Influence of finite Hund rules and charge transfer on properties of Haldane systems.

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We consider the Kondo-Hubbard model with ferromagnetic exchange coupling \(J_H\), showing that it is an approximate effective model for late transition metal-O linear systems. We study the dependence of the charge and spin gaps \(\Delta_C, \Delta_S\), and several spin-spin correlation functions, including the hidden order parameter \(Z(\pi)\), as functions of \(J_H/t\) and \(U/t\), by numerical diagonalization of finite systems. Except for \(Z(\pi)\), all properties converge slowly to the strong-coupling limit. When \(J_H/t \sim 2\) and \(U/t \sim 7\) (the effective parameters that we obtain for \(Y_2\)BaNiO\(_5\)), \(\Delta_S\) is roughly half of the value expected from a strong-coupling expansion.

I. INTRODUCTION

After Haldane’s conjecture that integer-spin antiferromagnetic Heisenberg chains should exhibit a gap in their excitation spectrum, there has been a considerable amount of research in spin \(S = 1\) systems. Fascinating aspects of these systems are the presence of free spin-1/2 excitations at the end of sufficiently long finite chains, and the presence of a hidden string-topological order.

The compound \(Y_2\)BaNiO\(_5\) is a candidate to a nearly ideal realization of the spin \(S = 1\) antiferromagnetic Heisenberg chain and stimulated intense research on the system recently. The 1D character is supported by experimental evidence which shows that the exchange couplings transverse to the chains are very small and unable to induce long range magnetic order. The representation of the two \(S = 1/2\) holes per Ni by a \(S = 1\) spin in the effective one-band model is, however, an intuitive but not clearly justified simplification, being the underlying assumption a large Hund rule acting on the two relevant Ni-orbitals. Such a point of view has been adopted in most theoretical works of the system, like an alternative interpretation of specific-heat experiments in Zn-doped \(Y_2\)BaNiO\(_5\) which raised doubts about the presence of free spin-1/2 excitations near the end of long chains. Theoretical work motivated by other experimental results for Ca-doped \(Y_2\)BaNiO\(_5\), for which the NiO chains are not broken, but doped with holes also retain only the ground state of the 3d\(^8\) configuration of Ni\(^{2+}\).

On general physical grounds one expects the effective Ni-Ni hopping (via O) to be of the order of the corresponding one in CuO chains \((t \sim 0.85\text{eV})\). Furthermore, spectroscopic data in atomic Ni show that the Hund rule leads to a ferromagnetic exchange \(J_H \sim 1.6\text{eV}\). Thus, it seems that not only the triplet ground state of the 3d\(^8\) configuration of Ni\(^{2+}\), but also the excited singlet should be taken into account for a realistic description of the system. Except for a brief discussion on the charge gap and Ni \(L_3\) x-ray absorption spectrum, this issue has been unexplored so far, to our knowledge. Even if the effective intratomic repulsion \(U\) is large compared with \(t\), as we shall show, the properties of the system differ from those of the strong-coupling limit. In particular, the expression \(\Delta_S = 0.410\text{eV} J\) for the spin gap in terms of the effective Ni-Ni exchange \(J\), is no longer valid (at least if \(J\) is calculated perturbatively, see section IV). Thus, at least a qualitative study of the effects of a realistic \(J_H\) (instead of infinite) on the properties of these systems seems necessary.

In this work we derive and study the Kondo-Hubbard model with ferromagnetic coupling, as an approximate (in the sense which will be clarified in the next section) effective model for linear transition metal-oxygen systems, in which the relevant transition-metal orbitals are the \(e_g\) ones. The model retains the effects of charge fluctuations at the transition-metal ions and finite Hund rules. Explicit effective parameters are calculated for \(Y_2\)BaNiO\(_5\). Its version with antiferromagnetic coupling \(J_H\) has been extensively studied in the context of heavy fermion systems, while the ferromagnetic case also acquired relevance in connection with the physics of the perovskite Mn oxides with giant magnetoresistance, being also closely related to the double-exchange model and other models used to study these compounds.

In section II, we explain the derivation of the Kondo-Hubbard model as a low-energy effective model, in which some terms of lower magnitude, were neglected for simplicity. Section III contains the results for charge and spin gaps, spin expectation values and several spin-spin correlation functions, obtained by numerical diagonalization. Section IV contains the conclusions.

II. THE LOW-ENERGY REDUCTION PROCEDURE

In the simplest and most usual perovskite structures, the transition metal atoms are in sites of nearly cubic \((O_h)\) symmetry, surrounded by six O atoms, lying in the directions \(\pm x, \pm y, \pm z\). In the particular case of \(Y_2\)BaNiO\(_5\), these octahedra are linked by their vertices
and form well separated chains, making a nearly ideal one-dimensional compound. Since by far, the largest contribution to crystal-field splitting is due to covalency near the end of the 3d series, the few holes present in the 3d shell of the transition metal enter the $e_g$ ($d_{x^2−y^2}$ or $d_{z^2}$) orbitals. This is due to their larger hybridization with the $2p_e$ orbitals (those pointing towards the transition metal atom) of the nearest-neighbor O atoms. The starting multiband Hamiltonian for the system should include the above mentioned orbitals and can be divided as follows:

$$H = H_d + H_p + H_{pd} + H_{pp},$$

where $H_d$ ($H_p$) describes the on-site correlations inside the 3d (2p) shell. $H_{pd}$ contains the transition metal-O hoppings and repulsions. The O-O hopping is described by $H_{pp}$. The last three terms of Eq. (1) are a trivial extension of similar terms extensively described and studied in multiband models for the cuprates and will be not reproduced here. The largest energies in the problem and the ingredients of the new physics when more than one relevant orbital per site is present, are contained in $H_d$. The Coulomb and exchange integrals among the $e_g$ spin-orbitals can be parameterized in terms of three Slater parameters $F_0$, $F_2$ and $F_4$, using usual methods in atomic physics. Denoting $a_{iσ}^+(b_{iσ}^\dagger)$ the creation operator for the $a_{iσ} g_{dz^2−y^2}$ ($b_{iσ} g_{d_{x^2−y^2}}$) orbital at site $i$ with spin $σ$, the result can be written in the form:

$$H_d = U_d \sum_i \{a_{iσ}^+ a_{iσ} a_{iσ}^+ a_{iσ} + b_{iσ}^+ b_{iσ} b_{iσ}^+ b_{iσ}\}
+ (U_d - J_H') \sum_{iσσ'} a_{iσ}^+ a_{iσ} b_{iσ'}^+ b_{iσ'}
+ J_H' \sum_i \{\sum_{σσ'} a_{iσ}^+ b_{iσ'} a_{iσ}^+ b_{iσ}\}
+ \{a_{iσ}^+ b_{iσ}^+ b_{iσ} H.c.\}],$$

where $U_d = F_0 + F_2 + 36 F_4$ and $J_H' = 8 F_2 + 30 F_4$. Because of the neglect of the $t_{2g}$ ($d_{xy}$, $d_{yz}$, $d_{zx}$) orbitals, $H_d$ lost the invariance under rotations of the atom, but retains cubic (O$_h$) symmetry. From the two lowest excitation energies of atomic Ni, we obtain $F_2 = 0.1600$eV and $F_4 = 0.0108$eV, leading to $J_H' = 1.60$eV. According to the theoretical interpretation of optical experiments in NiO, $U_d + J_H'/2 = 10 eV$. This is due to the second-order process which carries a 3$d_{z^2−y^2}$ hole to the same orbital of a nearest-neighbor Ni atom: $t = t_{pd}^2/\Delta$. However, the case $Δ < U_d$ is not representative of charge transfer systems like Y$_2$BaNiO$_5$, for which $Δ < U_d$. In this case, the states $a_{iσ}^+ b_{iσ}^\dagger b_{iσ}$ actually represent states with occupation close to one in the O $π$ orbitals.

As a consequence, $U$ is mainly determined by $Δ$ instead of $U_d$, and the hopping matrix elements become dependent on the occupation and spin of the two sites involved. As mentioned above, this dependence was neglected to keep a simple and more general form of $H_{KH}$. To estimate the parameters of the effective model for Y$_2$BaNiO$_5$, we took the values of $J_H'$ and $U_0$ mentioned above, and the (more uncertain) values of $Δ$ and the different hopping parameters in $H_{pd}$ and $H_{pp}$ were taken from work on NiO.[2] the $p_d−p$ hopping parameters scaled with distance $r$ as $r^{−7/2}$ and $r^{−2}$ respectively. The parameters of $H_{KH}$ which result from the mapping procedure are $U = 4.4 eV$, $J_H = 1.2 eV$ and $t ≈ 0.7 eV$. It is interesting to note that $J_H$ has a very
small sensitivity to the parameters of \( H \). Instead, changing \( \Delta \) and the hoppings of \( H \) within reasonable values affects \( U \) by \( \sim 20\% \) and \( t \) by \( \sim 30\% \).

III. RESULTS.

In this section, we study the behavior of the charge and spin gap, spin expectation values and spin-spin correlation functions of \( H_{KH} \), using Lanczos diagonalizations in periodic rings of length \( L = 4, 6 \) and \( 8 \). The rapid increase of the Hilbert space with \( L \) prevents us to study longer even chains with the present state of the art, but as we shall show, some trends are already clear. The unit of energy is chosen as \( t = 1 \).

A. Charge gap

In Fig. 1 we represent the charge gap \( \Delta_C = E(1) + E(-1) - 2E(0) \), where \( E(n) \) is the ground-state energy for \( n \) added holes to the stoichiometric system (which contains one \( a_{1g} \) and one \( b_{1g} \) hole per site). The result for \( L = 8 \) is compared to that of a polynomial extrapolation in \( 1/L \) to estimate finite-size effects. These effects are small for \( U \geq 4 \). As expected, the gap increases with \( U \) and \( J_H \). In the strong-coupling limit \( t = 0 \), the gap is \( \Delta_0 = U + J_H/2 \). As \( t \) is turned on, but kept small, the leading correction to \( E(0) \) is of order \( t^2/\Delta_0 \), while those of \( E(1), E(-1) \) are equal and of order \( t \). Assuming a Neel background (alternating spin projections 1 and -1) the correction for one added or one removed hole can be calculated and is \(-\sqrt{2}t \). In both cases, it is more convenient to align ferromagnetically the spin at the site of the added or removed hole with those of its nearest neighbors. Thus, for large \( U, J_H \), we estimate:

\[
\Delta_C = \Delta_0 - 2\sqrt{2}t. \tag{4}
\]

In Fig. 2 we represent \( \Delta_C - \Delta_0 \) as a function of \( U \) and \( J_H \). The results agree with Eq. (1) in the strong-coupling limit. In the opposite limit, for \( U = 0 \), and small values of \( J_H \), the results have important size effects, and a large positive value of \( \Delta_C - \Delta_0 \) is not reasonable. However, the extrapolated results show a reasonable behavior and tend to small values in the limit of \( J_H = 0 \). In any case, the results for \( U \geq 4 \) seem reliable. From the parameter estimates for \( Y_2BaNiO_5 \) given at the end of the previous section (\( U/t \approx 6.3, J_H/t \approx 1.7, t \approx 0.7eV \)), we obtain \( \Delta_C \sim 3eV \). This is somewhat larger than the experimental value \( \Delta_C \sim 2eV \). This discrepancy is probably due to the fact that the charge transfer gap and possibly the hopping parameters cannot be transferred directly from Ref. [12] (which is a theoretical interpretation of optical spectra in NiO) to \( Y_2BaNiO_5 \).

B. Spin gap

In Fig. 3, we show the spin gap \( \Delta_S \) as a function of \( J_H \) for several values of \( U \). For \( U = 0 \), the result for \( \Delta_S \) has already been reported [3]. Here, for the smaller values of \( U \) and \( J_H \), the finite-size effects are too large, and the extrapolated values to the thermodynamic limit (in some cases negative) are meaningless. However, for more realistic values of \( U \), our results allow us to extract some conclusions.

The qualitative behavior of \( \Delta_S \) as a function of \( J_H \) was to be expected from the limiting cases: if \( J_H = 0 \), the model is equivalent to the Hubbard model plus \( L \) free spin-1/2 states, and therefore \( \Delta_S = 0 \). For \( J_H \rightarrow 0 \), \( \Delta_S \sim J_H^2 \) has been obtained using bosonization [4]. In the limit of large \( J_H \), the low-energy physics of \( H_{KH} \) reduces to a spin-1 Heisenberg chain:

\[
H_{Heis} = J \sum_i S_i \cdot S_{i+1}, \quad J = \frac{t^2}{\Delta_0} = \frac{t^2}{U + J_H/2}, \tag{5}
\]

where \( S_i = S_{ia} + S_{ib} \). This model has a spin gap \( \Delta_{Heis} = c(L)J \), where the constant \( c(L) \) depends on the size of the system. In particular \( c(4) = 1, c(6) = 0.72, c(8) = 0.59, c(\infty) = 0.410492 \). [5] The first three values of \( c(L) \) coincide within 1% with our results extrapolated to infinite \( J_H \). As \( J_H \) increases, first \( \Delta_S \) increases from zero, and as the system approaches the strong-coupling limit, \( \Delta_S \) decreases with the effective spin-1 exchange \( J \).

In Fig. 4 we show \( \Delta_S/\Delta_{Heis} \) as a function of \( J_H \). For \( U > 4 \), the extrapolated values do not differ very much from those of \( L = 8 \). Note that even for large values of \( U \), the ratio \( \Delta_S/\Delta_{Heis} \) is considerably smaller than 1 if \( J_H \sim t \). In particular, for the parameters estimated for \( Y_2BaNiO_5 \), \( \Delta_S/\Delta_{Heis} \sim 0.5 \). However, this ratio was assumed 1 to estimate the value of \( J \) from experimental measurements of \( \Delta_S \). Using the same set of parameters, we obtain from the extrapolated values \( \Delta_S \sim 240K \), while the experimental value is \( \Delta_S \sim 100K \). In view of the approximations made in deriving \( H_{KH} \), the uncertainties in the parameters of \( H \), and the sensitivity of \( \Delta_S \) and \( J \) to these parameters, the result is satisfactory. Part of the overestimate is due to ferromagnetic corrections to \( J \) in second-order in the intercell hopping, which involve virtual quadruplet three-hole states. These states are contained in \( H \), but were projected out of the Hilbert space of \( H_{KH} \). We have calculated \( J \) by the cell-perturbation method, including these corrections. The effective \( J \) is reduced from 0.098eV to 0.088eV, but the result is quite sensitive to the parameters of \( H \). Comparison with exact diagonalizations of a \( Ni_2O_{11} \) cluster [6], shows that the second-order result of the cell-perturbation method is still an overestimation by a factor near 2, due to higher order corrections.

C. Spin expectation values

The behavior of the spin gap as a function of \( J_H \) and \( U \) displays a slow change from the weak to the strong-coupling regimes. In Fig. 5(a) we show the ratio of the spin gap to the effective exchange, as a function of \( U \) for \( L = 8 \) and different values of \( J_H \). For any non-zero value of \( J_H \), the strong-coupling limit is reached for sufficiently large \( U \) and the gap tends to the limit \( \Delta_{Heis}^H = 0.59J \). Fig 5(b) shows the corresponding change in the total spin of both itinerant (\( a_{1g} \)) and localized (\( b_{1g} \))
holes as $U$ is increased, in the lowest-energy state with total spin and projection $S_z = S^z_L = 1$. In the limit of small $J_H$, both types of holes are decoupled and it is easier to flip a localized hole rather than an itinerant one from the $S_z = 0$ ground state. As a consequence, $S_{zL} \approx 1 - S^z_L \approx 0$. In the opposite limit of very large $J_H$, the singlet states at each site $\langle (a_i^\dagger b_j^\dagger - a_j b_i) [0] \rangle$ can be projected out of the relevant Hilbert space, and in this case, the following equality among spin operators at a given site can be proved: $2S_{zL} = 2S_{zL}^L = S_L$. Summing over all sites: $2S_{zL} = 2S_{zL}^L = S_L$. Thus, $S_{zL}^2$ changes from 0 to 1/2 as $J_H$ increases and $S_{zL}^z = 1 - S_{zL}^z$. The effect of increasing $U$ is to localize the itinerant $a_{1g}$ holes and therefore, to contribute to the effect of $J_H$, reaching the strong-coupling limit. However, it is noticeable that the approach to this limit is very slow. Comparison of the quantities represented in Fig. 5 for different sizes suggests that this approach is even slower in the thermodynamic limit.

D. Spin-spin correlations

In addition to the spin-spin correlation functions

$$
S_1(l) = \langle (S^z_L + S^z_{L'}) (S^z_{L+l} + S^z_{L+l'}) \rangle,
$$
$$
S_2(l) = \langle (S^z_L - S^z_{L'}) (S^z_{L+l} - S^z_{L+l'}) \rangle,
$$

(6)

we also study in this section the string correlation function

$$
Z(j - i) = \langle S^z_i \exp(i\pi \sum_{l=i+1}^{j-1} S^z_i) S^z_j \rangle.
$$

(7)

This latter has been proposed as a hidden order parameter for $S = 1$ chains to describe a hidden $Z_2 \times Z_2$ symmetry breaking corresponding to the appearance of the Haldane gap. This symmetry has been first implicitly introduced in an elegant variational approach for the excited state. In Fig. 6, we show the different correlation functions. $S_2(l)$ has an on-site value $S_2(0) \approx 0.3$ and for other distances $S_2(\ell) < 0.02$ for the parameters of Fig. 6. The antiferromagnetic correlations are evident. They are larger for the localized holes than for the itinerant ones, as expected. For $U = 0$, a tendency to antiferromagnetic order with wave vector $q = \pi$ is expected from the form $\cos(2k_FR)$ of the oscillating Ruderman-Kittel-Kasuya-Yosida effective interaction between localized $b_{1g}$ holes at a distance $r$ mediated by the mobile $a_{1g}$ ones with Fermi wave vector $k_F = \pi/2$. In the strong-coupling limit, the effective model $H_{Heis}$ leads to the same type of short-range correlations.

The Fourier transform $S_1(q) = \sum_{l} e^{-iql} S_1(l)$, etc., of some of these correlation functions for wave vector $q = \pi$, is represented in Fig. 7. As $U$ increases, $S_1(\pi)$ and $S_2(\pi)$ approach slowly the asymptotic value in the strong-coupling limit, as it was the case of the spin gap and spin expectation values already discussed. Instead, $Z(\pi)$ seems to saturate faster to a fixed value as $J_H$ and $U$ increase.

In the strong-coupling limit, $Z(\pi)$ is a signature of the Haldane state. For our model, $Z(\pi)$ is a possible generalization of this order parameter, when local singlet states and charge fluctuations are allowed. The results of Fig. 7 are a hint that $Z(\pi)$ can be used as the corresponding parameter of a hidden order that also exists in the Kondo-Hubbard model $H_{KH}$. The difference in the behavior of $Z(\pi)$ as a function of $U$, $J_H$, in comparison with that of the other correlation functions, is an indication that $Z(\pi)$ is more sensitive to the transition to the spin-gap state. That is precisely what one expects from a quantity playing the role of an order parameter. The other spin-spin correlations should be short-range-like, due to the opening of the spin gap for finite $U$, $J_H$. Bosonization results indicate that this gap increases quadratically with the Hund coupling $J_H$, and is thus very small for $J_H \to 0$. In this regime, the correlation length is larger than the maximum system size that we have studied and we are unable to identify the change in the behavior of the correlation functions. For larger values of $J_H$, the change of regime is captured by our results, and more clearly from the behavior of $Z(\pi)$.

IV. SUMMARY AND DISCUSSION

We have studied charge and spin gap, spin expectation values, and several spin-spin correlation functions of a Kondo-Heisenberg model $H_{KH}$, for two particles per site. We have shown that the model can be considered as an approximate effective model for one-dimensional transition metal-O systems, in which only the $e_g$ orbitals of the transition metals are relevant. Without any adjustable parameters (taking the parameters of the original multiband Hamiltonian from NiO scaled appropriately with distance), we obtain from the effective $H_{KH}$, a charge and a spin gap of the correct order of magnitude for $Y_2BaNiO_5$. The model has also been used as a simplified model for the manganites, and our results should be qualitatively valid in the limit in which all Mn ions are Mn$^{3+}$.

For sufficiently large $U$ or $J_H$, the charge gap of $H_{KH}$ is approximately given by $\Delta_C \approx U + J_H / 2 - 2\sqrt{2}$. The effective model $H_{KH}$ contains the spin-1 antiferromagnetic Heisenberg model (also called Haldane chain) in the strong-coupling limit $t \ll J_H / U$. We obtain however that for realistic parameters for $Y_2BaNiO_5$ or when the effective Hund-rule exchange coupling $J_H$ is not much larger than the effective hopping $t$, several properties differ from the Haldane limit. In particular, the different dynamics of the itinerant and mobile $e_g$ holes (reflecting that they do not behave as part of the same spin-1 object) are clearly manifested in spin-spin correlation functions. In addition, the spin gap $\Delta_S$ is roughly half of that expected from a strong coupling expansions. This fact should be taken into account when the effective spin-1 exchange $J$ is extracted from experimental values of $\Delta_S$ and in the consistent interpretation of different thermodynamic experiments together with $\Delta_S$. One possible way to interpret our results for $\Delta_S$ when $U \gg J_H \sim t$, is that the effective spin-1 Heisenberg Hamiltonian Eq. (6) is still valid, but higher order corrections in $t$ reduce appreciably the second-order result $J = t^2 / (U + J_H / 2)$ for the effective exchange. Fourth-order corrections which include local singlet states as intermediate states are con-
sistent with this reduction. However, when \( t \sim J_H \), perturbation theory ceases to be valid, and it seems more adequate to include the local singlets \( \langle \epsilon_i^{\downarrow} b_i^{\dagger} \epsilon_i^{\uparrow} - \epsilon_i^{\uparrow} b_i^{\dagger} \epsilon_i^{\downarrow} \rangle \) in our notation) in the model Hamiltonian.

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35 This change of basis between the O \( p_z \) orbitals lying between Ni sites \( i \) and \( i+1 \) \( (p_{1/2,\sigma}) \) and the O Wannier functions \( \pi_{j,\sigma} \) centered at Ni site \( j \) is:
\[ p_{1/2,\sigma} = \sum_{j} (-1)^{j+1} \pi_{j,\sigma}. \]
If some or all of the four nearest O atoms to the transition-metal ion along the \( \pm x \) and \( \pm y \) directions are lacking, the low-energy reduction procedure and the form of \( H_{KH} \) (Eq. 3) are not substantially modified. However, if one of the mirror symmetries through the planes \( x = 0 \) or \( y = 0 \) is severely altered, the hopping of the “localized” \( b_{\alpha} \) holes, can no longer be neglected in \( H_{KH} \).
36 For example, a large contribution to the hopping between two nearest-neighbor cells with 2 and 3 holes respectively, is due to \( \pi_{i,\sigma} \) hopping which is favored if both cells have parallel total spin (antiparallel to that of the \( \pi_{j,\sigma} \) hole \( \sigma \)). The amount of \( \pi \) holes is much smaller in cells with 1 and 2 holes than in those with 3 holes.
37 H. Tsunetsugu, Y. Hatsugai, K. Ueda, and M. Sigrist, Phys. Rev. B 46, 3175 (1992).

FIGURE CAPTIONS

Fig. 1. Charge gap as a function of \( J_H \) for several values of \( U \) indicated inside the figure. Solid symbols are the result for \( L = 8 \) sites. Open symbols correspond to extrapolation to the thermodynamic limit from the results of \( L = 4, 6 \) and 8, using a quadratic polynomial in \( 1/L \).
**Fig. 2.** Same as in Fig. 1 for the charge gap minus its strong-coupling value $\Delta_0 = U + J_H/2$.

**Fig. 3.** Spin gap as a function of $J_H$ for several values of $U$. Solid symbols correspond to $L = 8$ and open symbols to the extrapolated value.

**Fig. 4.** Ratio of the spin gap $\Delta_S$ over its strong-coupling value ($\Delta_S^{\text{Heis}} = c(L)J$, where $J = t^2/(U + J_H/2)$, see text) as a function of $J_H$. The meaning of the symbols is the same as before.

**Fig. 5.** (a) Ratio of the spin gap to the effective exchange $\Delta_S/J$ as a function of $U$ for $L = 8$ and several values of $J_H$: $J_H = 2$ (circles), $J_H = 4$ (squares), $J_H = 6$ (diamonds) and $J_H = 20$ (dashed line). (b) $z$ component of the total spin of the $a_{1g}$ ($b_{1g}$) holes as a function of $U$ for $L = 8$ and several values of $J_H$ indicated by the same solid (open) symbols as above, in the lowest-energy state with total spin and $z$ component $S_t = S^z_t = 1$.

**Fig. 6.** Spin-spin correlation functions $\langle S^z_i S^z_{i+l} \rangle$ as a function of distance $l$ for $a_{1g}$ ($b_{1g}$) holes, the sum of both spins ($S_1(l)$), and that defined by Eq. (1), for $J_H = 2$ and two values of $U$: $U = 2$ (circles), and $U = 10$ (diamonds).

**Fig. 7.** Fourier transform of the correlation functions at momentum $\pi$ for the sum ($S_1(\pi)$) and difference ($S_2(\pi)$) of the spin of both types of holes at a given site, and the hidden order parameter $Z(\pi)$.

**Fig. 8.** Size dependence of $S_1(q)$ and $Z(q)$ for $J_H = 2$, $U = 10$. 
A.E. Feiguin et al., Fig. 1

The graph shows the relationship between $\Delta_C$ and $J_H$ for different values of $L$ and $U$. The lines are color-coded to distinguish between $L=\text{inf}$ and $L=8$, with different symbols and line styles for various values of $U$. The horizontal axis represents $J_H$, and the vertical axis represents $\Delta_C$. The graph indicates a linear increase in $\Delta_C$ with increasing $J_H$ for each set of conditions.
A.E. Feiguin et al., Fig. 2
A.E. Feiguin et al., Fig. 3
A.E. Feiguin et al., Fig. 4

\[ \frac{\Delta S}{\Delta \text{Heis}} \]

vs.

\[ J_H \]

Legend:
- \( L=8 \)
- \( L=\text{inf.} \)
- \( U=0 \)
- \( U=2 \)
- \( U=4 \)
- \( U=6 \)
- \( U=8 \)
A.E. Feiguin, et al. Fig. 6

$S_a(x)$

$S_b(x)$

$S_1(x)$

$Z(x)$
$J_H=2; U=10$

$S_1(q)$

$Z(q)$