EXACT DIAGONALIZATION STUDIES OF QUASIPARTICLES IN DOPED QUANTUM ANTIFERROMAGNETS

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INTRODUCTION

Due to their relevance for superconducting copper oxides[1], models for strongly correlated systems have been studied extensively in last two years. In spite of a number of analytical approaches applied to these models, and to models of the CuO_2 layers in particular, some of the crucial questions lack even a qualitative answer. In such a situation exact diagonalization studies of small correlated systems have proven to be very valuable. Employing this method several groups obtained important results on various models[2-10], representing the insulating state and the low doping regime in CuO_2 layers.

The essential limitation of the exact diagonalization approach is in the smallness of systems which can be investigated. The allowed size of the system is determined by the number of quantum states N_{st}, representing the basis for the ground state (or the excited state) wavefunction $|\Psi_0\rangle$. For most efficient numerical approaches it is required that N_{st} be substantially smaller than the available computer memory. The complexity can be estimated from the total number of states $N_{st}^0 = m^N$, where m is the number of quantum states per unit cell and N is the number of cells. This puts a severe restriction on the studies of models with larger m. Increasing in the complexity are thus: a) the Heisenberg model with $m = 2$ where sizes up to $N = 24$ have been reached by the Lanczos technique[2], b) the $t - J$ model with $m = 3$ and maximum size $N = 16$ (for a single hole state also $N = 18$) [3-8], c) the single band Hubbard model with $m = 4$ and typicaly $N = 12$ (using a different technique also calculations for $N = 16$ are presented at this conference)[9], d) the two (three) band model for CuO_2 layers with $m = 64$ and maximum size $N = 4$ [10]. These estimates give a clear motivation for the studies of simpler models.

In most diagonalization procedures the Lanczos method is used. Starting with a simple wave function $|\Phi_0\rangle$, a sequence of orthogonal functions $|\Phi_n\rangle$ is generated by the recursion relation :

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$$H \mid \Phi_n >= b_{n-1} \mid \Phi_{n-1} > + a_n \mid \Phi_n > + b_n \mid \Phi_{n+1} >, \tag{1}$$

where $b_{-1} = 0$. Usually less than 40 Lanczos steps are needed in order to have a good convergence of the ground state energy E_0 and the wavefunction $|\Psi_0\rangle$, which is obtained by the diagonalization of the tridiagonal matrix with elements a_n, b_n. It is then straightforward to use $|\Psi_0\rangle$ for the evaluation of static expectation values or correlation functions.

The Lanczos method can be easily extended also to the calculation of dynamic response functions.[6,8] We show this on the example of the frequency dependent conductivity $\sigma(\omega)$,[8] which can be studied in a finite system as an extrapolation for $q \to 0$ of

$$\sigma(\vec{q},\omega) = -\frac{1}{\pi\omega} ImG(\omega + i\epsilon), \tag{2a}$$

$$G(z) = \langle \Psi_0 | j_{-\vec{q}} (z + E_0 - H)^{-1} j_{\vec{q}} | \Psi_0 \rangle, \tag{2b}$$

In order to evaluate $G(z)$ we start the Lanczos procedure, Eq.(1), with an initial wavefunction $|\tilde{\Phi}_0\rangle = A\ j_{\vec{q}} |\Psi_0\rangle$. Then $G(z)$ can be expressed with Lanczos corresponding coefficients α_n, β_n in the form of continued fractions

$$G(z) = \frac{\| j_{\vec{q}}\ \Psi_0 \|^2}{z - \alpha_0 - \dfrac{\beta_1^2}{z - \alpha_1 - \dfrac{\beta_2^2}{z - \ldots}}}. \tag{3}$$

In a finite system $G(z)$ has poles on the real axis. Although the convergence of the entire spectrum is hard to reach, only a small number of Lanczos steps (< 50) is needed to reproduce essential features.[8]

In order to reduce N_{st} it is important to employ symmetry properties of the system. Whereas the total number of fermions N_f and the corresponding S^z_{tot} are easily taken into account, representations having well defined wavevector $\vec{q}$ are more difficult to implement for a larger number of holes. On the other hand, it seems that the direct inclusion of the conservation of S_{tot} is not practical.

COMPARISON OF MODELS

Let us first investigate the relation between several models proposed for the CuO_2 layers. The two band model introduced by Emery[11] assumes that only $Cu\ d_{x^2-y^2}$ orbitals and $O\ p_\sigma$ orbitals are essential for the electronic properties,

$$H_{H\,ubb} = -t_{pd} \sum_{(ij)s} c^\dagger_{is} c_{js} + \Delta_0 \sum_{(i\in p)} n_i + \sum_i U_i n_{i\uparrow} n_{i\downarrow} \tag{4}$$

where $c_{is}, c^\dagger_{is}$ 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 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 (1) 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 mobile, hopping through intermediate Cu sites (or 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,[12] treating t_{pd} as the smallest quantity. Models can be further symplified introducing for holes the Wannier functions[13] corresponding to the free hole hopping, but centered on Cu sites. Terms involving the antisymmetric orbitals couple only weakly to the more relevant symmetric subsystem and seem to be less important at low doping. With $\tilde{c}_{is}$ denoting the operators for these symmetric orbitals, we get the symmetrized hole-spin model,[13]

$$H_{sym} = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j - t_0 \sum_{(ij)s} \tilde{c}^\dagger_{is} \tilde{c}_{js} + V \sum_i \tilde{\vec{s}}_i \cdot \vec{S}_i + t_1 \sum_{(ij)\,ss'} \tfrac{1}{2} \vec{\sigma}_{ss'} \cdot \vec{S}_i (\tilde{c}^\dagger_{is} \tilde{c}_{js'} + \tilde{c}^\dagger_{js} \tilde{c}_{is'}), \tag{5}$$

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[14]. Neglecting higher energy triplet states, the generalized t-J model[14,13] is obtained

$$H_{tJ} = J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j - t \sum_{(ij)s} d^\dagger_{is} d_{js} - t' \sum_{((jk))s} d^\dagger_{js} d_{ks} + \varsigma \sum_{(i,j\neq k)ss'} \tfrac{1}{2} \vec{\sigma}_{ss'} \cdot \vec{S}_i d^\dagger_{js} d_{ks'} \tag{6}$$

with operators $d_{is}, d^\dagger_{is}$ 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) t_{pd} is not small enough compared to Δ_0 to ensure the perturbation derivation of Eq. (5), so as V is not large enough for a straighforward derivation of Eq. (6). Therefore we performed a quantitative comparison of models,[13] allowing deviations of parameters from their perturbational values. We adopted the view that effective models should reproduce as well as possible the low energy spectra of a single hole in the antiferroamgnet (AFM), i.e. a single quasiparticle (QP), of the original model, Eq. (4). Here we present results obtained by the exact diagonalization of a $d = 1$ system with $N_0 = 4$ cells.

Since the main open question is whether models are compatible in the mixed valence regime $t_{pd} \gtrsim \Delta_0$,[12] 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. Also we find that corrections to the simplest t-J model are small, i.e. t' and ς terms are even smaller than those derived from a single

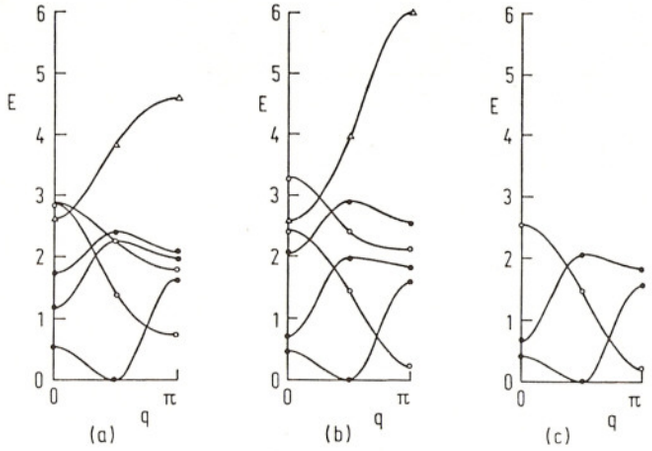

FIG. 1. The lowest lying branches for a system with a single QP on a chain of $N_0 = 4$ cells in a mixed valence regime, $\Delta_0 = 2$, $t_{pd} = 1.4$ and $U_{dd} = 7$. • represent the $S = \frac{1}{2}$, ∘ the $S = \frac{3}{2}$ and △ the $S = \frac{5}{2}$ levels, respectively. Lines are guides to the eye only. Here are: (a) two band Hubbard model, (b) symmetrized hole-spin model and (c) generalized t-J model.

band Hubbard model. It should be stressed however that the agreement between the Hubbard model and the Heisenberg model is less satisfactory in the mixed valence regime. In view of the existing experimental data[15] on magnetic properties, this could be an indication that real copper oxides are in the charge transfer regime $\Delta_0 \gg t_{pd}$.

SINGLE QUASIPARTICLE PROPERTIES

In the following we restrict our discussion to the prototype t-J model,[16] Eq. (6),

$$H = -t \sum_{<ij>s} d^{\dagger}_{is} d_{js} + J \sum_{<ij>} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right). \tag{7}$$

Here, we present a more detailed analysis[8] of the eigenstates of a single hole (QP) in a $d = 2$ system, which supplements the existing analytical and numerical results.[17,18,4,6] First, we calculate by the method of the diagonalization of finite $d = 2$ system the lowest branch of the QP energy dispersion $E(\vec{q})$. Whereas small 4×4 system can be diagonalized exactly, larger 8×4 systems are treated approximately, allowing only a finite number of spin flips $N_r \leq 6$ relative to the initial Néel AFM state.

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

$$\underline{\mu}^{-1} = \frac{1}{2t} \frac{\partial^2 E(\vec{k}_0 + \vec{p})}{\partial \vec{p} \partial \vec{p}} \bigg|_{\vec{p}=0}. \tag{8}$$

The enhancement is large along the AFM zone boundary (infinite for a 4×4 system), i.e. $\vec{p} \perp \vec{k}_0$ and finite $\mu_{\parallel} \equiv \mu$ for $\vec{p} \parallel \vec{k}_0$. Values for μ presented in Fig. 2 show an approximate $1/J$ dependence, as predicted theoretically.[17,18]

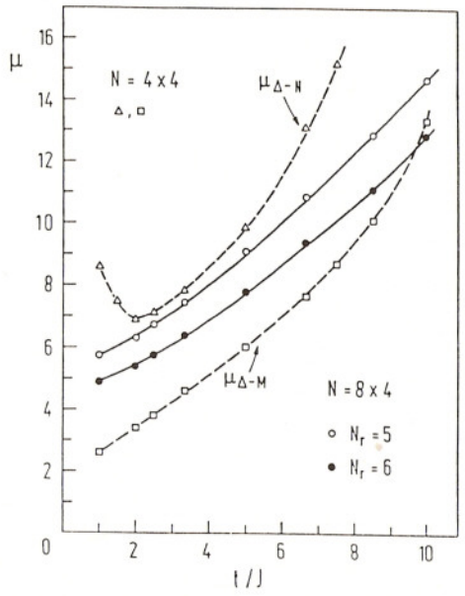

FIG. 2. Mass enhancement μ vs t/J for a) $N = 8 \times 4$ system for $N_r = 5$ and $N_r = 6$; b) for $N = 4 \times 4$ along $\vec{p} \parallel \vec{k}_0$. In the latter case the value of μ has been extracted from the variation along the $\Delta - N$ and the $\Delta - M$ line in a Brillouin zone.

The Lanczos method for the calculation of dynamical conductivity $\sigma(\omega)$ has been described in Sec.1. Since generally systems are too small for the evaluation of $q_x \to 0$, we compared two approaches:[8] a) By using the 8×4 system q_x becomes sufficiently small and an extrapolation $q_x \to 0$ can be performed for different parts of spectra. Results are however only aproximate due to restricted $N_r \lesssim 6$. b) Imposing $q = 0$ the conductivity sum rule is violated in a system with periodic boundary conditions. This can be however traced back to the disappearance of the lowest QP contribution from the spectra. Thus $q = 0$ results can be used for the investigation of the remaining part. Moreover smaller systems as 4×4 can be again used. Both methods give qualitatively similar results.

As seen in Fig. 3, where a typical plot of $\sigma(\omega)$ for finite but small q at $J/t = 0.2$ 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 into 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 $J \to 0$.[19] 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. It should be noted that our results are for $T = 0$, and that finite T would lead to the broadening of the coherent part and of the incoherent part. Whereas there are qualitative similarities between our and experimental results[29], measured $\sigma(\omega)$ show much broader features.

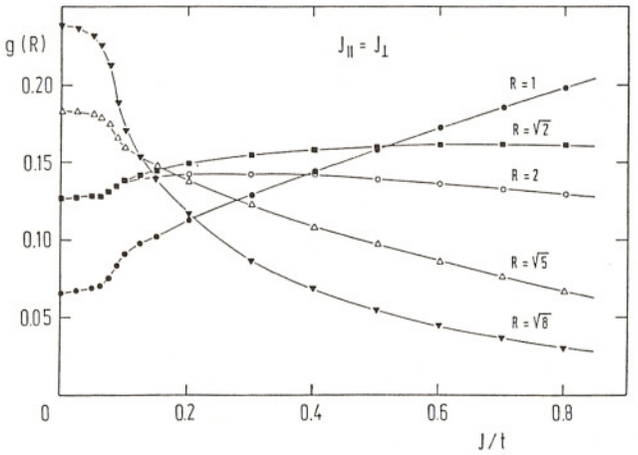

FIG. 3. Frequency dependent conductivity $\sigma(\omega)$ vs ω in units of t for $N = 8 \times 4$ and $J/t = 0.2$ ($N_r = 6$).

BINDING OF QUASIPARTICLES

We studied the binding of QP by numerically solving the t-J model with $N_h = 2$ holes on a 4×4 lattice.[4] 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[4,5], corresponding to $\vec{k}_0 = (0,0), (0,\pi)$ and $(\pi,0)$. In order to test the binding we calculate 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

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

$g(\vec{R})$ as presented in Fig. 4 as well as Δ 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. On the other hand the $S = 1$ hole pair state was found to be very weakly bound, i.e. $\Delta \sim 0$.

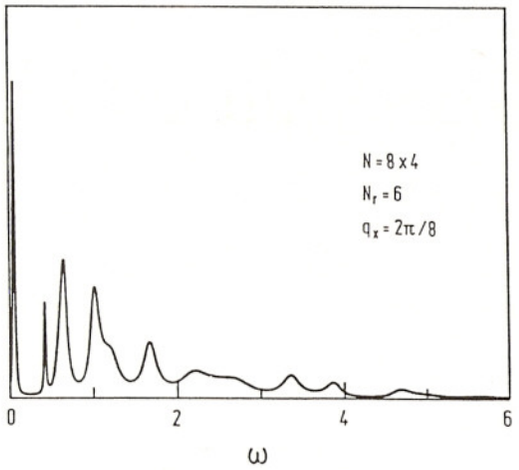

FIG. 4. Hole - density correlations $g(R)$ vs. J/t.

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 a situation can be simply explained by the formation of two oppositely polarized ferromagnetic spin polarons which repel each other, what is consistent with the attractive-repulsive transition observed in $g(R)$.[4]

The origin of a substantial hole binding for $J/t > 0.2$ regime is still not understood. Clearly, so large effect cannot be explained by a simple broken bond argument.[21] We investigate this question further by performing the diagonalization in a restricted basis set with a finite number of reversed spins N_r (relative to the Néel state). In Fig. 5 we present the result for the density correlations $g(R)$ as a function of N_r. It is quite surprising that the correct qualitative behaviour is obtained already with small $N_r > 1$. Moreover the $N_r \geq 2$ accounts well also for the attraction - repulsion transition at $J/t \sim 0.2$. Since at $N_r = 2$ the number of involved states is not large, the binding should be quite local phenomenon clearly related to the AFM correlated background. Our results stimulate the use of analytical approaches (cumulant expansion) using t/J as an expansion parameter. Our diagonalization results as well as preliminary cumulant expansion results indicate on several contributions to the hole binding: a) the static exchange bond contribution [21], b) the quantum interference effect [17], preventing the loss of kinetic energy of two holes to the order t^2/J, c) lowering of the kinetic energy of two holes due to the reduction of the local AFM order (spin bag effect).

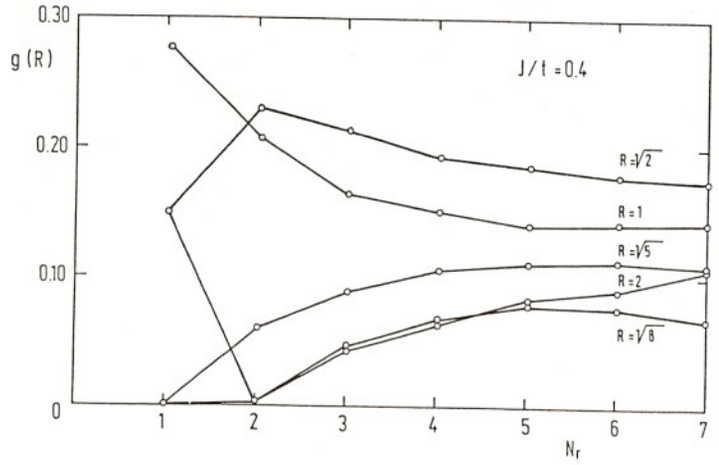

FIG. 5 Hole - density correlations $g(R)$ at fixed $J/t = 0.4$ as a function of the number of reversed spins N_r.

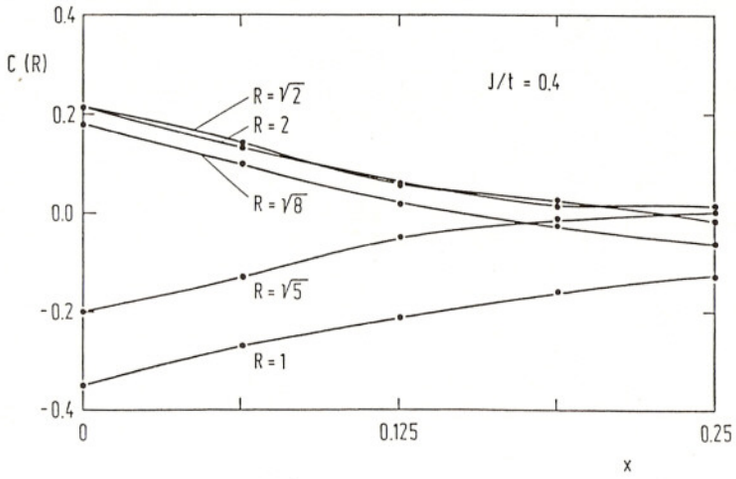

FIG. 6. Spin correlations $C(\vec{R})$ vs hole concentration x, at fixed $J/t = 0.4$.

HIGH DOPING REGIME

In order to investigate the many-hole state and the possible SC hole pairing, we also performed the exact diagonalization of the $N = 4 \times 4$ system with $N_h = 3, 4,$[7] 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. 6 as a function of the concentration x. Whereas at low doping $x < \frac{1}{16}$ correlations are qualitatively consistent with $C(R)$ in a layered quantum AFM, weak AFM correlations remain essentially only among nearest neighbours $R = 1$ 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

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

which would be related to the correlation length as $\tilde{C}_{AFM} = A\xi^2$, at least for $\xi \gg 1$. From our results in Fig. 6 we get $\tilde{C}_{AFM} \propto \frac{1}{x}$ in the relevant regime $x > \frac{1}{16}$. This is consistent with experiments and with a simple argument [15] that the 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

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

We present here G for four characteristic configurations, as shown in Fig. 7. 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 the many hole state is in certain properties very similar to a dilute fermion system with $N_f = N_h$ [7], 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 show that the exact diagonalization of small systems in spite of its deficiencies yields important results on the properties of a single hole in an AFM , on the nature of hole binding and on the nature of their collective state. Our analysis also shows that the effective t-J model exhibits attractive quasiparticle interactions and pairing phenomena and should be further considered as a possible model for superconductivity at high temperatures.

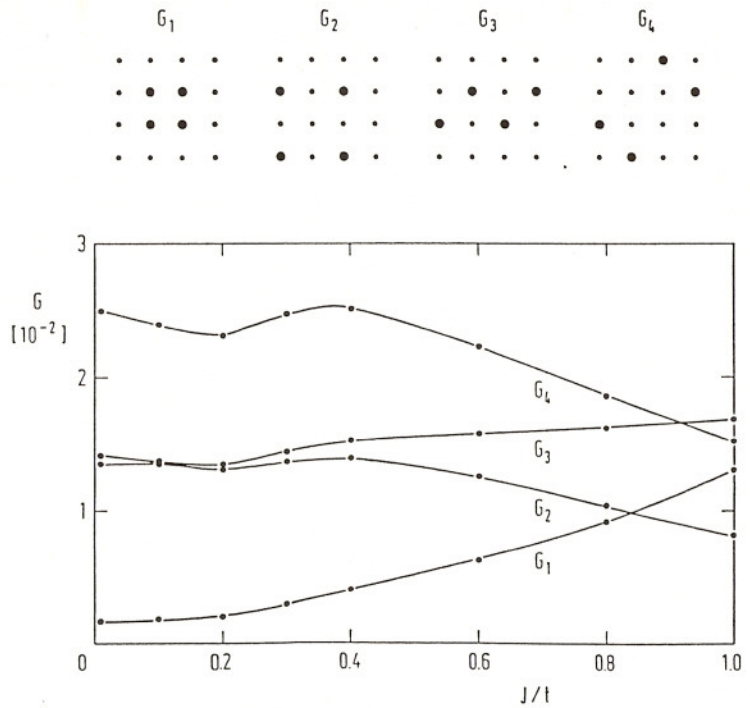

FIG. 7. The four-point density correlations for configurations G_1 to G_4 vs J/t, at fixed $x = \frac{1}{4}$.

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