Spin bonds in an insulator with both charge-transfer and Hubbard-Mott gaps

1992 J. Phys.: Condens. Matter 4 5989

(http://iopscience.iop.org/0953-8984/4/27/016)

J. Phys.: Condens. Matter 4 (1992) 5989–5996. Printed in the UK

Spin bonds in an insulator with both charge-transfer and Hubbard–Mott gaps

Shijie Xiong
CCAST (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China and Department of Physics, Nanjing University, Nanjing 210008, People's Republic of China

Received 15 July 1991, in final form 27 January 1992

Abstract. The effective spin bonds in a material with both charge-transfer and Hubbard–Mott gaps are investigated. With the assumption that there are localized spins which can be described by a spin-only Hamiltonian in real space, the spin-coupling strengths of the bonds are analytically calculated by an exact mapping from an extended Hubbard model to a Heisenberg model for both the undoped and the doped cases. The result also provides some information on the form of the spin-only Hamiltonian for the description of the spin degrees of freedom of the system.

1. Introduction

It has been commonly accepted that the spin degrees of freedom of electrons in a 3d transition-metal compound with a Hubbard–Mott gap at the insulating limit can be well described by the Heisenberg model with AF superexchange between the nearest spins. Mott [1] and Hubbard [2] have provided a basic solution to this problem by pointing out that, if the Coulomb and exchange energy U is large compared with the one-electron dispersional band width, the polarity fluctuations are suppressed and a correlation gap of order U occurs. This idea has formed the basis for the separation of the excitations into low (spin-only) and high (charge fluctuation) energy scales and also forms the basis for the very successful Anderson [3] theory of superexchange in describing the low-energy-scale properties in terms of spin-only Hamiltonians. Recently Zaanen and Sawatzky [4] have pointed out that the Mott–Hubbard theory implies that the band gap is a d–d gap which, although correct for the Ti and V compounds, probably is not the case for the late-transition-metal compounds where the gap variation with anion electronegativity strongly indicates a gap of charge-transfer type. The AF superexchange has been calculated for a three-centre model with a bond angle of 180° by the perturbation scheme [3, 5] and by consideration of the spin configuration [4]. More recently, the study of Cu–Cu bonds in copper oxides has been re-excited by the discovery of high-T_c superconductors, and the t–J model (a generalization of the spin-only Hamiltonian by including the charge fluctuation terms) has been extensively investigated for both the doped and the undoped cases [6]. However, there are still some puzzling details of the description of the spin degrees of freedom in these compounds. On the one hand, in the case with a charge-transfer gap, we need to know to what accuracy the low-energy-scale

0953-8984/92/275989 + 08 $04.50

properties can be regarded as processes which involve only the spin degrees of freedom. On the other hand, there is some controversy about the form of the spin-only Hamiltonian in the doped case; some models involve only Cu 3d spins [6] and others involve both Cu 3d and O 2p spins [7].

In this paper we present an exact mapping from a model with both charge-transfer and Hubbard–Mott gaps to a spin-only model at the insulating limit, in order to gain some insight into the above problems. The two kinds of spin-only models (one involving only the 3d spins and the other involving both the 3d and the 2p spins) are compared for the undoped case and the doped case. A projection coefficient in this mapping is used to describe the weight of 3d spin-only states in the original ground state.

2. Exact mapping for the undoped case at the insulating limit

As has been pointed out by Anderson [3] and others [5], at the insulating limit a nearest-neighbour magnetic bond with a bond angle of 180° in a transition–metal compound is only relevant to a three-centre model with two 3d orbitals and a 2p orbital in between:

$$H = t\sum_{i,\sigma}(p_\sigma^\dagger d_{i\sigma} + \text{HC}) + U\sum_{i,\sigma} n_{i\sigma}n_{i-\sigma} + \Delta\sum_{\sigma} p_\sigma^\dagger p_\sigma \tag{1}$$

where p_σ and $d_{i\sigma}$ are the hole operators for the 2p and the 3d states, respectively, $i = 1, 2$ is the site index for 3d orbitals, U is the Mott–Hubbard gap and $\Delta = \varepsilon_p - \varepsilon_d$ is the charge-transfer gap, $n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$. There are three levels: the lower Hubbard level, the upper Hubbard level and the charge-transfer level. The energy of the lower Hubbard level is set to zero, and the gaps U and Δ are both much larger than t to guarantee that the compound is an insulator.

In the undoped case, there are two holes in the three-centre model and the eigenstates of Hamiltonian (1) can be expressed by linear combinations of 15 basis vectors. By consideration of symmetry they can be separated into several groups and solved as follows.

For group 1, the total spin $S = 0$. There are six eigenstates which can be further decomposed into two subgroups.

(i) The first subgroup includes four eigenstates expressed as

$$\psi_i = a_{i1}x_1 + a_{i2}x_2 + a_{i3}x_3 + a_{i4}x_4 \qquad (i = 1, 2, 3, 4) \tag{2}$$

with

$$\begin{aligned} x_1 &= 2^{-1/2}(d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger - d_{1\downarrow}^\dagger d_{2\uparrow}^\dagger)|0\rangle \\ x_2 &= \tfrac{1}{2}(d_{1\uparrow}^\dagger p_\downarrow^\dagger - d_{1\downarrow}^\dagger p_\uparrow^\dagger + p_\uparrow^\dagger d_{2\downarrow}^\dagger - p_\downarrow^\dagger d_{2\uparrow}^\dagger)|0\rangle \\ x_3 &= 2^{-1/2}(d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger + d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger)|0\rangle \qquad x_4 = p_\uparrow^\dagger p_\downarrow^\dagger|0\rangle \end{aligned} \tag{3}$$

where $|0\rangle$ is the vacuum state for the holes. The secular equation for ψ_i is then

$$E(\Delta - E)(U - E)(2\Delta - E) + 4t^2(U - E)(\Delta - E) - 2t^2E(2\Delta + U - 2E) = 0. \tag{4}$$

This is a fourth-order algebraic equation which has analytical solutions. Here we do not

write the complicated expressions for these and only denote the eigenvalues as E_i ($i = 1$–4), corresponding to the eigenstates with the following normalized coefficients:

$a_{i1} = -2^{1/2}h_i/E_i \qquad a_{i2} = h_i/t \qquad a_{i3} = 2^{1/2}h_i/(U - E_i) \qquad a_{i4} = 2h_i/(2\Delta - E_i)$

with

$$h_i = [2E_i^{-2} + t^{-2} + 2(U - E_i)^{-2} + 4(2\Delta - E_i)^{-2}]^{-1/2}. \tag{5}$$

(ii) The second subgroup has two eigenstates; they are

$$\psi_i = a_{i5}x_5 + a_{i6}x_6 \qquad (i = 5, 6)$$

with

$$\begin{aligned} x_5 &= \tfrac{1}{2}(d_{1\uparrow}^{\dagger}p_{\downarrow}^{\dagger} - d_{1\downarrow}^{\dagger}p_{\uparrow}^{\dagger} - p_{\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} + p_{\downarrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle \\ x_6 &= 2^{-1/2}(d_{1\uparrow}^{\dagger}d_{1\downarrow}^{\dagger} - d_{2\uparrow}^{\dagger}d_{2\downarrow}^{\dagger})|0\rangle \end{aligned} \tag{6}$$

which have the eigenvalues

$$E_5 = \tfrac{1}{2}\{U + \Delta - [(U - \Delta)^2 + 8t^2]^{1/2}\} \qquad E_6 = \tfrac{1}{2}\{U + \Delta + [(U - \Delta)^2 + 8t^2]^{1/2}\} \tag{7}$$

and the coefficients

$$a_{i5} = 2h_i/(\Delta - E_i) \qquad a_{i6} = 2^{1/2}h_i/t \qquad (i = 5, 6)$$

with

$$h_i = [4(\Delta - E_i)^{-2} + 2t^{-2}]^{-1/2}. \tag{8}$$

Group 2 has total spin $S = 1$. There are three energy levels each of which has three degenerate eigenstates with the z component S_z of the total spin equal to 1, 0 and -1:

$$\begin{aligned} E_7 = E_{10} = E_{13} &= \tfrac{1}{2}[\Delta - (\Delta^2 + 8t^2)^{1/2}] \\ E_8 = E_{11} = E_{14} &= \tfrac{1}{2}[\Delta + (\Delta^2 + 8t^2)^{1/2}] \\ E_9 = E_{12} = E_{15} &= \Delta. \end{aligned} \tag{9}$$

(i) The states with $S_z = 0$ are

$$\psi_i = a_{i7}x_7 + a_{i8}x_8 \qquad (i = 7, 8)$$

with

$$\begin{aligned} x_7 &= 2^{-1/2}(d_{1\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} + d_{1\downarrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle \\ x_8 &= \tfrac{1}{2}(d_{1\uparrow}^{\dagger}p_{\downarrow}^{\dagger} + d_{1\downarrow}^{\dagger}p_{\uparrow}^{\dagger} + p_{\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} + p_{\downarrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle \end{aligned} \tag{10}$$

and the coefficients

$$a_{i7} = -2^{1/2}h_i/E_i \qquad a_{i8} = h_i/t$$

with

$$h_i = (2E_i^{-2} + t^{-2})^{-1/2} \tag{11}$$

$$\psi_9 = \tfrac{1}{2}(d_{1\uparrow}^{\dagger}p_{\downarrow}^{\dagger} + d_{1\downarrow}^{\dagger}p_{\uparrow}^{\dagger} - p_{\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} - p_{\downarrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle. \tag{12}$$

(ii) The states with $S_z = 1$ are

$$\psi_i = h_i[(1/E_i)d_{1\uparrow}^{\dagger}d_{2\uparrow}^{\dagger} + (1/2t)(d_{1\uparrow}^{\dagger}p_{\uparrow}^{\dagger} + p_{\uparrow}^{\dagger}d_{2\uparrow}^{\dagger})]|0\rangle \tag{13}$$

with

$$h_i = (E_i^{-2} + \tfrac{1}{2}t^{-2})^{-1/2} \qquad (i = 10, 11)$$

$$\psi_{12} = 2^{-1/2}(d_{1\uparrow}^{\dagger}p_{\uparrow}^{\dagger} - p_{\uparrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle. \tag{14}$$

(iii) The states with $S_z = -1$ are ψ_{13}, ψ_{14} and ψ_{15}, which are obtained from ψ_{10}, ψ_{11} and ψ_{12} by changing the spins from up to down, respectively.

Thus we have found all the eigenstates and their energy levels of Hamiltonian (1) in the undoped case. The four low-lying states are ψ_1, ψ_7, ψ_{10} and ψ_{13}. At the same time the spin-only Hamiltonian

$$H_1 = JS_1 \cdot S_2 \tag{15}$$

has four eigenstates: one singlet and three triplets

$$\begin{aligned} &\psi^{(1)}_{1,2} = 2^{-1/2}(d^\dagger_{1\uparrow} d^\dagger_{2\downarrow} \mp d^\dagger_{1\downarrow} d^\dagger_{2\uparrow})|0\rangle \\ &\psi^{(1)}_3 = d^\dagger_{1\uparrow} d^\dagger_{2\uparrow} |0\rangle \qquad \psi^{(1)}_4 = d^\dagger_{1\downarrow} d^\dagger_{2\downarrow} |0\rangle \end{aligned} \tag{16}$$

with eigenvalues

$$E^{(1)}_1 = -3J/4 \qquad E^{(1)}_{2,3,4} = J/4. \tag{17}$$

Because the spin-only excitations are the low-energy-scale processes [1, 2], we need to select only the four low-lying states of H to make the projection to the phase space of H_1. After that we find an exact one-to-one mapping:

$$\psi_1 \to \psi^{(1)}_1 \qquad \psi_7 \to \psi^{(1)}_2 \qquad \psi_{10} \to \psi^{(1)}_3 \qquad \psi_{13} \to \psi^{(1)}_4 \tag{18}$$

with the eigenvalue correspondences

$$E_1 \to E^{(1)}_1 \qquad E_{7,10,13} \to E^{(1)}_{2,3,4}.$$

From this the superexchange J can be derived as

$$J = E_{7,(10,13)} - E_1. \tag{19}$$

We should notice, however, that only a fraction of the low-lying states of H coincides with the corresponding states consisting of only Cu 3d orbitals. We can use the amplitude of the projection of the ground state of H to the corresponding Cu spin state to characterize the weight of the mapping:

$$g = |a_{11}|. \tag{20}$$

In figure 1 the variations in J and g with the values of U/t and Δ/t are illustrated. It can be seen that J is always AF like and is very sensitive to the value of the charge-transfer gap if $\Delta < U$. The parameter g approaches unity only when $U/t \to \infty$ and $\Delta/t \to \infty$. This means that the Cu spin-only states only partly reflect the spin degrees of freedom for finite gaps.

3. Exact mapping for the doped case at the insulating limit

In real crystals the three levels of Hamiltonian (1) are extended to three subbands with gaps U and Δ. In the doped case, the second subband is partially filled and the compound becomes a conductor. So the spins are not localized and the description of the spin degrees of freedom becomes complicated. However, if the hopping integrals are so small that spins can be regarded as localized, we can still use the spin-only Hamiltonian. In this case the three-centre model has three holes, and Hamiltonian (1) has 20 basis vectors. The eigenstates and eigenvalues can be solved similarly.

For $S = \frac{1}{2}$, $S_z = \frac{1}{2}$, there are eight eigenstates.

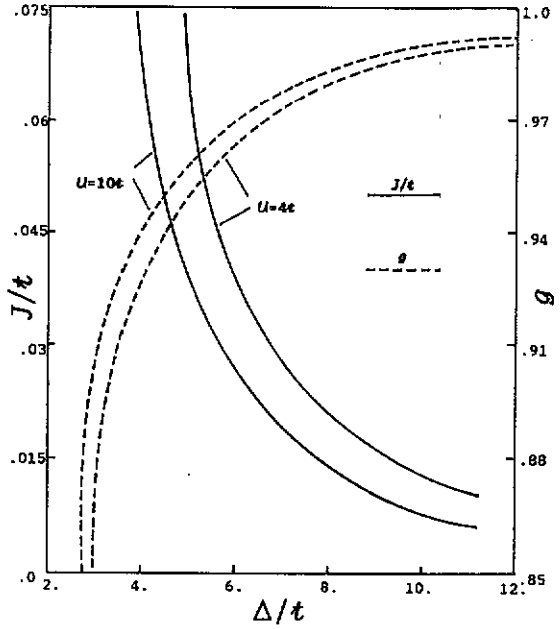

Figure 1. Variations in J and g with U/t and Δ/t in the undoped case.

(i)

$$\varphi_i = b_{i1}y_1 + b_{i2}y_2 + b_{i3}y_3 + b_{i4}y_4 \qquad (i = 1, 2, 3, 4)$$

with

$$\begin{aligned} y_1 &= 6^{-1/2}(d^\dagger_{1\uparrow}p^\dagger_\uparrow d^\dagger_{2\downarrow} + d^\dagger_{1\downarrow}p^\dagger_\uparrow d^\dagger_{2\uparrow} - 2d^\dagger_{1\uparrow}p^\dagger_\downarrow d^\dagger_{2\uparrow})|0\rangle \\ y_2 &= 2^{-1/2}(p^\dagger_\uparrow p^\dagger_\downarrow d^\dagger_{2\uparrow} - d^\dagger_{1\uparrow}p^\dagger_\uparrow p^\dagger_\downarrow)|0\rangle \\ y_3 &= 2^{-1/2}(d^\dagger_{1\uparrow}d^\dagger_{1\downarrow}d^\dagger_{2\uparrow} - d^\dagger_{1\uparrow}d^\dagger_{2\uparrow}d^\dagger_{2\downarrow}|0\rangle \\ y_4 &= 2^{-1/2}(d^\dagger_{1\uparrow}d^\dagger_{1\downarrow}p^\dagger_\uparrow - p^\dagger_\uparrow d^\dagger_{2\uparrow}d^\dagger_{2\downarrow})|0\rangle \end{aligned} \qquad (21)$$

and

$$b_{i1} = -3^{1/2}v_i(U + \Delta - E_i) \qquad b_{i2} = tv_i(3U + 4\Delta - 4E_i)/(2\Delta - E_i)$$
$$b_{i3} = tv_i(3U + 4\Delta - 4E_i)/(U - E_i) \qquad b_{i4} = v_i(\Delta - E_i)$$
$$v_i = [3(U + \Delta - E_i)^2 + t^2(3U + 4\Delta - 4E_i)^2[(2\Delta - E_i)^{-2} + (U - E_i)^{-2}] + (\Delta - E_i)^2]^{-1/2}.$$

The corresponding eigenvalues E_i $(i = 1, 2, 3, 4)$ are the four roots of the secular equation

$$(U-E)(2\Delta-E)(\Delta-E)(U+\Delta-E) - t^2(U+2\Delta-2E)(3U+4\Delta-4E) = 0. \qquad (22)$$

(ii)

$$\varphi_i = b_{i5}y_5 + b_{i6}y_6 + b_{i7}y_7 + b_{i8}y_8 \qquad (i = 5, 6, 7, 8)$$

with

$$\begin{aligned} y_5 &= 2^{-1/2}(d^\dagger_{1\uparrow} p^\dagger_\uparrow d^\dagger_{2\downarrow} - d^\dagger_{1\downarrow} p^\dagger_\uparrow d^\dagger_{2\uparrow})|0\rangle \\ y_6 &= 2^{-1/2}(p^\dagger_\uparrow p^\dagger_\downarrow d^\dagger_{2\uparrow} + d^\dagger_{1\uparrow} p^\dagger_\uparrow p^\dagger_\downarrow)|0\rangle \\ y_7 &= 2^{-1/2}(d^\dagger_{1\uparrow} d^\dagger_{1\downarrow} d^\dagger_{2\uparrow} + d^\dagger_{1\uparrow} d^\dagger_{2\uparrow} d^\dagger_{2\downarrow})|0\rangle \\ y_8 &= 2^{-1/2}(d^\dagger_{1\uparrow} d^\dagger_{1\downarrow} p^\dagger_\uparrow + p^\dagger_\uparrow d^\dagger_{2\uparrow} d^\dagger_{2\uparrow} d^\dagger_{2\downarrow})|0\rangle \end{aligned} \tag{23}$$

and

$$\begin{aligned} &b_{i5} = v_i(2\Delta - U) \qquad b_{i6} = v_i[2t^2 - (\Delta - E_i)(U - E_i)]/t \\ &b_{i7} = v_i[(\Delta - E_i)(2\Delta - E_i) - 2t^2]/t \\ &b_{i8} = v_i[(\Delta - E_i)(2\Delta + U - 2E_i) - 4t^2]/(U + \Delta - E_i) \\ &v_i = \{[(2\Delta - U)^2 + \{[2t^2 - (\Delta - E_i)(U - E_i)]^2 + [(\Delta - E_i)(2\Delta - E_i) - 2t^2]^2\}/t^2 \\ &\qquad + [(\Delta - E_i)(2\Delta + U - 2E_i) - 4t^2]^2/(U + \Delta - E_i)^2\}^{-1/2}. \end{aligned} \tag{24}$$

The corresponding eigenvalues E_i ($i = 5, 6, 7, 8$) are four roots of the secular equation

$$(U - E)(2\Delta - E)(\Delta - E)(U + \Delta - E) - t^2(U - 2\Delta - 2E)^2 + 4t^4 = 0. \tag{25}$$

For $S = \frac{1}{2}$, $S_z = -\frac{1}{2}$, the eight eigenstates (φ_i, $i = 9$–16) can be obtained from φ_1–φ_8 by exchanging spin up and spin down. The eigenvalues are

$$E_{i+8} = E_i \qquad \text{for } i \text{ from 1 to 8.} \tag{26}$$

For $S = 1\frac{1}{2}$, there are four degenerate states with eigenvalue

$$E_{17} = E_{18} = E_{19} = E_{20} = \Delta. \tag{27}$$

(i) The state with $S_z = \frac{1}{2}$ is

$$\varphi_{17} = 3^{-1/2}(d^\dagger_{1\uparrow} p^\dagger_\uparrow d^\dagger_{2\downarrow} + d^\dagger_{1\downarrow} p^\dagger_\uparrow d^\dagger_{2\uparrow} + d^\dagger_{1\uparrow} p^\dagger_\downarrow d^\dagger_{2\uparrow})|0\rangle. \tag{28}$$

(ii) The state with $S_z = -\frac{1}{2}$(φ_{18}) can be obtained from φ_{17} by exchanging spin up and spin down.

(iii) The state with $S_z = 1\frac{1}{2}$ is

$$\varphi_{19} = d^\dagger_{1\uparrow} p^\dagger_\uparrow d^\dagger_{2\uparrow}|0\rangle. \tag{29}$$

(iv) The state with $S_z = -1\frac{1}{2}$ is

$$\varphi_{20} = d^\dagger_{1\downarrow} p^\dagger_\downarrow d^\dagger_{2\downarrow}|0\rangle. \tag{30}$$

There is no correspondence between the four low-lying states (φ_1, φ_5, φ_9 and φ_{13}) and the eigenstates of H_1. We have to search for the correspondence between eight low-lying states (φ_1, φ_5, φ_9, φ_{13}, φ_{17}, φ_{18}, φ_{19} and φ_{20}) with the eigenstates of the following spin-only Hamiltonian:

$$H_2 = J_1 S_1 \cdot S_2 + J' \sum_{i=1,2} S_i \cdot s \tag{31}$$

where s is the spin at the 2p orbital. These eigenstates are

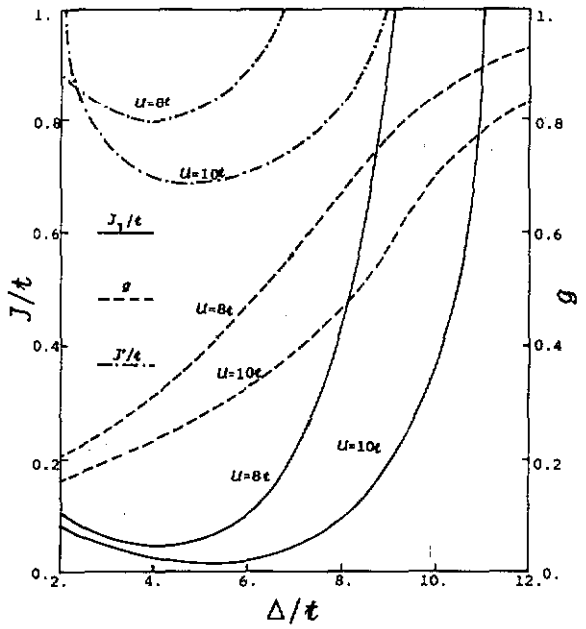

Figure 2. Variations in J_1, J' and g with U/t and Δ/t in the doped case.

$$\begin{aligned}
\varphi_1^{(2)} &= 6^{-1/2}(d_{1\uparrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} + d_{1\downarrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\uparrow}^{\dagger} - 2d_{1\uparrow}^{\dagger}p_{\downarrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle \\
\varphi_3^{(2)} &= 2^{-1/2}(d_{1\uparrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} - d_{1\downarrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle \\
\varphi_5^{(2)} &= 3^{-1/2}(d_{1\uparrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\downarrow}^{\dagger} + d_{1\uparrow}^{\dagger}p_{\downarrow}^{\dagger}d_{2\uparrow}^{\dagger} + d_{1\downarrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\uparrow}^{\dagger})|0\rangle \\
\varphi_7^{(2)} &= d_{1\uparrow}^{\dagger}p_{\uparrow}^{\dagger}d_{2\uparrow}^{\dagger}|0\rangle
\end{aligned} \tag{32}$$

and $\varphi_2^{(2)}$, $\varphi_4^{(2)}$, $\varphi_6^{(2)}$ and $\varphi_8^{(2)}$ are obtained from $\varphi_1^{(2)}$, $\varphi_3^{(2)}$, $\varphi_5^{(2)}$ and $\varphi_7^{(2)}$, respectively, by exchanging spin up and spin down. The corresponding eigenvalues are

$$\begin{aligned}
&E_1^{(2)} = E_2^{(2)} = J_1/4 - J' \qquad E_3^{(2)} = E_4^{(2)} = -3J_1/4 \\
&E_5^{(2)} = E_6^{(2)} = E_7^{(2)} = E_8^{(2)} = J_1/4 + J'/2.
\end{aligned} \tag{33}$$

After projecting the eight low-lying states of Hamiltonian (1) onto the space of Hamiltonian (31), we also find an exact one-to-one mapping:

$$\varphi_1 \to \varphi_1^{(2)} \qquad \varphi_9 \to \varphi_2^{(2)} \qquad \varphi_5 \to \varphi_3^{(2)} \qquad \varphi_{13} \to \varphi_4^{(2)}$$

with

$$\begin{aligned}
&\varphi_{17} \to \varphi_5^{(2)} \qquad \varphi_{18} \to \varphi_6^{(2)} \qquad \varphi_{19} \to \varphi_7^{(2)} \qquad \varphi_{20} \to \varphi_8^{(2)} \\
&E_{1,9} \to E_{1,2}^{(2)} \qquad E_{5,13} \to E_{3,4}^{(2)} \qquad E_{17,18,19,20} \to E_{5,6,7,8}^{(2)}.
\end{aligned} \tag{34}$$

The spin couplings in (31) can be determined as

$$J' = 2(E_{17,18,19,20} - E_{1,9})/3 \qquad J_1 = E_{1,9} - E_{5,13} + J'. \tag{35}$$

Similarly, we define the coefficient $|b_{11}| = g$ as a measure of the coincidence of the ground state of H with the corresponding Cu spin-only states.

In figure 2 we plot the variations in J_1, J' and g with U/t and Δ/t.

4. Discussion

We have described a new approach for mapping a three-centre system as a spin-only system with the assumption that the spin degrees of freedom can be regarded as localized in real space. We have also provided a parameter to characterize the weight of projection. In the undoped case, the three-centre system has four low-lying states which coincide with the states of the spin-only Hamiltonian (15) after projection. At the same time, in the doped case, the spin degrees of freedom of the eight low-lying states coincide with the spin configuration of the states of Hamiltonian (31). If we further project the eight states onto H_1 space, we can see that φ_5 and φ_{13} correspond to the singlet and the other six states are combinations of the triplet states. This means that, by doping, the triplet level of Hamiltonian H_1 is split into two levels: one is below the singlet level and the other is above. If we treat the 3d spins as Ising-like spins, the J'-term in H_2 can be transformed into an effective ferromagnetic interaction between the 3d spins, which leads to equivalence between H_1 and H_2, as suggested by Aharony *et al* [8].

Acknowledgments

The author would like to thank Professor C S Ting, J H Xu, W Z Wang and H T Wang for helpful discussions.

References

[1] Mott N F 1949 *Proc. Phys. Soc.* A **62** 416
[2] Hubbard J 1964 *Proc. R. Soc.* A **277** 237; 1964 *Proc. R. Soc.* A **281** 401
[3] Anderson P W 1959 *Phys. Rev.* **115** 2
[4] Zaanen J and Sawatzky G A 1987 *Can. J. Phys.* **65** 1262
[5] Oh S J, Allen J W, Lindau I and Mikkelsen J C 1982 *Phys. Rev.* B **26** 4845
[6] Zhang F C and Rice T M 1988 *Phys. Rev.* B **37** 3759
[7] Emery V J and Reiter G 1988 *Phys. Rev.* B **38** 4547
[8] Aharony A, Birgeneau R J, Coniglio A, Kastner M A and Stanley H E 1988 *Phys. Rev. Lett.* **60** 1330