-particle correlation functions. We attempt such analytic calculations and then

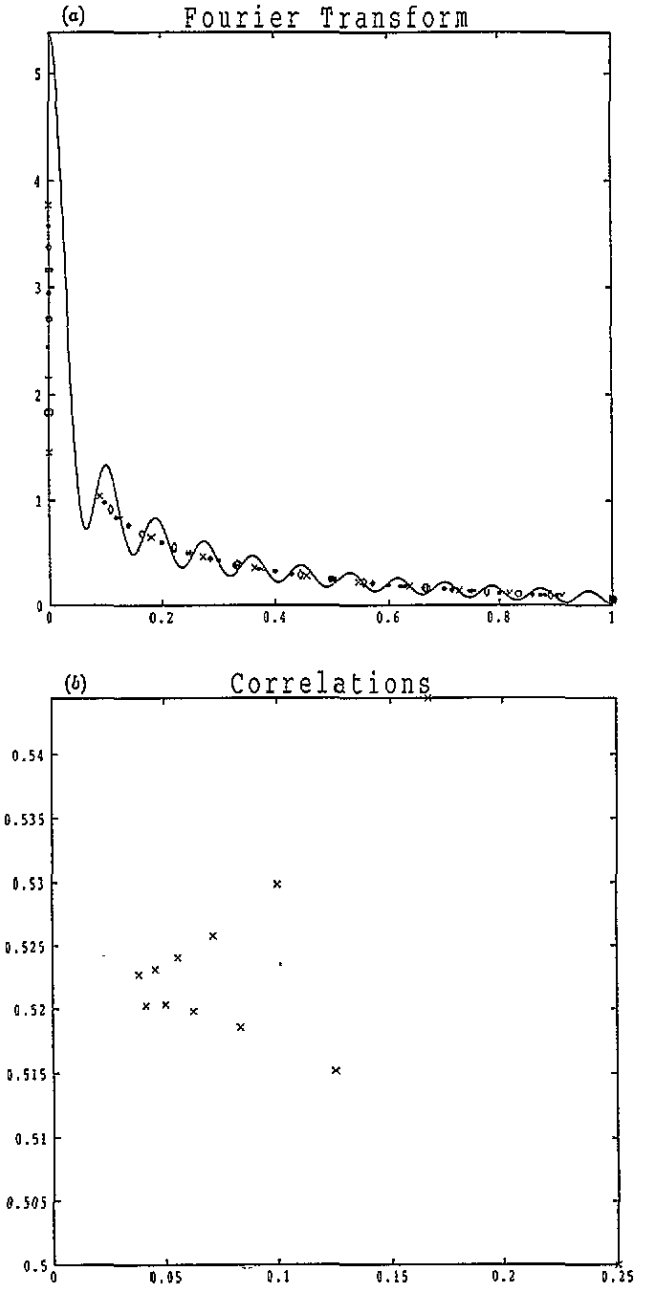

Figure 2. A mixture of analytical and finite-size exact diagonalization calculations for the spin–spin correlation functions of the one-dimensional x–y model. (*a*) The Fourier transform of the spin–spin correlations, $\sum_n e^{i\pi kn}\hat{S}_0 \cdot \hat{S}_n$, with many small systems superimposed (symbols) and the exact result truncated (solid line). (*b*) Finite-size scaling of the spin–spin correlations *diametrically across the loop*, $\hat{S}_0 \cdot \hat{S}_{N/2} \times N^{1/2}$, *as a function of inverse loop length*, N.

compare them with exact-diagonalization studies in order to test our predictive power with the computer.

The spin–spin correlations are straight forward to evaluate, if we note that

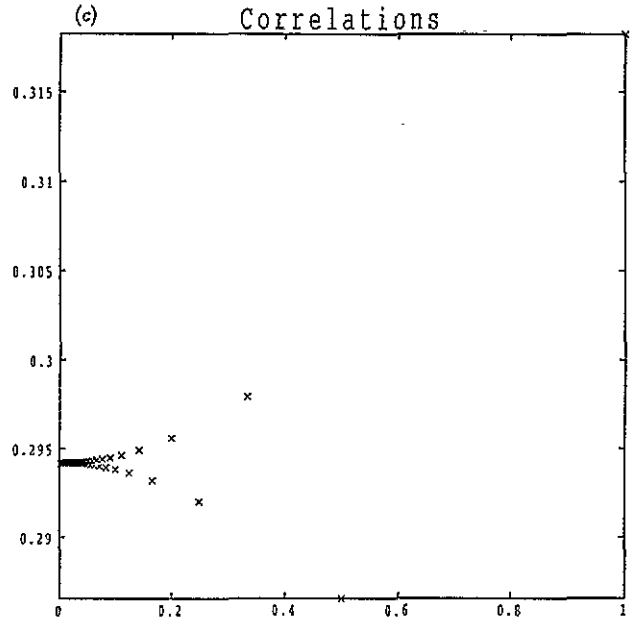

Figure 2. (*Continued.*) (*c*) Plot of the exact spin–spin correlations, $\hat{S}_0 \cdot \hat{S}_n \times n^{1/2}$, as a function of inverse range, n. If we have correctly chosen the power law, our plots should converge to a finite constant.

$$\langle b_0^\dagger b_n \rangle = \left\langle f_0^\dagger f_n \prod_{m=1}^{n-1} (1 - 2 f_m^\dagger f_m) \right\rangle \tag{2.5}$$

where $f_m^\dagger$ are the associated fermionic operators. This fermionic quantity can be evaluated as an $n \times n$ determinant, which can be found numerically for ranges of up to about 500 lattice spacings. In figure 2 we plot various spin–spin correlation quantities. The Fourier transform has a diverging peak at the origin, for the ferromagnetic case, which appears to come from a slow decay, $\hat{S}_0 \cdot \hat{S}_n \sim 1/n^{1/2}$, for the correlation functions. We have finite-size scaled the correlation function diametrically across the ring for our exact-diagonalization calculations, in the same way that we do for our later, less well controlled models. We plot the exact correlations, as deduced from our determinant calculations, for comparison and the two calculations agree very well. The numerical determinant calculations indicate that $\hat{S}_0 \cdot \hat{S}_n \sim 1/n^{1/2}$ is almost certainly exact, and has only negligible spatial corrections, that is no extraneous additional subdominant power laws.

The cyclic-permutation calculations are by no means as simple: it has proven impossible to find a representation for these correlation functions in terms of a single determinant. A representation which at first sight looked useful is

$$\langle R_n \rangle = \prod_{m=0}^{n-1} \left[\frac{\sqrt{5}+1}{2} - b_j^\dagger b_{j+1} - b_{j+1}^\dagger b_j \right] \left[\frac{\sqrt{5}-1}{2} + b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right] \tag{2.6}$$

but we could only make progress with

$$\langle R_n \rangle = \sum_{\chi^1=0}^{1} \cdots \sum_{\chi^{n-1}=0}^{n-1} \prod_{m=0}^{n-1} \left[\frac{1}{\sqrt{3}+1} + b_{m+\chi^m}^\dagger b_{m+1-\chi^m} \right] \left[\frac{1}{\sqrt{3}-1} - b_{m+1-\chi^m}^\dagger b_{m+\chi^m} \right]. \tag{2.7}$$

Obviously, the final representation involves 2^n $n \times n$ determinants and is therefore impressively computationally expensive. There is a second method for evaluating these correlation functions which is much less expensive numerically. It is based on the operators

$$\hat{\mathbf{P}}_{r,r+1} \equiv 1 - (f_r^\dagger - f_{r+1}^\dagger)(f_r - f_{r+1}) + 2f_r^\dagger f_r f_{r+1}^\dagger f_{r+1} \tag{2.8a}$$

$$\hat{\mathbf{A}}_{r,r+1} \equiv 1 - (f_r^\dagger - f_{r+1}^\dagger)(f_r - f_{r+1}) \tag{2.8b}$$

in terms of which we can rerepresent

$$\hat{\mathbf{R}}_n = \prod_{m=0}^{n-1} \hat{\mathbf{A}}_{m,m+1} + 2\sum_{r=0}^{n-1}\prod_{m=0}^{r-1} \hat{\mathbf{P}}_{m,m+1} f_r^\dagger f_r f_{r+1}^\dagger f_{r+1} \prod_{m'=r+1}^{n-1} \hat{\mathbf{A}}_{m',m'+1} \tag{2.9a}$$

which, using the commutation relations of the $f^\dagger$ collapses down to

$$\hat{\mathbf{R}}_n = \prod_{m=0}^{n-1} \hat{\mathbf{A}}_{m,m+1} + 2\sum_{r=0}^{n-1} f_0^\dagger(f_1 + f_0) f_1^\dagger(f_2 + f_1)\cdots f_{r-1}^\dagger(f_r + f_{r-1}) f_r^\dagger f_r$$
$$\times f_{r+1}^\dagger f_{r+1}(f_{r+1}^\dagger - f_{r+2}^\dagger) f_{r+2}\cdots(f_{n-1}^\dagger - f_n^\dagger) f_n \tag{2.9b}$$

each term of which can be independently evaluated as a determinant. This representation yields one $n \times n$ determinant and n different $(n+1) \times (n+1)$ determinants and a corresponding saving in computer time. In figure 3 we plot the corresponding quantities for cyclic permutations as we did for spin–spin correlations. We plot both the real part and the imaginary part, which are derived from different Q-values, which in turn correspond to different boundary conditions for cyclic-permutation 'periodicity'. It appears that the cyclic-permutation correlations decay rather faster than the spin–spin correlations, with a $\langle R_n \rangle \sim 1/n^{5/8}$ power law. The divergence is associated with the k-point half-way to the zone boundary, the 'Fermi surface' of the model. Once again, the accuracy that we can reach numerically indicates that $\langle R_n \rangle \sim 1/n^{5/8}$ is exact, but for this case there are clear subdominant power laws in the scaling.

For the current model, we would like to deduce that the classical spin-wave-like excitations are more relevant than the solitonic excitations. When we include longer-range hopping, this result is much less obvious, because the model changes its characteristics, developing a gap and eventually yielding a dimer ground state when $x \equiv J_2/J_1 = \frac{1}{2}$. For situations where the cyclic permutations are dominant, we are proposing that the phase transition to a gapped state occurs when the cyclic-permutation divergence is maximal. If the phase transition to the gapped phase is to be controlled by the solitons in the x–y model, then as the value of x is increased, we would require that the roles of the two types of correlations should reverse, and that the cyclic permutations should become dominant. Numerically this assertion appears to be confirmed.

If we consider the structure of the dispersion for excitations, it is easiest to believe that the phase transition is associated with a softening of the linear dispersion at the 'Fermi surface' to a quadratic dispersion which then 'lifts' off. The expected fluctuations in the ground state would be expected to be maximal at the phase transition, becoming *finite* in the gapped phase. In figure 4 we finite-size scale the value of the ratio x which corresponds to the maximum value of the cyclic-exchange correlations at the 'Fermi surface', that is the singular point. It is quite easy to believe that this maximum occurs at $x = \frac{1}{3}$. We will mention the state found at $x = \frac{1}{3}$ again later.

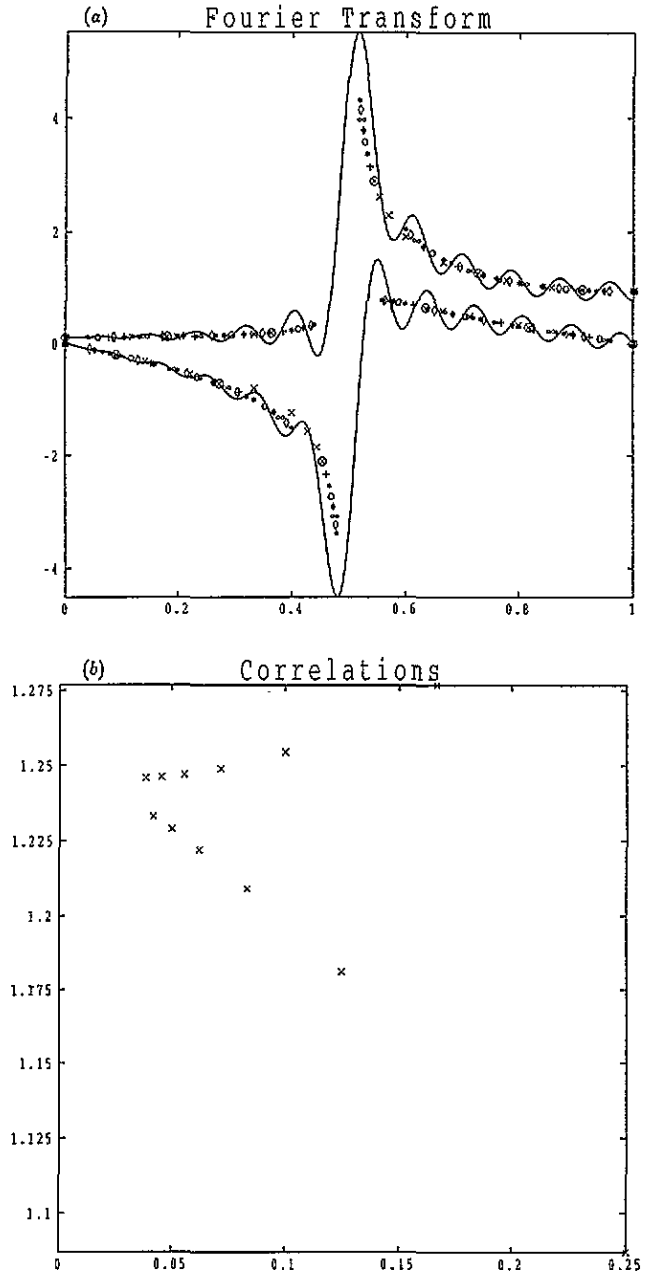

Figure 3. A mixture of analytical and finite-size exact diagonalization calculations for the cyclic-permutation correlation functions of the one-dimensional x–y model. (*a*) The real and imaginary parts of the Fourier transform of the cyclic-permutation correlations, $\sum_n e^{i\pi kn}\hat{\mathbf{R}}_n$, with many small systems superimposed (symbols) and the exact result truncated (solid line). (*b*) Finite-size scaling of the cyclic-permutation correlations diametrically across the loop, $\hat{\mathbf{R}}_{N/2} \times N^{5/8}$, as a function of inverse loop length, N.

2.4. The long-range cyclic-permutation model

Due to the attention lavished on the classical Néel state, we know a lot about the spin–spin

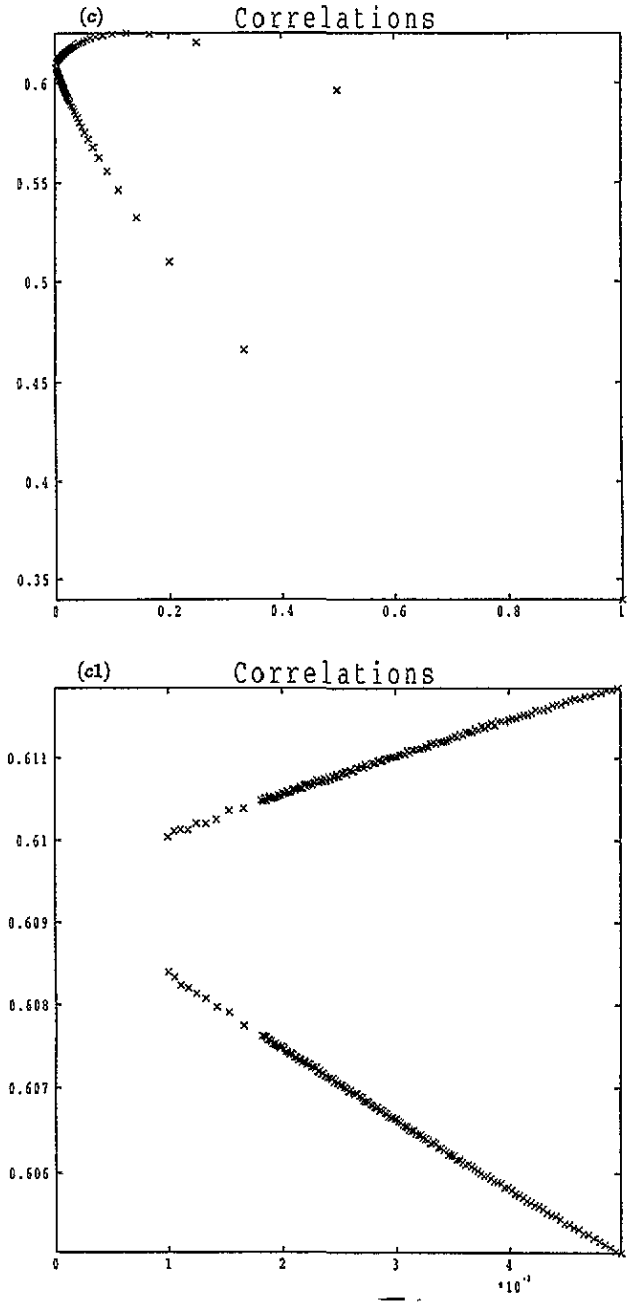

Figure 3. (*Continued.*) (*c*) Plot of the exact cyclic-permutation correlations, $\hat{\mathbf{R}}_n \times n^{5/8}$, as a function of inverse range, n. If we have correctly chosen the power law, our plots should converge to a finite constant.

correlations, even in the quantum-dominated systems. The same is not true for cyclic-permutation correlations. Even for a quantum system there is a total-spin-singlet analogue to the Néel state: we make the two natural sublattices have maximal spin and then add these spins together to form a total-spin singlet. The spin–spin correlations for such a state

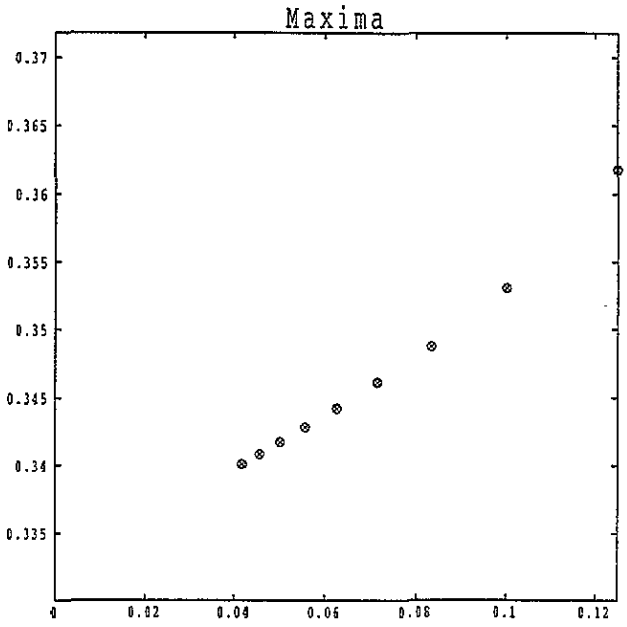

Figure 4. A finite-size-scaling calculation of the value of $x \equiv J_2/J_1$ at which the Fourier transform of the cyclic-permutation correlations calculated half-way to the zone boundary is maximum. The scatter comes from numerical inaccuracy, since this quantity is expensive to calculate numerically. It is easy to believe that this curve converges to $\frac{1}{3}$.

do not decay at all, simply oscillating between $\pm\frac{1}{4}$. This state constitutes the longest-range spin–spin correlations for a total-spin singlet. Which state yields the longest-range cyclic-permutation correlations for a total-spin singlet, and is there the equivalent of long-range order?

In order to gain some insight into the question of maximal range for cyclic-permutation correlations, we have studied the long-range Hamiltonian composed of the two Fourier components of the cyclic-permutation operators corresponding to $k = \pm k_f$:

$$H_{\pm} = \sum_{jn} \left[\mathrm{i}^{\pm n} \hat{\mathbf{R}}_{j;n} + \mathrm{cc} \right] \tag{2.10}$$

where $\hat{\mathbf{R}}_{j;n}$ is the cyclic exchange operator for $n+1$ particles starting at site j, and the $\pm$ degree of freedom corresponds to the two possible k-points and can be absorbed into a judicious choice of boundary conditions for a periodic system, since the real part and imaginary part of the Hamiltonian can usually be chosen to be proportional to each other. The fundamental cause of this simplification is that

$$\hat{\mathbf{R}}_{N-1} = \left[\hat{\mathbf{P}} \hat{\mathbf{T}} \right]^{N-1} \hat{\mathbf{T}}^{1-N} = \hat{\mathbf{T}}$$

and therefore that for a Bloch state the $\hat{\mathbf{R}}_n^{-1} \sim \mathrm{e}^{\mathrm{i}\phi} \hat{R}_{N-n-1}$ and for an even-membered loop, odd-length cyclic permutations have even-length cyclic permutations as their inverses, yielding a relationship between the real and imaginary parts.

It is straightforward to use exact diagonalization on finite systems, and we find a total-spin-singlet ground state reminiscent of the nearest-neighbour Heisenberg model ground

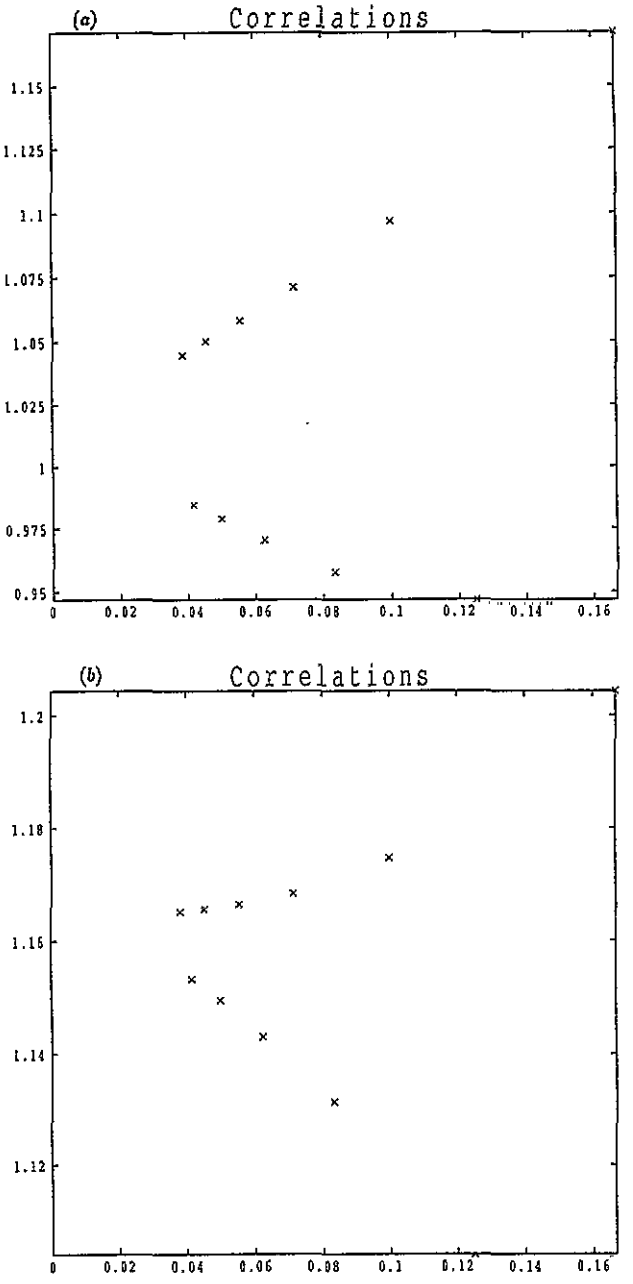

Figure 5. Finite-size-scaling calculations, using exact diagonalization for the long-range cyclic-permutation model, of (*a*) the spin–spin correlations diametrically across the ring $\hat{S}_0 \cdot \hat{S}_{N/2} \times N$ as a function of inverse loop length, N, and (*b*) the cyclic-permutation correlations diametrically across the ring $\hat{\mathsf{R}}_{N/2} \times N^{1/2}$ as a function of inverse loop length, N.

state. In figure 5 we finite-size scale both the spin–spin correlations and the cyclic-permutation correlations for the case of permutations diametrically across the loop. The spin–spin correlations are best fitted by a $S_n \sim 1/n$ power law, whereas the cyclic-exchange correlations are best fitted by a $R_n \sim 1/n^{1/2}$ power law.

It would appear that it is *impossible* to achieve long-range cyclic-permutation 'order'. The longest range would appear to be square-root decay. It should also be observed that in comparison to the x–y model, the role of the two types of correlation has *reversed*, with the cyclic-permutation correlations now being longer range.

2.5. *The J_1–J_2 Heisenberg model*

In this section we will look at the relationship between the cyclic-permutation correlations and the phase transition which is known to exist in the J_1–J_2 Heisenberg model.

A lot is known about two particular cases of this model: firstly, the case $J_2 = 0$ has been solved using the Bethe *ansatz* and the spin–spin correlations have been deduced from the continuum limit [2]. Secondly, the case $J_1 = 2J_2$ is trivially solvable [5] by a pure dimer state and most correlation functions can be calculated immediately. The nearest-neighbour Heisenberg model has a $1/n$ spin–spin correlation decay with logarithmic corrections, and the dimer state has exponential decay for both spin–spin and cyclic-permutation correlations. These results are consistent, in our interpretation scheme, with the nearest-neighbour Heisenberg model being gapless and the Hamiltonian yielding the dimer ground state having a gap. Somewhere in between these two systems the gap must open up at a phase transition.

Our first problem is that we do not know the behaviour of the cyclic-permutation correlations in the nearest-neighbour Heisenberg model. In figure 6 we finite-size scale these correlations yielding a prediction of a $1/n^{1/2}$ power law, much slower than the spin–spin correlations. Surprisingly, we find similar results to the long-range model and quite dissimilar results to the x–y model. We would naturally like to conclude that the low-energy excitations are quite different for the two models.

The spin–spin correlations for the Heisenberg model are problematic. Unlike the long-range model, a simple $S_n \sim 1/n$ power law is inappropriate; there are logarithmic corrections [10]. Unfortunately, our best fit is given by $S_n \sim (\ln n)^{1/4}/n$, the *wrong* logarithmic correction. We do not understand this anomaly at present. This result has been found previously in Monte Carlo simulations [11], but at that time there was no field-theory prediction to cause concern.

When we start to consider a prediction for where the phase transition might occur, we are led to a very surprising result. Unlike the x–y model, where the value of J_2/J_1 at which the maximum of $R_{k=k_F}$ occurs varies as a function of loop-size, $R_{k=k_F}$ is a maximum *exactly* when $J_1 = 4J_2$ for all loop sizes. A possibly related fact is that when $4J_2 = -J_1 > 0$ there is an exact degeneracy between a maximum-spin state and a minimum-spin state for all values of loop size, yielding another phase transition in the system. We believe that the phase transition in this Heisenberg model occurs exactly when $J_1 = 4J_2$.

When we look at this special value of the parameters, we see another fairly surprising fact: the solution to the Heisenberg model is almost identical to the solution of the long-range cyclic-permutation model of the preceeding section. The correlation functions for our largest system (26 sites) agree to 0.01% for example, and the overlap between the long-range ground state and the $J_1 = 4J_2$ ground state is 0.99996!

If we return briefly to the x–y model, then a study of the special case when $J_1 = 3J_2$, that is the point at which we predict the phase transition, once again we find a state very similar to the long-range-model ground state, with correlation-function agreement to about 2% for our largest system (26 sites).

We would suggest that these phase transitions to a gapped phase are all the same phenomenon, being controlled by proliferation of solitonic spin excitations. The natural correlation functions to study are the cyclic permutations, and power-law singularities in

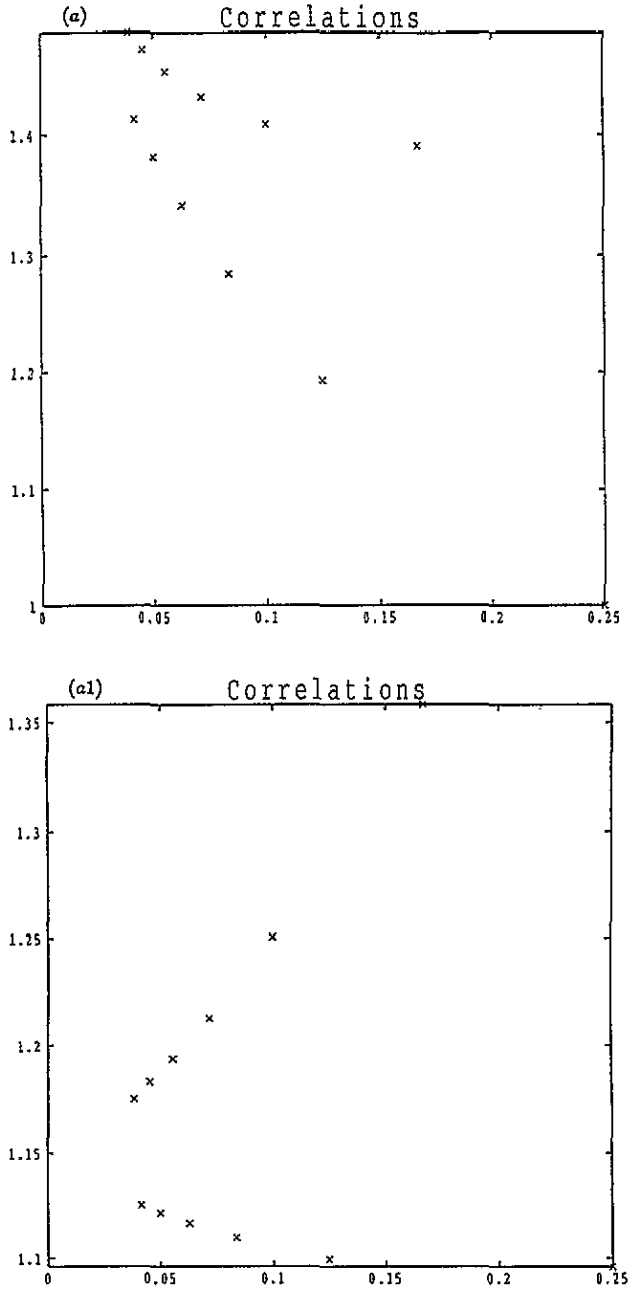

Figure 6. Finite-size-scaling calculations using exact diagonalization for the nearest-neighbour Heisenberg model. (*a*) The spin–spin correlations diametrically across the ring $\hat{S}_0 \cdot \hat{S}_{N/2} \times N$ as a function of inverse loop length, N. (*a*1) $\hat{S}_0 \cdot \hat{S}_{N/2} \times N/(\ln(N/2))^{1/4}$, as a function of inverse loop length, N. The power $\frac{1}{4}$ should be $\frac{1}{2}$.

these quantities control the physical behaviour. The phase transition itself may have an as-yet unprobed relationship to the long-range model that we considered.

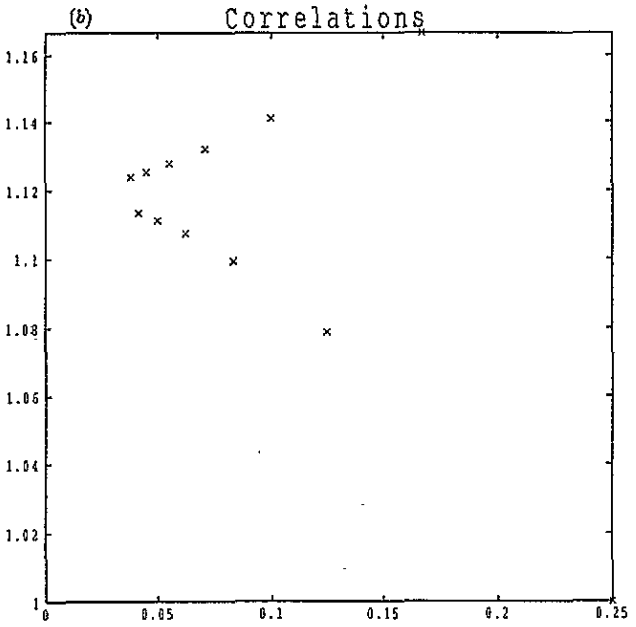

Figure 6. (*Continued.*) (*b*) The cyclic-permutation correlations diametrically across the ring $\hat{\mathbf{R}}_{N/2} \times N^{1/2}$ as a function of inverse loop length, N.

3. Hubbard models and cyclic permutations

The relevance of cyclic permutations to the Hubbard model comes from a particular representation of the Hubbard model which is of use when the ground state is 'spin–charge separated': the idea is that the spin degrees of freedom and the charge degrees of freedom decouple leading to 'independent' excitations. In one dimension, where this behaviour is best understood, we can use the order of the electrons along the chain to label the spin degrees of freedom, a labelling which does not change in the fast 'concertinaing' of electrons, but only in the slow exchange processes where the order of the electrons changes. The basis we use is

$$c^{\dagger}_{i_1\sigma_1} c^{\dagger}_{i_2\sigma_2} \cdots c^{\dagger}_{i_n\sigma_n} |0\rangle \equiv f^{\dagger}_{i_1} f^{\dagger}_{i_2} \cdots f^{\dagger}_{i_n} |\sigma_1\sigma_2\cdots\sigma_n\rangle \tag{3.1}$$

where $c^{\dagger}_{i\sigma}$ create the original electrons, $f^{\dagger}_{i}$ are fermion creation operators for the charge only, and n is the total number of electrons. In terms of this we can write down a general state as

$$\sum_{\chi^1=0}^{1} \cdots \sum_{\chi^N=0}^{1} C_{\chi^1\cdots\chi^N} \prod_{i=1}^{N} \left[f^{\dagger}_{i} \right]^{\chi^i} |0\rangle \sum_{\sigma_1} \cdots \sum_{\sigma_n} \hat{S}^{\chi^1\cdots\chi^N}_{\sigma_1\cdots\sigma_n} |\sigma_1 \cdots \sigma_n\rangle \tag{3.2}$$

where N is the total number of atoms, χ_j are variables which 'count' whether or not an electron is present on a site, $n = \sum_{i=1}^{N} \chi^i$ ensures that we have the correct number of electrons, C_{χ} is a charge wavefunction which does *not* depend on spin, and $\hat{S}^{\chi}_{\sigma}$ is a spin wavefunction which does (in general) depend on the charge configuration. *This*

representation is quite general, and we can write down the original hopping amplitudes in this basis:

$$c_{i\sigma}^{\dagger}c_{i+m\sigma} = f_i^{\dagger}f_{i+m}\sum_{\chi^{i+1}=0}^{1}\sum_{\chi^{i+2}=0}^{1}\cdots\sum_{\chi^{i+m-1}=0}^{1}\prod_{l=1}^{m-1}\left[f_{i+l}^{\dagger}f_{i+l}\right]^{\chi^{i+l}}\left[1-f_{i+l}^{\dagger}f_{i+l}\right]^{1-\chi^{i+l}}$$
$$\times\frac{1}{2}\left[1+\sigma\hat{S}_{\alpha_i}^{z}\right]\times\hat{\mathbf{R}}_{\alpha_i;\alpha_{i+m}-\alpha_i-1} \tag{3.3}$$

where the χ_l measure whether or not an electron is on a particular site i, and in terms of which the $\alpha_m = \sum_{l=1}^{m}\chi_l$ 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 our cyclic-permutation operator $\hat{\mathbf{R}}_{i;n}$. This representation has been studied before [12].

A 'spin–charge-separated' solution would involve only irrelevant dependence of the spin wavefunction on the charge configuration: although we would expect some differences between the spin wavefunctions, local enhancements of some spin–spin correlations when charges bunch up for example, we would expect each spin wavefunction to have a strong overlap with the others, allowing the charges to move around independently from the spins. Indeed, we can envisage a sort of 'average' spin wavefunction which controls the spin physics, and then irrelevant hybridization into other spin configurations locally, as the charge bunches up, in a very similar manner to the way in which quantum fluctuations 'renormalize' a classical antiferromagnetic solution. If the spin wavefunction did not depend on the charge configuration, then we could evaluate the charge correlation functions, controlled by the $f_i^{\dagger}$, and cyclic-permutation functions independently and form the single-particle correlation functions as a sort of 'convolution'; the strength of the contribution from a particular cyclic permutation depending on the probability of finding the correct number of particles between the hop. We would find

$$\sum_{\sigma}\langle c_{i\sigma}^{\dagger}c_{i+m\sigma}\rangle = \sum_{r=0}^{m-1}\sum_{\chi^{i+1}=0}^{1}\cdots\sum_{\chi^{i+m-1}=0}^{1}\delta\left(\sum_{j=1}^{m-1}\chi^{i+j}-r\right)\langle S|\hat{\mathbf{R}}_r|S\rangle$$
$$\times\langle C|f_i^{\dagger}f_{i+m}\prod_{l=1}^{m-1}\left[f_{i+l}^{\dagger}f_{i+l}\right]^{\chi^{i+l}}\left[1-f_{i+l}^{\dagger}f_{i+l}\right]^{1-\chi^{i+l}}|C\rangle \tag{3.4}$$

where $|C\rangle$ is the charge wavefunction and $|S\rangle$ is the spin wavefunction. For the particular case of the infinite-U Hubbard model when all but the nearest-neighbour hopping is infinitesimal, this result is exact [12].

If we insert the Fourier transform of the cyclic-permutation correlations, then

$$\sum_{\sigma}\langle c_{i\sigma}^{\dagger}c_{i+m\sigma}\rangle = \frac{1}{N}\sum_{q}\langle S|\hat{\mathbf{R}}_q|S\rangle\times\tilde{n}_m(q) \tag{3.5a}$$

with

$$\tilde{n}_m(q) = \sum_{\chi^{i+1}=0}^{1}\cdots\sum_{\chi^{i+m-1}=0}^{1}e^{-iq\sum_{j=1}^{m-1}\chi^{i+j}}\langle C|f_i^{\dagger}f_{i+m}\prod_{l=1}^{m-1}\left[f_{i+l}^{\dagger}f_{i+l}\right]^{\chi^{i+l}}\left[1-f_{i+l}^{\dagger}f_{i+l}\right]^{1-\chi^{i+l}}|C\rangle \tag{3.5b}$$

$$\tilde{n}_m(q) \equiv \langle C|f_i^{\dagger}f_{i+m}\prod_{l=1}^{m-1}\left[1-f_{i+l}^{\dagger}f_{i+l}+e^{-iq}f_{i+l}^{\dagger}f_{i+l}\right]|C\rangle \tag{3.5c}$$

where we recognise the single-particle correlation function for *anyonic* statistics! When our particle is transferred from site $i+m$ to site i, it picks up a phase of $(-1)e^{-iq}$, for each particle passed over. If we choose to work with anyonic particles with statistical phase $e^{i(\pi-q)}$, then this phase would be compensated and we would evaluate $\langle C|\tilde{f}_i^\dagger \tilde{f}_{i+m}|C\rangle$, the single-particle occupancy for anyonic particles. The final Fourier transform yields

$$n_k = \frac{1}{N}\sum_q \langle S|\hat{\mathbf{R}}_q|S\rangle \times \tilde{n}_k(q) \tag{3.6}$$

with each possible statistics being weighted by the relevant component of the cyclic-permutation correlations. This result is quite general and depends only upon the assumption that the spin wavefunction does not depend on the charge wavefunction. Obviously this assumption can only be expected to be true for very long-range correlations in general.

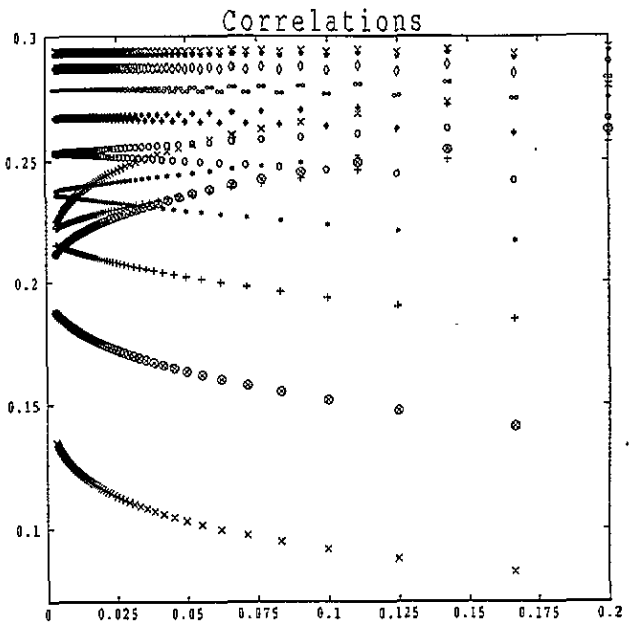

Figure 7. Scaling of $m^{1-q/\pi+1/2(q/\pi)^2} \times |\tilde{n}_m(q)|$ as a function of $1/m$, for the values $q = (0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0)\pi$. The particular choice of band filling is half filled, and the residual long-range oscillation is related to this choice: the 'pairs-of-curves' aspect can be understood from the likelihood of finding odd and even numbers of electrons between the two chosen end-points of the transfer. The fact that all superimposed plots tend to a constant indicates that the power law proposed is correct. The fact that the 'constant' depends on q indicates that there is additional dependence which has not been understood.

For the elementary case of infinitesimal longer-range hopping in the infinite-U Hubbard model, this separation becomes exact, and further the charge wavefunction reduces to that of the spinless-fermion ground state. It is possible to evaluate the relevant anyonic correlation functions as determinants:

$$\tilde{n}_m(q) = a(q)^{m+1} \begin{bmatrix} n_1 & n_2 & n_3 & \cdots & n_{m-1} & n_m \\ n_0 - 1/a(q) & n_1 & n_2 & \cdots & n_{m-2} & n_{m-1} \\ n_1 & n_0 - 1/a(q) & n_1 & \cdots & n_{m-3} & n_{m-2} \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & \cdots & & \\ n_{m-3} & n_{m-4} & n_{m-5} & \cdots & n_1 & n_2 \\ n_{m-2} & n_{m-3} & n_{m-4} & \cdots & n_0 - 1/a(q) & n_1 \end{bmatrix} \tag{3.7}$$

where $a(q) \equiv 1 - e^{-iq}$ and $n_r \equiv \langle f_i^\dagger f_{i+r} \rangle = \sin \pi n_0 r / \pi r$. A numerical analysis of these quantities reveals that

$$\tilde{n}_m(q) \propto \frac{e^{-iqn_0 m}}{m^{1-q/\pi+1/2(q/\pi)^2}} \tag{3.8}$$

which is deduced from figure 7. The phase factor is easy to understand, being the phase picked up from the *average* number of particles between the end-points of the hop, but the power law is difficult to understand. Obviously, fermions ($q = 0$) and bosons ($q = \pi$) yield the correct results as deduced from our previous calculations. The Fourier transform yields

$$\tilde{n}_k(q) \propto |k - n_0 q|^{-q/\pi+1/2(q/\pi)^2} \qquad (q > 0) \tag{3.9}$$

and hence

$$n_k \propto \frac{1}{N} \sum_q \langle S|\hat{\mathbf{R}}_q|S\rangle |k - n_0 q|^{-q/\pi+1/2(q/\pi)^2} \tag{3.10}$$

a 'sort-of' convolution. Our previous analysis of the Heisenberg model suggests that

$$\langle S|\hat{\mathbf{R}}_q|S\rangle \propto \frac{1}{|q - \pi/2|^s} \tag{3.11}$$

with $s = \frac{1}{2}$ for the nearest-neighbour Heisenberg model. This in turn predicts

$$\begin{aligned} n_k &\propto \int \mathrm{d}q \frac{1}{|q - \pi/2|^{1/2}} |k - n_0 q|^{-q/\pi+1/2(q/\pi)^2} \\ &\propto \int \mathrm{d}x |k - n_0 \frac{\pi}{2} - n_0 x^2|^{-3/8 - x^2/2\pi + x^4/2\pi^2} \\ &\propto \left| k - n_0 \frac{\pi}{2} \right|^{1/8} \end{aligned} \tag{3.12}$$

to leading order, in complete agreement with the results previously obtained from field theory [13].

Obviously, for infinitesimal longer-range hopping the charge wavefunction is invariant and so the behaviour of the number occupancy is controlled by the spin wavefunction. The nearest-neighbour Heisenberg model yields $s = \frac{1}{2}$, but as next-nearest-neighbour interactions become important we might expect the power to change. Numerical work suggests that s increases without bound as $-J_2/J_1 \mapsto \infty$, although the numerics are not conclusive.

The only assumption which underpins our results is that the spin wavefunction does not depend on charge. In order to look more closely at this assumption and to make a connection with previous work [14], we have analysed the single-hole problem in some detail.

In this article we will be dominantly concerned with a single hole in the infinite-U Hubbard model. This ensures that the 'number-fluctuation' aspect is irrelevant, since there is only one hole. Enforcing Bloch's theorem then eliminates the charge degrees of freedom completely, and we are left with

$$\sum_{\sigma}\langle c^{\dagger}_{i\sigma}c_{i+m\sigma}\rangle = \frac{(-1)}{N}\langle S^{i+m}|\hat{\mathsf{R}}_{i;m-1}|S^{i}\rangle \tag{3.13}$$

where we have left the dependence of the spin wavefunction on the position of the hole explicit. For this case, the *change* in the occupation number because of the hole is *identically* a Fourier transform of cyclic-permutation operators. The spin wavefunction is no longer translationally invariant, being 'centred' around the hole, however Bloch's theorem on the original system does imply that we find the *same* spin wavefunction for each hole position once the wavefunction has been translated to yield the same position for the hole.

We perform calculations on the t_1–t_2 model with a single hole, evaluating the function n_k from (3.13). We use the *non*-translationally invariant spin wavefunction when necessary. For the limiting cases of $t_1 \mapsto 0$ or $t_2 \mapsto 0$, the hole moves so far in between the minor degeneracy-breaking interactions that there is no point in distorting the spin structure around the hole and we rigorously find a translationally invariant spin state. For the case of $t_2 \mapsto 0$ we find the Heisenberg ground state, and so the relevant cyclic-permutation correlations are *precisely* those of the quantum-spin systems of the previous section. For the case of $t_1 \mapsto 0$ we find a state reminiscent of the Heisenberg ground state but ordered on the Möbius connectivity of a single sublattice [14]. For situations with t_1 and t_2 of similar magnitude, there is a strong local spin distortion in the vicinity of the hole, but this distortion does not appear to spread over a large distance. The spin correlations in the 'background' spin state far from the hole can be long range, and it is to these correlations that we attribute most of the finite-size effects that we have observed.

There is an important difference between the cyclic-permutation Fourier transform relevant to quantum-spin systems and that for the Hubbard model: the hop to nearest neighbours does *not* permute any spins, and so the non-trivial correlations only occur at next-nearest-neighbour hopping. The initial contribution controls the overall shape of the occupation number, forcing the electrons into the best energetic areas for a short-range-hopping model. In figure 8 we plot n_k for the t_1–t_2 model with one additional hole away from half filling, in the limit $t_2 \mapsto 0$ for a system with 26 spins. The singularity at the non-interacting Fermi surface is clearly growing, together with the uniform real-space features that one would anticipate from the energetics. This is the case where the spin wavefunction is translationally invariant and so we find the pure Heisenberg state with the corresponding long-range singularity.

When we consider longer-range hopping for the energetics of the hole, that is $t_2 \not\mapsto 0$, then things change. Firstly, the short-range cyclic-permutation correlations change so as to optimize the relevant energetics. In figure 9 we plot n_k for the opposite limit of $t_1 \mapsto 0$, and it is clearly seen that the periodicity has effectively doubled leading to *four* Fermi points as might be anticipated from the free-electron-gas solution. The divergences still appear to be present. Secondly, it is possible for the spin physics to change completely [14]. In figure 10 we plot n_k for the case $t_2 = 2t_1$, for a system with 22 spins. There is

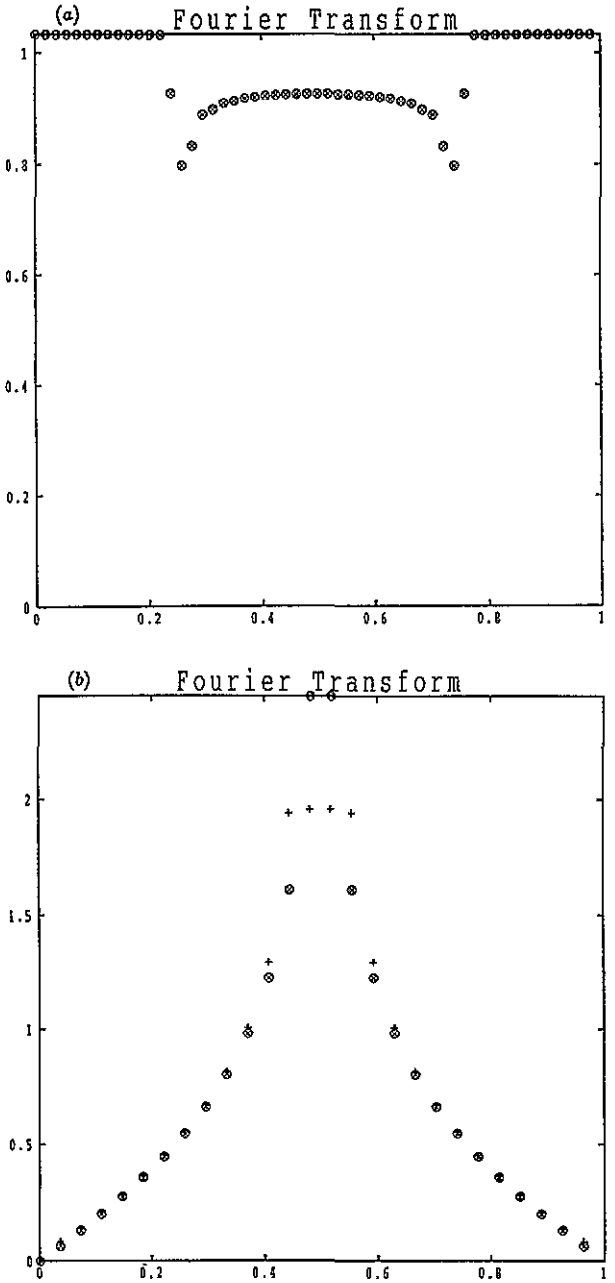

Figure 8. (*a*) The occupation number, n_k, for one full period, and (*b*) the Fourier transform of the spin–spin correlations, also for one full period, for a single hole in the infinite-U t_1–t_2 Hubbard model in the limit that $t_2 \mapsto 0$. We calculated this quantity for a system of 27 atoms and 26 electrons. The calculations have clearly not converged, there being a singularity either half way to the zone boundary, or at the zone boundary.

no long-range contribution, since the spin wavefunction has spontaneous broken symmetry and only short-range correlations present.

We believe that the behaviour of n_k is controlled by cyclic-permutation correlations in

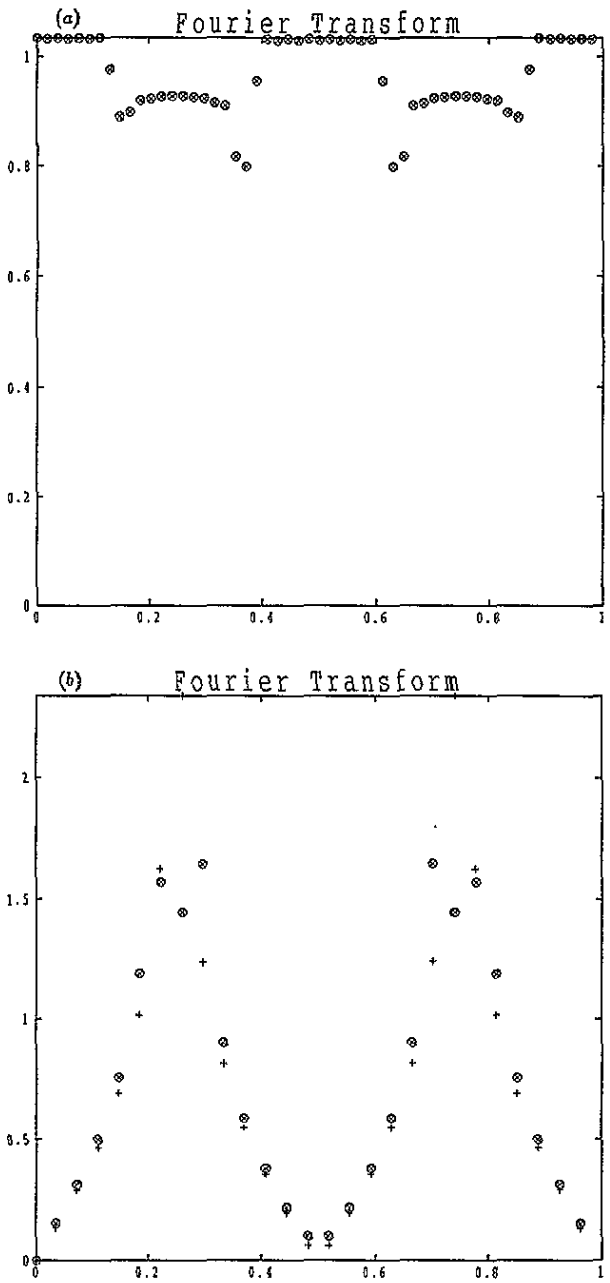

Figure 9. (*a*) The occupation number, n_k, for one full period, and (*b*) the Fourier transform of the spin–spin correlations, also for one full period, for a single hole in the infinite-U t_1–t_2 Hubbard model in the limit that $t_1 \mapsto 0$. We calculated this quantity for a system of 27 atoms and 26 electrons. The calculations have clearly not converged, there being a singularity either quarter way to the zone boundary, or half way to the zone boundary.

a spin–charge separated system. If the spin wavefunction has a divergence then we are led to a 'Luttinger liquid' [8], but if the spin wavefunction has only short-range correlations then we are led to a system with no singularity in n_k and rather more exotic behaviour.

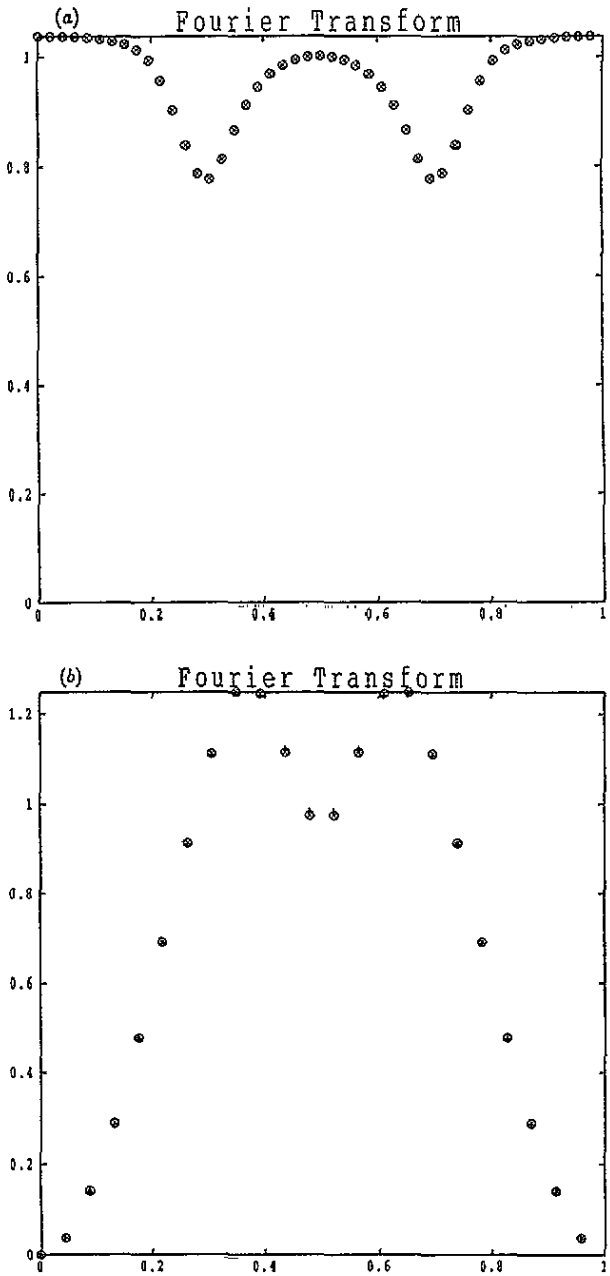

Figure 10. (*a*) The occupation number, n_k, for one full period, and (*b*) the Fourier transform of the spin–spin correlations, also for one full period, for a single hole in the infinite-U t_1–t_2 Hubbard model in the limit that $t_2 = 2t_1$.We calculated this quantity for a system of 23 atoms and 22 electrons. The calculations have converged because there are only short-range correlations.

4. Conclusions

We believe that cyclic-permutation correlations are an important concept in the understanding of topological 'defects' in quantum-spin systems. We believe, admittedly with

little analytical support, that cyclic permutations are directly related to topological excitations and are a measure of the susceptibility to excitations for *short-range* Hamiltonians. We anticipate a similar relationship between fluctuations in 'long-range' classical order leading to low-energy spin waves, and fluctuations in 'long-range' cyclic-permutation correlations leading to low-energy 'spinons'.

In quantum-spin systems with power-law correlations, we associate singularities in the Fourier transform of cyclic permutations with a zero in the spinon dispersion. Further, for a phase transition caused by a softening of such a spinon dispersion, we anticipate a 'maximum' in the relevant cyclic-permutation correlations. We have used this idea to predict that the phase transition in the J_1–J_2 Heisenberg model occurs exactly at $J_2 = 4J_1$, the classical phase transition-point.

In 'spin–charge'-separated solutions to the infinite-U Hubbard model, we associate 'Luttinger-liquid' singularities with divergences in the cyclic-permutation correlations, predicting the relationship between the electron density and the motion of the singularity. We envisage as many different types of behaviour as there are possible types of spin wavefunction, including power-law singularities and dimer ground states. For systems with dominant charge motion, we anticipate that the low-temperature behaviour will be controlled by the weaker spin physics, with the phase changes in the one-dimensional Hubbard model being controlled by changes in the spin subsystem.

Our charge-motion analysis is subject to the exact decoupling of the spin from the charge. For the specific case of one hole, we examine this decoupling, finding that the coupling between the system is strong, but restricted to the near vicinity of the hole, consequently being irrelevant to the low-energy arguments.

We provide a relationship between singularities encountered in the Hubbard-model occupation number to singularities in the independent spin and charge subsystems. Although the free-fermion-gas calculations are under control, the corresponding Heisenberg-model calculations require much more analysis, with severe problems encountered in recognising the difference between power laws and logarithmic corrections.

Our analysis suggests that the dominant changes to be expected in spin–charge separated systems should come from the spin degrees of freedom, where the robust spinless-fermion charge motion is replaced by subtle weak interactions between spins, controlled by the various exchange processes, which strongly depend on the electron density, and which are permitted by longer-range hops.

This article suffers from a lack of the formal mathematics required to make the physical ideas concrete. We believe that such mathematics can be developed and will yield a framework in which to study quantum problems involving solitonic excitations and their related phase transitions.

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