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DIFFERENCES BETWEEN ONE- AND MULTIBAND HUBBARD MODELS

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Abstract. We investigate the large U limit of the one- and the three-band Hubbard model. It is found that the dynamics of a hole concerning the stabilization of spin fluctuations differs essentially in the two models. We therefore propose an alternative approach of mapping the three-band model onto an effective one-band Hamiltonian which describes the motion of an additional oxygen hole, in contrast to the usual mapping where the hopping of the Cu–O singlet is reduced to the motion of the Cu hole alone.

Key words: Hubbard model, antiferromagnet, spin-polarons.

INTRODUCTION

A common feature of high-T_c perovskite compounds such as La_2CuO_4 and $YBa_2Cu_3O_6$ is that they are highly correlated AF-ordered insulators in an undoped case. Upon doping the systems by either chemical or photoexcitational methods the additional holes strongly couple to their magnetic surrounding, leading to a metal-insulator transition at relatively small concentrations. This fact and the simultaneous persistence of two-dimensional spin ordering up to high charge carrier concentrations has been explained earlier by one of the authors [1] within the model of microscopic percolative phase separation. This model is based on the idea that the doping of CuO_2 planes with holes leads to the creation of small spin-polarized clusters (magnetic polarons, ferrons). These clusters have but low mobility, whereas the holes inside the clusters can move freely. As a result, on increasing the hole concentration and due to the diffusion of clusters, the latter start overlapping and a (fractal) metallic-like percolation network is built up. This leads to the destruction of the AF order and to the appearance of metallic-like conductivity or, below T_c, to superconductivity, within the percolation network [1]. This spin-cluster

model allows also the explanation of recent experimental data on time- and temperature-dependent phase separation in weakly doped $La_2CuO_{4+\delta}$ and $La_{2-x}Sr_xCuO_4$ samples [2, 3]. Also, magnetic susceptibility measurements [2] show the existence of small spin-polarized (superparamagnetic) particles associated with holes. Recently, the existence of spin-polarized clusters in $La_2CuO_{4+\delta}$ has been demonstrated by EPR measurements [4]. In addition, the magnetic resonance signals measured in $RBa_2Cu_3O_x$ (R=Y, Gd) have been attributed to clusters with a magnetic ordering [5]. A review about the experiments on phase separation is given in [6, 7].

Concerning the calculation of spin-cluster states, two models have been established which are used to describe the low-energy features of CuO_2 planes. The first one is the large U limit of the one-band Hubbard model ($t - J$ model), which in the context of cuprate superconductors has been proposed by Anderson [8]. The existence of spin-polarized states within the $t - J$ model has been proved by several groups [9, 10]. The second model was simultaneously proposed by Emery [11] and it takes into account the hybridization between the oxygen $p_{x/y}$ and the Cu $d_{x^2-y^2}$ orbital, the latter being additionally subjected to a strong Hubbard repulsion. Within this model, as we will see later, the formation of magnetic polarons is strongly favoured, compared with the $t - J$ model. The binding energy and the polarization of the spin clusters have been obtained by various methods in [1, 12–14]. It has been shown by Zhang and Rice [15] that in a certain limit of parameters an exact mapping of the three-band model onto the $t - J$ model is possible. However, an important point of criticism in connection with this one-band mapping is the fact that the derivation of the $t - J$ model does not depend on the magnetic ordering which strongly influences the transport properties of an oxygen hole. It has been pointed out by Hizhnyakov et al. [16] that in a one-band model the kinetic energy should be described by a spin-conditioned hopping term instead of the usual conditional hopping Hamiltonian like in the $t - J$ model.

In the present article, we study the motion of a doped oxygen hole in an AF-ordered CuO_2 plane. Starting from the Emery model, we will derive an effective Hamiltonian for the oxygen holes alone. To account for the AF-ordered Cu-spin background we will formulate the Hamiltonian in a similar way as has been done by Varma and Schmitt-Rink (VSR) [17] for the $t - J$ model. The hole dynamics in our Hamiltonian will be seen to differ essentially from that of VSR, as it contains the motion of spin clusters and the motion of holes inside these clusters from the very beginning.

2. THREE-BAND HUBBARD MODEL

We start from the Emery model mentioned above, writing it as follows:

$$H = \sum_{\sigma} H_{0\sigma} + H_{int}, \tag{1}$$

where

$$H_{0\sigma}=\sum_n \epsilon_d n^d_{n\sigma} + \epsilon_p \sum_m n^p_{m\sigma} + U \sum_n n_{n\uparrow} n_{n\downarrow} +$$
$$+T \sum_{nm} (1 - n^d_{n-\sigma}) \left(d^\dagger_{n\sigma} p_{m\sigma} + h.c. \right), \quad (2)$$

$$H_{int}=T \sum_{nm} n^d_{n-\sigma} \left(d^\dagger_{n\sigma} p_{m\sigma} + h.c. \right). \quad (3)$$

Like in [18], we will remove Cu states with double occupancy by the following unitary transformation:

$$S = \frac{T}{U-\epsilon} \sum_{nm} n_{d-\sigma} \left(d^\dagger_{n\sigma} p_{m\sigma} - h.c. \right), \quad (4)$$

with $\epsilon = \epsilon_d - \epsilon_p$. This leads to an effective Hamiltonian which contains essential elements up to the fourth order:

$$H=\sum_{n\sigma} \epsilon_d n^d_{n\sigma} + \epsilon_p \sum_m n^p_{m\sigma} + T \sum_{nm\sigma} (1 - n_{d-\sigma}) \left(d^\dagger_{n\sigma} p_{m\sigma} + h.c. \right) +$$
$$+J^K \sum_m \left(\mathbf{S}^{\mathbf{d}}_{\mathbf{m}} \mathbf{S}^{\mathbf{P}}_{\mathbf{m}} - \frac{1}{4} n^d_m N^P_m \right) + J^{dd} \sum_{(nm)} \left(\mathbf{S}^{\mathbf{d}}_{\mathbf{n}} \mathbf{S}^{\mathbf{d}}_{\mathbf{m}} - \frac{1}{4} n^d_n n^d_m \right). \quad (5)$$

$\mathbf{S}^{\mathbf{d}}_{\mathbf{m}}$ and $\mathbf{S}^{\mathbf{P}}_{\mathbf{m}}$ are Cu and O spin operators introduced as usual according to

$$d^\dagger_{m\uparrow} d_{m\downarrow} = \mathbf{S}^{\mathbf{d}}_{\mathbf{xm}} + i \mathbf{S}^{\mathbf{d}}_{\mathbf{ym}}, \; d^\dagger_{m\uparrow} d_{m\uparrow} = \frac{1}{2} n^d_m + \mathbf{S}^{\mathbf{d}}_{\mathbf{zm}}, \quad (6)$$

$$P^\dagger_{m\uparrow} P_{m\downarrow} = \mathbf{S}^{\mathbf{P}}_{\mathbf{xm}} + i \mathbf{S}^{\mathbf{P}}_{\mathbf{ym}}, \; P^\dagger_{m\uparrow} P_{m\uparrow} = \frac{1}{2} N^P_m + \mathbf{S}^{\mathbf{P}}_{\mathbf{zm}}. \quad (7)$$

$$P^\dagger_{m\sigma} = \frac{1}{2} \sum_{m'} p^\dagger_{m\sigma} \quad (8)$$

is a totally symmetric oxygen electron operator of a CuO_4 plaquette, (m') denotes the sum over four oxygen sites which are nearest to the mth Cu site. The term $\sim J^K$ describes a Kondo-type Cu–O spin–spin coupling; it differs from zero if there is a hole on an oxygen site. The interaction constant is given by

$$J^K = 8 \frac{T^2}{U-\epsilon}. \quad (9)$$

In the limit $U \to \infty, \epsilon \to \infty$, where the mapping from the three-band model to the $t-J$ one becomes exact, J^K is equivalent to the energy gain due to the singlet formation of an oxygen hole with a Cu hole.

The term $\sim J^{dd}$ describes a Cu–Cu spin–spin interaction which causes an AF order in the system. The interaction parameter reads as follows:

$$J^{dd} = \frac{2T^4}{(U-\epsilon)^3} \left(1 + \frac{2(U-\epsilon)}{U + \frac{8T^2}{U-\epsilon}} \right). \quad (10)$$

The main interaction term in H ($\sim T$) describes the spin-conditioned hopping of the electron or hole between the nearest neighbour Cu and O ions. As has been pointed out by Hizhnyakov et al. in [16], this process differs essentially from the analogous process in the $t-J$ model. In our case the single hole motion $\sim T$ depends on spin orientation on Cu sites already in the second order, while such dependence in the $t-J$ model first appears in the fourth order [19]. In the latter model the dynamics of the system is reduced to the Cu–Cu hole motion alone. Indeed, when one considers a hole in a three-band model initially being located at a Cu site, there is no restriction concerning the spin ordering for the motion to the next nearest Cu site. A Cu hole in this sense behaves like in a one-band model, whereas an oxygen hole does not. However, as the doped holes are mainly of an oxygen type, it is important to account for their dynamical properties when constructing a one-band model.

3. ONE-BAND MODEL

In this section we derive an effective one-band Hamiltonian for the oxygen hole motion which takes into account the effect of spin-conditioned hopping between Cu and O sites. By using the Wannier operators

$$P'_{m\sigma}=\frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}m} P'_{\mathbf{k}\sigma}, \tag{11}$$

$$Q_{m\sigma}=\frac{1}{N}\sum_{\mathbf{k}} e^{i\mathbf{k}m} Q_{\mathbf{k}\sigma}, \tag{12}$$

with

$$P'_{\mathbf{k}\sigma}=\frac{1}{2}\beta_{\mathbf{k}}[P_{x,\mathbf{k}\sigma}(1+e^{ik_y})+P_{y,\mathbf{k}\sigma}(1+e^{-ik_x})], \tag{13}$$

$$Q_{\mathbf{k}\sigma}=\frac{1}{2}\beta_{\mathbf{k}}[P_{x,\mathbf{k}\sigma}(1+e^{ik_y})-P_{y,\mathbf{k}\sigma}(1+e^{-ik_x})], \tag{14}$$

$$P_{\alpha,\mathbf{k}\sigma}=\sum_{m} e^{i\mathbf{k}m} P_{\alpha,m\sigma}, \tag{15}$$

$$\beta_{\mathbf{k}}=\sqrt{1+\frac{1}{2}(\cos k_x+\cos k_y)} \tag{16}$$

(indices $\alpha = x, y$ describe two oxygen states in the mth cell), Hamiltonian (5) can be represented in the form [1]

$$H=\sum_{n\sigma}\{\epsilon_d n^d_{n\sigma}+\epsilon_p P'^{\dagger}_{n\sigma}P'_{n\sigma}+2T_0(1-n^d_{n-\sigma})\left(d^{\dagger}_{n\sigma}P'_{n\sigma}+h.c.\right)\}+$$

$$+2T_1\sum_{(nm)}(1-n^d_{n-\sigma})\left(d^{\dagger}_{n\sigma}P'_{m\sigma}+h.c.\right)+J^K\sum_{m}\left(\mathbf{S}^{\mathbf{d}}_{\mathbf{m}}\mathbf{S}^{\mathbf{P}}_{\mathbf{m}}-\frac{1}{4}n^d_m N^P_m\right)+$$

$$+J^{dd}\sum_{(nm)}\left(\mathbf{S}^{\mathbf{d}}_{\mathbf{n}}\mathbf{S}^{\mathbf{d}}_{\mathbf{m}}-\frac{1}{4}n^d_n n^d_m\right), \tag{17}$$

where the transfer matrix elements are defined via

$$T_0 = 0.96\,T, \tag{18}$$

$$T_1 = 0.14\,T. \tag{19}$$

The unit cell now consists of a Cu and a symmetric oxygen state $|P'\rangle$, respectively. The hybridization between these states in the cell is given by T_0, between the neighbouring cells, by T_1.

When we restrict ourselves to the motion of a single hole in the CuO_2 plane, the second-order process of moving the oxygen hole from one cell to the next one is given by

$$H^{(2)} = \frac{4T_0T_1}{\epsilon} \sum_{(mm')\sigma\sigma'} (-1)^{1-\sigma-\sigma'} Y_{m'}^{-\sigma',2}(X_m^{\sigma'\sigma} + X_{m'}^{\sigma'\sigma})Y_m^{2,-\sigma}. \tag{20}$$

Here X_m and Y_m denote Hubbard projection operators for Cu and oxygen states, respectively.

Hamiltonian (20) is projected on the AF-ordered Neel state by means of the following definitions:

In a unit cell where the Cu spin has $\uparrow$ orientation, we define

$$X_m^{\uparrow\downarrow} = S_{d,m}^{+}, \tag{21}$$

$$Y_m^{\uparrow\downarrow} = S_{p,m}^{+} \tag{22}$$

and complex conjugate at sites of the other sublattice. For the Cu spin operators the usual Holstein–Primakoff bosonization scheme is applied with $S_{d,m}^{+} = b_m$. To get a better insight into the physical properties of the system and to provide a better starting point for the treatment of spin fluctuations, we will also decouple the charge and the spin of the oxygen hole. This is done by means of the mapping:

$$Y_m^{2,\uparrow} = h_m S_{p,m}^{+}, \tag{23}$$

$$Y_m^{2,\downarrow} = h_m \tag{24}$$

at a lattice site with Cu spin $\uparrow$ orientation. We also bosonize the oxygen spin via $S_{p,m}^{+} = k_m$. Additionally the constraints

$$Y_m^{\downarrow\downarrow} = h_m^{\dagger} h_m (1 - k_m^{\dagger} k_m), \tag{25}$$

$$0 = k_m^{\dagger} k_m (1 - h_m^{\dagger} h_m) \tag{26}$$

have to be satisfied.

Within these definitions it can be seen that Hamiltonian (20) transforms to

$$H^T = -\tilde{t} \sum_{mm'} h_{m'}^{\dagger} h_m \{k_{m'}^{\dagger} + k_m - k_{m'}^{\dagger} k_m (b_m + b_{m'}^{\dagger}) - k_m b_m^{\dagger} b_m - k_{m'}^{\dagger} b_{m'}^{\dagger} b_{m'} + (b_m^{\dagger} + b_{m'})\}. \tag{27}$$

The Cu–Cu and Kondo-type spin–spin interaction can also be presented in terms of the new basis which gives

$$H^{dd}=J^{dd}\sum_{ij}\left[b_i^\dagger b_i+\frac{1}{2}(b_i b_j+b_i^\dagger b_j^\dagger)\right], \tag{28}$$

$$H^K=\frac{J^K}{2}\sum_i h_i^\dagger h_i\left\{k_i^\dagger k_i(1-b_i^\dagger b_i)+b_i^\dagger b_i(1-k_i^\dagger k_i)+(b_i k_i+b_i^\dagger k_i^\dagger)\right\}. \tag{29}$$

We have set the zero of energy equal to half of the singlet binding energy. As can be seen from (29), only the Kondo-type interaction is active when a hole is present and it gives a positive contribution when either a k or a b fluctuation appears (which means nothing but a parallel spin alignment between oxygen and Cu).

The effective Hamiltonian constituted by H^T, H^{dd}, and H^K differs essentially from the analogous treatment of the $t-J$ model by Schmitt-Rink, Varma, and Ruckenstein [17] and Kane, Lee, and Read [20] concerning the process of stabilizing a spin fluctuation $b_i^\dagger$. In these papers the motion of a hole in a single-band quantum antiferromagnet is described by the Hamiltonian

$$H=-t\sum_{(mm')}h_{m'}^\dagger h_m(b_m^\dagger+b_{m'})+$$
$$+J\sum_{(ij)}\left[b_i^\dagger b_i+\frac{1}{2}(b_i b_j+b_i^\dagger b_j^\dagger)\right]. \tag{30}$$

In (30), the simultaneous occupancy of a site with a Cu spin fluctuation and a hole is forbidden, whereas in (27) it is not, which is naturally connected with the fact that in our case the hole is of an oxygen type.

Consider first the elementary stabilization process of a spin fluctuation in (30) for the situation that hole and boson are diagonally neighbouring. As can be seen from Fig. 1*a*, the hole will restore the spin configuration after one walk on the square where in intermediate states two bosons are present. To restore the spin configuration without an initial boson (Fig. 1*b*) one needs three walks on the same square where now up to three bosons are created during these walks. Thus it is the gain in kinetic energy on the square connected with a reduced number of bosonic excitations, which stabilizes the spin fluctuation (or magnetic polaron) in the $t-J$ model.

In Hamiltonian (27) this scenario works as well. However, due to spin-conditioned hopping a much stronger stabilization process starts to work.

Consider first the hole in the Neel-ordered state without any fluctuations present. It can either create a k boson at the next site or leave a Cu-spin fluctuation ($b^\dagger$) behind. The first of these two processes is energetically clearly less favourable. By the second one we have created a spin-cluster state for which the magnetic energy $\sim J^{dd}$ has to be paid.

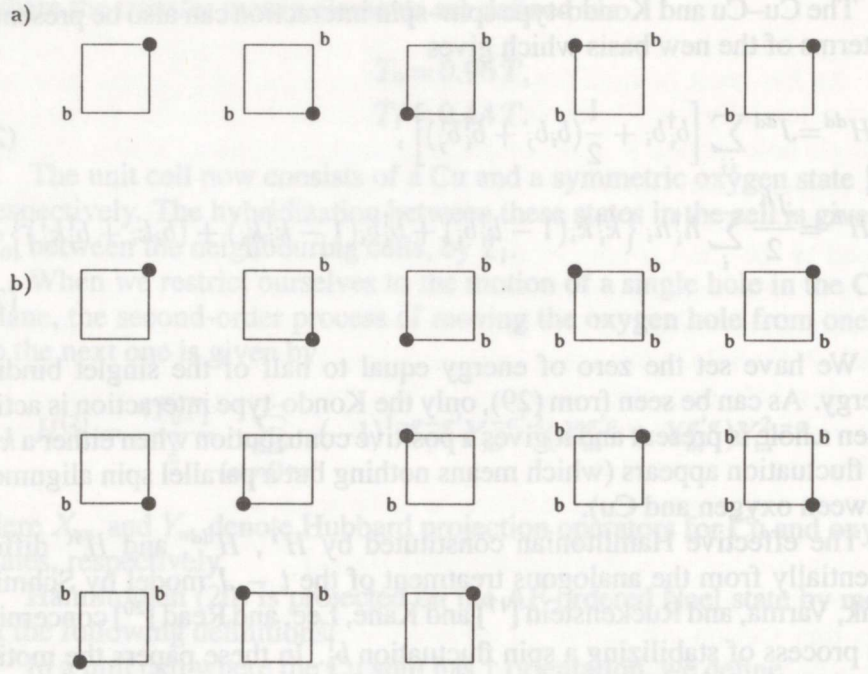

Fig. 1. a) Stabilization process for a spin fluctuation in a single-band quantum antiferromagnet. b) Walk on a square when no fluctuation is initially present.

In Hamiltonian (27) the term

$$H^{del} = \tilde{t} \sum_{mm'} h^{\dagger}_{m'} h_m \left(k_m b^{\dagger}_m b_m + k^{\dagger}_{m'} b^{\dagger}_{m'} b_{m'} \right) \tag{31}$$

provides the delocalization of the hole within a region consisting of the site with the Cu-spin fluctuation and its four nearest neighbours without an additional cost of magnetic energy. Note that when the hole is moved to the same site as the Cu-spin fluctuation, also a k boson is created which prevents the Kondo exchange to become active. Thus, the kinetic stabilization process in this model is of the second order rather than of the fourth order, as it is in the $t - J$ model.

A further process which provides the stabilization of spin-cluster states is also explicitly contained in (27). It is the hopping of the spin cluster itself which is described by

$$H^{trans} = \tilde{t} \sum_{mm'} h^{\dagger}_{m'} h_m k^{\dagger}_{m'} k_m (b_m + b^{\dagger}_{m'}). \tag{32}$$

As can be seen from Fig. 2, the successive operation with H^{trans} on a spin-cluster state $|h^{\dagger} b^{\dagger} k^{\dagger}\rangle$ moves this state to the next nearest site with an intermediate creation of a k boson indicating the large effective mass of these clusters.

We have checked our results in a one-dimensional model, restricting ourselves to the subspace with only one b boson present. We have found

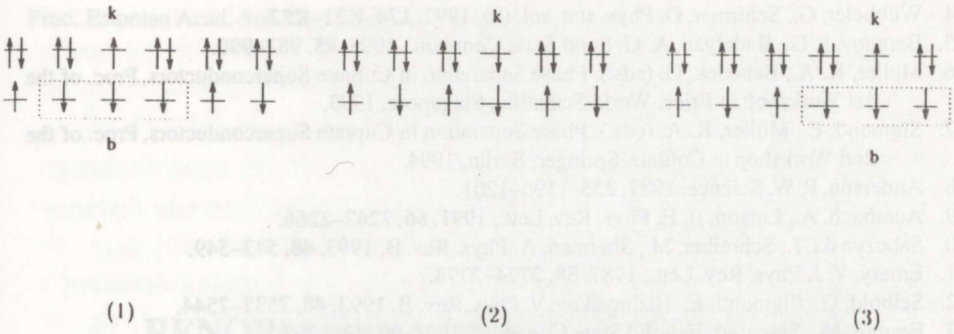

Fig. 2. Hopping process of a spin cluster. The first action of (32) on state (1) restores as an intermediate step the AF order which has a k boson with the hole. The second action ends up with state (3) where the cluster has been shifted by two sites compared with (1).

that already in this simplified model $\sim 70\%$ of the ground state belongs to a coherent spin-cluster state $|(h^+k^+b^+)_q\rangle$ with the wave vector $\mathbf{q}$, whereas in the $t-J$ model no spin polaron formation in 1D is possible.

4. CONCLUSIONS

We have discussed the motion of a single hole in the large U limit of a single- and a three-band Hubbard model, respectively. It has turned out that the dynamical processes stabilizing a spin fluctuation are basically different in the two systems. To account for the spin-conditioned hopping in the three-band model we have derived an effective one-band Hamiltonian which describes the motion of only oxygen holes. A spin fluctuation in this model is stabilized by a second-order process rather than a fourth-order process like in the $t-J$ model. Therefore a question arises whether the $t-J$ model is appropriate to describe the low-energy physics of cuprate superconductors. Especially the experimentally observed results such as electronic phase separation become clearly more pronounced in a three-band than in a single-band model.

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REFERENCES

1. Hizhnyakov, V., Sigmund, E. Physica C, 1988, **156**, 655–666.
2. Kremer, R. K., Sigmund, E., Hizhnyakov, V., Hentsch, F., Simon, A., Müller, K. A., Mehring, M. Z. Phys. B, Condensed Matter, 1992, **86**, 319–324.
3. Taliani, C., Pal, A., Ruani, G., Zamboni, R., Wei, X., Vardeny, Z. V. – In: Kuzmany, H., Mehring, M., Fink, J. (eds.). Electronic Properties of High-T_c Superconductors and Related Compounds. Springer Series in Solid State Sciences 99, Berlin, 1990.

4. Wübbeler, G., Schirmer, O. Phys. stat. sol. (b), 1992, **174**, K21–K22.
5. Baranov, P. G., Badalyan, A. G. Solid State Commun., 1993, **85**, 987–990.
6. Müller, K. A., Benedek, G. (eds.). Phase Separation in Cuprate Superconductors, Proc. of the 1st Workshop in Erice. World Scientific, Singapore, 1993.
7. Sigmund, E., Müller, K. A. (eds.). Phase Separation in Cuprate Superconductors, Proc. of the 2nd Workshop in Cottbus. Springer, Berlin, 1994.
8. Anderson, P. W. Science, 1987, **235**, 1196–1201.
9. Auerbach, A., Larson, B. E. Phys. Rev. Lett., 1991, **66**, 2262–2266.
10. Sabczynski, J., Schreiber, M., Sherman, A. Phys. Rev. B, 1993, **48**, 543–549.
11. Emery, V. J. Phys. Rev. Lett., 1987, **58**, 2794–2798.
12. Seibold, G., Sigmund, E., Hizhnyakov, V. Phys. Rev. B, 1993, **48**, 7537–7544.
13. Eremin, M., Sigmund, E. Solid State Commun., 1994, **90**, 795–797.
14. Klemm, D., Letz, M., Sigmund, E. Phys. Rev. B, 1994, **50**, 7046–7052.
15. Zhang, F. C., Rice, T. M. Phys. Rev. B, 1988, **37**, 3759–3761.
16. Hizhnyakov, V., Sigmund, E., Seibold, G.: see in Ref. 7, p. 50–65.
17. Schmitt-Rink, S., Varma, C. M., Ruckenstein, A. E. Phys. Rev. Lett., 1988, **60**, 2793–2797.
18. Hizhnyakov, V., Sigmund, E., Schneider, M. Phys. Rev. B, 1991, **44**, 795–803.
19. Brinkman, W. E., Rice, T. M. Phys. Rev. B, 1976, **2**, 1324–1338.
20. Kane, C. L., Lee, P. A., Read, N. Phys. Rev. B, 1989, **39**, 6880–6992.

ERINEVUSED ÜHE- JA MITMETSOONILISE HUBBARDI MUDELI VAHEL

Götz SEIBOLD, Ernst SIGMUND

On uuritud ühe- ja kolmetsoonilist Hubbardi mudelit suure U piirjuhul ning leitud, et spinnfluktuatsioonide stabiliseerumise osas erineb aukude dünaamika oluliselt mõlemas mudelis. Seetõttu on esitatud alternatiivne käsitlus kolmetsoonilise mudeli kujutamiseks ühetsoonilise efektiivse hamiltoniaani kaudu, mis kirjeldab hapniku lisaaugu liikumist erinevalt tavalisest kujutamisest, kus Cu–O singleti ülekandumine taandub ainuüksi Cu augu liikumisele.

РАЗЛИЧИЯ МЕЖДУ ОДНО- И МНОГОЗОННОЙ МОДЕЛЯМИ ХАББАРДА

Гэц ЗАЙБОЛД, Эрнст ЗИГМУНД

Исследованы одно- и трехзонная модели Хаббарда в пределе большого U. Найдено, что в части стабилизации спиновых флуктуаций динамика дырок в обеих моделях существенно отличается. Поэтому предложен альтернативный подход к изображению трехзонной модели через эффективный однозонный гамильтониан, описывающий движение добавочной кислородной дырки в отличие от привычного изображения, где перенос Cu–O-синглета редуцирован к движению единственной Cu-дырки.