direct hoppings h between σ and π orbitals on adjacent oxygen sites. One can see that for the ground state $G_S>$ the singularity of the density of state moves towards the band center when the amplitude h becomes greate. Nevertheless for $h < 0.7\tau$ the peak of the density of state remains and lies near the band bottom as it is shown in fig.1.

Our consideration provides a good starting point for a set of theories which explain high-T_c material properties and are based on the assumption of presence of a narrow carrier band.

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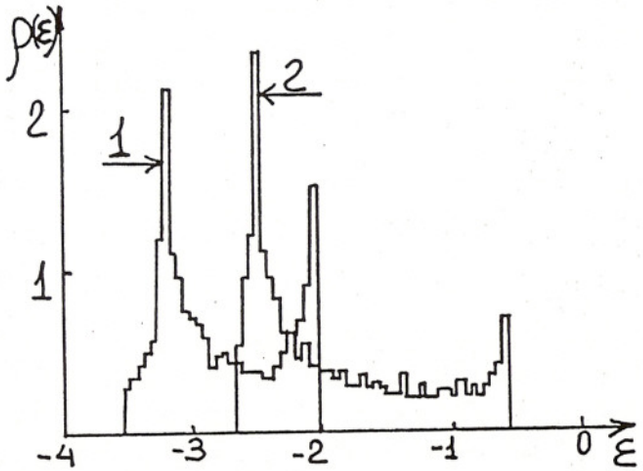

Fig.1. Density of states $\rho(\varepsilon)$ for $G> = G_N>$ and 47 basis functions. *1 - $J = 0.25\tau$; 2 - $J = 0.5\tau$.*

QUASIPARTICLE PROPERTIES IN EFFECTIVE MODELS FOR COPPER OXIDES

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ABSTRACT

Several effective models for CuO_2 layers are first compared. It is shown that the hole-spin models and generalized effective single-band (t-J) model reproduce well quasiparticle spectra of the two-band Hubbard model. Results for the quasiparticle properties in a planar t-J model, as obtained by the exact diagonalization of small systems, are then presented. Discussed are the coherent effective mass and the optical conductivity of a single hole in a quantum antiferromagnet, the binding of two holes and the possibility of pairing in the high doping regime.

1. MODELS

Models for strongly correlated systems are at present in the focus of theoretical investigations due to their relevance to copper oxides, these being superconducting (SC) at high temperatures.[1] One of the challenging questions is to understand the properties of the CuO_2 layers, doped with a small concentration of holes. Whereas the antiferromagnetic (AFM) character of the undoped system is now well established, the properties of a quasiparticle (QP), i.e. a mobile hole within the perturbed spin background, and especially the nature of two-hole and many-hole states are far from being settled. In this paper we will review some of our results on the QP properties in the doped quantum AFM, as obtained by the method of the exact diagonalization of small systems. We first establish the relation between several models proposed in this connection.

Assuming that in CuO_2 layers $Cu\ d_{x^2-y^2}$ orbitals and $O\ p_\sigma$ orbitals are essential for the electronic properties, the two band Hubbard model has been introduced by Emery,[2]

$$H_{Hubb} = -t_{pd} \sum_{\langle ij \rangle_\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \Delta_0 \sum_{(i \in p)} n_i + \sum_i U_i n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

where $c_{i\sigma}, c^\dagger_{i\sigma}$ represent hole operators on $Cu\ d$ and $O\ p$ sublattices, with a corresponding vacuum of filled shells $Cu\ d^{10}, O\ p^6$. Here, we take into account only

the hybridization (t_{pd}) contribution, the charge transfer (Δ_0) term and the onsite Coulomb repulsions with $U_i = U_{pp}, U_{dd}$.

For the undoped system with $\Delta_0 > 0$ and $U_{dd} \gg t_{pd}$ it is expected that the model can be described well by the Heisenberg model with only spin degrees on the Cu sites. Additional holes introduced by doping (mainly) on O sites can be however mobile, hopping through intermediate Cu sites (or even directly by the $O-O$ hopping). For this case, the mobile holes and localized spins on Cu sites are relevant degrees of freedom and coupled hole-spin models have been derived,[3-5] treating t_{pd} as the smallest quantity. The model can be further symplified if we introduce for holes the ordinary Wannier functions corresponding to the free hole hopping, but centered on d sites

$$\tilde{c}^{\gamma}_{i\sigma} = \sum_{l} w^{\gamma}_{i,l} c_{l\sigma}, \qquad \gamma = (s, a). \tag{2}$$

Terms involving the antisymmetric orbitals ($\gamma = a$) couple only weakly to the more relevant symmetric subsystem and seem to be less important at low doping. With $\tilde{c}^{s}_{i\sigma} = \tilde{c}_{i\sigma}$, we thus get the symmetrized hole-spin model,[6]

$$\begin{aligned} H_{sym} = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j - t_0 \sum_{(ij)\sigma} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + V \sum_{i} \tilde{\vec{s}}_i \cdot \vec{S}_i \\ + t_1 \sum_{(ij)\sigma\sigma'} \tfrac{1}{2} \vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_i (\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma'} + \tilde{c}^{\dagger}_{j\sigma} \tilde{c}_{i\sigma'}), \end{aligned} \tag{3}$$

where some less important terms have been omitted. For large V a local singlet state, formed out of the local d hole and the symmetrized p hole, can be used as a new vacuum[7]

$$|\tilde{0}_i\rangle = \frac{1}{\sqrt{2}} \left(\tilde{c}^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} - \tilde{c}^{\dagger}_{i\downarrow} c^{\dagger}_{i\uparrow} \right) |0\rangle. \tag{4}$$

When the participation of higher energy triplet states is neglected, we obtain the generalized t-J model[7,6].

$$H_{tJ} = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j - t \sum_{(ij)\sigma} d^{\dagger}_{i\sigma} d_{j\sigma} - t' \sum_{((jk))\sigma} d^{\dagger}_{j\sigma} d_{k\sigma} + \varsigma \sum_{(i,j\neq k)\sigma\sigma'} \tfrac{1}{2} \vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_i d^{\dagger}_{j\sigma} d_{k\sigma'} \tag{5}$$

with operators $d_{i\sigma}$, $d^{\dagger}_{i\sigma}$ acting on a subspace with no doubly occupied sites. Included are the nnn ((jk)) hopping terms with the (t') spin independent hopping and the (ς) hopping dependent on the intermediate spin $\vec{S}_i$.

In Eq. (1) the hybridization (t_{pd}) is not small enough compared to Δ_0 to ensure the perturbation derivation of Eq. (3), so as V is not large enough for a straighforward derivation of Eq. (5). Therefore we perform a quantitative comparison of models,[6] allowing deviations of parameters from their perturbational values. We adopt the view that effective models should reproduce as well as possible the low energy single QP spectra of the original Hubbard model, Eq. (1). Here we present results obtained by the exact diagonalization of a one-dimensional system with $N_0 = 4$ cells. Still we do not expect that relations between parameters would crucially depend on the dimensionality of the lattice.

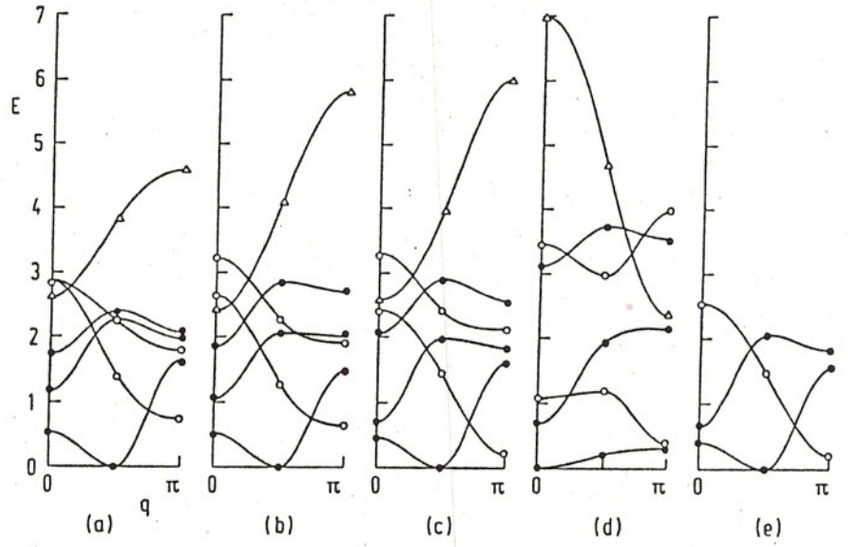

FIG. 1. The lowest lying branches for a system with a single additional hole on a chain of $N_0 = 4$ cells for different models corresponding to mixed valence regime, $\Delta_0 = 2$, $t_{pd} = 1.4$ and $U_{dd} = 7$. Full circles • represent the $S = \frac{1}{2}$ energy levels, ○ correspond to the $S = \frac{3}{2}$ and △ to the $S = \frac{5}{2}$ levels, respectively. The solid lines between the points are only a guide to the eye. (a) Two band Hubbard model; (b) Hole-spin model; (c) Symmetrized hole-spin model; (d) Kondo-lattice model; (e) Generalized t-J model.

Since the main open question is whether models are compatible in the mixed valence regime $t_{pd} \gtrsim \Delta_0$,[4] we present in Fig. 1 results in the latter regime. With the use of the appropriate renormalized parameters the agreement is even quantitative, especially for the lowest QP branch. The deviations are larger for the reduced (Kondo-lattice) model[3], (d), where in Eq. (3) only the first three terms are taken into account, with the Kondo-type coupling between both kinds of spins. Also we find that corrections to the simplest t-J model are small, i.e. t' and

rms are even smaller than those derived from a single band Hubbard model.[8] hould be stressed however a less satisfactory agreement between the Hubbard del and the Heisenberg model in the mixed valence regime with respect to the energy spectra for the undoped system (without mobile holes). In view of ting experimental data[9] on magnetic properties, this could be an indication t real copper oxides are in the charge transfer regime $\Delta_0 \gg t_{pd}$.

2. SINGLE QUASIPARTICLE PROPERTIES

In the following we restrict our discussion to the prototype t-J model,[7,10] (5),

$$H_0 = -t \sum_{<ij>,s} d^\dagger_{is} d_{js} + J \sum_{<ij>} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right), \tag{6}$$

ch has been shown to be a good representation of the model (1), at least for le QP spectra. Here, we present a more detailed analysis[11] of the eigenstates QP in a $d = 2$ system, which supplements the existing analytical and numerical lts[12-14]. First, we calculate by the method of the diagonalization of finite 2 system the lowest branch of the QP (single hole) energy dispersion $E(\vec{q})$. reas small 4×4 system can be diagonalized exactly, larger 8×4 systems are ted approximately, allowing only a finite number of spin flips $N_e \leq 6$ relative ie initial Néel AFM state.

In a t-J model on a $N = 4 \times 4$ system a single hole state is degenerate along AFM Brillouin zone boundary , i.e. at $\vec{k}_0 = (\pm\pi/2, \pm\pi/2)$, $(\pi, 0)$ and $(0, \pi)$. same near degeneracy persists for a larger system, with the lowest energy at $\vec{k}_0 = (\pm\pi/2, \pm\pi/2)$. Thus the effective mass and consequently the mass ncement $\underline{\mu}$ are highly anisotropic tensors,

$$\underline{\mu}^{-1} = \frac{1}{2t} \frac{\partial^2 E(\vec{k}_0 + \vec{p})}{\partial \vec{p} \partial \vec{p}} \bigg|_{\vec{p}=0}. \tag{7}$$

ncement is infinite along the AFM zone boundary, i.e. $\vec{p} \perp \vec{k}_0$ and finite μ for $\vec{p} \parallel \vec{k}_0$. Values for μ presented in Fig. 2 show an approximate $1/J$ idence, as predicted theoretically.[12-14]

The frequency dependent conductivity $\sigma(\omega)$ can be studied in a finite system extrapolation for $q \to 0$ of

$$\sigma(\vec{q}, \omega) = -\frac{1}{\pi\omega} Im G(\omega + i\epsilon), \tag{8a}$$

$$G(z) = \langle \Psi_0 | j_{-\vec{q}} (z + E_0 - H)^{-1} j_{\vec{q}} | \Psi_0 \rangle, \tag{8b}$$

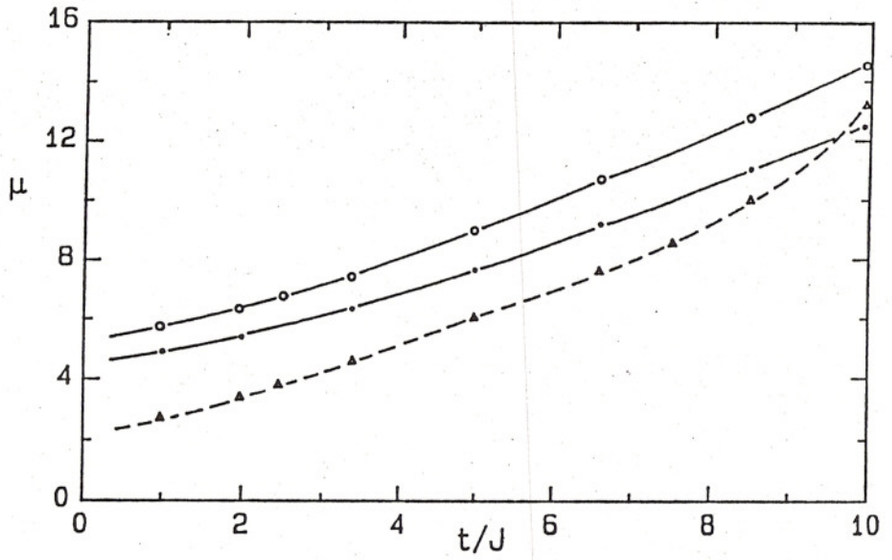

FIG. 2. Mass enhancement μ vs t/J for a) $N = 8 \times 4$ system for $N_e = 5$ (o) and $N_e = 6$ (•) respectively; b) for $N = 4 \times 4$ along $\vec{p} \parallel \vec{k}_0$ (△).

where $j_{\vec{q}}$ is the current operator and $|\Psi_0\rangle$ is the ground state wave function. In order to evaluate $G(z)$ we start the Lanczos procedure with an initial normalized wavefunction $|\tilde{\Psi}_0\rangle = A\, j_{\vec{q}} |\Psi_0\rangle$. Then $G(z)$ has a representation in terms of Lanczos coefficients α_n, β_n as a continued fraction in z. Since α_n, β_n are found to converge for $n \gg 1$, we use this property to sum analytically higher order fractions and to get continuous $\sigma(\omega)$ in the higher frequency regime.

As seen in Fig. 3, where a typical plot of $\sigma(\omega)$ for $J/t = 0.2$ is presented, the spectra show two distinct parts: a) an undamped QP peak, which would approach $\omega \to 0$ for $q \to 0$ and is expected to broaden to a Drude peak only at $T > 0$, and b) the higher frequency part due to the incoherent hopping of the hole, where excitations have mainly the magnon character. We note that at finite J the lower magnon peaks are still well pronounced, the lowest being at $\omega \sim 2J$, in contrast to the smooth variation $\sigma \propto 1/\omega$ expected for $J \to 0$.[15] The optical sum rule is mainly exhausted by the incoherent part, since the QP peak takes only the fraction $1/\mu$ of the total intensity.

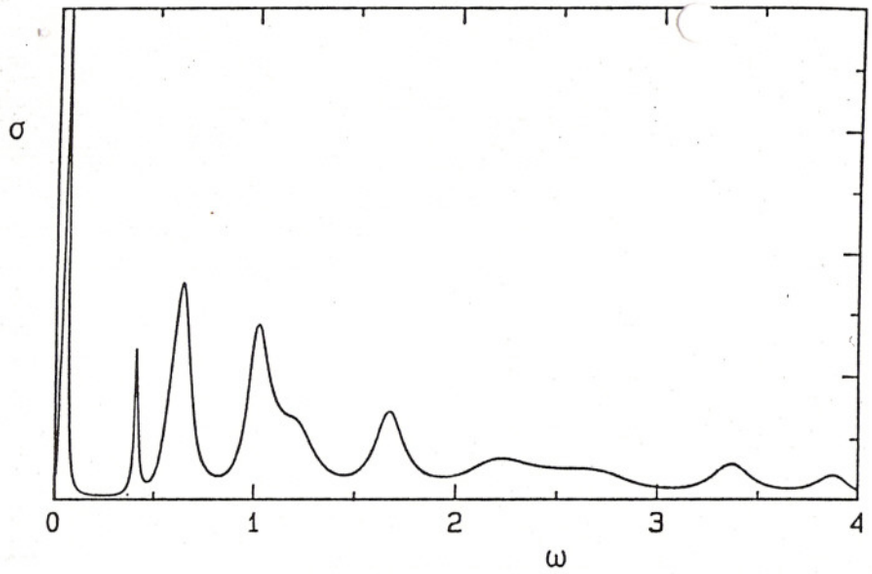

FIG. 3. Frequency dependent conductivity $\sigma(\omega)$ vs ω in units of t for $N = 8 \times 4$ and $J/t = 0.2$ ($N_c = 6$).

3. BINDING AND PAIRING OF QUASIPARTICLES

We study the binding of QP by diagonalizing exactly the t-J model with $N_h = 2$ holes on a 4×4 lattice.[16] In the whole regime of J/t that we investigated, the $N_h = 2$ ground state was found to be a spin singlet $S = 0$ and triply degenerate, corresponding to $\vec{q} = (0,0)$, $(0,\pi)$ and $(\pi,0)$. To test the binding of holes we calculate two quantities, i.e. the binding energy of the hole pair,

$$\Delta = E_0\,(N_h = 2) - 2E_0\,(N_h = 1) + E_0\,(N_h = 0)\,, \tag{9}$$

and the hole density correlation function

$$g(\vec{R}) = \sum_i \langle \Psi_0 | n_h(\vec{R}_i) n_h(\vec{R}_i + \vec{R}) | \Psi_0 \rangle. \tag{10}$$

Δ as presented in Fig. 4 as well as $g(\vec{R})$ clearly indicate on the bound state of a hole pair at $J/t > 0.2$. Whereas $\Delta \simeq J$ in this regime, the hole density correlations fall off with distance so that the finite size effects seem not to be crucial. Note that the $S = 1$ hole pair state was found to be very weakly bound, i.e. $\Delta \approx 0$.

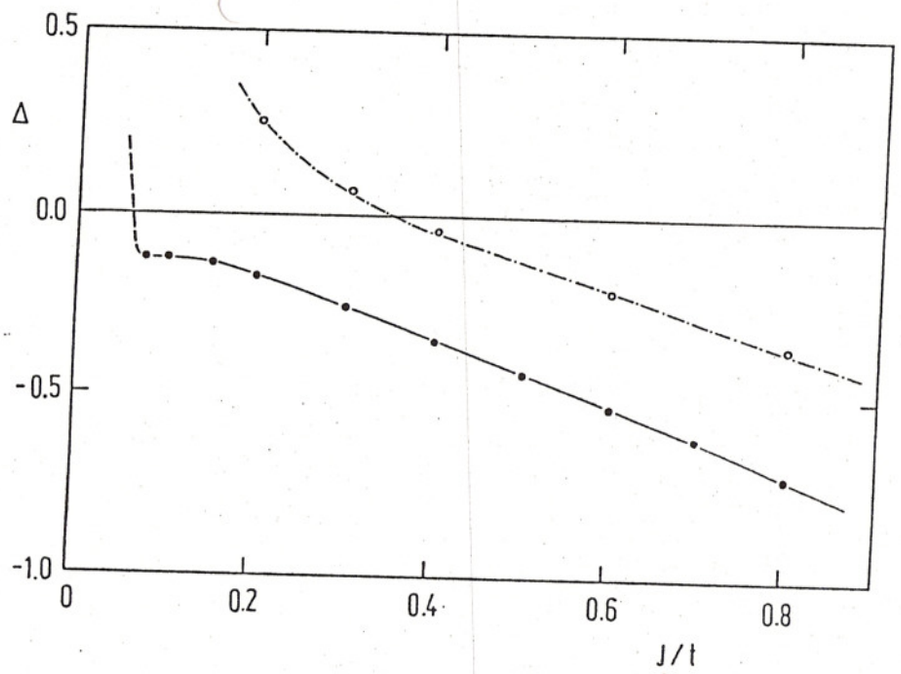

FIG. 4. Effective binding energy Δ of two holes (in units of t) vs J/t. Dashed line represents the $J_\perp = 0$ case .

A gradual change to an entirely different state below $J/t < 0.1$ is evident also from nearest neighbour spin correlations $C(\vec{R})$,

$$C(\vec{R}) = \sum_i \langle \Psi_0 | \vec{S}(\vec{R}_i) \cdot \vec{S}(\vec{R}_i + \vec{R}) | \Psi_0 \rangle, \tag{11}$$

which become ferromagnetic-like for nearest neighbours below $J/t < 0.1$. Such situation can be simply explained by the formation of two oppositely polarized FM spin polarons which repel each other, what is consistent with the attractive-repulsive transition observed in $g(R)$.[16] On the other hand, the origin of rather large hole binding in the $J/t > 0.2$ regime is still not well understood. Clearly, such large effect cannot be explained by the simple broken bond argument, which neglects the hole kinetic energy and even then yields $|\Delta| < J$. It is rather connected with the quantum frustration effect,[12] for we found that holes remain bound even if we allow only a very small number of spin flips relative to the original Néel AFM configuration.

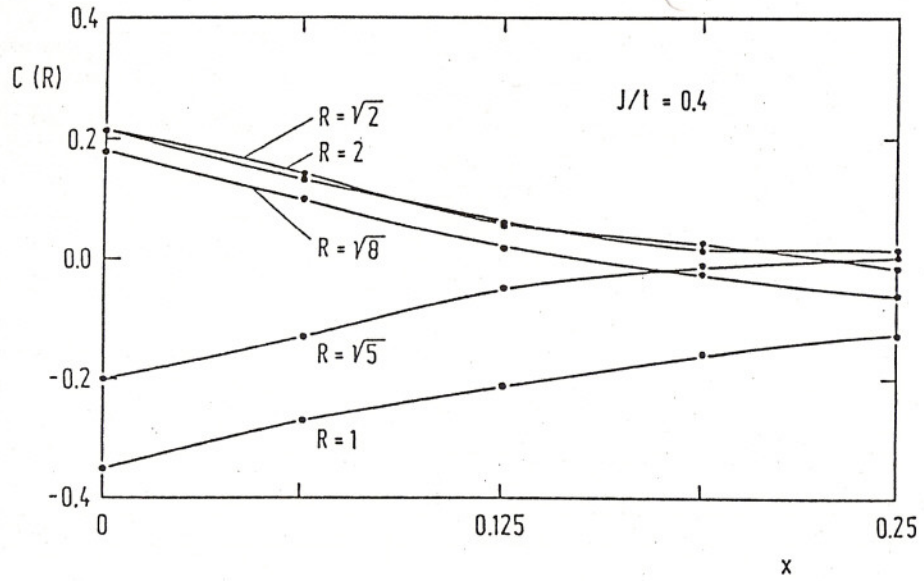

FIG. 5. Spin correlations $C(\vec{R})$ vs hole concentration x, at fixed $J/t = 0.4$.

In order to investigate the many-hole state and the possible SC hole pairing, we study by the exact diagonalization the $N = 4 \times 4$ system with more holes, $N_h = 3, 4$,[17] corresponding to concentrations $x = N_h/N < 0.25$ representing in real copper oxides the substances with highest T_c. For $N_h = 4$ we found in the whole regime the ground state to be again a spin singlet $S = 0$. A clear effect of higher doping is the reduction of spin correlations $C(R)$ as shown in Fig. 5 as a function of the concentration x. Whereas at low doping $x < \frac{1}{16}$ they are qualitatively consistent with $C(R)$ in a layered quantum AFM, weak AFM correlations remain essentially only among nearest neighbors $R = 1$ at high doping $x = \frac{1}{4}$. A decrease of the AFM correlation length ξ can be in our system tested also by the AFM Fourier component

$$\tilde{C}_{AFM} = \sum_i e^{i\vec{q}\cdot\vec{R}} C(R), \quad \vec{q}_0 = (\pi, \pi), \tag{12}$$

which would be related to the correlation length as $\tilde{C}_{AFM} = A\xi^2$, at least for $\xi \gg 1$. It follows from our results shown in Fig. 5 that approximately $\tilde{C}_{AFM} \propto \frac{1}{x}$ in the relevant regime $x > \frac{1}{16}$. This is in agreement with the simple argument being also consistent with experiments,[9] that the linear average distance between holes determines the AFM correlation length, i.e. $\xi \propto \frac{1}{\sqrt{x}}$.

An information on the collective state of holes in a $N_h = 4$ system can be gained from the four-point density correlations

$$G(\vec{R}_1, \vec{R}_2, \vec{R}_3) = \sum_i \langle \Psi_0 | n_h(\vec{R}_i) n_h(\vec{R}_i + \vec{R}_1) n_h(\vec{R}_i + \vec{R}_2) n_h(\vec{R}_i + \vec{R}_3) | \Psi_0 \rangle. \tag{13}$$

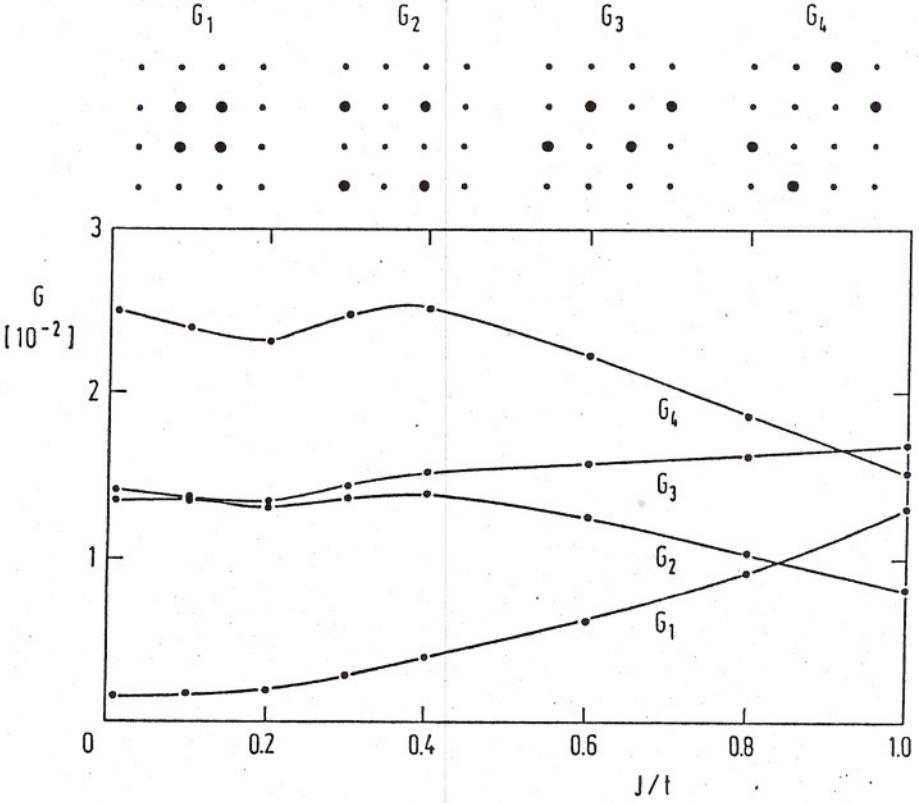

FIG. 6. The four-point density correlations for configurations G_1 to G_4 vs J/t, at fixed $x = \frac{1}{4}$.

We present here G for four characteristic configurations, as shown in Fig. 6. At very large $J/t > 1.2$, G_1 gives the largest contribution what shows that the model becomes unstable against the formation of droplets in this unrealistic regime. G_1 is strongly suppressed with decreasing J/t and the G_4 correlation becomes dominant. This can be interpreted as an indication for a paired state, where pairs with the interhole distance $R = \sqrt{2}$, being the most probable in this regime, are at the largest possible interpair distance in such a small system. We note also that G_4

is the largest at the intermediate $J/t = 0.4$. Although many hole state is in certain properties very similar to a dilute fermion system with $N_f = N_h$, e.g. in hole density correlations $g(R)$, G correlations are substantially different. The main difference is in the exchanged role of G_4 and G_2, so that N_f system does not show a tendency towards pairing while $N_h = 4$ does.

Our results thus support the opinion that the effective t-J model shows attractive quasiparticle interactions and pairing phenomena and should be further considered as a possible model for superconductivity at high temperatures.

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ENTANGLE LUXOID LIQUID STATES IN HIGH Tc SUPERCONDUCTING BiCaSrCuO

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ABSTRACT

The remanent magnetization in high Tc superconducting BiCaSrCuO was measured by using BTi SQUID susceptometer as a function of time (t) and temperature (T). It was found to decay with ln(t). The decay rate, r = (dM/Mo)/(dt/t), was found to increase with T initially, to have two maxima with a dip near 20K for the magnetic field H = 300G before it was turned off, and to vanish at the critical temperature Tc. The dip in r is attributed to the entangled fluxoid liquid states rather than strong pinning centers.

INTRODUCTION

One of many fascinations with high Tc superconductors is the time dependendent remanent magnetization, M(t,T), due to fluxes trapped after the applied magnetic field is turned off. M was observed to decay with ln(t) in BaLaCuO, and the decay rate r increased with T and with magnetic field cubed H^3, suggesting a superconducting glassy state (1). Theoretically, the disorder induced vertex glassy state is proposed for this slow process (2), where the fluxoids were pinned and the zero resistance state can be realized. However, somewhat different results were observed in BaYCuO (3,4) and in BaErCuO (5), where r increased with T initially, had a maximum, and then vanished near Tc. This behaviour of r can be understood in terms of thermally activated creeping flux bundle (6), by introducing the effective volume occupied by fluxoid (5) or the distribution of activation energies (7,8). As an alternative to the glassy state, the giant flux creep was suggested (4).

In this paper, the decay rate of magnetization due to fluxoids trapped in a superconducting BiCaSrCuO is discussed.