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Interacting holes in CuO cyclic chains

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Abstract. The Kondo-reduced Emery model is investigated for cyclic CuO chains. When the spin–exchange coupling is zero, the model is exactly solvable in terms of spinless fermion operators. In the general case we find that the ground state energy has an unconventional dependence on an external magnetic flux. This behaviour can be interpreted as due to an induced statistical flux. The strong-coupling behaviour can be explained in terms of compound particles, which allows some rigorous results in this limit.

1. Introduction

In the last few years many people have been interested in the properties of strongly correlated fermionic systems. To a large extent this interest was associated with the phenomenon of high-T_c superconductivity (HTS) discovered at the end of 1986 by Bednorz and Müller [1]. In spite of an enormous experimental and theoretical activity since then no great progress has been made in understanding the mechanism of HTS.

It is now generally accepted that regular CuO_2 planes are responsible for HTS. Both components, Cu and O, seem to be important in the strong antiferromagnetic and superconducting properties of the HTS family. Anderson [2] was the first to suggest that the simple Hubbard model could be a good candidate to describe this system. Although the majority of theoreticians today deal with strongly correlated models, their interests are no longer attached to a very definite model. Instead, many are involved in investigating the models according to their own prejudices.

Among these other models, one can find those involving only one sublattice represented by Cu sites. This approach supposes the Cu-ion state to be strongly correlated with the electronic configuration of O ions from its environment. We do not wish to discuss the question of advantages and disadvantages of concrete models, but our choice is associated with what we call the Kondo-reduced Emery (KRE) model. It and other similar models [4, 5] originate from the Emery model [3], where a conventional 'vacuum' corresponds to the ionic states Cu^+ and O^{2-}. Single hole excitations will transform them into Cu^{2+} and O^-, respectively, while for the Cu^{3+} and neutral O states one needs to include the on-site Coulomb repulsion terms. The wave functions on Cu and O sites are strongly hybridized. This is equivalent to including in the Hamiltonian a Cu–O hopping term of rather strong amplitude. Because a single-hole energy level on an O site is a few eV above that on a Cu site, the former would be approximately empty of holes if there were no doping.

The KRE model can be derived in second order of the perturbation theory from the original Emery model when the expansion proceeds in a small parameter, which is the

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ratio of a hopping amplitude over the energy gap [6,7]. According to this model all Cu sites are treated as if they are Cu^{2+} ions. Hence, these ions are responsible for strong antiferromagnetic correlations in HT superconductors. The carriers due to doping preferential occupy O sites, transforming them into the O^- state. In the framework of the KRE model, the Cu–O hopping amplitude transforms into the effective O–O hopping term which includes a spin scattering on the intermediate Cu site. Actually, such a hopping amplitude differs from that due to a simple kinetic-energy term, but this O–O charge transfer is more reminiscent of a two-particle interaction. The same- (second-) order perturbation theory leads to the spin–exchange interaction of holes on the nearest O and Cu sites. In short, one can say that KRE model reflects the low-energy properties and neglects all the contributions due to upper Cu and O bands, i.e. two-hole on-site states are excluded.

The Hamiltonian of the KRE model has the following form:

$$H = \tau \sum_{\langle r_1 \neq r_2, R\rangle} p^{\dagger}_{r_2,\alpha} d^{\dagger}_{R,\beta} d_{R,\alpha} p_{r_1,\beta} + J \sum_{\langle r,R\rangle} p^{\dagger}_{r,\alpha} d^{\dagger}_{R,\beta} d_{R,\alpha} p_{r,\beta} \tag{1}$$

where $p^{\dagger}_{r,\alpha}$ creates a hole on the O site r with spin projection α while $d^{\dagger}_{R,\beta}$ creates one on the Cu site R with spin projection β. In the first term one sums over all Cu sites R and the nearest O sites labelled by r_1 and r_2. This represents O holes hopping in the localized background of Cu spins. The second term gives a spin exchange of Cu and O holes situated at the nearest sites. In figure 1 the effect of the Hamiltonian on a state consisting of one O and four Cu spins is shown.

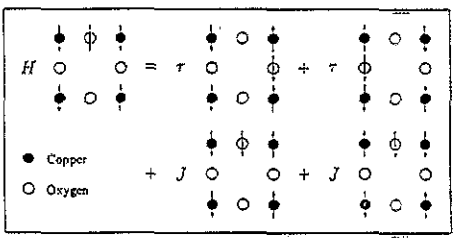

Figure 1. The effect of the Hamiltonian of the Kondo-reduced Emery model on a state consisting of one O and four Cu spins.

In this work we are interested in the properties of CuO alternating chains. This problem seems to be very far from giving any explanation of HTS mechanisms. However, such chain fragments are very common in O-deficient planes of $YBa_2Cu_3O_{6+x}$ and similar HTS compounds. Nowadays there is a real possibility for direct neutron measurements of a spin density on Cu sites belonging to the short chain fragments. This is equivalent to the collective contribution of Cu spins to the paramagnetic susceptibility [8]. In addition, short chain fragments enclosed periodically demonstrate very interesting properties, which could be interpreted in terms of spinless carriers with a local statistical field attached [9, 10]. This fact points to the possibility that O carriers in the regular CuO_2 planes can be quasi-autolocalized with a statistical field attached in order to gain energy. A similar statistical flux is also seen in the t–J model [11–13] and the connection to anyons and fractional statistics has been pointed out [14, 15].

This work is organized as follows. In section 2 we present an exact solution of the KRE model with the spin–exchange term neglected. This allows is to extract the statistical field contribution to the energy of the spinless fermions. It is noteworthy, as has been demonstrated in [16], that such a model can to be generalized by introducing the

special exchange interaction which keeps the magnetic and spinless fermionic degrees of freedom separated. In section 3 we return to the more realistic case of non-zero magnetic-coupling constant J and obtain numerically the ground-state energies of small cyclic chains in an external magnetic field. Similarly to the situation in the exactly solvable model, the statistical field that determines the carrier-band motion still persists. Some numerical results concerning the density–density and correlation functions of carriers are presented in section 4. Surprisingly, they are found to be almost completely independent of the coupling constant J. We also calculate Cu–Cu spin correlation functions. These are found to be more sensitive to the spin–exchange coupling. In section 5 we consider the strong-coupling limit when a carrier is effectively transformed into a compound particle due to the strong magnetic interaction with the Cu spins surrounding the O hole. We can then obtain an exact solution of the model for chains with $N = 3$ and $N = 4$ Cu spins, which confirms our previous numerical results.

2. Exact solution for zero spin–exchange coupling

We consider an alternating ring of N Cu sites and N O sites. The Cu ions are situated on the half-integer-numbered sites $\frac{1}{2}, \frac{3}{2}, \ldots$ between the O sites at $1, 2, \ldots, N$. There is a localized spin-$\frac{1}{2}$ d hole on every Cu site and we consider n spin-$\frac{1}{2}$ O p holes hopping between the O sites.

We will first consider the simplest case when spin–exchange coupling $J = 0$. The Hamiltonian (1) can then be written as

$$H = \tau \sum_{i=1}^{N} p_{i,\alpha}^{\dagger} d_{i+\frac{1}{2},\beta}^{\dagger} d_{i+\frac{1}{2},\alpha} p_{i+1,\beta} + \text{HC.} \tag{2}$$

and we will impose periodic boundary conditions

$$d_{N+\frac{1}{2}} = d_{\frac{1}{2}} \qquad p_{N+1} = p_1. \tag{3}$$

The Hamiltonian changes the position of the O holes, but it never changes the spin sequence $\{\sigma_1, \sigma_2, \ldots, \sigma_{N+n}\}$. So the subspace of states which have the same spin configurations or one that is obtained by applying the cyclic permutation operator P:

$$P\{\sigma_1, \sigma_2, \ldots, \sigma_{N+n}\} = \{\sigma_2, \sigma_3, \ldots, \sigma_{N+n}, \sigma_1\}$$

is invariant under the action of the Hamiltonian. Using this special symmetry of the corresponding wave functions, this model has recently been solved exactly and found to be equivalent to a system of non-interacting spinless fermions [10].

A more compact solution will be presented here. It is very similar to the exact solution of the one-dimensional Hubbard model in the limit $U \to \infty$ obtained by Caspers and Iske [17]. In both cases there are effectively n spin-$\frac{1}{2}$ particles on N sites, and the sequence of spins is not changed by the Hamiltonian. The difference is that in the above Kondo-reduced model the spin sequence consists of $n + N$ spins and the holes change their spins when moving between O sites. Nevertheless it is possible to construct almost the same effective Hamiltonian in both cases.

Using $p_\sigma^\dagger$ and $d_\sigma^\dagger$ as creation operators of holes of spin σ on O and Cu sites, a general state with n holes on the O sites $j_1, j_2, ..., j_n$ can be written

$$|\Omega_{j_1 j_2 \ldots j_n}(\sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle = d^\dagger_{\frac{1}{2},\sigma_1} d^\dagger_{\frac{3}{2},\sigma_2} \ldots d^\dagger_{j_1-\frac{1}{2},\sigma_{j_1}} p^\dagger_{j_1,\sigma_{j_1+1}} d^\dagger_{j_1+\frac{1}{2},\sigma_{j_1+2}} \ldots d^\dagger_{j_2-\frac{1}{2},\sigma_{j_2+1}} p^\dagger_{j_2,\sigma_{j_2+2}} d^\dagger_{j_2+\frac{1}{2},\sigma_{j_2+3}} \ldots d^\dagger_{N-\frac{1}{2},\sigma_{N+n}} |0\rangle. \tag{4}$$

We now find it convenient to introduce a state which is the Fourier sum over the cyclic permutations of the spins. When it has wave number k, it can be written as

$$|\Phi_{j_1 j_2 \ldots j_n}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle = \frac{1}{\sqrt{n'}} \sum_{m=0}^{n'-1} e^{(imk)} |\Omega_{j_1 j_2 \ldots j_n}[P^m(\sigma_1, \sigma_2, ..., \sigma_{N+n})]\rangle$$

$$= \frac{1}{\sqrt{n'}}\big[|\Omega_{j_1 j_2 \ldots j_n}(\sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle + e^{(ik)}|\Omega_{j_1 j_2 \ldots j_n}(\sigma_2, \sigma_3, ..., \sigma_1)\rangle + \ldots + e^{ik(n'-1)}|\Omega_{j_1 j_2 \ldots j_n}(\sigma_{n'}, \sigma_{n'+1}, ..., \sigma_{n'-1})\rangle\big]$$

where $n' \leqslant N + n$ is such that

$$P^{n'}\{\sigma_1, \sigma_2, ..., \sigma_{N+n}\} = \{\sigma_{n'+1}, \sigma_{n'+2}, ..., \sigma_{n'}\} = \{\sigma_1, \sigma_2, ..., \sigma_{N+n}\}$$

and the wave number takes the values

$$k = (2\pi/n')\,\mu \qquad \mu = 0, 1, 2, ..., n' - 1. \tag{5}$$

To find the effect of the Hamiltonian (2) on the states we consider the three different cases:

I: $\quad 1 < j_1 < j_2 < \ldots < j_n < N$

IIa: $\quad 1 = j_1 < j_2 < \ldots < j_n < N$

IIb: $\quad 1 < j_1 < j_2 < \ldots < j_n = N.$

In the first case the Hamiltonian is simply changing the indices j as in the Hubbard model and we have

$$H|\Phi_{j_1 j_2 \ldots j_n}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle = -\tau\big[|\Phi_{j_1-1 j_2 \ldots j_n}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle + |\Phi_{j_1+1 j_2 \ldots j_n}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle + \ldots + |\Phi_{j_1 j_2 \ldots j_n+1}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle\big]$$

If $j_1 + 1 = j_2$ there will be no $|\Phi_{j_1+1 j_2 \ldots j_n}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle$ term and this state is forbidden.

Now we define the new set of states $|\Psi_{j_1 j_2 \ldots j_n}\rangle$ where the quantum numbers k and σ_j are not involved and a corresponding effective Hamiltonian H_{eff}, such that the effect of H_{eff} on $|\Psi_{j_1 j_2 \ldots j_n}\rangle$ is the same as the effect of H on $|\Phi_{j_1 j_2 \ldots j_n}(k; \sigma_1, \sigma_2, ..., \sigma_{N+n})\rangle$. This is obtained by

$$|\Psi_{j_1 j_2 \ldots j_n}\rangle = c^\dagger_{j_1} c^\dagger_{j_2} \ldots c^\dagger_{j_n} |0\rangle \tag{6}$$

$$H_{\text{eff}} = -\tau \sum_{j=1}^{N-1} (c^\dagger_j c_{j+1} + c^\dagger_{j+1} c_j) \tag{7}$$

in which c_j are fermion operators.

We now consider the case II*a*. The only difference from case I is when the Hamiltonian (2) moves a hole from O site 1 to site N. Then we have

$$\begin{aligned} H_{1\to N}|\Omega_{1j_2\ldots j_n}(\sigma_1,\sigma_2,\ldots,\sigma_{N+n})\rangle &= -\tau p^\dagger_{N,\sigma_1} d^\dagger_{N+\frac{1}{2},\sigma_2} p_{N+1,\sigma_2} d_{N+\frac{1}{2},\sigma_1} d^\dagger_{\frac{1}{2},\sigma_1} p^\dagger_{1,\sigma_2} d^\dagger_{\frac{3}{2},\sigma_3}\ldots d^\dagger_{N-\frac{1}{2},\sigma_{N+n}}|0\rangle \\ &= -\tau p^\dagger_{N,\sigma_1} d^\dagger_{\frac{1}{2},\sigma_2} d^\dagger_{\frac{3}{2},\sigma_3}\ldots d^\dagger_{N-\frac{1}{2},\sigma_{N+n}}|0\rangle \\ &= -\tau(-1)^{N+n-1} d^\dagger_{\frac{1}{2},\sigma_2} d^\dagger_{\frac{3}{2},\sigma_3}\ldots d^\dagger_{N-\frac{1}{2},\sigma_{N+n}} p^\dagger_{N,\sigma_1}|0\rangle \\ &= -\tau(-1)^{N+n-1}|\Omega_{j_2\ldots j_nN}(\sigma_2,\sigma_3,\ldots,\sigma_{N+n},\sigma_1)\rangle. \end{aligned}$$

This gives

$$H_{1\to N}|\Phi_{1j_2\ldots j_n}(k;\sigma_1,\sigma_2,\ldots,\sigma_{N+n})\rangle = -\tau(-1)^{N+n-1}e^{(-ik)}|\Phi_{j_2j_3\ldots j_nN}(k;\sigma_1,\sigma_2,\ldots,\sigma_{N+n})\rangle$$

and corresponds to an additional term in the effective Hamiltonian. It is simply seen to be

$$H_{\text{eff}}(1\to N) = -\tau(-1)^N e^{(-ik)} c^\dagger_N c_1$$

since then

$$H_{\text{eff}}(1\to N)|\Psi_{1j_2\ldots j_n}\rangle = -\tau(-1)^N e^{(-ik)} c^\dagger_N c^\dagger_{j_2}\ldots c^\dagger_{j_n}|0\rangle = -\tau(-1)^{N+n-1}e^{(-ik)}|\Psi_{j_2\ldots j_nN}\rangle.$$

Repeating this argument for case II*b*, it follows that the effect of H on the arbitrary state $|\Phi_{j_1j_2\ldots j_n}(k;\sigma_1,\sigma_2,\ldots,\sigma_{N+n})\rangle$ is again the same as the effect of H_{eff} on the state $|\Psi_{j_1j_2\ldots j_n}\rangle$ where now the full, effective Hamiltonian with the above boundary piece is

$$H_{\text{eff}} = -\tau\left(\sum_{j=1}^{N-1}(c^\dagger_j c_{j+1} + c^\dagger_{j+1}c_j) + (-1)^N e^{(-ik)} c^\dagger_N c_1 + (-1)^N e^{(ik)} c^\dagger_1 c_N\right) \tag{8}$$

The only difference between this effective Hamiltonian and that of the single-band Hubbard model is the factor $(-1)^N$ and the possible values k can take.

We can make this Hamiltonian translationally invariant by the local gauge transformation

$$c_j = e^{(i\theta_j)} a_j \qquad c^\dagger_j = e^{(-i\theta_j)} a^\dagger_j \tag{9}$$

when the phase angle takes the special value $\theta_j = j\Delta$. When the parameter Δ satisfies the condition

$$e^{\{i[k+(N-1)\Delta]\}} = e^{[-i(\Delta-\pi N)]} \tag{10}$$

which is equivalent to $\Delta = -k/N + \pi$, the effective Hamiltonian takes the form of the tight-binding model

$$H_{\text{eff}} = -\tau\sum_{j=1}^{N}[e^{(i\Delta)} a^\dagger_j a_{j+1} + e^{(-i\Delta)} a^\dagger_{j+1} a_j]. \tag{11}$$

It is easily diagonalized in momentum space where it becomes

$$H_{\text{eff}} = -2\tau \sum_q \cos(q + \Delta) a_q^\dagger a_q \tag{12}$$

with the quantized momenta

$$q = (2\pi/N)\,\nu \qquad \nu = 0, 1, \ldots, N-1. \tag{13}$$

The number operator $n_q = a_q^\dagger a_q$ has eigenvalues $n_q = 0, 1$ so the eigenvalues of the Hamiltonian are

$$E_{\{n_q\}} = 2\tau \sum_q \cos\left(q - \frac{k}{N}\right) n_q \tag{14}$$

where the set of quantum numbers $\{n_q\}$ has to satisfy the constraint

$$\sum_q n_q = n. \tag{15}$$

We see that the energy spectrum is identical to the spectrum of the single-band Hubbard model [17] except for the overall minus sign and the possible values (5) the wave number k can take.

We are now also able to calculate the ground state correlation function for two O holes in a system with N Cu holes. The ground state will be of the form

$$|\psi_0\rangle = a_{q_1}^\dagger a_{q_2}^\dagger |0\rangle \tag{16}$$

and has the energy

$$E_0 = 2\tau\left(\cos\eta_1 + \cos\eta_2\right)$$

where $\eta_i = q_i - k/N$ with the constraint $q_1 \neq q_2$. In the ground state the quantum numbers must be chosen such that both η_1 and η_2 are as close as possible to π. This is obtained when the difference $\eta_1 - \eta_2$ is as small as possible. Thus we have $q_1 - q_2 = \pm 2\pi/N$. The correlation function is given by

$$\langle n_{j_1} n_{j_2}\rangle_N = \langle\psi_0|a_{j_1}^\dagger a_{j_1} a_{j_2}^\dagger a_{j_2}|\psi_0\rangle = 2\left[1 - \cos\left(q_1 - q_2\right)\left(j_1 - j_2\right)\right]/N^2. \tag{17}$$

when $j_1 \neq j_2$. With the above result for $q_1 - q_2$ in the ground state, it then becomes

$$\langle n_{j_1} n_{j_2}\rangle_N = 2\left[1 - \cos(2\pi/N)\left(j_1 - j_2\right)\right]/N^2. \tag{18}$$

When $j_1 = j_2$, we have simply

$$\langle n_{j_1} n_{j_1}\rangle_N = \langle n_{j_1}\rangle_N = 2/N$$

which is simply the density of two O holes on N sites.

A homogeneous magnetic flux ϕ through the ring leads to the appearance of a phase factor $e^{(i\phi/N)}$ in the hopping term τ. This changes the energy spectrum (14) to

$$E_{\{n_q\}} = 2\tau \sum_q \cos\left(q - \frac{k}{N} + \frac{\phi}{N}\right) n_q. \tag{19}$$

We see that the term $-k/N$ appears in the energy in the same way as the external flux. It is therefore natural to consider it some kind of induced flux due to the dynamics of the quantum spins. Under interchange of holes it was shown in [10] that it also shows up in a phase factor, which is consistent with this interpretation. One can therefore also call this induced term a statistical flux.

The correlation function does not depend on the magnetic flux since the difference $\eta_1 - \eta_2$ is independent of it.

3. Ground-state energies

When the spin–exchange coupling $J \neq 0$, the Hamiltonian (1) does not have an exact solution. We have instead performed numerical calculations of the ground-state energy (GSE) using the Dagotto–Moreo algorithm [18]. We have considered systems characterized by different numbers of Cu and O holes and a homogeneous magnetic flux ϕ through the ring. To find the ground state for an even number of spins we used as a basis all possible states with $S_z = 0$, and for an odd number of spins we chose as a basis all states with $S_z = -1$, for convenience spin is measured in integer units. In figure 2 the ground state of a chain consisting of one O and six Cu holes is plotted as a function of external magnetic flux. The upper curve corresponds to $J = 0$ and can also be obtained from (19). It changes gradually as J is increased to $J = 0.1$. The shape of the GSE is similar for all $J \geqslant 0.1$. There are absolute minima in the energy at $\phi/2\pi \simeq 0.28$ and $\phi/2\pi \simeq 0.72$ and at the other periodically equivalent points.

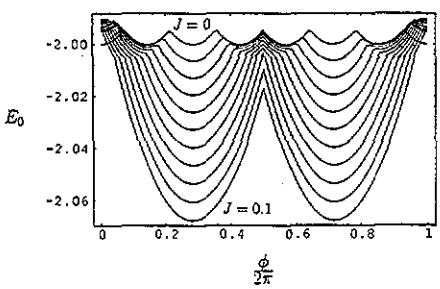

Figure 2. Ground-state energy E_0 as a function of magnetic flux in a system consisting of one O and six Cu holes. The coupling constant J is changed from 0 to 0.1 in steps of 0.01.

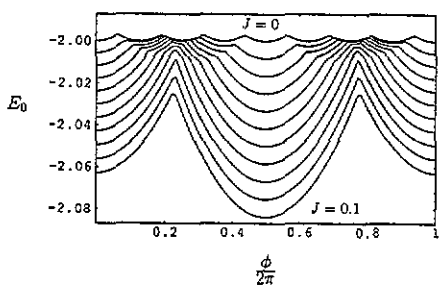

Figure 3. Ground-state energy E_0 as a function of magnetic flux in a system consisting of one O and seven Cu holes. The coupling constant J is changed from 0 to 0.1 in steps of 0.01.

When the number of Cu spins increases by one, we find the new energies shown in figure 3. There is now an absolute minimum at $\phi/2\pi = 0.5$ and slightly higher minima

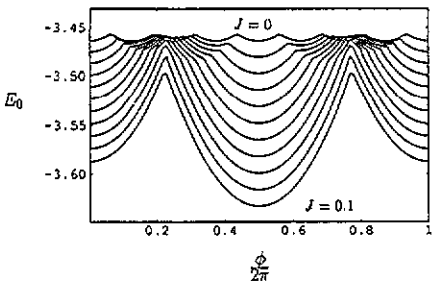

Figure 4. Ground state energy as a function of magnetic flux in a system consisting of two O and six Cu holes. The coupling constant J is changed from 0 to 0.1 in steps of 0.01.

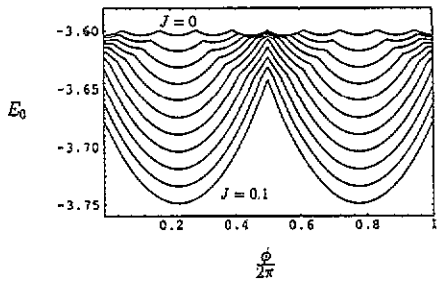

Figure 5. Ground state energy E_0 as a function of magnetic flux in a system consisting of two O and seven Cu holes. The coupling constant J is changed from 0 to 0.1 in steps of 0.01.

at $\phi/2\pi = 0.1$. Qualitatively the same behaviour is found with two holes moving in a background of six Cu spins, shown in figure 4. With two holes among seven Cu spins, shown in figure 5, we again find a dependence on the external flux similar to the case shown in figure 2 with one O hole and six Cu spins.

The effect of the external flux is seen to depend in a significant way on the total number of spins in the system, i.e. the number of mobile O holes plus the number of localized Cu spins. We see that the most important changes in the energy occur when J increases from 0 to 0.1 in units of τ. For further increases in J the variation of the GSE with the flux does not change substantially, simply the magnitude of the energy. In section 5 we will explain this behaviour in the strong-coupling limit in terms of a compound particle consisting of an O hole and its two nearest Cu spin neighbours.

From these results we may also conjecture about the behaviour of such systems in the thermodynamic limit. Figures 3 and 4 indicate that the local minima of the GSE will persist at integer and half-integer values for the magnetic flux $\phi/2\pi$. When increasing the length of the chain, these minima are expected to tend to the same limit. This would then be evidence for a superconducting state of the one-dimensional ring according to the Byers–Yang theorem [19]. Similar results are obtained for the attractive and repulsive Hubbard model and a t–J-like model on cyclic chains [20]. The situation with odd numbers of spins in figures 2 and 5 in the thermodynamic limit seems even more intriguing, because the GSE minima are situated at the magnetic flux values $\phi/2\pi = \frac{1}{4}(2n \pm 1)$. The periodicity of $E_0(\phi)$ in this case again signals the appearance of superconductivity at $T = 0$. Perhaps the unusual shift of the minima is connected with a constant induced flux of magnitude $\phi/2\pi = \frac{1}{4}$.

4. Correlation functions

Numerically it is straightforward to calculate the correlation function between two O holes. With zero spin–exchange coupling the correlation function was found to be independent of the flux in the analytical result (18). When the spin–exchange coupling J is different from zero, the correlation functions are found to be almost independent of the magnetic flux. They change by at most 1% or 2% as the flux is varied and we will therefore take the flux to be zero.

We have numerically calculated the charge correlation function $C_{ij} = \langle n_i n_j \rangle$ for the O holes. At $J = 0$ the two holes were found to repel each other. With increasing coupling J

this repulsion increases as seen in figure 6, where the correlation functions are calculated for a system consisting of two O holes and five Cu spins. When $J \geqslant 50$ there is almost zero probability for the two holes to be nearest neighbours and $\langle n_1 n_3 \rangle$ approaches the upper limit $\frac{1}{5}$. This asymptotic value is consistent with two equally distanced holes distributed over five possible sites. For $J = 0$ the numerically calculated correlation functions agree with the analytical result of (18).

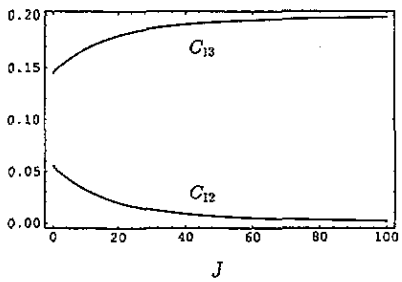

Figure 6. Oxygen hole correlation functions in a system consisting of two O and five Cu holes with zero magnetic field.

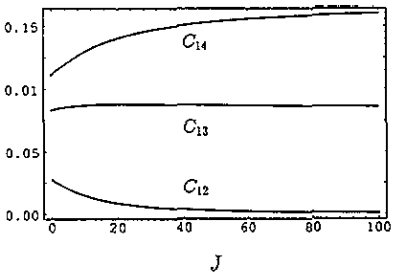

Figure 7. Oxygen hole correlation functions in a system consisting of two O and six Cu holes and with zero magnetic field.

In figure 7 the number of Cu holes is increased by one. Now there are three different possible distances between the two O holes. Again we see that the correlation functions increase with the hole separation. The repulsion becomes stronger as the spin–exchange coupling increases, but the next-nearest-neighbour correlation remains small and almost constant. The reason for such an excluded-volume effect will be elucidated in section 5 where the concept of a compound particle makes a strong O–O repulsion at the nearest sites clear.

To obtain some information about the spin configurations we have also calculated the spin correlation functions of the Cu spins. When $J = 0$ these correlations are irrelevant since the Hamiltonian does not change the spin sequence. However, when $J > 0$, the configurations are mixed and non-trivial correlations will arise. In figure 8 we plot the different correlation functions versus J in a system consisting of one O and six Cu spins. They are calculated with magnetic flux $\phi/2\pi = 0.2$. The correlation functions are defined as

$$S_{mn} = \langle s_m s_n \rangle - \langle s_m \rangle \langle s_n \rangle \tag{20}$$

where s_m is the spin projection of the spin on the mth Cu site and s_n the projection of the spin on the nth Cu site. The Cu spin expectation value $\langle s \rangle$ is also calculated and we see that somewhat surprisingly $\langle s \rangle \neq -\frac{1}{7}$. This means that $\langle s \rangle$ and the O-spin expectation value $\langle \sigma \rangle$ are not equal. The O spin tends to have a positive spin projection when $\langle s \rangle$ is negative. This means that the O spin tends to arrange the nearest Cu spins antiferromagnetically.

In figure 9 one Cu spin is added and $\langle s \rangle = \langle \sigma \rangle = 0$ because the number of spins up and down are equal and the state is symmetric with respect to the spin projection. Here the tendency to antiferromagnetic ordering is even more clear.

The correlation functions are plotted in figure 10 as a function of the magnetic flux when the spin–exchange coupling $J = 0.1$. The step-like behaviour at $\phi/2\pi = 0.22$ and

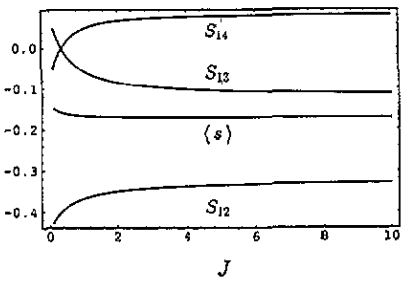

Figure 8. Copper spin correlation functions as function of spin–exchange coupling J with magnetic flux $\phi/2\pi = 0.2$. The system consists of a cyclic chain of one O and six Cu spins.

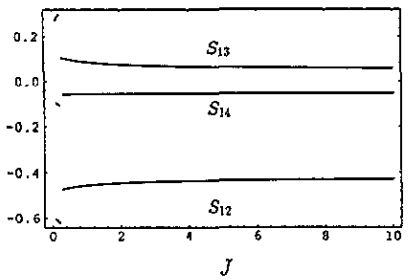

Figure 9. Copper spin correlation functions as function of spin–exchange coupling J with magnetic flux $\phi/2\pi = 0.2$. The system consists of a cyclic chain of one O and seven Cu spins.

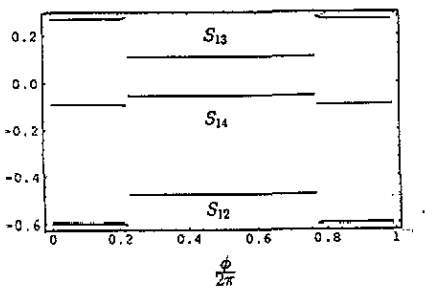

Figure 10. Copper spin correlation functions as a function of magnetic flux with spin–exchange coupling $J = 0.1$. The system consists of a cyclic chain of one O and seven Cu spins.

0.78 corresponds to the sharp peaks in the lowest plot of the elsewhere smooth ground state in figure 3. This is because the ground-state wave function changes at these values of the flux. A similar situation appears in figure 9 in a narrow region around $J = 0$.

Concluding this section we wish to discuss the possibility of application of the conformal field theory ideas to estimate the exponents of the spin–spin correlation function [21, 22]. In order to realize this program for the spin-$\frac{1}{2}$ Heisenberg model, we need to perform a finite-size calculation of the leading terms in the GSE and of the first excited energy level. Extrapolations performed for the lattice size up to 18 spins give a reasonable, but not perfect, estimate of the exponent mentioned above. However, a similar estimate is problematic in the present model. Therefore, let us consider carrier concentration $\frac{1}{3}$. Corresponding chain fragments are (3 Cu, 1 O), (6 Cu, 2 O) and (9 Cu, 3O). Certainly, this information is not enough to extract the terms proportional to N and N^{-1} (N is the total number of Cu sites). It is noteworthy that computer size limits the use of numerical methods to find the GSE for chain fragments consisting of more than 10 Cu sites.

5. Compound particles in the strong-coupling limit

The concept of compound particles has been discussed after the remark of Anderson [23] that the Emery model can be mapped on a single band model. Such a mapping was carried out by Zhang and Rice [24]. They interpreted a compound particle as an O hole attached to the O plaquette surrounding the central Cu site. Emery and Reiter [25] also used the idea of a compound particle, however, they involved in the complex particle one O hole and two Cu spins. So, our consideration is more of the Emery–Reiter type than of that due to

Zhang and Rice. The intrinsic structure of the complex involving the O hole, which tends to localize in its environment some paramagnetic configuration, is known after the estimate by the variational method by Glazman and Ioselevich [26] and relates also to the Emery-Reiter type of interpretation. In this section we present one more example of a compound particle model for which an exact solution exists.

When the spin–exchange coupling J is much larger than the amplitude of the hopping amplitude τ, one O hole and the two Cu holes surrounding it are bound in a compound particle due to the strong Cu–O exchange force. In the leading order such a compound particle is localized. However, due to the hopping amplitude, the O hole can be transferred onto the nearest O site, destroying the coherent spin state and creating a new compound particle at the new site. The effective hopping amplitude of such a compound particle obviously depends on the spin arrangement.

One can easily check that the ground state wave function of one O spin-$\frac{1}{2}$ hole, coupled antiferromagnetically with the two Cu spins surrounding it, is a spin doublet. When this compound particle is situated at site m and has a positive spin projection, it is represented by the operator

$$C^{\dagger}_{m,\uparrow} = (1/\sqrt{6})\Big(2d^{\dagger}_{m-1/2,\uparrow}p^{\dagger}_{m,\downarrow}d^{\dagger}_{m+1/2,\uparrow} - d^{\dagger}_{m-1/2,\downarrow}p^{\dagger}_{m,\uparrow}d^{\dagger}_{m+1/2,\uparrow} - d^{\dagger}_{m-1/2,\uparrow}p^{\dagger}_{m,\uparrow}d^{\dagger}_{m+1/2,\downarrow}\Big)$$

The GSE for such a compound particle is equal to $-J$ if the exchange operator has the form $J\hat{P}$ where $\hat{P}$ is the spin permutation operator.

We will now calculate the amplitudes of the effective hopping terms. Starting with a sequence of spins $C^{\dagger}_{m,\uparrow}d^{\dagger}_{m+\frac{3}{2},\uparrow}$, it is changed by the Hamiltonian into

$$\begin{aligned} C^{\dagger}_{m,\uparrow}d^{\dagger}_{m+\frac{3}{2},\uparrow} \rightarrow (1/\sqrt{6})\Big(&-2d^{\dagger}_{m-1/2,\uparrow}d^{\dagger}_{m+1/2,\downarrow}p^{\dagger}_{m+1,\uparrow}d^{\dagger}_{m+\frac{3}{2},\uparrow} \\ &+ d^{\dagger}_{m-1/2,\downarrow}d^{\dagger}_{m+1/2,\uparrow}p^{\dagger}_{m+1,\uparrow}d^{\dagger}_{m+\frac{3}{2},\uparrow} \\ &+ d^{\dagger}_{m-1/2,\uparrow}d^{\dagger}_{m+1/2,\uparrow}p^{\dagger}_{m+1,\downarrow}d^{\dagger}_{m+\frac{3}{2},\uparrow}\Big) \Rightarrow \tfrac{2}{3}\,d^{\dagger}_{m-1/2,\uparrow}C^{\dagger}_{m+1,\uparrow} \end{aligned}$$

when the amplitudes are measured in units of τ and we have projected the resulting state onto the compound particle again. For the sequence of spins $C^{\dagger}_{m,\uparrow}d^{\dagger}_{m+\frac{3}{2},\downarrow}$ the analogous calculation results in

$$\begin{aligned} C^{\dagger}_{m,\uparrow}d^{\dagger}_{m+\frac{3}{2},\downarrow} \rightarrow (1/\sqrt{6})\Big(&-2d^{\dagger}_{m-1/2,\uparrow}d^{\dagger}_{m+1/2,\downarrow}p^{\dagger}_{m+1,\uparrow}d^{\dagger}_{m+\frac{3}{2},\downarrow} \\ &+ d^{\dagger}_{m-1/2,\downarrow}d^{\dagger}_{m+1/2,\uparrow}p^{\dagger}_{m+1,\uparrow}d^{\dagger}_{m+\frac{3}{2},\downarrow} + d^{\dagger}_{m-1/2,\uparrow}d^{\dagger}_{m+1/2,\uparrow}p^{\dagger}_{m+1,\downarrow}d^{\dagger}_{m+\frac{3}{2},\downarrow}\Big) \\ \Rightarrow\ &-\tfrac{5}{6}\,d^{\dagger}_{m-1/2,\uparrow}C^{\dagger}_{m+1,\downarrow} - \tfrac{1}{6}\,d^{\dagger}_{m-1/2,\downarrow}C^{\dagger}_{m+1,\uparrow}. \end{aligned}$$

The corresponding equations describing how $C^{\dagger}_{m,\downarrow}d^{\dagger}_{m+\frac{3}{2},\uparrow}$ and $C^{\dagger}_{m,\downarrow}d^{\dagger}_{m+\frac{3}{2},\downarrow}$ transform are now evident.

Most likely, a single compound particle problem defined in terms of these hopping matrix elements cannot be solved exactly for an arbitrary Cu magnetic arrangement. However, we can solve it for some special backgrounds. The simplest is the ferromagnetic case when we can take the basis states to be the following:

$$
\begin{aligned}
|\psi_1\rangle &= C^\dagger_{1,\uparrow} d^\dagger_{5/2,\uparrow} \dots d^\dagger_{N-1/2,\uparrow}|0\rangle \\
|\psi_2\rangle &= d^\dagger_{1/2,\uparrow} C^\dagger_{2,\uparrow} d^\dagger_{7/2,\uparrow} \dots d^\dagger_{N-1/2,\uparrow}|0\rangle \\
&\vdots \\
|\psi_{N-1}\rangle &= d^\dagger_{1/2,\uparrow} \dots d^\dagger_{N-5/2,\uparrow} C^\dagger_{N-1,\uparrow}|0\rangle \\
|\psi_N\rangle &= C^\dagger_{N,\uparrow} d^\dagger_{\frac{3}{2},\uparrow} \dots d^\dagger_{N-\frac{3}{2},\uparrow}|0\rangle.
\end{aligned}
$$

Now using the derived hopping amplitudes for the compound particle applied to these states, we find for the corresponding wave functions

$$\mathcal{H}\psi_m = \tfrac{2}{3}(\psi_{m-1} + \psi_{m+1}) \qquad 2 \leqslant m \leqslant N-1$$

where $\mathcal{H}$ is the effective Hamiltonian acting in this space of projected states. Similarly, hopping from the first and last states in the above sequence results in

$$\mathcal{H}\psi_1 = \tfrac{2}{3}\big[\psi_2 + (-1)^N \psi_N\big] \qquad \mathcal{H}\psi_N = \tfrac{2}{3}\big[\psi_{N-1} + (-1)^N \psi_1\big].$$

This is simplified after the local gauge transformation

$$\psi_m \to (-1)^m \, \mathrm{e}^{(\mathrm{i}\alpha m)} \overline{\psi}_m \tag{21}$$

which restores translational invariance. Then we have for all states

$$\mathcal{H}\overline{\psi}_m = -\tfrac{2}{3}\big[\mathrm{e}^{(-\mathrm{i}\alpha)}\overline{\psi}_{m-1} + \mathrm{e}^{(\mathrm{i}\alpha)}\overline{\psi}_{m+1}\big]. \tag{22}$$

We can now impose periodic boundary conditions which yield $\alpha = (2\pi/N)n$ where n is an integer. The resulting energy eigenvalues are therefore

$$\varepsilon = -\tfrac{4}{3}\cos(2\pi n/N + \phi/N) \tag{23}$$

where we again have included the effect of an external magnetic flux ϕ and we now measure the energy in units of τ. In addition to this term we will have the uninteresting, but much larger energy $-J$ of the compound particle. The energies (23) are very similar to what would result for a single particle in a periodic lattice in the tight-binding approximation. This should be expected as long as the Cu spin background remains undisturbed. Since the total spin of this system is very high, the result cannot be compared with the previously obtained GSE since these were calculated for the states with the smallest spin.

We can also obtain an analytic solution in the somewhat more realistic case involving a compound particle and a flipped spin. Now we define the set of basis eigenfunctions as follows:

$$|\psi^{>}_{m,n+1/2}\rangle = \ldots C^{\dagger}_{m,\uparrow}\ldots d^{\dagger}_{n+1/2,\downarrow}\ldots|0\rangle \qquad 1 \leqslant m \leqslant n-1 \qquad n < N$$

$$|\psi^{<}_{m,n-1/2}\rangle = \ldots d^{\dagger}_{n-1/2,\downarrow}\ldots C^{\dagger}_{m,\uparrow}\ldots|0\rangle \qquad 1 \leqslant n \leqslant m-1 \qquad m < N$$

$$|\psi_{N,n+1/2}\rangle = C^{\dagger}_{N,\uparrow}\ldots d^{\dagger}_{n+1/2,\downarrow}\ldots|0\rangle \qquad 1 \leqslant n < N-1$$

$$|\psi_{m}\rangle = \ldots C^{\dagger}_{m,\downarrow}\ldots|0\rangle \qquad 1 \leqslant m < N$$

$$|\psi_{N}\rangle = C^{\dagger}_{N,\downarrow}\ldots|0\rangle.$$

In order to use these states in a translationally invariant form, we subject the corresponding amplitudes to a local gauge transformation as in (21):

$$\psi_{m,r} \to (-1)^{m}\mathrm{e}^{(\mathrm{i}\alpha m)}\overline{\psi}_{m,r} \qquad \psi_{m} \to (-1)^{m}\mathrm{e}^{(\mathrm{i}\alpha m)}\overline{\psi}_{m} \tag{24}$$

with $\alpha = 2\pi l/N$. When the effective hopping Hamiltonian now acts on these states, we find that it gives

$$\mathcal{H}\overline{\psi}_{m,r} = -\tfrac{2}{3}\left(\mathrm{e}^{(-\mathrm{i}\gamma)}\overline{\psi}_{m-1,r} + \mathrm{e}^{(\mathrm{i}\gamma)}\overline{\psi}_{m+1,r}\right) \tag{25}$$

where r is some half integer labeling the site of a Cu spin and satisfying the conditions $|r-m| > \frac{3}{2}$ and $|r-m| < N-\frac{3}{2}$. Then the compound particle is outside the range where it can interact with the flipped spin. If it is not, then we obtain instead

$$\mathcal{H}\overline{\psi}_{m,m\pm\frac{3}{2}} = \tfrac{1}{6}\,\mathrm{e}^{(\pm\mathrm{i}\gamma)}\overline{\psi}_{m\pm1,m\mp1/2} + \tfrac{5}{6}\,\mathrm{e}^{(\pm\mathrm{i}\gamma)}\overline{\psi}_{m\pm1} - \tfrac{2}{3}\,\mathrm{e}^{(\mp\mathrm{i}\gamma)}\overline{\psi}_{m\mp1,m\pm\frac{3}{2}} \tag{26}$$

$$\mathcal{H}\overline{\psi}_{m} = \tfrac{1}{6}\left[\mathrm{e}^{(\mathrm{i}\gamma)}\overline{\psi}_{m+1} + \mathrm{e}^{(-\mathrm{i}\gamma)}\overline{\psi}_{m-1}\right] + \tfrac{5}{6}\left[\mathrm{e}^{(\mathrm{i}\gamma)}\overline{\psi}_{m+1,m-1/2} + \mathrm{e}^{(-\mathrm{i}\gamma)}\overline{\psi}_{m-1,m+1/2}\right] \tag{27}$$

Here we have introduced $\gamma = \alpha + \phi/N$ when the system is in an external flux ϕ. The solutions of these equations are now translationally invariant and will depend on the distance between the compound particle and the spin flip.

We can now solve this eigenvalue problem. Writing the eigenvalues in the form

$$\varepsilon = -\tfrac{2}{3}(e^{q} + e^{-q}) \tag{28}$$

one can easily check that eigenstates will be of the form

$$\overline{\psi}_{m,m+\frac{3}{2}} = A\mathrm{e}^{[-q(N-3)]} + B$$

$$\overline{\psi}_{m-1,m+\frac{3}{2}} = \mathrm{e}^{(\mathrm{i}\gamma)}[Ae^{-q(N-3)}\mathrm{e}^{q} + B\mathrm{e}^{(-q)}]$$

$$\vdots$$

$$\overline{\psi}_{m+3,m+\frac{3}{2}} = \mathrm{e}^{[\mathrm{i}\gamma(N-3)]}\left\{A + B\mathrm{e}^{[-q(N-3)]}\right\}.$$

Substituting these amplitudes into (26), we obtain the two equations

$$\left\{e^{[i\gamma(N-2)]} + 4e^{[-q(N-2)]}\right\}A + \left\{4e^{q} + e^{[i\gamma(N-2)]}e^{[-q(N-3)]}\right\}B + 5e^{(i\gamma)}\psi = 0$$
$$\left\{4e^{q} + e^{[-i\gamma(N-2)]}e^{[-q(N-3)]}\right\}A + \left\{e^{[-i\gamma(N-2)]} + 4e^{[-q(N-2)]}\right\}B + 5e^{[-i\gamma(N-2)]}\psi = 0$$

where now $\overline{\psi}_m$ = constant = ψ. Similarly, we obtain from (27)

$$5\left\{e^{[i\gamma(N-2)]} + e^{(-i\gamma)}e^{[-q(N-3)]}\right\}A + 5\left\{e^{(-i\gamma)} + e^{[i\gamma(N-2)]}e^{[-q(N-3)]}\right\}B + \left\{2\cos\gamma + 4\left[(e^{q} + e^{(-q)}\right]\right\}\psi = 0$$

completing the set of three linear equations for the three unknowns A, B and ψ. The solution will give us $q(\gamma)$ and, hence, the energy of the interacting state. We note that the quantity $e^{[\pm i\gamma(N-2)]}$ entering the equations can be transformed into $e^{[\pm i(\phi-2\gamma)]}$.

In the limit of a very long chain the effect of periodicity disappears. After some elementary calculations the above eigenvalue problem then simplifies to

$$16z^4 + 8z^3\cos\gamma - 35z^2 + 12z\cos\gamma - 1 = 0 \tag{29}$$

where $z = \exp q$. Naturally, the energy must depend on the generalized wave number γ. When $\gamma = 0$ we reproduce the GSE as in the case of the compound particle in the ferromagnetic background. However, non-zero γ values will lower the energy. Its minimum is $\varepsilon = -1.609$ when $\gamma = \pi$. Most likely, the energy spectrum will become lower and lower with increasing number of spin flips. In the infinite-chain limit it probably becomes a non-dispersion level with no periodic dependence on the external flux.

Finite rings are good candidates for studying the behaviour of complex systems that include particles and their spin environment. We can now compare the above analytical results for one compound particle and one spin flip with our numerical results for one O particle on the background consisting of three and four Cu spins. In both of these cases the GSE of the system should then result. For such small systems it is not possible to neglect the terms proportional to $\exp(-qN)$.

For a ring with $N = 3$ Cu spins, the determinant for the above set of linear equations simplifies to

$$25\cos^2\gamma = \left\{\cos\gamma + 2\left[(e^{q} + e^{(-q)})\right]\right\}^2$$

which has the solutions

$$\varepsilon = 2\cos\gamma \qquad \varepsilon = -\tfrac{4}{3}\cos\gamma. \tag{30}$$

When the number of Cu spins is $N = 4$, the determinant gives the polynomial equation

$$16z^6 + 8z^5\cos\gamma + (-19 + 8\cos 2\gamma)z^4 + (20\cos\gamma + 4\cos\gamma\cos 2\gamma - 50\cos 3\gamma)z^3 + (-19 + 8\cos 2\gamma)z^2 + 8z\cos\gamma + 16 = 0$$

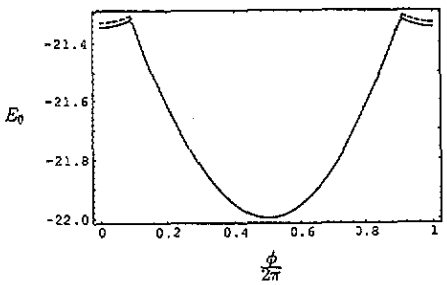

Figure 11. Ground state energy of a system consisting of one O and three Cu spins as a function of magnetic flux with $J = 20$. The broken curve corresponds to the compound particle and the full curve to the numerical results.

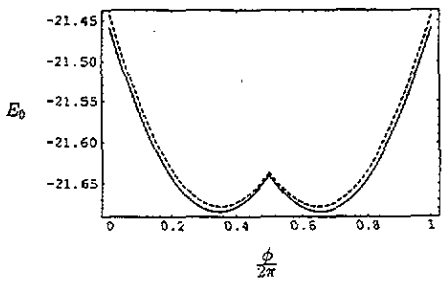

Figure 12. Ground state energy of a system consisting of one O and four Cu spins as a function of magnetic flux with $J = 20$. The broken curve corresponds to the compound particle and the full curve to the numerical results.

which has the analytical solutions

$$\varepsilon = \tfrac{1}{6}\left(5\cos\gamma \pm \sqrt{75 - 71\cos^2\gamma}\right) \qquad \varepsilon = -\tfrac{4}{3}\cos\gamma. \tag{31}$$

Since the generalized wave number $\gamma = \alpha + \phi/N$, these energies are functions of the flux ϕ.

In figure 11 we compare the GSE of a system consisting of one O and three Cu spins found from equation (30) using $E_0 = -J + \varepsilon$ with our previous numerical results. The parameters of the Hamiltonian are $J = 20$ and $\tau = 1$. The broken curve corresponds to the numerical results and we see that it coincides with the full curve corresponding to the analytical results in the central part of the figure. The results for a ring with $N = 4$ Cu spins are shown in figure 12. The true numerical GSE lies slightly below the analytical result of equation (31), but the agreement is still surprisingly good.

6. Conclusions

The KRE model is probably typical of various strongly correlated fermionic models. We have here restricted our considerations to finite rings, consisting of alternating atoms as in Cu–O chain fragments. This problem is not completely academic because in real HT superconductors like Y–Ba–Cu–O the chain fragments form O deficient planes and are responsible for the charge-transfer mechanism and some other normal properties of such substances. Among several interesting properties of the model, we would like to mention the unusual dependence of the GSE on the external flux. We explain this in terms of a dynamically induced statistical field. It probably allows a superconducting state at zero temperature for infinite chains.

The paper starts with the rigorous analysis of the KRE model when the spin–exchange coupling J is negligible. In this limit one can separate the charge and spin degrees of freedom and the model can be solved exactly in terms of free fermions. In addition, the ground state wave function has a well defined form for any value of the external flux, which allows us to perform perturbative calculations over a small parameter J. There is a possibility for a straightforward, but tedious analytical calculation of the minima in the GSE using perturbation theory when $J \ll \tau$.

For general values of the spin–exchange coupling we calculate the GSE numerically for small chains using the variationally based algorithm of Dagotto and Moreo. We can then also obtain the charge and spin correlation functions. These calculations can be extended to also determine the first excited state. Using finite-size scaling we can then extrapolate to large systems where results from conformal field theory can be used. One can then hope to estimate the exponents of the correlation functions in this limit.

In the last part of the paper we consider the opposite limit of a rather small Kondo-hopping term where the spin–exchange dominates the dynamics. In this case the compound-particle concept is applied to reformulated the initial model in terms of a modified, but also strongly correlated, model. This allows a fairly simple solution for $N = 3$ and $N = 4$ Cu spins which explains our numerical results in this limit. The problem of compound particles in larger systems should also be addressed. Its solution will give much needed insight and understanding of such strongly correlated fermion systems.

Acknowledgments

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