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Analytic correlation functions for the one-dimensional Hubbard model with short-range hopping in the strong-coupling limit

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Abstract. In the limit of dominant nearest-neighbour hopping and infinitesimal second- and third-nearest-neighbour hopping, the Hubbard model is solvable in the sense that it separates into two models which have previously been analysed in the literature. The solutions are spin–charge separated and involve highly correlated motion of the electrons. Although in general the solutions are too complicated to analyse, there are two quite specific states which are amenable to direct analytical attack: the phase boundary between the quantum paramagnet and the Nagaoka ferromagnet, and the 'dimer' phase where all spins pair up into nearest-neighbour singlets. We have been able to evaluate both $\langle n(k) \rangle$ and $\langle S_{-k} \cdot S_k \rangle$ accurately enough to deduce the qualitative behaviour for the two types of state in question. The second of these correlation functions is directly relevant to neutron-scattering studies. Although the solutions are highly correlated and spin–charge separated, the correlations are reminiscent of the non-interacting 'spinfull' free-electron gas solution, the spin response exhibiting a divergence where the non-interacting susceptibility does, for example.

1. Introduction

The behaviour of strongly correlated electrons is a central theme in many-body physics. Perhaps the simplest model for which the strong-coupling limit is considered is the Hubbard model [1], and there is currently a great deal of theoretical interest in the low-temperature behaviour inherent to this model. Unfortunately, the model is rather subtle, and the current rigorous knowledge is restricted mainly to one dimension, where the Bethe *ansatz* has been used to find the spectrum for the model with nearest-neighbour hopping [2]. These exact solutions are a great advance, but in some respects they are not complete. The complexity of the mathematics is such that even quite elementary correlation functions, that one would consider routinely for a non-interacting solution, are inaccessible. In this article we will calculate some correlation functions for the Hubbard model in a limit for which the mathematics is rather less formidable, although the solution retains the fundamental characteristic of being spin–charge separated.

Recently the present authors have developed a new method for solving a class of one-dimensional Hubbard models, in a strong-coupling but restricted limit [3]. The solution involves taking the $U = \infty$ case, where the charge motion is that of spinless fermions but the spin physics remains degenerate, and then focusing on the manner in which the spin degeneracy is lifted by additional interactions. Although we can handle the natural case of $U < \infty$ perturbatively, we have thought more about the role of longer-range hopping, a situation which cannot be handled by the Bethe *ansatz*. In this article we will focus on

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two quite simple spin states and evaluate some correlation functions associated with the original electronic degrees of freedom, namely the Bloch distribution function, $\langle n(k) \rangle$, and the spin–spin correlation function, $\langle S_{-k} \cdot S_k \rangle$.

Although the physics of the $U = \infty$ square-lattice Hubbard model remains a mystery, there are some concrete ideas which appear relevant: in the limit very close to half filling, where the physics is controlled by a few well separated holes, Nagaoka ferromagnetism [4] may well be relevant and in the nearly empty limit, where the physics is controlled by a few well separated electrons, Kanamori paramagnetism should be relevant [5]. One can envisage the physics, as a function of doping, as being a competition between these two phenomena with some form of transition between the two distinct regions of dominance. For our chosen limit there is a definite ferromagnetic phase, and we are studying the phase that the ferromagnet transits into at the phase boundary, and consequently we are looking at the region of maximum competition.

There has been an enormous effort in the literature devoted to attempting to calculate and understand the quantity, $\langle n(k) \rangle$, for low-dimensional systems. The existence or non-existence of a discontinuity has been associated with 'Fermi-liquid' behaviour, and for the exactly solved one-dimensional models there is a singularity at the Fermi energy but *not* a discontinuity. The calculations that we have made for this quantity do not even show a singularity at the Fermi energy, and we attribute this behaviour to the characteristics of the underlying spin physics. One should not necessarily expect all spin–charge-separated solutions to have similar behaviour to the Bethe *ansatz* solvable one-dimensional models.

In section 2 we explain the solutions in our chosen limit, focusing on the particular parameters that we will deal with. In section 3 we evaluate our chosen correlation functions in terms of determinants, in section 4 we interpret our results, and in section 5 we conclude.

2. Exact solutions

The Hubbard model in the limit that the Hubbard repulsion diverges, $U = \infty$, reduces to a one-parameter model, the t-model:

$$H = -t_1 \sum_{\langle ii' \rangle \sigma} (1 - c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}}) c^\dagger_{i\sigma} c_{i'\sigma} (1 - c^\dagger_{i'\bar{\sigma}} c_{i'\bar{\sigma}}) \tag{2.1}$$

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 the atom. The motion of the electrons is dominated by 'bumping' into each other in this limit, and in one dimension there is no way for electrons to pass each other at all. The charge motion is controlled by the matrix element t_1, and the spin order along the chain is conserved on this energy scale and is lifted on a much weaker energy scale; in this article by weak longer-range hopping.

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:

$$c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} \ldots c^\dagger_{i_n\sigma_n} |0\rangle \equiv f^\dagger_{i_1} f^\dagger_{i_2} \ldots f^\dagger_{i_n} |\sigma_1\sigma_2 \ldots \sigma_n\rangle \tag{2.2}$$

where the $f_i^\dagger$ 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, in the thermodynamic limit

$$c_{i\sigma}^\dagger c_{i+n\sigma} = f_i^\dagger f_{i+n} \sum_{\chi_i=0}^{1} \sum_{\chi_{i+1}=0}^{1} \cdots \sum_{\chi_{i+n-1}=0}^{1} \prod_{m=1}^{n-1} \left[f_{i+m}^\dagger f_{i+m} \right]^{\chi_{i+m}} \left[1 - f_{i+m}^\dagger f_{i+m} \right]^{1-\chi_{i+m}} \times \tfrac{1}{2} \left[1 + \sigma \hat{S}_{\alpha_i}^z \right] \hat{R}_{\alpha_i, \alpha_{i+n}-1} \tag{2.3}$$

where the χ_i 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

$$\hat{R}_{\alpha,\alpha+n} = \prod_{\beta=\alpha}^{\alpha+n-1} \left[\tfrac{1}{2} + 2\hat{S}_\beta \cdot \hat{S}_{\beta+1} \right] \tag{2.4}$$

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:

$$H_1 = -\sum_{n>1} t_n \sum_{i\sigma} \left((1 - c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}}) c_{i\sigma}^\dagger c_{i+n\sigma} (1 - c_{i+n\bar{\sigma}}^\dagger c_{i+n\bar{\sigma}}) + \text{cc} \right) \tag{2.5}$$

where the t_n are infinitesimal matrix elements of variable *relative* magnitudes. Although the solution to our chosen limit of finite t_1 and infinitesimal t_n ($n > 1$) was dealt with in previous work [3], we will swiftly review the argument here. In our chosen basis the dominant nearest-neighbour hopping becomes

$$H_0 = -t_1 \sum_i (f_i^\dagger f_{i+1} + \text{cc}) \tag{2.6}$$

which lifts the charge degeneracy to yield a non-interacting spinless fermion gas, but which leaves the spin degrees of freedom degenerate. The low-energy spin physics is then decided by the infinitesimal longer-range hopping, which in degenerate perturbation theory yields an effective spin interaction. To leading order the charge motion remains unaffected, and so the form of the effective spin interaction can be deduced immediately from (2.3) to be

$$H_{\text{deg}} = K_0 + \sum_n K_n \sum_\alpha \left[\hat{R}_{\alpha,\alpha+n} + \text{cc} \right] \tag{2.7}$$

where the matrix elements, K_n, are the amplitudes for electrons to hop past specific numbers of other electrons in the spinless fermion ground state. Simply substituting (2.3) into (2.5) *immediately yields*

$$K_n = -\sum_{r=n+1}^{\infty} t_r \left\langle f_0^\dagger f_r \sum_{\chi_1=0}^{1} \cdots \sum_{\chi_{r-1}=0}^{1} \delta\left(\sum_{s=1}^{r-1} \chi_s - n\right) \prod_{m=1}^{r-1} \left[f_m^\dagger f_m\right]^{\chi_m} \left[1 - f_m^\dagger f_m\right]^{1-\chi_m} \right\rangle \tag{2.8}$$

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 and structure of this result can easily be understood physically: for our basis, a longer-range hop carries an electron over any electrons in between the two end points of the hop. This amounts to a ring exchange acting on the spin wavefunction, but involving the number of electrons between the two end points, which is a *variable*. Although it is clear that the action on the spin wavefunction is just ring exchanges of different lengths, the range of the exchange and the amplitude must be deduced. Obviously, the maximum number of spins which can be involved occurs when the chain is completely filled between the end points of the hop. This explains why we only get a contribution to the ring exchange amplitudes, K_n, from hops of longer range than the number of spins involved. The *amplitude* of the ring exchange is more subtle, because it depends on both the probability of finding exactly the correct number of electrons between the end points, *and* the likelihood of finding the new charge configuration once the electron has actually been moved in the original ground state. These probabilities obviously depend on what the electrons are doing in the charge ground state, viz. the spinless-fermion gas. The matrix elements in equation (2.8) are precisely the likelihoods of the electron hopping between the two end points and simultaneously finding exactly the correct number of electrons required in between in order to achieve a ring exchange involving the desired number of spins. Each individual contribution can be found in terms of a single determinant involving the single-particle correlation functions, as is proved in the appendix. Obviously this procedure is numerically intensive, and we have not gone beyond about twentieth-nearest-neighbours without employing 'tricks'.

In a previous article we considered next- and next-next-nearest-neighbour hopping, deducing the spin Hamiltonian and then recognising it in terms of models solved previously in the literature [3]. Here we will briefly indicate how the argument works in order to give the current calculations more foundation, since they build on these previous results.

The next-nearest-neighbour hopping takes the form

$$H_1 = -t_2 \sum_i \left[f_i^\dagger f_{i+2}(1 - f_{i+1}^\dagger f_{i+1} + f_{i+1}^\dagger f_{i+1} \hat{R}_{\alpha_i,\alpha_{i+1}}) + \text{cc} \right] \tag{2.9a}$$

while the third-nearest-neighbour hopping takes the form

$$H_2 = -t_3 \sum_i \Big[f_i^\dagger f_{i+3} \Big(\Big(1 - f_{i+1}^\dagger f_{i+1}\Big)\Big(1 - f_{i+2}^\dagger f_{i+2}\Big) + \Big[\Big(1 - f_{i+1}^\dagger f_{i+1}\Big) f_{i+2}^\dagger f_{i+2} + f_{i+1}^\dagger f_{i+1}\Big(1 - f_{i+2}^\dagger f_{i+2}\Big)\Big] \hat{R}_{\alpha_i,\alpha_{i+1}} + f_{i+1}^\dagger f_{i+1} f_{i+2}^\dagger f_{i+2} \hat{R}_{\alpha_i,\alpha_{i+2}} \Big) + \text{cc} \Big] \tag{2.9b}$$

in our new basis. In degenerate perturbation theory this immediately reduces to

$$\begin{aligned} H_{\mathrm{deg}} &= K_0 + K_1 \sum_\alpha \left[\hat{R}_{\alpha,\alpha+1} + \mathrm{cc}\right] + K_2 \sum_\alpha \left[\hat{R}_{\alpha,\alpha+2} + \mathrm{cc}\right] \\ &= K_0 + K_1 \sum_\alpha (1 + 4\boldsymbol{S}_\alpha \cdot \boldsymbol{S}_{\alpha+1}) \\ &+ K_2 \sum_\alpha \left[(\tfrac{1}{2} + 2\boldsymbol{S}_\alpha \cdot \boldsymbol{S}_{\alpha+1})(\tfrac{1}{2} + 2\boldsymbol{S}_{\alpha+1} \cdot \boldsymbol{S}_{\alpha+2}) + \mathrm{cc}\right] \\ &= K_0 + \sum_\alpha \left[K_1 + \frac{K_2}{2}\right] \\ &+ 4(K_1 + K_2) \sum_\alpha \boldsymbol{S}_\alpha \cdot \boldsymbol{S}_{\alpha+1} + 2K_2 \sum_\alpha \boldsymbol{S}_\alpha \cdot \boldsymbol{S}_{\alpha+2} \end{aligned} \tag{2.10}$$

where we have used a spin identity to deduce the final result. We immediately recognize the one-dimensional J_1–J_2 model, with the nearest-neighbour spin interaction $J_1 = 4(K_1 + K_2)$ and the second-nearest neighbour interaction $J_2 = 2K_2$. In general we have t_2/t_3 and the electron concentration as parameters, and J_1 and J_2 have strong dependence on these parameters [3].

In practice, the J_1–J_2 Hamiltonian is much too difficult to treat rigorously, with the exception of a few special cases. We will ignore the immensely complicated Bethe *ansatz* solutions, and in this article we focus on two particular cases and generalise the current result to correlation functions for such ground states. We are restricting attention to next-nearest- and next-next-nearest-neighbour hopping, because longer-range hops include longer-range ring-exchange interactions and we cannot solve such interactions. The two particular cases are firstly, the state for which the spins form the quantum analogue of the Néel state (viz. $J_1 = 0$ and $J_2 > 0$, and hence, $0 > K_1 = -K_2 \neq 0$ and other amplitudes K vanish), and secondly the 'dimer' phase with nearest neighbours paired into singlets (viz. $J_1 = 2J_2 > 0$, and hence $K_1 = 0$, $0 < K_2 \neq 0$ and other amplitudes K vanish). The state with $J_2 > 0$ and $0 < J_1 \mapsto 0$ achieves long-range Néel order *in the limit*, with the two sublattices becoming saturated and antiparallel. The state with $2J_2 = J_1$ yields the famous Majumdar–Ghosh nearest-neighbour paired-valence-bond ground state.

Previously, we considered either next- or next-next-nearest-neighbour hopping independently, but here we will permit a competition between the two in order to allow our chosen phases to become stable over a range of band filling. Our final task is to find the particular parameters that correspond to our chosen ground states. For our chosen model the relevant correlation functions from the spinless fermion gas are

$$\begin{aligned} K_1 &= -t_2\langle f_0^\dagger f_2 f_1^\dagger f_1\rangle - t_3\left\langle f_0^\dagger f_3\left[f_1^\dagger f_1(1 - f_2^\dagger f_2) + (1 - f_1^\dagger f_1) f_2^\dagger f_2\right]\right\rangle \\ K_2 &= -t_3\langle f_0^\dagger f_3 f_1^\dagger f_1 f_2^\dagger f_2\rangle \end{aligned} \tag{2.11}$$

in terms of simple correlation functions which can readily be evaluated. We can readily find the lines in parameter space for which our chosen states are stable by forcing the relevant constraints on the amplitudes K of (2.11). Setting $K_1 + K_2 = 0$ yields the phase boundary between ferromagnetism and paramagnetism, and setting $K_1 = 0$ yields the parameterization for which the 'dimer' phase is the ground state. We depict these two lines in figure 1. Although we have plotted these two lines on the same graph, bear in mind that the *signs* of

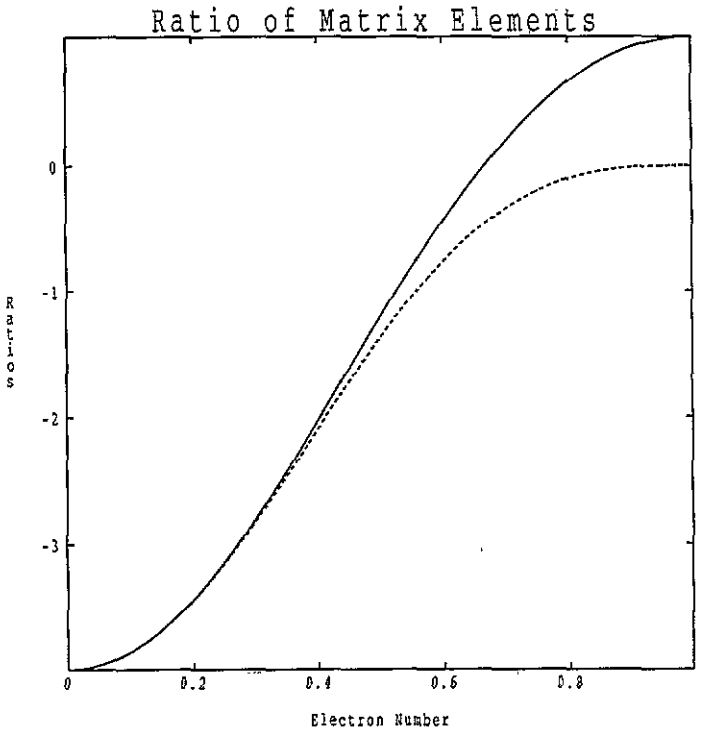

Figure 1. *The ratios of the second-nearest-neighbour hopping matrix element to the third-*nearest-neighbour hopping matrix element (t_2/t_3), for the Néel state (solid line) and dimer state (dashed line). For the Néel state the third-nearest-neighbour matrix element has the same sign as the nearest neighbour, while for the dimer state the phases are opposite.

the pair of matrix elements are reversed, with the Néel state involving the same sign for the nearest-neighbour and next-next-nearest-neighbour matrix elements, and with the 'dimer' state finding opposite signs. This figure indicates that there are realizations of our chosen ground states for all possible choices of band filling, but it does not indicate whether or not these particular realizations are probable.

We are able to evaluate correlation functions for a range of infinite-U Hubbard models with dominant nearest-neighbour and infinitesimal next-nearest- and next-next-nearest-neighbour hopping. We allow *any* concentration of electrons, but force the ratio of the two infinitesimal hopping matrix elements to lie on the curves depicted in figure 1. For the long-range-ordered antiferromagnetic spin state we have $t_1 > 0$ and $t_3 > 0$, with t_2 being defined by the full line of figure 1. For the dimer state we have $t_1 > 0$ and $t_3 < 0$, with t_2 being defined by the dashed line of figure 1. To be physically relevant, we would prefer to work with a bipartite lattice, and so the most 'interesting' region of parametrization is where the solid line passes through zero (the relative phase for the dimer phase matrix elements is *always* frustrated, since $t_1 t_3 < 0$).

Having explained our choice of ground states, we now set a physical context for them. The usual way to interpret the Hubbard-model phase diagram is in terms of the electron concentration, with the physical process of doping the system being the motivation. In this picture the matrix elements, t_n, are presumed fixed, unlike the collection of states we are currently considering. For the usual bipartite systems, the expected picture is

for paramagnetism at low concentration, where only pairs exchange, becoming unstable to ferromagnetism at high concentration where only triples exchange. Our Néel state corresponds precisely to the phase transition between these two phenomena, but examined from the paramagnetic side. The only unfrustrated geometry available to us is the case $t_2 = 0$ and $t_3 > 0$. This case shows precisely the expected behaviour, with the transition occuring at $n_c \sim 0.6675$. In order to stabilize our Néel state to other concentrations, we have resorted to including some frustrated bonds into the system. Using $t_2 > 0$ stabilizes paramagnetism whereas $t_2 < 0$ stabilizes ferromagnetism.

A couple of relatively easy to understand limits are as follows. (1) The nearly empty but strongly correlated limit, where the spin degeneracy is lifted by electrons coming together rarely. There is four times the chance of hopping past an electron with a third-neighbour hop than with a second-neighbour hop, and so the hops compensate when $4t_2 + t_3 = 0$. (2) The nearly full limit, where a single hole locally controls the spin degeneracy. Second-neighbour hops promote singlets while third-neighbour hops promote ferromagnetism, and so the hops compensate when $t_2 = t_3$.

Having chosen our ground states, we now move on to a calculation of our chosen correlation functions.

3. Correlation functions

At first sight, one might think that we could evaluate the current correlation functions for any values of the parameters, but this is not the case. The problem is not the mapping, which remains valid, but the solution to the resulting spin Hamiltonian which is in general too hard to find. Even for the case of the nearest-neighbour Heisenberg model, which has been solved via the Bethe *ansatz*, we would need the spin–spin and ring-exchange correlations as a function of range, and to our knowledge these correlation functions have not been evaluated in the literature. The only cases that we can handle are those for which the resulting spin state is effectively trivial, and this restricts attention to the two states that we have focused on.

The first correlation function that we will consider is the single-particle Bloch-momentum density, $\langle n_k \rangle = \sum_\sigma \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle$, which would have a discontinuity at the Fermi surface if the system were a Fermi liquid. We have already developed the mathematics, and all that is now required is to evaluate the correlations in the ground-state charge and spin wavefunctions. The quantity that we need to consider is

$$\sum_\sigma \langle c^\dagger_{i\sigma} c_{i+n\sigma} \rangle = \left\langle f^\dagger_0 f_n \sum_{\chi_1=0}^{1} \cdots \sum_{\chi_{n-1}=0}^{1} \prod_{m=1}^{n-1} \left[f^\dagger_m f_m \right]^{\chi_m} \left[1 - f^\dagger_m f_m \right]^{1-\chi_m} \right\rangle \langle \hat{R}_{\alpha_0,\alpha_n} \rangle \tag{3.1}$$

where the charge ground state is the non-interacting spinless-fermion gas, and the spin wavefunction is either the quantum Néel state or the 'dimer' paired state. At first sight, one might think that one may find a closed-form solution, but in fact this is impractical. Indeed, even to evaluate the correlation function for length n, we have been forced into numerically evaluating an equivalent $n \times n$ determinant. Taken at face value, a direct numerical evaluation of (3.1) would entail 2^{n-1} different $n \times n$ determinants, a computationally extremely intensive task. Fortunately, for the two states central to the current investigation, we can re-express the correlation functions in terms of a single $n \times n$ determinant.

First let us consider the quantum Néel state: the state for which the two sublattices are saturated and combined in a total-spin singlet. It is elementary to calculate the ring-exchange correlations, which all vanish, since no matter what the range of the exchange,

at least one spin is transferred to the other sublattice yielding an orthogonal spin-state. For this case the only non-vanishing contribution comes from when no particles are exchanged, viz. when the order of the particles is invariant and particles only hop across vacant atoms. The correlation functions reduce to

$$\sum_{\sigma}\langle c^{\dagger}_{i\sigma}c_{i+n\sigma}\rangle = \left\langle f^{\dagger}_{0}f_{n}\prod_{m=1}^{n-1}[1-f^{\dagger}_{m}f_{m}]\right\rangle \tag{3.2}$$

which is evaluated as a determinant in the appendix. We have plotted the Fourier transform in figure 2 for a spread of band fillings. The plots may be treated as being effectively exact, since the chosen correlation functions decay exponentially and can therefore be calculated on all relevant length scales. Although one can see a remnant of the spinfull Fermi step function, the sharp structure has been completely 'washed out' and only a smooth curve remains. Interpretation will be attempted in the next section.

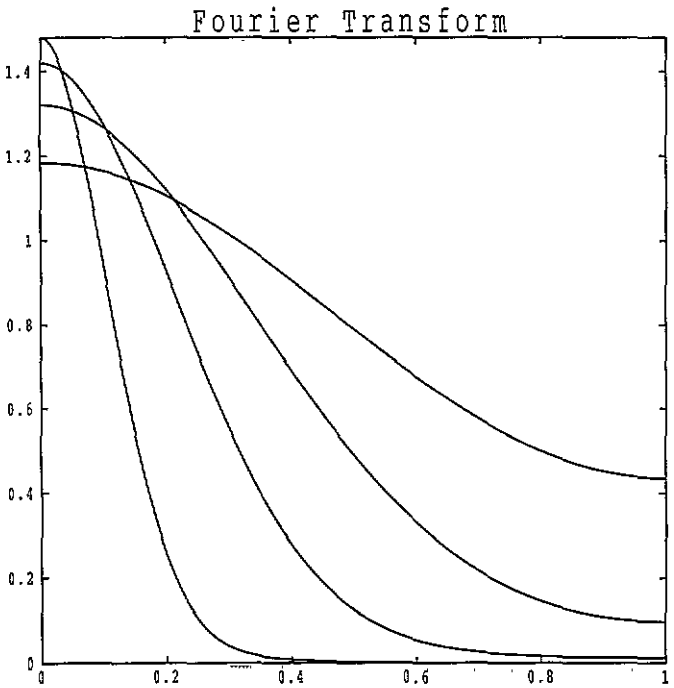

Figure 2. Plots of $\langle n(k)\rangle$, for band fillings of $n_0 = 0.2, 0.4, 0.6$ and 0.8, in the Néel-state phase. The higher concentrations yield a larger contribution at the zone boundary.

The situation for the dimer phase is more subtle, since the ring-exchange correlations do not vanish. Using the fairly well known result that the overlap between two distinct valence bond configurations is $\pm 1/2^{d-1}$, where d is the number of inequivalent valence bonds in one configuration, it is possible to show that

$$\langle \hat{R}_{0,2n}\rangle = \frac{(-1)^n}{2^n} \tag{3.3a}$$

$$\langle \hat{R}_{0,2n-1}\rangle = \frac{(-1)^n}{2^{n+1}} \tag{3.3b}$$

for $n > 0$. After a brief consideration of how to tell whether one has an odd or even number of electrons on a region of the lattice, one is drawn inexorably to the conclusion that

$$\sum_{\sigma}\langle c_{i\sigma}^{\dagger}c_{i+n\sigma}\rangle = \mathrm{Re}\left(\left[1-\frac{\mathrm{i}}{2\sqrt{2}}\right]\left[1+\frac{\mathrm{i}}{\sqrt{2}}\right]^{n-1}(-1)^{n-1}\left\langle f_0^{\dagger}f_n\prod_{m=1}^{n-1}\left[f_m^{\dagger}f_m-\frac{2-\sqrt{2}\mathrm{i}}{3}\right]\right\rangle\right) \tag{3.4}$$

where i is the square root of (-1). Once again, this expression can be rewritten as a single determinant as shown in the appendix. We have plotted the Fourier transform in figure 3 for a range of band fillings. The plots are seen to be smooth, but there is much more structure as will be commented on in the next section.

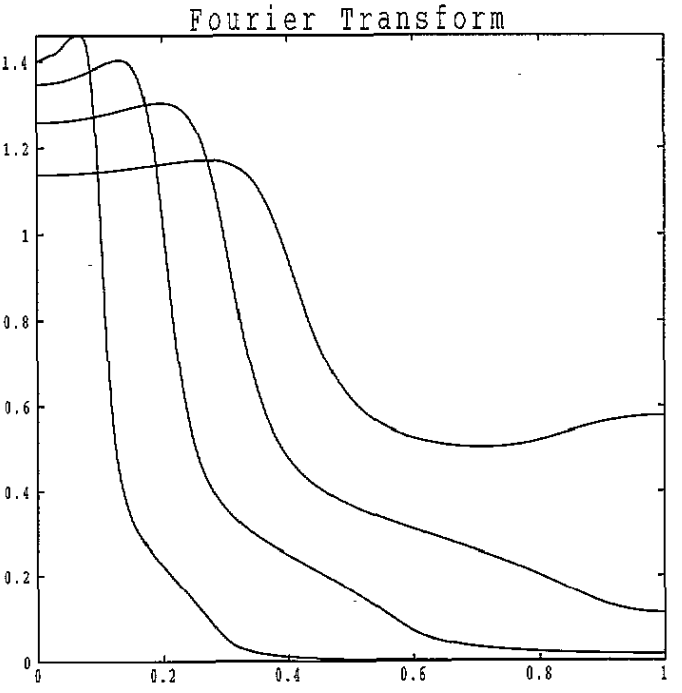

Figure 3. Plots of $\langle n(k)\rangle$, for band fillings of $n_0 = 0.2, 0.4, 0.6$ and 0.8, in the dimer-state phase. The higher concentrations yield a larger contribution at the zone boundary.

We now turn our attention to the spin–spin correlation functions, $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+n}\rangle$. Since there is no actual transportation of electrons for this process, we do not have to consider ring exchange. In fact, all we need to do is measure the correlations between the spins which happen to be on the relevant atoms. This is simply

$$\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+n}\rangle = \left\langle f_0^{\dagger}f_0 f_n^{\dagger}f_n \sum_{\chi_1=0}^{1}\cdots\sum_{\chi_{n-1}=0}^{1}\prod_{m=1}^{n-1}\left[f_m^{\dagger}f_m\right]^{\chi_m}\left[1-f_m^{\dagger}f_m\right]^{1-\chi_m}\right\rangle \langle \boldsymbol{S}_{\alpha_0}\cdot\boldsymbol{S}_{\alpha_n}\rangle \tag{3.5}$$

where the complications arise because it depends how many electrons are between the two atoms as to which spins are to be correlated. In order to make use of this result, we need to

be able to evaluate the spin–spin correlations for our spin wavefunction, which is elementary for both of our chosen solutions.

For the quantum Néel state, the spin–spin correlation functions are those of the classical Néel state:

$$\langle S_{\alpha_0} \cdot S_{\alpha_n} \rangle = \frac{(-1)^n}{4} \tag{3.6}$$

and so, once again, it is important to be able to evaluate the probability that there is either an even or an odd number of electrons on a particular set of atoms. With a little algebra, it can be shown that

$$\langle S_i \cdot S_{i+n} \rangle = \frac{(-1)}{16} \left[P_{n-1} - 2P_n + P_{n+1} \right] \tag{3.7}$$

for $n > 0$, with $\langle S_i \cdot S_i \rangle = \frac{3}{4} \langle f_0^\dagger f_0 \rangle$, in terms of the average 'fermionic phase change' operator:

$$P_n = \left\langle \prod_{m=1}^{n} (1 - 2 f_m^\dagger f_m) \right\rangle \tag{3.8}$$

for $n > 0$ and with $P_0 = 1$, which measures the average phase that a fermion picks up when hopping past n atoms. Once again, this type of correlation function can be expressed as a determinant, as explained in the appendix. In figure 4 we have plotted the spin–spin correlation function for various band fillings, and unlike previous calculations, the results are *not* effectively exact. There is a divergence which is clearly visible, and our truncation of the Fourier transform at finite range has both cut off this divergence and included some artificial oscillations into the functions. We will comment on this result in the next section.

For the dimer state, the spin–spin correlations are precipitously short range, vanishing for next-next-nearest neighbours and beyond. This result restricts the contributions to those where there are vacant atoms between the two spins, which leads quite directly to

$$\langle S_i \cdot S_{i+n} \rangle = \frac{(-3)}{8} \left[Q_{n-1} - 2Q_n + Q_{n+1} \right] \tag{3.9}$$

for $n > 0$, with $\langle S_i \cdot S_i \rangle = \frac{3}{4} \langle f_0^\dagger f_0 \rangle$, in terms of the probability that a length of chain happens to be vacant:

$$Q_n = \left\langle \prod_{m=1}^{n} (1 - f_m^\dagger f_m) \right\rangle \tag{3.10}$$

for $n > 0$ and with $Q_0 = 1$. Once again, we find a representation which is amenable to calculation via a single determinant, as shown in the appendix. We have plotted some examples in figure 5, for various band fillings, and will comment on the form in the next section.

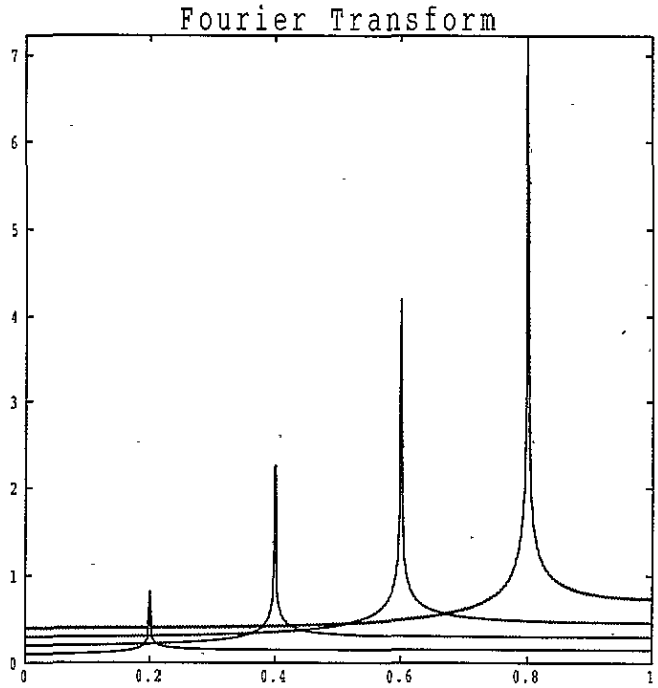

Figure 4. Plots of $\langle S_{-k} \cdot S_k \rangle$, for band fillings of $n_0 = 0.2, 0.4, 0.6$ and 0.8, in the Néel-state phase. The calculations have *not* converged, we used a range of about 400 atoms, and the 'spikes' are believed to diverge logarithmically in the limit that the range diverges. The higher concentrations yield a larger contribution at the zone boundary.

4. Interpretation

For a spin–charge-separated system an evaluation of $\langle n(k) \rangle$ might at first sight appear absurd, but there are a couple of motivating facts. Firstly, for a Fermi liquid it is believed that this quantity will have a 'step-like' discontinuity and this behaviour can be discounted by direct calculation and the likely behaviour inserted in place. Secondly, since the chosen Hamiltonian involves hopping over various ranges, this quantity is a fairly direct measure of where in reciprocal-space kinetic energy is gained and where it is lost.

In the standard discussions of one-dimensional models, one often finds residual singularities at the Fermi wavevector [6]. We find no such behaviour, since our real-space contributions decay exponentially yielding smooth behaviour at the Fermi momentum. The cause is obvious: the ring-exchange correlations for our two states are precipitous, while the corresponding correlations for the Heisenberg ground state, found in the nearest-neighbour Hubbard model, have long-range character [7]. It is the spin wavefunction which controls this behaviour, and we have chosen quite different spin states to those previously considered. Obviously it is important to decide which of the two options is more relevant to consider for a two-dimensional system, but we have been unable to resolve this issue, having little basic understanding of the likely spin wavefunction in two dimensions.

The kinetic energy issue is rather more interesting, involving the use of the spin degrees of freedom in order to optimize the shape of $\langle n(k) \rangle$. The dominant nearest-neighbour hopping acts as an *integral constraint* on this function, because the charge ground state is invariantly the spinless fermion ground state, leading to an unchanging overlap with $\cos \pi k$.

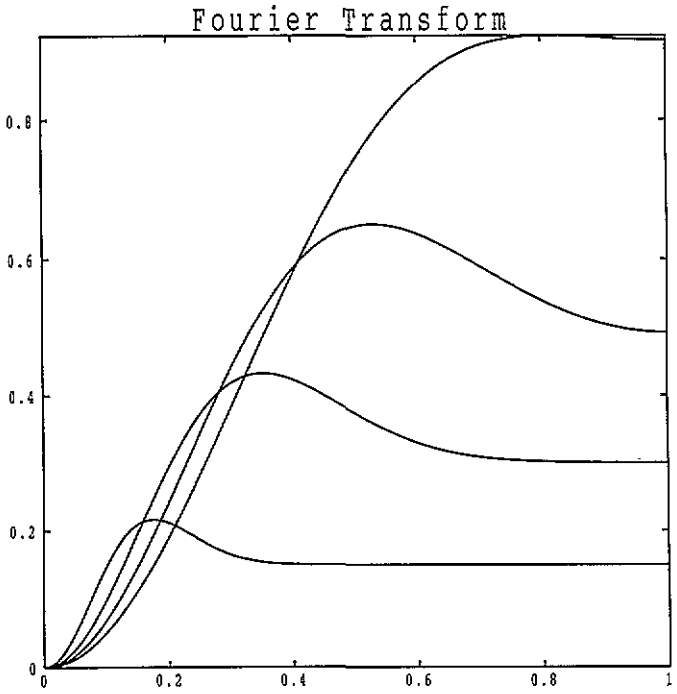

Figure 5. Plots of $\langle S_{-k} \cdot S_k \rangle$, for band fillings of $n_0 = 0.2, 0.4, 0.6$ and 0.8, in the dimer-state phase. The higher concentrations yield a larger contribution at the zone boundary.

Only the higher Fourier components are affected by the lifting of the spin degeneracy, and of these only the first two make a contribution to the energy. In figure 6 we plot the contribution to the kinetic energy which lifts the degeneracy for a particular case of the dimer phase. Comparison with the $\langle f_i^\dagger f_i \rangle = 0.8$ curve in figure 3 shows that the electrons are peaked in the best regions, as expected. These considerations lead to a fairly direct interpretation of the content of our calculations: we are trying to find the spin state which yields the maximum degree of short-range hopping with the chosen strengths, or equivalently with the maximum degree of overlap with the degeneracy-breaking kinetic-energy dispersion in reciprocal space. The difficult physical constraint is that the state chosen must be a quantum spin-half state, and solving the equivalent quantum spin problem is difficult.

The spin–spin correlation functions are physically more interesting, and indicate what might be expected from neutron-scattering experiments. Although the two spin wavefunctions that we are dealing with are elementary, the observed spin correlations are more subtle, because the neutron sees the spin dependence of the *atoms* and not the ordered electrons. Although the spins in the Néel phase have long-range order, the atoms on which they are found are spaced out according to the band filling and fluctuate according to the fast spinless fermion motion. In practice we observe a *convolution* of the spin wavefunction 'averaged' over the charge motion. Due to some subtleties associated with the Néel state, we will deal with the dimer phase first.

The spin correlations in the dimer phase exist only between neighbouring electrons, and so the range of the observed spin correlations is controlled by the probability function for finding neighbouring electrons a certain distance apart. Also, the ground state is a total-spin singlet and so there can be no long-range ferromagnetic spin correlations. We would

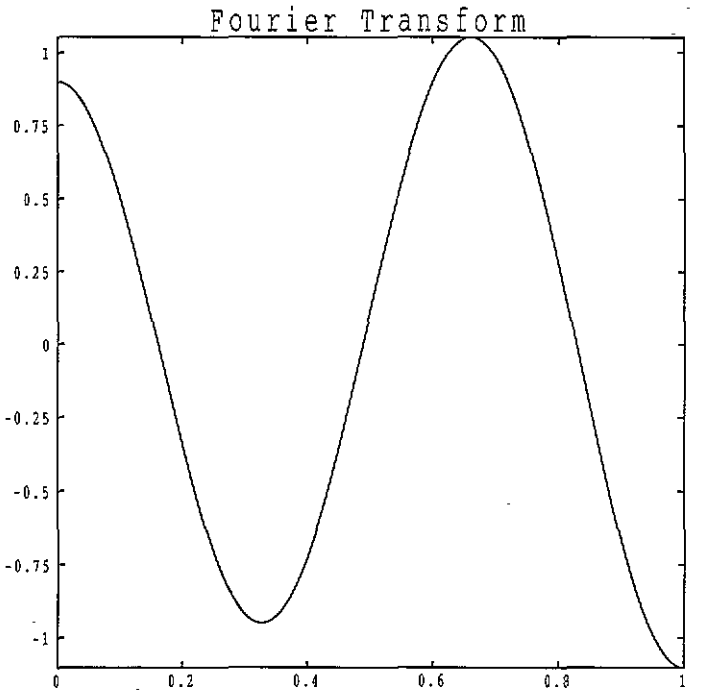

Figure 6. The dispersion that lifts the spin degeneracy for the case of the dimer-state phase with a band filling of $n_0 = 0.8$. The 'troughs' in the dispersions clearly coincide with the peaks in the relevant plot in figure 3.

expect to see an antiferromagnetic response, peaking at the average inverse separation of the electrons, and this is exactly what is observed.

The Néel phase is more subtle. Firstly, although for finite systems the quantum Néel state is a total-spin singlet, in the limit where the system size diverges we find the *classical* Néel state on all finite length scales. Although the point $k = 0$ is special, there is a limiting contribution yielding short-range ferromagnetic correlations. Secondly, immediately obvious from figure 4 is a divergence in the spin density. This is caused by the fact that the long-range correlations inherent in the spin wavefunction are being convoluted with less obvious long-range correlations in the charge wavefunction. Although the spinless Fermi gas is metallic, there are very long-range correlations associated with the state where we have equidistant fermions. These correlations show up in the quantity P_n, which measures (indirectly) the average number of particles in a region of length n: there are long-range contributions associated with the average. It is this fact which causes the divergence. Neutrons will see the Néel ground state on a length scale associated with the average distance apart of the electrons. The weakness of the divergence comes from the metallic behaviour of the charges, which fluctuate in position, but not enough to wash out the divergence altogether. Interestingly, the observed spin correlations are remarkably similar to the susceptibility of the spinfull free-electron gas, which has a similar logarithmic divergence at $2k_F$. We have plotted the spin–spin correlations, $\langle S_{-k} \cdot S_k \rangle$, and the spin-susceptibility for the non-interacting free-electron gas in figure 7, for a band-filling of $n_0 = 0.8$, and the similarity with figure 4 is clear. We cannot say that we understand *why* the interacting spin correlations are similar to the non-interacting spin *susceptibility*, but we do feel that the

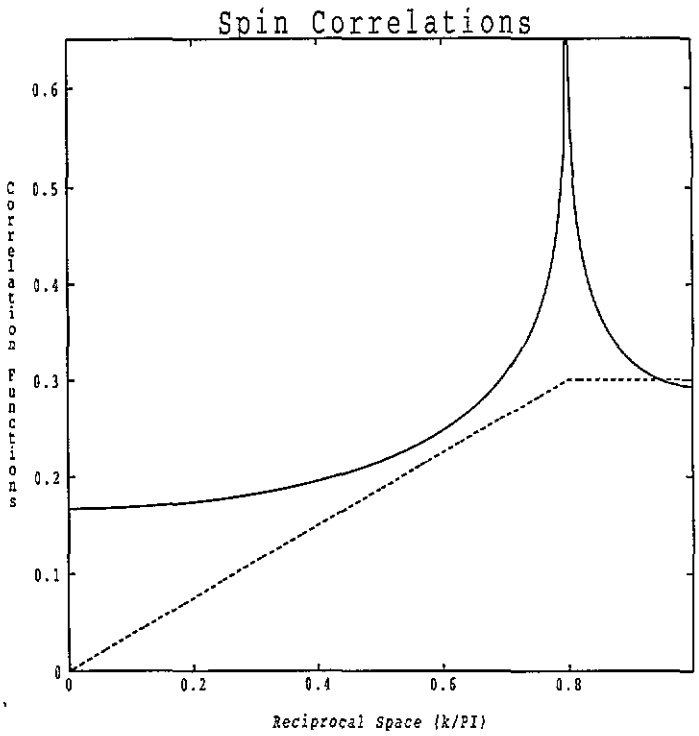

Figure 7. The spin–spin correlations (dotted line), $\langle S_{-k} \cdot S_k \rangle$, and spin susceptibility (full line) or Lindhard function for the non-interacting free-electron gas at band filling $n_0 = 0.8$. The logarithmic divergence at $2k_F$ is clearly reminiscent of the divergence present in our spin–charge separated calculations of the spin–spin correlations (figure 4).

result is interesting.

Another relevant fact is that one can associate these spin correlations with the spiralling discussed in the weakly doped perovskite superconductors [8], which has a similar natural interpretation: the Néel correlations found in the parent compound become spread out by the doped holes, which act as spacers changing the pitch of the spiral.

It is crucial to try to understand what might be expected in the square-lattice geometry of current interest: would we expect similar long-range spin correlations? The cause of the spin–spin divergence in our model is clearly partly related to the one-dimensional nature of the system: as well as the long-range Néel spin order, there are also long-range charge correlations present in P_n of (3.8). Independent of whether we can predict the spin wavefunction, we would not expect such long-range charge correlations, because the two-dimensional motion eliminates such linear one-dimensional correlations. Direct calculation verifies that electron-number fluctuations in a fixed area in two dimensions are also stronger than the corresponding fluctuations in one dimension. Any corresponding effects would be controlled by more subtle arguments than has been presented here, and so we have no pertinent evidence for the behaviour of a two-dimensional system.

The cause of the long-range spin correlations is partly the very uniform distribution of charge in the system. If the electronic charge motion were more highly correlated, then we might expect a change in this divergence. In order to examine this question we have performed some 'Hartree–Fock' calculations on the model with *finite* longer-range hopping.

We will not go into the details of the calculations, but just give a broad outline. We make two uncontrolled approximations: firstly, we assume that the spin–charge separation is complete, and that the spin and charge wavefunctions are independent. Secondly, we cannot solve the resulting charge Hamiltonian exactly, and so we perform a Hartree–Fock analysis for the correlations, namely, we presume that the ground state can be described by a non-interacting fermion state, although we do allow pairing correlations. For the system currently under consideration, the effective spin Hamiltonian is still the J_1–J_2 Heisenberg model, and so we can tune our parameters to ensure that the spin wavefunction is the Néel state. The resulting charge Hamiltonian involves hopping only across vacant atoms, and so pairing correlations are induced to promote a higher probability of finding such regions. The resulting additional charge motion, which corresponds to superconductivity in higher dimensions, would be expected to decorrelate the long-range uniformity of charge and to eliminate the divergence in the spin correlations. A particular case is plotted in figure 8, and the loss of the divergence is readily seen. The additional complexity involved in the evaluation of the determinant is briefly mentioned in the appendix.

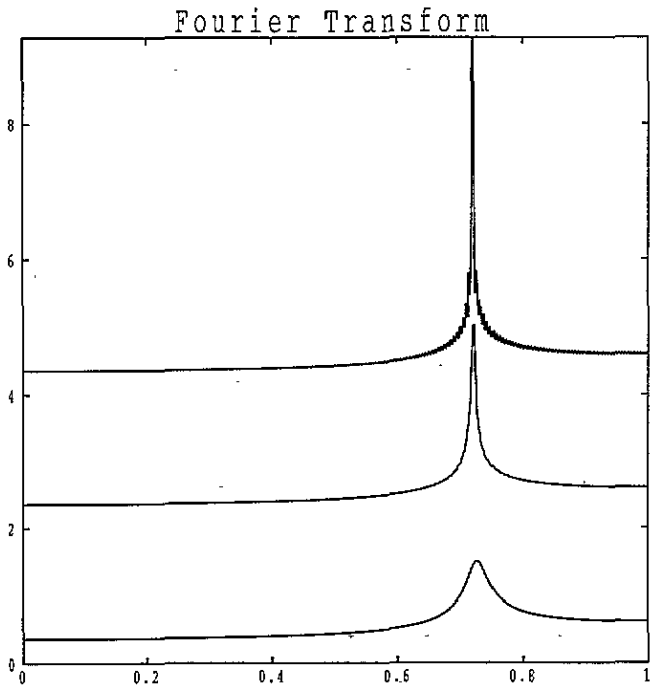

Figure 8. Plots of $\langle S_{-k} \cdot S_k \rangle$, for the Néel-state phase for the trio of cases $(t_1, t_2, t_3) = (1.0, 0.3, 1.0)$, $(t_1, t_2, t_3) = (1.0, 0.225, 0.75)$ and $(t_1, t_2, t_3) = (1.0, 0.15, 0.5)$. We have separated the curves via additive constants of two, because otherwise they would lie on top of each other. Although the stronger hopping cases have converged, the weakest case has longer-range correlations than we have calculated. The stronger values of hopping clearly yield only short-range spin–spin correlations.

5. Conclusions

For a particular class of Hubbard models in quite restrictive limits, we have been able

to deduce the form of some electronic correlation functions. The systems are all one dimensional and spin–charge separated, and the spin wavefunctions are fairly extreme cases. The physics suggested by the calculations is, however, quite instructive.

The limit that we examine is that of a nearest-neighbour $U = \infty$ Hubbard model in one dimension, which is solved up to spin degeneracy by the spinless Fermi gas. We are interested in how additional interactions then lift the spin degeneracy and which types of state are stabilized. Longer-range hopping can stabilize various types of spin state, and we have selected two very simple examples to study: firstly, we have looked at the quantum Néel state which is found on the border between paramagnetism and ferromagnetism, a particularly important region of parameters for the experiments, and secondly we have looked at the 'dimer' phase which might be relevant to a highly frustrated geometry.

We looked at $\langle n(k) \rangle$, which has little obvious experimental significance, but is central to some theoretical bickering and measures the degree of success that the Hubbard model has in making use of the additional hopping degrees of freedom. The results for both states are similar, in the sense that the curves are completely smooth and involve no singularities as have been predicted by Luttinger liquid theory [9]. The reason is straightforward: for both states the *relevant* spin correlations decay exponentially and although the charge wavefunction has helpful characteristics, the spin wavefunction washes the correlations out. The behaviour of our systems might be deemed pathological, but this remains to be seen. One thing that is clearly true is that the low-lying excitations for the Néel system are spin waves and *not* spinons, which may be another way to explain why no Fermi singularity might be expected. The low-lying excitations for the dimer system are solitons at the relevant Fermi wavevector, but the existence of a spin gap is probably sufficient to eliminate singularities at the Fermi energy for the ground state. Only in systems for which the low-lying excitations are collective 'shuffling' modes might we expect a singularity at the Fermi surface, as in the nearest-neighbour Heisenberg model for example [10]. Unfortunately, systems controlled by 'collective' phenomena are more difficult to analyse than the systems under current investigation.

In the standard discussion of the singularity in $\langle n(k) \rangle$, a power law is expected, where, for the Hubbard model, the power ranges from one-eighth in the strong coupling limit down to zero in the weak-coupling limit. We presume, for next-nearest-neighbour hopping, that for our model this power varies smoothly from one-eighth in the low-density limit, where the spin system is the Heisenberg ground state, up to unity at the boundary with ferromagnetism, where the spin system is the Néel state. This rather different behaviour stems from the rather stronger physics inherent in longer-range hopping.

We also looked at $\langle S_{-k} \cdot S_k \rangle$, the spin–spin correlation function. Due to the precipitous spin correlations in the dimer phase, the system exhibits short-range antiferromagnetic correlations, as might be expected. The Néel system is rather more interesting. Although the long-range correlations in the spin wavefunction do not show up in the ring exchange, they do show up in two-particle correlations, like the spin susceptibility. We find long-range spiralling correlations, as are predicted by classical considerations [8], which can be understood in terms of 'smearing out' the antiferromagnetism over the spaced out electrons, with the pitch of the spiral being controlled by the average electron separation. Due to long-range charge correlations there is a divergence in this spin-response, but charge fluctuations expected for finite longer-range hopping should wash this out, leaving only short-range correlations to be expected experimentally. An approximation scheme alluded to in the main test bears out this hypothesis.

Perhaps the most important consideration is whether or not these calculations tell us what to expect for the two-dimensional system of current experimental interest: Perovskite

superconductors. Unfortunately, any deductions are too tenuous at present, although various things ought to be said. The first and most important consideration is whether or not the two-dimensional Hubbard model is in fact spin–charge separated: This problem is way beyond the technical expertise of the authors, although at least one of us believes that it probably is. Secondly, *if* the Hubbard model is spin–charge separated, what is the nature of the two components? One would expect that the charge degrees of freedom would be a bosonic condensate [11], but thinking about the spin degrees of freedom is much worse. The existence of the 'Fermi surface' in photoemission suggests spin-half excitations and a collective picture for the spin physics: the most difficult possibility to deal with.

In conclusion, we have looked at some spin–charge-separated systems which exhibit quite different behaviour to that usually prescribed for so-called Luttinger liquids [9]. One should not presume that non-Fermi-liquid behaviour is a unique type of behaviour, but rather perhaps that any possible combination of spin and charge physics can exist in particular cases. The physics of spin–charge separation is probably fairly involved.

Appendix

In this appendix we write down two results that are elementary to prove for the free-fermion gas, but we believe to be true for the free-fermion gas *plus* pairing correlations. The method of proof is direct, involving the basic idea that for a free-fermion gas *all* correlation functions can be evaluated by adding together the contributions from every possible way to pair up the operators in a particular expression. The pair correlation functions form a matrix, and the summation, combined with the Fermi minus signs, lead directly to the observation that the terms can be resummed into a *determinant*.

In terms of the single-particle correlations

$$n_j = \langle f_i^\dagger f_{i+j} \rangle$$

and the pairing correlations

$$\delta_j = \langle f_i^\dagger f_{i+j}^\dagger \rangle$$

we find that moving a single fermion over a certain range, with a strength depending upon how many of the intermediate sites are filled, yields

$$\left\langle f_i^\dagger f_{i+n} \prod_{j=1}^{n-1} (f_{i+j}^\dagger f_{i+J} - \alpha_j) \right\rangle =$$

$$\text{Even} \begin{bmatrix} n_1 - \delta_1 & n_2 - \delta_2 & n_3 - \delta_3 & \cdots & n_{n-1} - \delta_{n-1} & n_n \\ n_0 - \alpha_1 & n_1 - \delta_1 & n_2 - \delta_2 & \cdots & n_{n-2} - \delta_{n-2} & n_{n-1} - \delta_{n-1} \\ n_1 + \delta_1 & n_0 - \alpha_2 & n_1 - \delta_1 & \cdots & n_{n-3} - \delta_{n-3} & n_{n-2} - \delta_{n-2} \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ & & & \cdots & & \\ n_{n-3} + \delta_{n-3} & n_{n-4} + \delta_{n-4} & n_{n-5} + \delta_{n-5} & \cdots & n_1 - \delta_1 & n_2 - \delta_2 \\ n_{n-2} + \delta_{n-2} & n_{n-3} + \delta_{n-3} & n_{n-4} + \delta_{n-4} & \cdots & n_0 - \alpha_{n-1} & n_1 - \delta_1 \end{bmatrix} \tag{A1}$$

where Even indicates that we only include even numbers of pairing correlations, while the probability of finding certain configurations of fermions yields

$$\left\langle \prod_{j=1}^{n} (f_{i+j}^{\dagger} f_{i+j} - \alpha_j) \right\rangle$$

$$= \begin{bmatrix} n_0 - \alpha_1 & n_1 - \delta_1 & n_2 - \delta_2 & \dots & n_{n-2} - \delta_{n-2} & n_{n-1} - \delta_{n-1} \\ n_1 + \delta_1 & n_0 - \alpha_2 & n_1 - \delta_1 & \dots & n_{n-3} - \delta_{n-3} & n_{n-2} - \delta_{n-2} \\ n_2 + \delta_2 & n_1 + \delta_1 & n_0 - \alpha_3 & \dots & n_{n-4} - \delta_{n-4} & n_{n-3} - \delta_{n-3} \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ & & & \dots & & \\ n_{n-2} + \delta_{n-2} & n_{n-3} + \delta_{n-3} & n_{n-4} + \delta_{n-4} & \dots & n_0 - \alpha_{n-1} & n_1 - \delta_1 \\ n_{n-1} + \delta_{n-1} & n_{n-2} + \delta_{n-2} & n_{n-3} + \delta_{n-3} & \dots & n_1 + \delta_1 & n_0 - \alpha_n \end{bmatrix} \tag{A2}$$

We have found it difficult to formalize the method of the proof in a convenient way, but in short, we associate pairing contributions indirectly with the non-pairing contributions, with the non-interacting 'paths' between pairing contributions being spatially reversed. We appreciate that this explanation does little to assist the reader, but you may like to try to prove it for yourself.

All the correlation functions found in the main text are of one of these two basic formats.

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