QUASIPARTICLES IN DOPED QUANTUM ANTIFERROMAGNETS

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ABSTRACT

Results for few holes in the quantum antiferromagnet, as obtained within the $t-J$ model by the methods of the exact diagonalization and the cumulant expansion, are reviewed. In particular, we discuss properties of a single hole, the origin of the binding of two holes and the behaviour at higher doping.

1. INTRODUCTION

Systems of strongly correlated electrons have been extensively studied in recent years mainly in connection with copper-oxide-based superconductors [1]. In spite of a number of theoretical approaches applied to the models for such systems, with an emphasis on the models for CuO_2 layers, some of the crucial questions lack even a qualitative answer. In such a situation exact diagonalization studies and perturbation expansion methods, as will be described in this talk, have proven to be very valuable.

A possible approach to the understanding of strongly correlated electrons is to start with an antiferromagnetic (AFM) insulator as a reference and introduce charge carriers by doping a system with low concentration of holes. Holes are strongly coupled to the AFM spin background and behave as well defined mobile quasiparticles (QP). Their individual static and dynamical properties, e.g. effective masses, related spin distortions of the AFM background etc., form the basis for the understanding of the QP interactions and of the possible superconducting pairing.

Among the models for strongly correlated systems the $t-J$ model [2] represents conceptually the simplest model, taking into account the essential ingrediants: mobile character of fermions and a strong on-site electron-electron repulsion,

$$H = -t \sum_{<ij>s} (c^{\dagger}_{is} c_{js} + c^{\dagger}_{js} c_{is}) + J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j, \qquad (1)$$

describing the hopping of electrons in the presence of empty sites in a spin system with the AFM Heisenberg interaction, where $\vec{S}_i = \frac{1}{2} \sum_{ss'} c^{\dagger}_{is} \vec{\sigma}_{ss'} c_{is'}$. Here, $c^{\dagger}_{is}, c_{is}$

are projected fermion operators, taking into account the requirement of strong correlation that a double occupancy of sites is not allowed.

The $t-J$ model has been and remains the subject of numerous theoretical studies, with an emphasis on $d=2$ systems. The properties of a single hole in planar AFM seem to be now at least qualitatively understood due to analytical [3,4,5], in particular selfconsistent [6] approaches, and due to numerical exact diagonalization studies [7,8,9]. Beyond the Nagaoka regime at very small $J/t \ll 1$ the dynamics of a hole is governed by spin flips in the AFM background [5,6], i.e. $m^* \propto 1/J$. Less clear is the existence and the origin of the real space binding of two holes in an AFM, as observed in exact diagonalization studies [7,8] even for modest $J/t > 0.2$. Regime of finite (larger) concentration of holes x, which is most relevant for oxide superconductors, has been treated with various mean-field, variational and field-theory approaches [2]. The relation of these analytical approaches to the exact results for small systems [10] is still rather unclear. However these questions are mainly beyond the scope of this review.

So far even a clear qualitative understanding of a phase diagram in a parameter space $J/t - x$ is missing. Whereas at $J/t \ll 1$ and $x \ll 1$ a Nagaoka - type behaviour with short-range ferromagnetic (FM) correlations seems to dominate, instabilities in the form of phase separation are expected for $J \gg 1$ [11].

2. EXACT DIAGONALIZATION AND CUMULANT EXPANSION METHOD

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 roughly determined by the number of quantum states N_{st}, representing the basis for the ground 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 thus 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 shows a clear motivation for studies of simplest models of correlated systems, i.e. of the $t-J$ model with the smallest basis $m=3$ and a typical size $N=16$, as compared to the single band Hubbard model with $m=4$ (where recently also results for $N=16$ were obtained [13]) and to the two (three) band model with $m=64$.

In most diagonalization procedures [7-10] the Lanczos method is used, where the ground state energy E_0 and the wavefunction $|\Psi_0\rangle$ are calculated. 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 calcu-

lation of dynamical quantities [9], in particular response functions as the frequency dependent conductivity $\sigma(\omega)$ [14], dynamical spin correlation functions [11] etc.

One of disadvantages of small finite sizes is also a small set of allowed $\vec{k}$ points in the Brillouin zone . This set can be expanded into a continuous variation by introducing into the kinetic term phase factors, corresponding to the effect of a vector potential [15,16]

$$H_t = -t \sum_{<ij>s} (e^{i\vec{\theta}\cdot\vec{n}_{ij}} c^\dagger_{is} c_{js} + h.c.), \tag{2}$$

where $\vec{n}_{ij}$ is the unit vector between neighbouring sites. Varying $\vec{\theta} = \delta\vec{k}$ the entire Brillouin zone can be probed.

The $t-J$ model as such is nonperturbative in both limit $J/t \ll 1$ and $J/t \gg 1$. An expansion can be performed if the spin exchange J is assumed to be anisotropic. Hence we divide the $t-J$ model into the unperturbed (Ising) part

$$H_0 = -J \sum_{<ij>} S^z_i S^z_j \tag{3}$$

and the perturbation $H' = H_t + H_\gamma$,

$$H_t = -t \sum_{ijs} c^\dagger_{is} c_{js}, \quad H_\gamma = \frac{\gamma}{2} J \sum_{ij} S^+_i S^-_j, \tag{4}$$

with the fermion hopping part H_t and the spin-flip part H_γ.

An expansion in t/J and γ is now possible, in particular for a small finite number of holes in a reference Néel AFM. We present here results [17] for a single hole $N_h = 1$ and a hole pair $N_h = 2$. We follow the standard cumulant expansion procedure for the ground state energy [18]. The final result for n holes [17] is the series for the energy ϵ_n, expressed relative to the undoped AFM ground energy for chosen $\vec{k}$

$$\epsilon_n(\vec{k}) = -J \sum_{n,m} a_{n,m}(\vec{k}) (\frac{t}{J})^n \gamma^m. \tag{5}$$

For a single hole $N_h = 1$ the unperturbed (localized) ground state $| \emptyset_i >$ of H_0 represents just a hole in a reference Néel spin state. For $N_h = 2$ the ground state of H_0 is a bound pair of holes, i.e. the Néel configuration $| \emptyset >$ with two neighbouring empty sites,

$$| \emptyset_{i,r} > = c_{i\downarrow} c_{i+r\uparrow} | \emptyset >, \tag{6}$$

where $\tau = x+,\ x-,\ y+,\ y-$. The above states are used to construct the local states having the s, p, d - type rotational symmetries, e.g.

$$| \emptyset_{i,s} >= \tfrac{1}{2}(| \emptyset_{i,x+} > + | \emptyset_{i,y+} > + | \emptyset_{i,x-} > + | \emptyset_{i,y-} >),$$

$$| \emptyset_{i,d} >= \tfrac{1}{2}(| \emptyset_{i,x+} > - | \emptyset_{i,y+} > + | \emptyset_{i,x-} > - | \emptyset_{i,y-} >). \qquad (7)$$

Due to the translational symmetry, the properly chosen unperturbed (as well as intermediate) states are of the Bloch-type $| \emptyset_{\vec{k}} >$, characterized by the momentum $\vec{k}$.

The fermionic sign does not appear for $N_h = 1$, while it already plays an essential role for $N_h = 2$. Still it is not necessary to follow the sign through all intermediate state, since it can be deduced from the final state. Namely, a pair of holes (in its initial state $| \emptyset_{i,\tau} >$) behaves as an oriented bond. Both holes can be tagged and remain distinguishable, hence the overall sign of the final stage depends merely on the final position and on the orientation of the bond. The analogy of states $| \emptyset_{i,\tau} >$ with p - type wavefunctions for two spinless fermions is thus evident, although the many-body state is much more involved in the intermediate state.

We also note that there are close similarities between the cumulant expansion as discussed and the exact diagonalization of small systems using the Lanczos method. The Lanczos method with M steps, starting from a reference Néel state, is essentially equivalent to the cumulant expansion of the same order. For small systems with a limited total number of quantum basis states there are no serious limitations in the number of Lanczos steps, results are however dominated by finite size effects. On the other hand, for larger systems the Lanczos method would generate on each step a prohibitive number of new basis states, mainly due to unlinked processes. In this respect the cumulant expansion is more efficient, since only linked processes contribute. In this way larger (infinite) systems can be studied. Still the number of processes (diagrams) increases very fast with the order. The cumulant expansion can thus supplement the exact diagonalization results, yielding the finite size corrections [17] and allowing for more transparent interpretation by considering different contributions order by order. In our calculations we reach up to $n = 12$ order in t/J and $m = 6$ in γ for $N_h = 1, 2$. Various techniques, in particular the method of Padé approximants, can be used to extend analytically the power series onto the whole regime of J/t and γ.

3. SINGLE QUASIPARTICLE PROPERTIES

Let us first discuss the lowest branch of the energy dispersion for a single QP $\epsilon_1(\vec{k})$. In a $t - J$ model on a $N = 4 \times 4$ lattice it appears that the ground state of

a single QP is degenerate at $\vec{k}_0 = (\pm\pi/2, \pm\pi/2)$ (Δ point), $\vec{k}_0 = (\pi, 0)$ (X point) and $\vec{k}_0 = (0, \pi)$ [7,8]. Introducing the continuous $\vec{k}$ variation via the phase method, it appears that minimum energy state is actually outside the high symmetry point, i.e. the minimum is near the line $\Delta - X$ for $J/t < 1$ [16]. This effect can be explained by the fact that a single hole in a finite system rather simulates the effect of finite doping.

One of the most important quantitities characterizing the QP is its coherent mass enhancement tensor $\underline{\mu}$ and the corresponding coherent hopping integral t_c^*, defined through the dispersion

$$t\,\underline{\mu}^{-1} = \underline{t}_c^* = \frac{1}{2}\frac{\partial^2 \epsilon_1(\vec{k}_0 + \vec{p})}{\partial \vec{p}\,\partial \vec{p}}|_{p=0}. \qquad (8)$$

On the other hand $< H_t >= -2\,d\,t_i^*$ can be used as a definition of the incoherent effective hopping t_i^*. In a system with periodic boundary conditions both effective hoppings are related via the optical conductivity sum rule [16]

$$t_c^* = t_i^* - \sum_{m\neq 0} \frac{|< \Psi_m \mid j \mid \Psi_0 >|^2}{E_m - E_0} = t_i^* - \int_0^\infty \sigma(\omega) d\omega, \qquad (8)$$

Let us first discuss the QP masses in $d = 1$ and $d = 2$ system. In order to determine t_c^* and t_i^* we have studied [16] single hole states in a $d = 1$ chain by diagonalizing exactly using the Lanczos method systems with up to $N = 20$ sites, and then performing the scaling to $N \to \infty$. Results show that the coherent hopping is nearly unperturbed $t_c^* \sim t$ in the whole range of J/t and thus unaffected by the AFM short range spin correlations. In particular, for $J = 2t$ an exact solution is obtained by the Bethe Ansatz method [16] with $t_c^*/t = 0.938$. This property of the $t - J$ model on a chain can be understood starting from the limit $J/t \to 0$ where the incoherent hopping equals the free value $t_i^*/t = 1$ [4]. At the same time $[H, j] = 0$ so that the current j is conserved. Eq.(8) then implies that $t_c^* = t_i^*$. The equality does not seem to persist for finite $J/t > 0$, but the difference has been found to be very small in the entire regime J/t, i.e. $(t_c^* - t_i^*)/t_c^* < 0.02$.

Alternative explanation is related to the observation that for odd chains the mobile hole cannot spoil the AFM correlations. Hence we are dealing with a very mobile holon representing a typical domain wall (soliton) in the $d = 1$ AFM. Also for even chains with an additional spinon in a system, the current is almost conserved.

This indicates that the QP behaviour is essentially different from $d = 2$, where the ratio $t_c^*/t_i^* \propto J/t$ approaches zero [5-7] for $J/t \to 0$ outside the regime

of the Nagaoka FM polaron $J/t \ll 1$, and the coherent contribution to $\sigma(\omega)$ is vanishing in this limit. The latter result is now qualitatively established by several approaches. Since the exact diagonalization results are deficient due to quite evident finite size effects, we present here the cumulant expansion analysis [17], which clarifies the origin of mass renormalization and its anisotropy.

In the Ising case $\gamma = 0$ the QP coherent mass is extremely high since up to the $m = 6$ order in hopping [5] the hole has to return to the starting site. I.e., the QP is bound to the origin by a string of overturned spins. For $\gamma > 0$ the dispersion appears already in low orders (n, m). The lowest process involves two hops and a connected spin flip which clears the path before or after the hole passage. The corresponding coefficient is

$$a_{2,1} = \frac{16}{15}(cos\ q_x + cos\ q_y)^2 - \frac{16}{15}, \tag{9}$$

showing a minimum along the AFM zone boundary. This is just the degeneracy of the exact diagonalization studies of the 4×4 system [7,8]. The degeneracy is lifted in the cumulant expansion in all higher orders, e.g.

$$a_{2,2} = 0.0781 - 0.4029(cos\ q_x + cos\ q_y)^2 + 0.1896(cos\ q_x - cos\ q_y)^2, \tag{10}$$

We notice that all $a_{n,1}$ terms introduce only a weak perturbation to the simple form, Eq.(9), while $a_{n,2}$ terms lead to a substantial stabilization of the QP ground state at the Δ point, consistent with partial diagonalization of larger systems [14] and with the selfconsistent approaches [5,6]. Results of a more complete analysis up to $n = 12$ and $m = 6$, supplemented by the extrapolation to the regime $J/t < 1$ using the Padé approximant, are given in Ref.(17). In Fig.1 we present only the final result for the mass enhancement tensor, i.e. for the longitudinal $\mu_\parallel$ ($\vec{p} \| \vec{q}$) and for the mass ratio $\mu_\perp/\mu_\parallel$. Whereas the ratio does not change qualitatively in the whole regime of J/t, $\mu_\parallel$ increase in both limits, in particular for $J/t \ll 1$ we get $\mu_\parallel \sim 2.3t/J$.

4. QUASIPARTICLE INTERACTION

An information on the QP interaction can be gained by studying the ground state of two QP. We calculate the latter by solving the $t - J$ model with $N_h = 2$ holes on a 4×4 lattice [7,8]. In the whole regime of J/t the $N_h = 2$ ground state was found to be a spin singlet $S = 0$ and triply degenerate, corresponding to $\vec{k}_0 = (0,0), (0,\pi), (\pi,0)$. A test of the pair binding is the binding energy

$$\Delta_0 = \epsilon_2 - 2\epsilon_1, \tag{11}$$

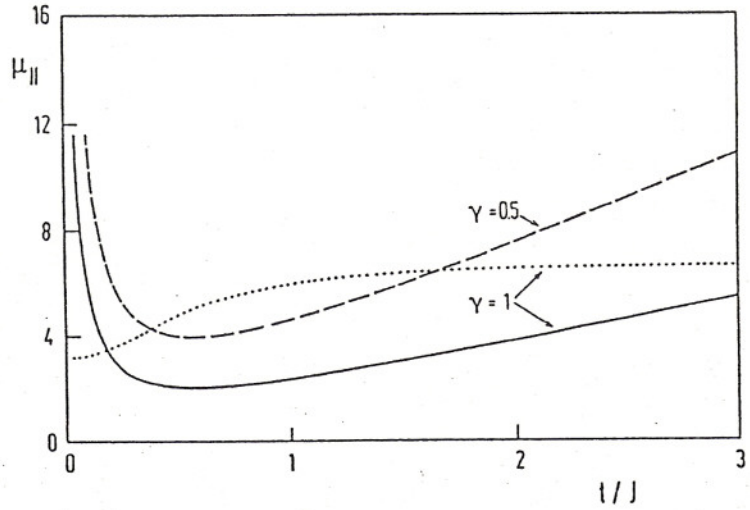

Fig. 1 Mass enhancement $\mu_{\|}$ vs.J/t for two different anisotropies γ. The mass ratio $\mu_{\perp}/\mu_{\|}$ is shown by a dotted curve.

where we should assume in ϵ_1 and ϵ_2 the appropriate $\vec{q}_1, \vec{q}_2$ corresponding to the ground states of $N_h = 1,2$, respectively. Additional information can be gained from the hole density correlation function [7,8]

$$g(\vec{R}) = \langle \Psi_0 | n_h(0) n_h(\vec{R}) | \Psi_0 \rangle. \tag{12}$$

Δ_0 and the density correlations $g(\vec{R})$, presented in Fig. 2, clearly indicate on the bound state of a hole pair at $J/t > 0.2$. The hole density correlations fall off with the distance, whereas $\Delta_0 \simeq -J$ in this regime.

A gradual change to an entirely different state is evident also from the spin correlations $C(\vec{R}) = \langle \Psi_0 | \vec{S}(0) \cdot \vec{S}(\vec{R}) | \Psi_0 \rangle$. They become FM - like for nearest neighbours at $J/t < 0.1$. Such a 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 $g(R)$.

To understand the origin of the hole binding, the cumulant expansion [17] offers a systematic approach where different contributions can be clearly located. Although the expansion starts at $J/t \gg 1$ and $\gamma \ll 1$, exact diagonalization results support the idea that there is no essential change in the binding mechanism up to $J/t \sim 0.2$ where a transition to a different (Nagaoka-type) regime happens. Within our perturbation expansion we evaluate the power series for Δ_0,

$$\Delta_0 = J \sum_{n,m} c_{n,m} (\frac{t}{J})^n \gamma^m, \tag{13}$$

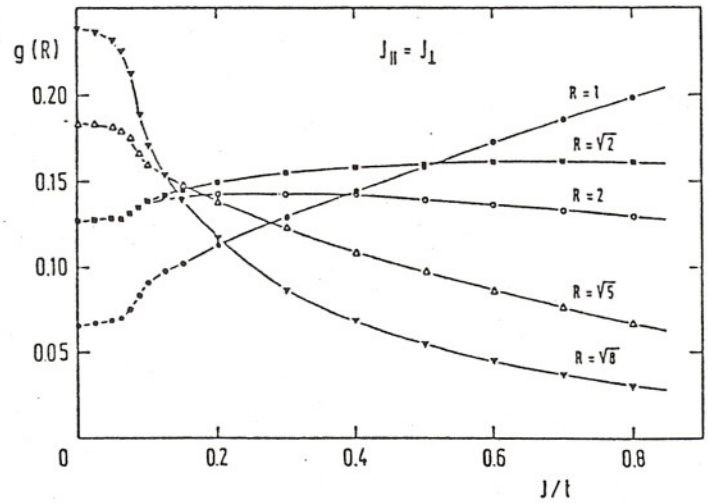

FIG. 2 Hole - density correlations $g(R)$ vs. J/t for $N_h = 2$, from Ref.(7).

Our results for $c_{n,m}$ (obtained up to $m = 6$ and $n = 8$) show that at least for $J/t > 1$ the hole - pair ground state corresponds to the d - type symmetry and $q_2 = 0$.

The binding of two static holes, with $t = 0, n = 0$ can be explained with the simple broken bond argument [7], i.e. a hole pair (holes on neighbouring sites) breaks 7 AFM bonds, while separated holes break 8 bonds. This would amount to the binding $\Delta_0/J = b_{0,0} = -\frac{1}{4}$. Corrections for $t = 0$ as determined by $c_{0,m}$ coefficients are all negative but small, yielding for the isotropic $\gamma = 1$ case $\Delta_0/J = -0.2764$.

For finite hopping $t > 0$ we first notice that within the order $n = 2, m = 0$ there is an attractive contribution, but also a large degeneracy of the ground state. The origin of this effect is due to the fact that a hole pair is quite mobile, in contrast to a single hole. Since the bond behaves as an oriented entity, there is an important interference between partial states of the wavefunction.

Higher order $n > 2, m = 0$ terms lift the degeneracy and the $q = 0, d$ state remains the lowest one for a hole pair. In this respect $n > 2$ terms already present finite size corrections to the exact diagonalization results for the 4×4 system [7,8], where the ground state is triply degenerate. $c_{n,m}$ values for $\gamma > 0$ indicate that in the leading order spin fluctuations enhance the binding. Using again a Padé approximant for the extension of series we get for Δ_0/J the result presented in Fig.3. In the $J/t < 1$ regime it shows even a relative enhancement over the static

hole case, both for $\gamma = 0$ and $\gamma = 1$. The exact diagonalization clearly yields a larger binding for $\gamma = 1$, what can be attributed to the finite size effects. It should be however noted that at $J/t \ll 1$ a crossover to a different single hole and hole pair state is expected leading to the unbinding of a hole pair [7].

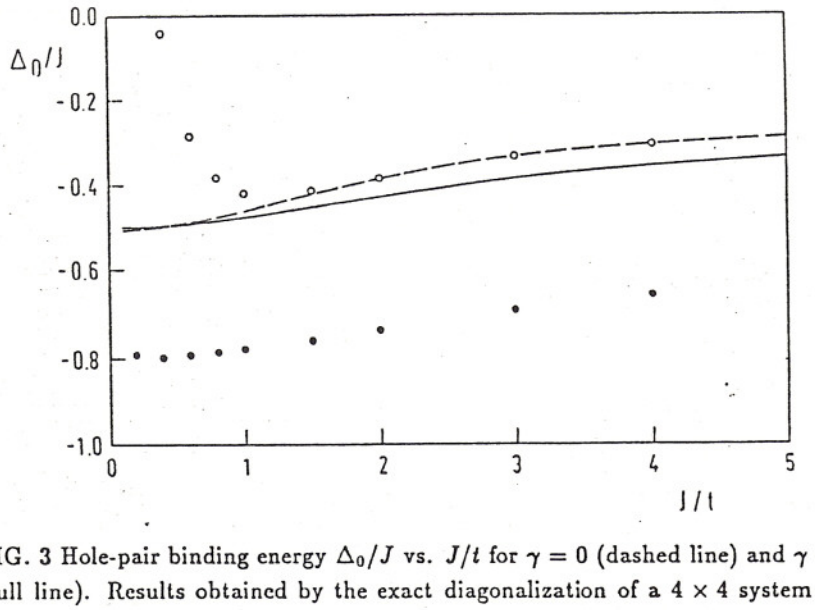

FIG. 3 Hole-pair binding energy Δ_0/J vs. J/t for $\gamma = 0$ (dashed line) and $\gamma = 1$ (full line). Results obtained by the exact diagonalization of a 4×4 system are presented by light and heavy dots, respectively.

4. MANY - HOLE STATES

Whether some characteristics of a single QP and the nature of QP interaction remain valid even at finite (higher) concentration of holes is one of the central questions in the theory of strongly correlated systems. Some aspects of this problem have been tested by the exact diagonalization. The system with $N_h = 3, 4$ holes on a 4×4 lattice has been investigated by the present authors [10,11]. Note that $N_h = 4$, corresponds to the concentration $x = N_h/N = 0.25$, representing in real copper oxides the materials with highest T_c.

For $N_h = 4$ we find for $J/t > 0.2$ the ground state to be again a spin singlet $S = 0$. A clear effect of higher doping is the reduction of spin correlations $C(R)$ with x [10]. Whereas at low doping $x \leq \frac{1}{16}$ correlations are qualitatively consistent with $C(R)$ in a layered quantum AFM, at high doping $x = \frac{1}{4}$ AFM correlations remain (only) among nearest neighbours $R = 1$. This result agrees

with experiments [19] and with a simple argument 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 [10] which show that the model becomes unstable against the hole droplet formation for $J/t \gg 1$, which is an manifestation of the phase separation instability [12] in a $t-J$ model. So far we have no indications for such separation in the physical regime $J/t < 1$. In particular the cumulant expansion method clearly shows that the introduction of hopping $t > 0$ prevents the binding of more holes $N_h = 3, 4$ etc. into a droplet, in contrast to the case of a hole-pair $N_h = 2$.

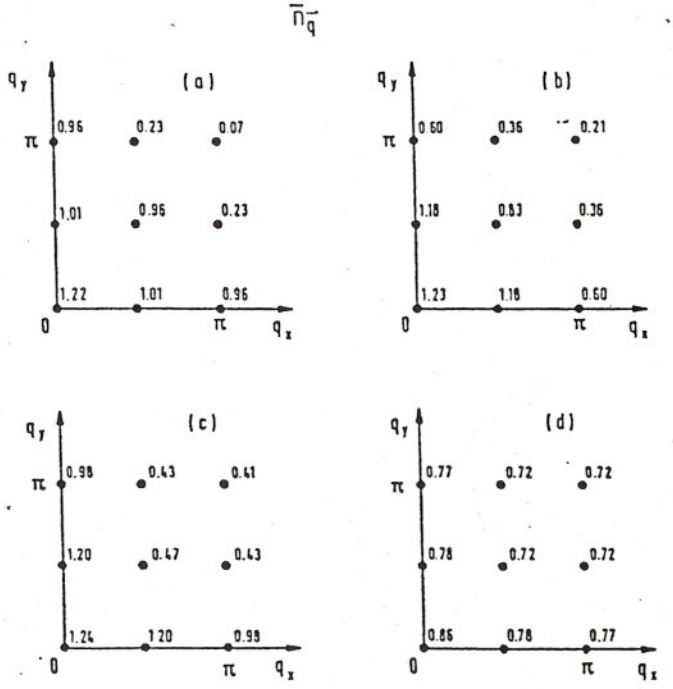

FIG. 4 The momentum distribution function $\bar{n}_{\vec{q}}$ for $N_h = 4$ holes on a 4×4 lattice at: a) $J = 0$, b) $J/t = 0.1$, c) $J/t = 0.8$ and d) $J/t = 10$.

A possibility of the Fermi-liquid behavior at higher doping is one of the most interesting open questions in correlated systems. Our results [11] for a small system can add some qualitative insight through the fermionic momentum distribution $\bar{n}_{\vec{q}}$.

In Fig. 4 we show $\bar{n}_{\vec{q}}$ in our system with fixed $N_h = 4$, i.e. with $N_f = N - N_h = 12$ fermions, for various values of J/t. At $J = 0$ with highly polarized ($S = 5$) ground state (Fig. 4a), $\bar{n}_{\vec{q}}$ is similar to the distribution for noninteracting spinless fermions. At $J/t = 0.1$, $\bar{n}_{\vec{q}}$ is more continuously decreasing from $\vec{q} = (0,0)$ towards the Brillouin zone edge. The shape of the distribution function is weakly dependent on J/t in the corresponding interval $0.048 < J/t < 0.35$. The latter holds also in the region $0.35 < J/t < 1.00$. From Fig. 4c we notice however ($J/t = 0.8$) that here $\bar{n}_{\vec{q}}$ is very close to the one expected in a Fermi liquid. The volume of the inner region with $\bar{n}_{\vec{q}} \gtrsim 1$ corresponds qualitatively to the volume for noninteracting fermions. The less occupied region $\bar{n}_{\vec{q}} < 0.5$ contains also the point $\vec{q} = (\frac{\pi}{2}, \frac{\pi}{2})$. This latter result is consistent with photoemission experiments [20] and can be interpreted simply using the fact that single holes preferably enter the $\vec{q} = (\frac{\pi}{2}, \frac{\pi}{2})$ state at low doping. At very large $J/t \gtrsim 10$ the situation is qualitatively different as shown in Fig. 1d. The distribution is almost constant for all $\vec{q}$ indicating the localization of fermions and the formation of hole rich droplets. The analogous variation of $n_{\vec{q}}$ is expected as a function of doping. Namely, at $x \ll 1$ and $J/t < 1$ the holes are nearly self-trapped due to the large coherent mass, and $\bar{n}_{\vec{q}}$ would appear nearly constant.

Four-point density correlations also indicate on the possibility of the paired state in the regime $0.4 < J/t < 1.0$, where pairs with the interhole distance $R = \sqrt{2}$ and $R = 1$ are the most probable. Still there are gradual changes in character of hole pairing. Whereas for $N_h = 2$ the pairing correlation functions are clearly dominated by the d-wave character [7,8], the s - wave function increase with doping and reaches the value of the d- type function in the most relevant regime $x = 0.25$ [11].

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