Quasiparticle properties in effective models for strongly correlated electrons

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The single-hole states are studied by the exact diagonalization method in two models for strongly correlated systems: the single-band effective (*t-J*) model and the Kondo-lattice model. The coherent mass m^* of the quasiparticle and the frequency-dependent conductivity $\sigma(\omega)$ are calculated for clusters with 4×4 and 8×4 sites. In particular, $\sigma(\omega)$ shows an isolated quasiparticle peak of weak intensity at small ω and a broad but structured incoherent part at higher ω.

I. INTRODUCTION

Strongly correlated systems are at present one of the most challenging theoretical problems in condensed-matter physics. Due to their connection with superconducting (SC) oxides, the main goal is the understanding of the quasiparticle (hole) interactions and the possibility of the SC pairing of an entirely electronic origin in these systems. Properties of a quasiparticle (QP) in a low-doping regime, i.e., a single hole in the reference antiferromagnetic (AFM) system, are much simpler to investigate and yet they are not fully understood.

Several models have been introduced for the description of layered strongly correlated systems, as realized in CuO_2 layers in oxide SC. The effective single-band (t-J) model[1–3] has been shown to represent well a more complete two-band Hubbard model.[4–6] In this prototype model the properties of a single mobile hole added to the quantum AFM system have been studied by a number of authors.[7–13] It has been shown that such a QP has an essentially different dispersion, as compared to the free fermion. Although it has only weakly reduced kinetic energy, i.e., rather small incoherent mass,[7] quite enhanced coherent mass m^* shows up in the optical conductivity response and in other low-frequency transport properties. m^* depends crucially on the transverse exchange coupling $J_\perp$,[8,10] which has been used as an expansion parameter in analytical approaches yielding the large enhancement μ over the bare electron band mass m_0, $\mu=m^*/m_0\propto t/J>>1$. In spite of several analytical[10] and numerical calculations,[8,9,11–13] the value of μ cannot be considered as settled in the relevant parameter regime $J/t<1$.

The optical conductivity $\sigma(\omega)$, which is at low frequencies closely related to the QP coherent mass, is a quantity accessible experimentally.[14] Measurements show at low temperatures a narrow Drude peak, having a small spectral weight and a broader part, which could be attributed to the incoherent motion. So far only the latter part has been described analytically within the retraceable path approximation for the limiting case $J/t\rightarrow0$.[15]

An alternative representation of the two-band Hubbard model are hole-spin models,[16–19] which describe the mobile hole, predominantly on O sites in the CuO_2 layers, and the localized spins on Cu sites as separate, but coupled degrees of freedom. These models have a conceptual and possibly also a technical advantage, that one can study the behavior of the system by varying the hole-spin coupling, the t-J model being a limiting case. Among the versions of the hole-spin models, the Kondo-lattice model is the simplest one and has been already studied[18,19] in connection with single-hole properties and the possibility of the SC pairing.

In this paper we study the Kondo-lattice model and the t-J model by the method of numerical diagonalization of small systems. We use the Lanczos method to determine both the ground-state dispersion of a single-hole state, and hence the coherent mass m^*, as well as the frequency-dependent conductivity $\sigma(\omega)$. Whereas one-dimensional ($d=1$) systems of sufficient length can be diagonalized exactly, on the square lattice ($d=2$) one has to use certain restrictions in the number of allowed states to reach sufficient system sizes. The idea is to start from a hole in a Néel state and add in a controlled way the states with reversed spins. In this procedure, the Kondo-lattice and the t-J model behave differently.

In Sec. II we present the models and our calculational procedure for mass enhancement μ and for $\sigma(\omega)$. Sections III and IV are devoted, respectively, to the presentation of results for μ and $\sigma(\omega)$. A summary of our results and conclusions are given in Sec. V.

II. MODELS AND METHODS

The effective single-band (t-J) model[1–3]

$$H_{t\text{-}J}=-t\sum_{\langle ij\rangle s}(c_{is}^\dagger c_{js}+c_{js}^\dagger c_{is})+J\sum_{\langle ij\rangle}\left[S_i^zS_j^z+\frac{\gamma}{2}(S_i^+S_j^-+S_i^-S_j^+)\right], \qquad (1)$$

where $\gamma=J_\perp/J_\parallel$ and $J=J_\parallel$ describes the hopping of electrons in the presence of a finite concentration of empty sites in a quantum AFM, as represented by (in general) an anisotropic Heisenberg exchange model for spin operators $\mathbf{S}_i=\sum_{ss'}c_{is}^\dagger\sigma_{ss'}c_{is'}$. $c_{is}^\dagger(c_{is})$ are here projected fermion operators, taking into account that double occupancy of sites is not allowed.

The Kondo-lattice model[16,18,19]

$$H=-t\sum_{\langle ij\rangle s}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is})+V\sum_{i}\mathbf{s}_i\cdot\mathbf{S}_i$$
$$+J\sum_{\langle ij\rangle}\left[S_i^zS_j^z+\frac{\gamma}{2}(S_i^+S_j^-+S_i^-S_j^+)\right] \quad (2)$$

treats holes, as represented by operators $c_{is}^{\dagger}(c_{is})$, and the localized spins $\mathbf{S}_i$ as separate degrees of freedom. On increasing V the model changes its character from an independent system of free holes in a quantum AFM system at $V\to 0$, to the t-J model at $V\gg t$ with a corresponding effective $\tilde{t}=t/2$, representing the matrix element for the hopping of a local singlet. The relation between the generalized hole-spin model (2) and the t-J model (1) has been established by several authors.[5,6] It has been shown that single-hole properties agree even quantitatively,[6] if one adds to Eq. (2) a spin-dependent nn hopping term. In the absence of this term there are some differences in the energy dispersion $E(\mathbf{k})$; i.e., in the t-J model the minimum has been found to be degenerate at $\mathbf{k}_0=(\pm\pi/2,\pm\pi/2)$, $\mathbf{k}_0=(0,\pi)$, and $(\pi,0)$ for a 4×4 and isotropic $\gamma=1$ system, while a hole in the model (2) is stable at $\mathbf{k}_0=(0,0)$ for $V<V_c$, where $V_c/t\gg 1$.

We study the lowest branch $E(\mathbf{k})$ of single-hole ($N_h=1$) states by the exact diagonalization of a finite system with N sites and periodic boundary conditions.[9,11] We use the Lanczos procedure and basis states expressed in the real space, taking into account a single representation among states related by the translation symmetry and thus directly monitoring $\mathbf{k}$ as a good quantum number. Starting with a hole in a Néel AFM configuration, we also keep track of the number of reversed spins N_r. Note that in both models the degenerate AFM states exist, characterized by $N_r=N$ in the Kondo-lattice model and $N_r=N-1$ in the t-J model, respectively. In the study of larger systems $N>16$ one is faced with an enormous number of basis states which have to be taken into account. Thus, e.g., for the next interesting cluster size 6×4, the dimension of the relevant basis (for the t-J model) exceeds 3.2×10^7. A way out is to restrict the number of reversed spins to $N_r<N_c$ or $N_r>N-N_c$, where $N_c=N/2$ for the Kondo-lattice model and $N_c=N/2-1$ for the t-J model. In the anisotropic $\gamma=0$ case this amounts to neglecting the configurations with long strings of overturned spins. Since such configurations are energetically unfavorable we expect the results for the ground-state energy $E_0=E(\mathbf{k}_0)$ and the corresponding wave function $|\Psi_0\rangle$ to be quite reliable. In the isotropic $\gamma=1$ case, however, only a small fraction of the available states assist the hole in its motion. The majority of states represent configurations where spins are flipped away (i.e., disconnected) from the neighborhood of a hole and thus only contribute corrections to the ground-state energy of the Heisenberg AFM. Since the states involved in the hopping of a hole are similar as for $\gamma=0$, supplemented by those states which dynamically erase too long strings of overturned spins appended to a hole, we do not expect the results to be less reliable than for the $\gamma=0$ case.

The frequency-dependent conductivity $\sigma(\omega)$ can be studied in a finite system as an extrapolation $\mathbf{q}\to 0$ (Refs. 18–20) of

$$\sigma(\mathbf{q},\omega)=-\frac{1}{\pi\omega}\mathrm{Im}G(\omega+i\delta)\ , \quad (3)$$

$$G(z)=\langle\Psi_0|j_{-\mathbf{q}}(z+E_0-H)^{-1}j_{\mathbf{q}}|\Psi_0\rangle\ , \quad (4)$$

where for definiteness we investigate only a component along one axis (for a $d=2$ system)

$$j_{\mathbf{q}}\equiv j_x(\mathbf{q})$$
$$=it\sum_{is}(c_{is}^{\dagger}c_{i+e_x,s}-c_{i+e_x,s}^{\dagger}c_{is})e^{i\mathbf{q}\cdot\mathbf{R}_i}\ . \quad (5)$$

Here e_x denotes neighbors in the positive x direction in $d=2$. In order to evaluate $G(z)$ we start the Lanczos procedure with a new normalized wave function[20]

$$|\Phi_0\rangle=j_{\mathbf{q}}|\Psi_0\rangle/\langle\Psi_0|j_{-\mathbf{q}}j_{\mathbf{q}}|\Psi_0\rangle\ ,$$

so that for a general term $n>1$

$$H|\Phi_n\rangle=\beta_{n-1}|\Phi_{n-1}\rangle+\alpha_n|\Phi_n\rangle+\beta_n|\Phi_{n+1}\rangle\ , \quad (6)$$

$$\alpha_n=\langle\Phi_n|H|\Phi_n\rangle\ ,$$
$$\beta_n=\langle\Phi_{n+1}|H|\Phi_n\rangle\ , \quad (7)$$

while $\beta_0=0$. $G(z)$ can be now expressed in terms of α_n,β_n as a continued fraction

$$G(z)=\cfrac{\|j_{\mathbf{q}}\Psi_0\|^2}{z-\alpha_0-\cfrac{\beta_1^2}{z-\alpha_1-\cfrac{\beta_2^2}{z-\ddots}}}\ . \quad (8)$$

In a finite system fractions, in principle, end up when one exhausts the number N_{st} of basis states ϕ_n. Then $G(z)$ shows poles only on the real axis, hence $\sigma(\omega)$ is a sum of δ functions.[18] N_{st} is however very large as compared to $n_L\sim 30$ Lanczos steps used in the calculation, so we will adopt the procedure appropriate for an infinite system. In nearly all cases considered we observe that α_n, β_n converge approximately to fixed values $\alpha_\infty,\beta_\infty$, for $n\gg 1$, so that higher-order fractions can be summed analytically and $\sigma(\omega)$ becomes continuous above a lower cutoff $\omega>\omega_c>0$.

It is important to note that in order to resolve the undamped QP peak at $\omega=\varepsilon(\mathbf{q})=E(\mathbf{k}_0+\mathbf{q})-E(\mathbf{k}_0)$ from the incoherent part connected to magnetic excitations at $\omega>\omega_c\propto J$, it is crucial to deal with a system of sufficient linear dimensions, i.e., $q=2\pi/L\ll q_{\max}$, so that $\varepsilon(\mathbf{q})<J$. Another possibility appropriate also for a smaller system is to investigate directly the $\mathbf{q}=0$ response. Although the general f-sum rule[18] (derived explicitly for the Kondo-lattice model) is not satisfied in this case, the interpretation of such $\tilde{\sigma}(\omega)$ is straightforward and has been checked on the results for the $N=8\times 4$ system. The QP peak is disappearing from the spectra, while the incoherent part $\omega>\omega_c$ seems to represent the correct $\mathbf{q}\to 0$ extrapolation of the $\mathbf{q}>0$ spectra.[21]

We investigate models both on a chain and on a $d=2$ square lattice with $N=L_x\times L_y$. In $d=1$ a system with $N\le 18$ is diagonalized exactly and allows for a sufficient

q resolution. On the other hand, in $d=2$ we investigate several sizes, in particular an 8×4 system with $N_r\le6$, where we are limited by the dimension of basis states $N_{st}<200\,000$.

III. EFFECTIVE MASSES

In a t-J model on a chain we found that the ground state with a single hole ($N=16$) corresponds to $k_0=\pm\pi/2$, analogous to the situation in $d=2$. The dispersion $E(k)$ appears to be more cusplike than parabolic around $k=k_0$, hence the effective mass is not well defined. This behavior is presumably related to typical $d=1$ instabilities and seems to be consistent with analytical findings.[10] Note also that the current operator j_0 commutes with the Hamiltonian for $J=0$ in $d=1$.[7,15] On the other hand, the Kondo-lattice model does not show such phenomena and the dispersion around the minimum appears to be parabolic.

In $d=2$ the behavior of $E(\mathbf{k})$ is not anomalous. In an infinite system the long range AFM order persists even in the presence of a hole[22] and effective masses are well defined. Since linear dimensions L_x are quite small, we are restricted to approximations or to some special cases: (a) In both models a single hole in the extreme anisotropic AFM with $\gamma=0$ (Ising case) can be studied much more efficiently. Even in large systems, e.g., for $N=8\times4$, the hopping hole generates in each Lanczos step only a tractable number of new configurations and the convergence of $|\Psi_0\rangle$, and consequently of the effective-mass tensor m^*, is satisfactory. (b) In the isotropic case $\gamma=1$ the number of new configurations multiplies in each Lanczos step, so quite restrictive N_r should be used for large systems, e.g., $N_r=6$ for $N=8\times4$. We still expect that such effective mass m^* is reliable, since the dispersion $E(\mathbf{k})$ is calculated consistently. In a large (strictly speaking infinite) system restricting N_r amounts to taking into account only contributions of clusters of reversed spins satisfying the constraint. Thus in the spirit of cluster expansion one would even expect that the results for the larger system should be more reliable since at fixed N_r the phase space available is less affected by the periodic boundary conditions. (c) For a smaller system, i.e., $N=4\times4$, we can get exact results for $E(\mathbf{k})$. Due to small L_x we can evaluate m^* only by assuming some simple form for the dispersion and so relate m^* to the corresponding bandwidth.[9,11-13]

In an isotropic t-J model and an $N=4\times4$ system, a single-hole ground state is degenerate along the AFM Brillouin zone boundary.[9,11] Thus, the effective mass and hence the mass enhancement tensor $\underline{\mu}$ are highly anisotropic quantities. Here, we define the enhancement relative to the unperturbed band mass $m_0=1/2t$ as

$$\underline{\mu}^{-1}=\frac{1}{2t}\frac{\partial^2E(\mathbf{k}_0+\mathbf{q})}{\partial\mathbf{q}\partial\mathbf{q}}\bigg|_{\mathbf{q}=0}. \tag{9}$$

For a 4×4 system the enhancement $\mu_\perp$ is infinite along the AFM zone boundary, $\mathbf{q}\perp\mathbf{k}_0$, and finite $\mu_\parallel\equiv\mu$ for $\mathbf{q}\parallel\mathbf{k}_0$. The same near degeneracy persists for the larger system, $N=8\times4$, where the state with $\mathbf{k}_0=(\pm\pi/2,\pm\pi/2)$ is found to have the lowest energy.

In Fig. 1 we present the values of μ, as calculated for the t-J model and $N=4\times4$, from the energy differences along the lines Δ-M (see inset) and Δ-N, respectively, where μ is shown as a function of the maximum allowed number of reversed spins N_r. In calculating μ we assume the simplest form for the dispersion $E(\mathbf{k})=2t^*(\cos k_x+\cos k_y)^2$ having the proper symmetry, i.e., the minimum along the X-Y line (for a 4×4 lattice). The result indicates that in general an increase of N_r leads to a gradual, but small decrease of μ. Another effect of increasing N_r is the splitting of the degeneracy at the points M and N (as well as at Γ and S), which appears (for $N=4\times4$) at $N_r=N_c$ due to the coupling between both Néel AFM configurations. Still an extrapolation of $\mu_{\Delta\text{-}N}(\mu_{\Delta\text{-}M})$ from $N_r<N_c$ to $N_r=N_c$ would yield a meaningful value, i.e., approximately the mean value between both nondegenerate $\mu_{\Delta\text{-}N}$ and $\mu_{\Delta\text{-}M}$.

These considerations give also a further justification for the use of $N_r<N_c$ for the larger 8×4 system, with the results presented in Fig. 2. We observe that in the intermediate regime $2<t/J<6$ results for the 4×4 and 8×4 systems are consistent, while at $t/J>6$ the larger system indicates on a smaller mass, especially in view of the decreasing tendency of μ with respect to N_r.

As seen from Fig. 2, the dependence of μ on t/J is in a broad range of $1<t/J<10$ close to being linear, in particular for the case $N=8\times4$. Such behavior is in agreement with results obtained by analytical approaches.[8,10] For the 4×4 system and $0.1<J/t<0.4$ a fit of the form $\mu^{-1}\propto J^\alpha$ for $J>0.075$ (note that for $J<0.075$ $S>\frac{1}{2}$ in the ground state[9]) and $\alpha\approx0.7$ is obtained, in agreement with the results reported by others.[12] For the larger system a similar fit over the whole region of t/J considered

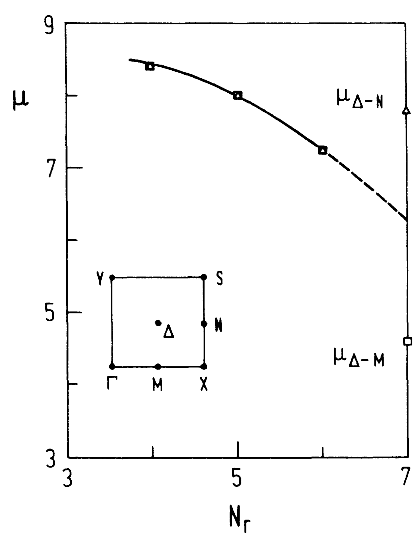

FIG. 1. The mass enhancement μ vs number of reversed spins N_r in the t-J model on a 4×4 lattice for $J=0.3$, $\gamma=1$ as calculated from the bandwidths along the lines in (one quarter of) the Brillouin zone as indicated in the inset. Here and in Figs. 2 and 3 the lines are a guide to the eye only.

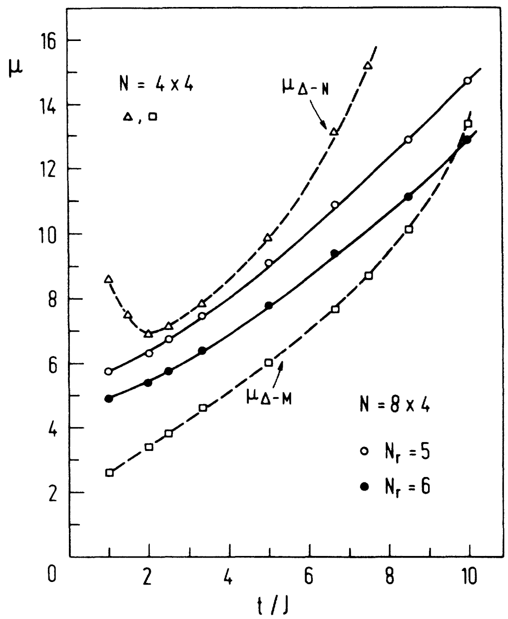

FIG. 2. μ vs t/J in the t-J model for the 4×4 and 8×4 systems.

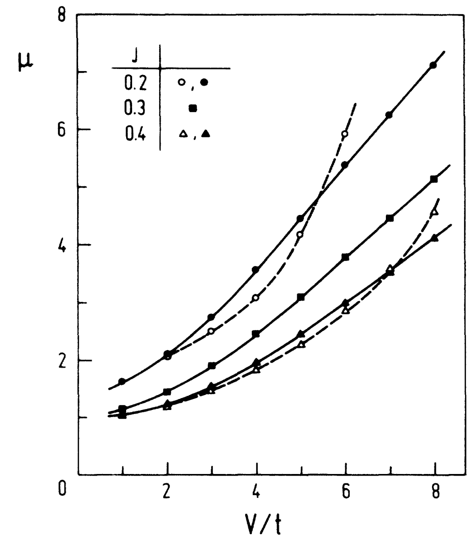

FIG. 3. μ vs V/t for the 8×4 Kondo-lattice model for three different values of J; empty symbols, $\gamma=1$; solid symbols, $\gamma=0$.

here results in $\alpha\approx0.8-0.9$. It should be noted that our analysis becomes less reliable in the $J/t<0.1$ regime, since the size of the magnetically perturbed region might exceed the size of the system, while also larger N_r are needed. In this paper we also do not discuss the regime $J/t>1$, where μ is expected to increase again.[13]

For the 4×4 system we have in the same way analyzed the Ising $\gamma=0$ case. Here the QP minimum is at $\mathbf{k}_0=0$, while $E(\mathbf{k})$ can be still approximately fitted to the same functional form with $t^*<0$. As expected, the enhancement μ (isotropic for $\mathbf{k}_0=0$), determined by Eq. (9), is very large in this case. We obtain, for example, by adjusting the energy difference between the $\Gamma-X$ points, the values $\mu=9.5$, 17.7, and 45.5 for $J/t=0.2$, 0.4, and 0.8, respectively.

The ground state of a single hole in a Kondo-lattice model is for $N=8\times4$ and $N_r\leq6$ still doubly degenerate, with $\mathbf{k}_0=0$ and $\mathbf{k}_0=(\pi,\pi)$, i.e., the degeneracy characteristic of the Néel state is not removed. For $N=4\times4$, however, the spectrum can again be computed exactly and one finds that the degeneracy is lifted, with $\mathbf{k}$ of the ground state at $\mathbf{k}_0=0$ for $V<V_c(J)$, and at $\mathbf{k}_0=(\pi,\pi)$ for $V>V_c$. For very large V the ground state should acquire $\mathbf{k}_0=(\pm\pi/2,\pm\pi/2)$ since in that limit the Kondo-lattice model should become equivalent to the t-J model. Thus, e.g., for $J/t=0.4$ we get $V_c\approx2.75t$, but for $V/t=15.0$ the ground state is found to be definitely t-J-like, i.e., with $\mathbf{k}_0=(\pm\pi/2,\pm\pi/2)$. Here we consider only values of $V\leq8t$ for which the gap from $E_\Gamma(E_S)$ to E_Δ is rather large, so that we expect no significant change in the behavior of μ due to crossover from $\mathbf{k}_0=0$ to $\mathbf{k}_0=(\pi,\pi)$ of the ground state. As seen from Fig. 3, representing both the Ising ($\gamma=0$) case and the isotropic ($\gamma=1$) case, μ shows a continuous increase with V, i.e., a quadratic dependence at small V/t, consistent with the perturbation expansion result, with $\mu\propto V^2/Jt$.[16,18] Although the perturbation expansion breaks down for $\mu\gtrsim2$, numerical results suggest its qualitative validity even beyond that limit.

IV. FREQUENCY-DEPENDENT CONDUCTIVITY

We have numerically calculated $\sigma(\omega)$ both in $d=1$ and $d=2$ for the t-J model as well as for the Kondo-lattice model. Typical examples of such spectra are shown in Figs. 4–6. Below we consider each of them in some de-

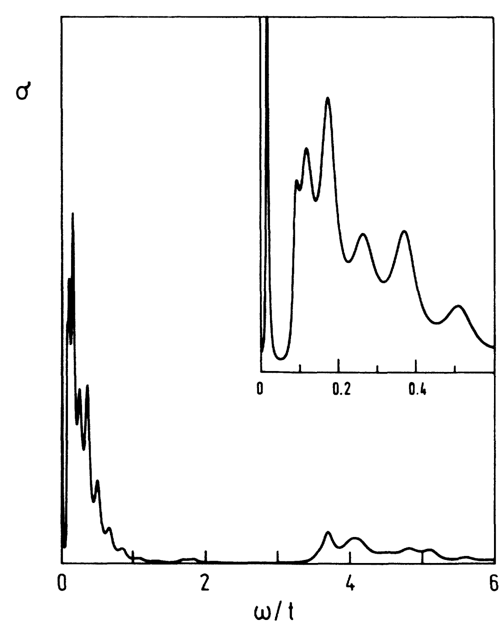

FIG. 4. Frequency-dependent conductivity $\sigma(\omega)$ vs ω for the Kondo-lattice model on a chain with $N=18$, $V/t=6.0$, $J/t=0.4$, and $\gamma=0$. In the inset the low-frequency part of the spectrum is shown where the quasiparticle peak is clearly seen.

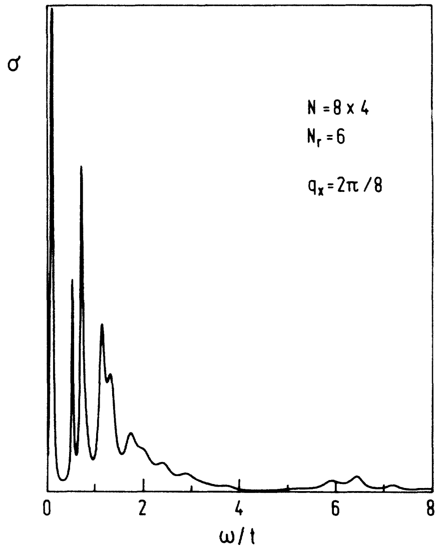

FIG. 5. $\sigma(\omega)$ vs ω in the Kondo-lattice model for an 8×4 cluster with $N_r=6$. Here $V/t=6.0, J/t=0.2$, and $\gamma=1$.

tail but here we would like to point to the common features shared by all of the spectra: (a) an undamped QP peak, whose position ω_{QP} should approach zero as $\mathbf{q}\rightarrow0$, and which is expected to broaden into a Drude peak only at finite temperatures, and (b) a broad and rather structured incoherent part clearly separated from the QP peak and extending in some cases to quite large ω.

In Fig. 4 $\sigma(\omega)$ is presented for the Kondo-lattice model on a chain of $N=18$ sites for $V/t=4.0$, $J/t=0.3$, and the anisotropic case $\gamma=0$. The ground state in this case is at $k_0=0$ (as for all other J at $\gamma=0$) and, according to the criterion mentioned at the end of Sec. II, the minimum nonzero $q=2\pi/18$ is sufficiently small to allow for the consideration of quite small $J\geq0.06$. The mass enhancement in this case is $\mu\approx6.0$. As the relative weight of the QP peak is $\propto 1/\mu$, it follows that the f-sum rule[18] is mainly exhausted by the two incoherent and rather broad peaks, having origin in the strong coupling of the hole with spin excitations. Also note that the second broad peak is centered around $\omega\sim V$ and can be attributed to excitations of the local singlet to the triplet state. It takes away approximately half of the spectral weight, i.e., of $\mathrm{Im}G(\omega)$ [not of $\sigma(\omega)$]. Well resolved is the lower edge of the incoherent part at $\omega_c\approx J/2$. This low-energy excitation is specific to the $1-d$ model and can be traced back to the hopping of a hole accompanied simultaneously by one AFM domain wall with an energy $\Delta\varepsilon=J/2$. Note also that the incoherent part shows a trend $\sigma(\omega)\propto1/\omega$ at $\omega<t$, as in fact obtained analytically for systems with relatively flat density of states and roughly constant current matrix elements.[15]

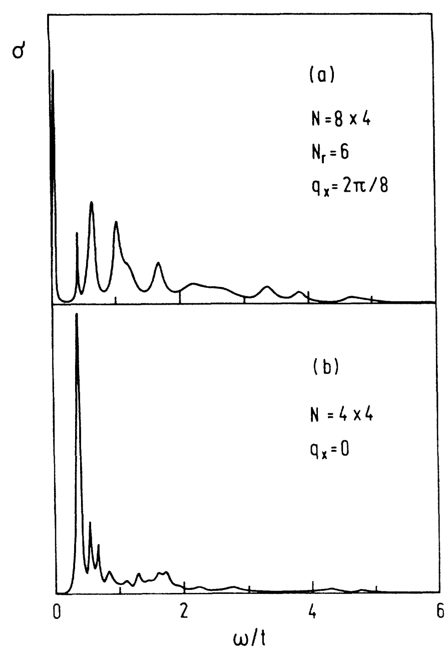

FIG. 6. $\sigma(\omega)$ vs ω in the t-J model in the isotropic case $J/t=0.2$, $\gamma=1$: (a) $N=8\times4$, $N_r=6$, and $\mathbf{q}=(2\pi/8,0)$; (b) exactly calculated $\sigma(\omega)$ for a 4×4 cluster at $\mathbf{q}=0$.

Typical plots of $\sigma(\omega)$ in $d=2$ for the $N=8\times4$ system are presented in Fig. 5, for the Kondo-lattice model with $V/t=6.0$, and in Fig. 6(a), for the t-J model. In both cases $J/t=0.2$, $\gamma=1$, and $N_r=6$. There is a great deal of similarity among the t-J and the Kondo-lattice spectra, apart from the position of the spikes, which for the t-J model are somewhat shifted towards lower ω. Thus in both examples presented, i.e., Fig. 5 (Kondo-lattice) and Fig. 6(a) (t-J model), the QP peak is well separated from the broad incoherent part of predominantly magnon character. Note that at finite J the lower magnon peaks are rather well pronounced, the lowest being at $\omega\sim2J$. This contrasts the smooth variation $\sigma\sim1/\omega$ expected for $J\rightarrow0$.[15] As before, the f-sum rule is mainly exhausted by the incoherent part. In the Kondo-lattice case there is a hint of a shallow and broad peak visible in Fig. 5 at $\omega\sim V$. Its weight is, unlike in the case of $d=1$, Fig. 4, almost negligible. The reason is that here we deal with the isotropic spin interaction and since the ground-state wave function has good spin $S=\frac{1}{2}$, the other band, centered around $\omega\sim V$ cannot carry away any significant part of the weight due to rather large V.

In Fig. 6(b) we show the corresponding $\sigma(\omega)$ for $\mathbf{q}=0$, calculated without approximations, i.e., with $N_r=N_c$, for $N=4\times4$. Clearly the QP peak is missing in the spectra. In spite of differences between details in the incoherent parts of spectra, the well pronounced onset ω_c is equal in both Figs. 6(a) and 6(b).

Before concluding one final remark should be made. Our continuation of the continued fraction expression for $G(z)$ [Eq. (4)] beyond $n=n_L$, as implied by the discussion in Sec. II, amounts to what is known as the constant-chain approximation. As a result, the spectral function $A(\omega)$ entering Eq. (3) is a superposition of contributions of poles resulting from the exactly treated part of $G(z)$ and the square-root-like $A_0(\omega)$ arising from the constant-chain part. Since the latter is zero below $\omega_c=-E_0+\alpha_\infty-2\beta_\infty$ (a branch point), it is reassuring to find that ω_c is always well above the QP peak and just slightly below the first pole contributing to the incoherent part of $\sigma(\omega)$ in the finite system considered here. Thus, the asymptotic values α_∞ and β_∞ through $A_0(\omega)$ mimic the continuous density of states coming from spin excitations of a much larger system.

V. CONCLUSIONS

In the paper we have discussed the properties of a single hole in an AFM, as determined by the *t-J* model and the Kondo-lattice model. In the $d=2$ system both models give several common features for the QP. Although the QP dispersion is not the same, the effective masses and the mass enhancement μ become comparable in both models, after assuming that the Kondo coupling is large, $V/t \gg 1$. The $\sigma(\omega)$ spectra are very similar, consisting of the undamped QP peak (of small intensity $\propto 1/\mu$) and the incoherent part at $\omega > \omega_c$, with an additional high ω structure in the Kondo-lattice model due to internal excitations of the singlet. In both models the incoherent part is not smooth but shows rather well-pronounced magnon resonances. There are also substantial differences. In the Kondo-lattice model the anisotropy γ is not playing such a role, since even in the extreme anisotropic case $\gamma=0$ the coherent mass is for $V/t \gg 1$ governed by a nonvanishing effective next neighbor hopping $\tilde{t} \propto t^2/V$, resulting in a finite μ. This gives the justification for the numerical study of the Ising case $\gamma=0$, which yields qualitatively similar results for μ and $\sigma(\omega)$, whereas the problems encountered in the diagonalization are drastically reduced. Namely, the number of basis states involved increases only slowly with the number of Lanczos steps, the convergence is better, etc. On the other hand our results confirm a well-established fact that in the *t-J* model the QP properties depend crucially on γ-μ in particular.

Our results for the conductivity are valid only for $T=0$. At $T>0$ the QP peak is expected to broaden into the low-frequency Drude with finite, but small width, as found also experimentally.[14] It should be noted that our results give a consistent intensity $\propto 1/\mu$ of this part. We expect also some smearing of the quite pronounced magnon structure in the incoherent part, which is in our calculation enhanced by finite size and finite N_r effects. Since the energy range remains large compared to characteristic kT, some features should persist in the spectra. Thus, a quasigap of the appropriate energy $\Delta\varepsilon=0.1$ eV is observed at low T in Y-Ba-Cu-O,[14] which roughly agrees with our result $\Delta\varepsilon=2J$. An absence of the structure above this energy can be, however, still a sign that either J is smaller as currently believed ($J \sim 0.1$ eV), or that additional degrees of freedom contribute to the formation of the quasiparticle.

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