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FERROMAGNETIC GROUND STATE OF TWO-BAND HUBBARD MODEL WITH ONE ELECTRON PER SITE

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We study the multiband mechanism to favour a ferromagnetic insulating ground state within a two-band Hubbard model. Besides perturbation theory we use exact diagonalization studies to examine the ground state of chains and 2D-lattices. According to second order perturbation theory the exact diagonalization yields a fully polarized ferromagnetic ground state, if the hopping between two ground state orbitals of neighbouring atoms t_{gg} is small and the hopping between a ground state orbital and an excited orbital t_{ge} dominates. However, in contrast to the suggestion from the second order perturbation theory this ferromagnetic state is stable only for very small hopping integrals $U \gg t_{ge} > t_{gg}$. For larger t_{ge} quantum interference effects lead to complex magnetic structures.

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Superexchange in insulators usually leads to a dominant antiferromagnetic coupling between magnetic ions. La_2CuO_4 and many similar compounds are of this type and show antiferromagnetic behaviour. Nevertheless there also exist ferromagnetic compounds with the same lattice structure, e.g. K_2CuF_4. As pointed out by Goodenough, Kanamori and Anderson (GKA) a special symmetry of ground- and excited state orbitals can produce a ferromagnetic coupling [1]. This GKA mechanism is responsible for the ferromagnetic interaction in the CuF_2-layer of K_2CuF_4, where the hopping between ground state orbitals of two magnetic ions is not allowed because of symmetry [2–4] and the ferromagnetic exchange is realized by hopping between ground state and excited state orbitals. In the same compound a ferromagnetic coupling between magnetic ions of different layers also exists. Here the exchange between ground state orbitals is reduced by destructive interference [5]. Both mechanisms can be discussed in a Hubbard model with more than one orbital, if the effective hopping between ground state orbitals is reduced for some reasons and the ferromagnetic interaction to a higher orbital dominates.

To study the interplay of effective hopping between two ground state orbitals t_{gg} and between a ground state and an excited state orbital t_{ge}, we discuss numerical and analytical results for the simplest Hubbard-type model with two orbitals

$$H = t_{gg} \sum_{\langle i,j\rangle,\sigma} c^+_{ig\sigma} c_{jg\sigma} + t_{ge} \sum_{\langle i,j\rangle,\sigma} (c^+_{ig\sigma} c_{je\sigma} + c^+_{ie\sigma} c_{jg\sigma}) + \epsilon \sum_{i\sigma} c^+_{ie\sigma} c_{je\sigma}$$
$$+ \frac{U}{2} \sum_{iab\sigma\sigma'} c^+_{ia\sigma} c^+_{ib\sigma'} c_{ib\sigma'} c_{ia\sigma} - \frac{J_H}{2} \sum_{i,a\neq b,\sigma\sigma'} c^+_{ia\sigma} c^+_{ib\sigma'} c_{ia\sigma'} c_{ib\sigma}. \tag{1}$$

Here $\langle i,j\rangle$ denotes nearest neighbours. $c^+_{ia\sigma}$ ($c_{ia\sigma}$) creates (annihilates) an electron with spin σ on site i and orbital a. There are two possible orbitals: g for the ground state orbital and e for the excited state orbital. Negative J_H leads to a ferromagnetic Hund's rule coupling between orbitals at the same site which can be seen by rewriting the one-site correlation term of Eq. (1)

$$H_V = U \sum_{i,a} n_{ia\uparrow} n_{ia\downarrow} + \frac{U}{2} \sum_{i,a\neq b} n_{ia} n_{ib} + J_H \sum_{i,a\neq b} \left(\boldsymbol{S}_{ia} \boldsymbol{S}_{ib} + \frac{n_{ia} n_{ib}}{4} \right). \tag{2}$$

Here $\boldsymbol{S}_{ia}$ denotes the spin operator and $n_{ia} = n_{ia\uparrow} + n_{ia\downarrow}$ the number operator. The Hamiltonian (1) is invariant under spin rotation and commutes with the z component S^z of the total spin $\boldsymbol{S}$ and also with the square of the total spin $\boldsymbol{S}^2$. These commutations allow us to restrict the numerical calculations to the subspace of $S^z = 0$. As discussed in Ref. [5] in the case of equivalent hoppings t_{gg} and t_{ge} the ferromagnetic exchange $J_{ge} \approx -(|J_H|/U) J_{gg}$ is smaller than the antiferromagnetic exchange between the ground state orbitals J_{gg}. As pointed out above the reduction of t_{gg} (i.e. J_{gg}) can favour a ferromagnetic coupling.

To study this mechanism in more details we have analyzed the ground state properties of model (1) by exact diagonalization and perturbation theory. We use the following parameters: $U = 8$, $\epsilon = 0.5$, $J_H = -1$ which corresponds to the situation in K_2CuF_4 [5]. We have calculated the ground state for linear chains and square lattices up to $N = 10$ sites for different hopping parameters. For more than three sites the ground state phase diagrams looks qualitatively very similar. Figure 1 shows the instability line of the ferromagnetic ground state for the linear chain and the square lattice for $N = 8$. For small hopping t_{ge} and $t_{gg} < t_{ge}$ the ground state is ferromagnetic which corresponds to the qualitative discussion given above. Let us discuss the breakdown of the ferromagnetic ground state in more details.

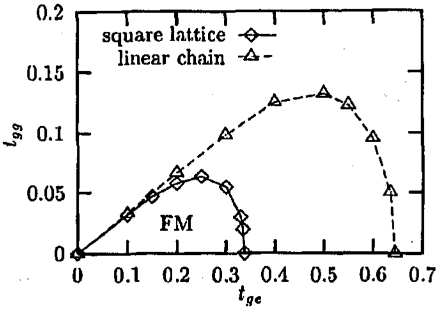

Fig. 1. Range of ferromagnetic ground state for a 8-site square lattice (solid line) and a 8-site linear chain (dashed line) with $U = 8$, $\epsilon = 0.5$ and $J_H = -1$.

First we consider a small hopping t_{ge} (smaller than 0.1 for square lattices and smaller than 0.3 for linear chains). In this limit the instability line is a straight line with a slope independent of the lattice and the transition goes from a fully polarized ferromagnetic to a quantum antiferromagnetic state. It can be easily calculated by perturbation theory in the second order in the hopping integrals. In Eq. (3) we have written the exchange energy as difference between the triplet and singlet state energy of a two site model

$$J_1^{(2)} = \frac{4t_{gg}^2}{U} + \frac{2t_{ge}^2}{U+\epsilon-J_H} - \frac{2t_{ge}^2}{U+\epsilon+J_H}. \tag{3}$$

The lower index denotes the nearest neighbour exchange and the upper index denotes the order of perturbation. Using above parameters for the instability line ($J_1^{(2)} = 0$) we get $t_{gg} = 0.335t_{ge}$. This result agrees precisely with the straight line in Fig. 1.

Second we turn to larger hopping t_{ge}. Obviously the qualitative picture given above is not appropriate and a Heisenberg model with only the nearest neighbour exchange J_1 is not sufficient to describe the more complicated ground state features. To simplify the discussion let us focus on $t_{gg} = 0$. In difference to the GKA picture we find a critical t_{ge}, where the ground state becomes a singlet with a complicated magnetic structure. For instance in the case of a linear chain a singlet ground state appears for $t_{ge} > 0.64$, where the nearest neighbour spin–spin correlation $\langle S_i S_{i+1}\rangle$ is ferromagnetic but the second nearest neighbour spin–spin correlation $\langle S_i S_{i+2}\rangle$ is weakly antiferromagnetic (Fig. 2). For $t_{ge} > 0.67$ this ground state changes to another state with a very small correlation $\langle S_i S_{i+1}\rangle$ and with a strong antiferromagnetic correlation $\langle S_i S_{i+2}\rangle$. This behaviour suggests to compare model (1) with a J_1–J_2 Heisenberg model with the ferromagnetic nearest neighbour exchange J_1 and antiferromagnetic second nearest neighbour exchange J_2. To show this analogy we have plotted the spin–spin correlations for the J_1–J_2 Heisenberg chain with $N = 8$ in Fig. 3. An increasing antiferromagnetic bond J_2

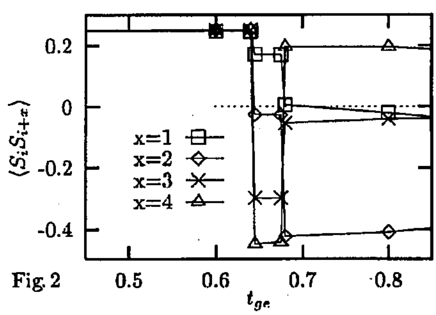

Fig. 2

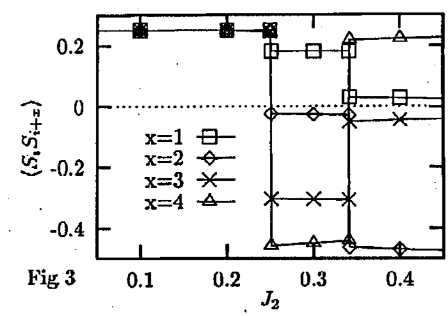

Fig 3

Fig. 2. Spin–spin correlations for the ground state of a 8-site linear chain with two orbitals ($U = 8$, $\epsilon = 0.5$, $J_H = -1$ and $t_{gg} = 0.01$).

Fig. 3. Spin–spin correlations for the ground state of a 8-site Heisenberg linear chain with ferromagnetic nearest neighbour exchange $J_1 = 1$ and antiferromagnetic second nearest neighbour exchange J_2.

leads to several spiral phases (see Fig. 3, $J_2 > 0.25J_1$ and $J_2 > 0.34J_1$).

The exchange coupling between second nearest neighbours J_2 first appears in fourth order perturbation theory. This exchange coupling is antiferromagnetic for all t_{ge}

$$J_2^{(4)} = \frac{4t_{\mathrm{ge}}^4}{(\epsilon+U)^2(3U+2\epsilon+J_H)} + \frac{2t_{\mathrm{ge}}^4}{(\epsilon+U)^2 U}. \tag{4}$$

The exchange coupling J_2 is also responsible for the difference between the linear chain and the square lattices for larger t_{ge}. Opposite to the linear chain in the square lattice the exchange coupling between the second nearest (diagonal) neighbours and third nearest neighbours are from the same order. Therefore we find the transition to the spiral phase for smaller t_{ge}.

In summary, we have shown that according to the GKA mechanism an insulating ferromagnetic ground state of a Hubbard type model with two orbitals can be realized if the hopping between ground- and excited state orbitals dominates over the hopping between ground state orbitals. However, for larger hopping integrals the GKA picture fails and the system becomes frustrated. In this case the spin correlations are described quite well by a Heisenberg model with the ferromagnetic nearest exchange couplings and antiferromagnetic second nearest (and third nearest for the square lattice) exchange coupling.

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