PHYSICAL REVIEW B VOLUME 47, NUMBER 6 1 FEBRUARY 1993-II

Single-hole spectral density in an antiferromagnetic background

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(Received 7 August 1992)

The dynamical spectral function of a single hole moving in a two-dimensional antiferromagnet is calculated on clusters of up to 26 sites. Quasiparticle peaks in the spectral function show up unambiguously at the bottom of the continuum. In some limited region of **k** space vague structures in the spectral density might be reminiscent of excited string levels. Our data for the Z factor of the t-J model are in excellent agreement with the self-consistent Born approximation.

The discovery of superconductivity in copper-oxide-based materials by Bednorz and Müller[1] has initiated an enormous theoretical effort on strongly correlated fermions in two dimensions (2D). The interplay between strong correlations and low dimensionality is a fascinating issue. Nevertheless, it is still not clear whether a Fermi-liquid-like picture, with electron-like quasiparticles (QP), applies in this case. In particular, it has been suggested that the breakdown of the QP picture (which is well established in one dimension) might also take place in 2D.[2]

In this paper, we address the question of Fermi-liquid-like behavior in the case of a single hole moving in a classical (Néel) or quantum antiferromagnetic (AF) background. The single-hole spectral function and density of states are calculated by exactly diagonalizing small clusters of the t-J_z and t-J Hamiltonians by a Lanczos algorithm. Clusters of square geometry are chosen with $N = 16$, 18, 20, and 26 sites. This is the first attempt of finite size scaling of *dynamical* correlations for spin-fermion models.[3] It extends previous work of finite size scaling for the ground state (GS) energies of the Heisenberg[4] and the t-J models.[5]

In standard notations the Hamiltonian is

$$\mathcal{H} = J_z \sum_{\mathbf{i},\vec{\epsilon}} S^z_{\mathbf{i}} S^z_{\mathbf{i}+\vec{\epsilon}} + \tfrac{1}{2} J_\perp \sum_{\mathbf{i},\vec{\epsilon}} (S^+_{\mathbf{i}} S^-_{\mathbf{i}+\vec{\epsilon}} + S^-_{\mathbf{i}} S^+_{\mathbf{i}+\vec{\epsilon}}) - t \sum_{\mathbf{i},\vec{\epsilon},\sigma} (c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{i}+\vec{\epsilon},\sigma} + \text{H.c.}). \quad (1)$$

The sum over $\mathbf{i}, \vec{\epsilon}$ is restricted to nearest neighbor bonds along $\vec{x}$ and $\vec{y}$ on a 2D square lattice. We have explicitly separated the longitudinal (J_z) and transverse ($J_\perp$) antiferromagnetic couplings, and shall consider two important cases: (i) the Ising limit $J_\perp = 0$ (no quantum spin fluctuations) and (ii) the isotropic case $J_\perp = J_z$.

The existence of a coherent propagation of the single hole in the classical or quantum AF backgrounds is very controversial. Two scenarios have been proposed: (i) a conventional picture based on the Fermi liquid theory which basically assumes the QP nature of the low energy excitations, and (ii) a more exotic picture where, like in 1D, spin and charge are deconfined. While the self-consistent Born approximation[6] (SCBA) predicts QP peaks with a dispersion proportional to J, in a Luttinger liquid[2] or a "marginal" Fermi liquid,[2,7] on the other

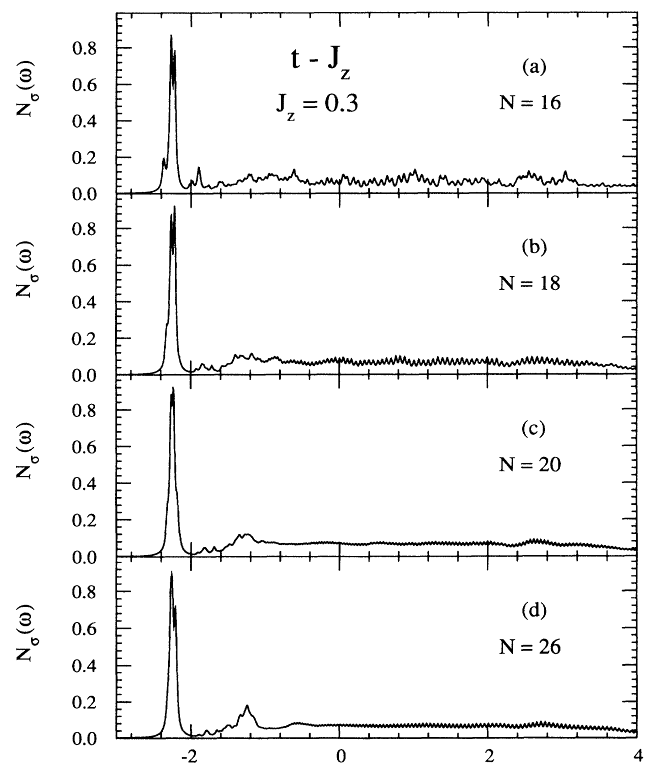


FIG. 1. Density of state of a single hole in the classical Néel state. Here and in Fig. 2, the spurious "fast oscillations" occurring at high energies are due to the finite number of Lanczos steps used. All energies are measured in units of t.

hand, there are overdamped QP excitations which have vanishing QP weight ($Z_{\mathbf{k}} = 0$) at low energies. Early numerical calculations of the single-hole spectral function on 16-site[8] and 20-site clusters[9] have given partial indications in favor of QP peaks which seem also to exist at finite hole density.[10,11] However, as will be seen below, for such small clusters finite-size effects are still rather large, and more conclusive results can be reached comparing clusters of different sizes.

The single-hole spectral function is defined by

$$A_{\mathbf{k},\sigma}(\omega) = \sum_m \mid \langle \Psi_{m,\sigma}^{N-1}(\mathbf{k}) \mid c_{\mathbf{k},\sigma} \mid \Psi_0^N \rangle \mid^2 \delta(\omega + E_0^N - E_m^{N-1}(\mathbf{k})). \tag{2}$$

Here $\mid \Psi_0^N \rangle$ is the GS at half-filling (N spins on N sites) which can be either, the classical Néel GS (Ising limit) or the quantum Heisenberg GS (isotropic case), and E_0^N is the corresponding energy. The set $\{\Psi_{m,\sigma}^{N-1}(\mathbf{k})\}$ is that of one hole eigenstates ($N-1$ spins), with corresponding energies $E_m^{N-1}(\mathbf{k})$. In the numerical results below a small $\epsilon = 0.02$ gives a small width to the δ functions. Note that, for symmetric $\mathbf{k}$ points in the Brillouin zone (BZ) like $\mathbf{k} = \mathbf{0}$, $\mathbf{Q}_0$, etc., due to selection rules the manifold $\{\Psi_{m,\sigma}^{N-1}(\mathbf{k})\}$ is in fact restricted to the most symmetric irreducible representation of the point group (like s wave). For $N \to \infty$, long range AF order implies a doubling of the unit cell and, in particular, $E_0^{N-1}(\mathbf{k} + \mathbf{Q_0}) = E_0^{N-1}(\mathbf{k})$ [$\mathbf{Q_0} = (\pi,\pi)$]. In the thermodynamic limit, while most of the δ functions lead to a continuum, a true δ peak persisting at the bottom of the spectrum will be the signature of a QP excitation. Its relative amplitude (that should remain finite when $N \to \infty$) is simply given by the matrix element of the hole operator between the lowest exact one-hole eigenstate ($m = 0$) and the initial half-filled GS,[12]

$$Z_{\mathbf{k}} = \sum_\sigma \mid \langle \Psi_{0,\sigma}^{N-1}(\mathbf{k}) \mid c_{\mathbf{k},\sigma} \mid \Psi_0^N \rangle \mid^2 . \tag{3}$$

Physically, $Z_{\mathbf{k}}$ corresponds to the relative spectral weight (between 0 and 1) located in the low energy peak. Alternatively, it can be seen as the discontinuity in the occupation number $n_{\mathbf{p},\alpha} = \langle \Psi_{0,\alpha}^{N-1}(\mathbf{k}) | \sum_\sigma c_{\mathbf{p},\sigma}^\dagger c_{\mathbf{p},\sigma} | \Psi_{0,\alpha}^{N-1}(\mathbf{k}) \rangle$ in the one-hole GS at $\mathbf{p} = \mathbf{k}$.[13] It should be noted that, increasing N from 16 to 26, the GS momentum $\mathbf{k}^*$ changes discontinuously although we expect the momentum of a hole in an antiferromagnet to be $(\pi/2, \pi/2)$. The 16-, 18-, 20-, and 26-site clusters have GS momenta $\mathbf{k}^*$ $(\pi/2, \pi/2)$, $(\pi, \pi/3)$, $(4\pi/5, 2\pi/5)$, and $(9\pi/13, 7\pi/13)$, respectively. Apart from the 16-site cluster the GS momenta are not located exactly on the Fermi surface (FS). On the other hand the largest 18-, 20-, and 26-site clusters no longer show extra hidden symmetry that could have biased the results of the 16-site cluster.

Since clusters of different sizes have different sets of discrete momenta it is convenient to define the single-hole density of state (per spin) as $N_\sigma(\omega) = \frac{1}{N} \sum_{\mathbf{k}} A_{\mathbf{k},\sigma}(\omega)$. Due to the sum over $\mathbf{k}$ the hole density is expected to have a weak size dependence. Note that it fulfills the sum rule $\sum_\sigma \int d\omega \, N_\sigma(\omega) = 1$.

The spectral densities (2) are calculated directly by a continued-fraction expansion (truncated after ~ 300 iterations) based on the Lanczos algorithm.[14] Handling the 26-site cluster (with 5.2 million configurations compared to only 6435 for $N = 16$) is a technically difficult step which requires ~ 6 Gbytes of disk space.

The hole density of states $N_\sigma(\omega)$ of the t-J_z model is shown in Fig. 1. First, we observe a QP band (see below) at the bottom of the spectrum whose amplitude increases slightly with system size. It is important to notice that this amplitude seems to *saturate* when the system size N reaches a characteristic size $N_c \sim 6\, J_z^{-2/3}$ which corresponds to the spatial extension of the hole wave function.[15] A similar scaling behavior was actually found for the GS energy.[5] Secondly, the hole density shows a large uniform incoherent background which decreases with increasing J_z. This can be attributed to the motion of the hole along retraceable paths[16] which preserve the initial Néel order. A third feature is of particular interest: a broad structure develops with increasing size and increasing J_z just above the QP band. It is tempting to associate this maximum with an excited state of the hole in a confining "string" potential, the existence of which was pointed out by Shraiman and Siggia[15] and investigated by numerical calculations.[17,5] Strictly speaking, one would then expect a series of discrete levels.[15,6] This picture is in fact not completely correct since there are special processes where the hole hops around the plaquette one and a half times.[18] This enables the hole to propagate coherently (along the diagonal of the plaquette) and gives a finite lifetime to the excited localized levels, in agreement with the broad feature at $\omega \approx -1.2$. It is interesting to notice that the GS energy shows roughly a $J_z^{2/3}$ behavior,[17,5] compatible with the string scenario.

Let us turn now to the isotropic case, i.e., $J_\perp = J_z$. Figure 2 shows the evolution of the spectral density with increasing system size. We observe first that the band at the bottom of the spectrum [located between the smallest arrows in Figs. 2(c) and 2(d)] is robust when N increases so that we can interpret it as a QP band as for $J_\perp = 0$. The largest arrow on Fig. 2 indicates a spurious peak in the continuum of the spectral function $A_{\mathbf{k},\sigma}$ for $\mathbf{k} = \mathbf{0}$ which broadens and eventually disappears for the 26-site cluster. We stress that a finite-size analysis is crucial here in order to be able to distinguish between genuine features of the spectral density and spurious finite size effects. Indeed, we observe that, in general, all sharp features (apart from the coherent band) existing for the smaller cluster evolve into a continuum with increasing N (e.g., the peaks located around $\omega \sim 2.2$ in Fig. 2). Since the spin-flip term $J_\perp$ allows a complete delocalization of the hole, the broad structures that might be reminiscent of string levels become (i) of very small amplitude (compared to the QP peak) and (ii) are only restricted to

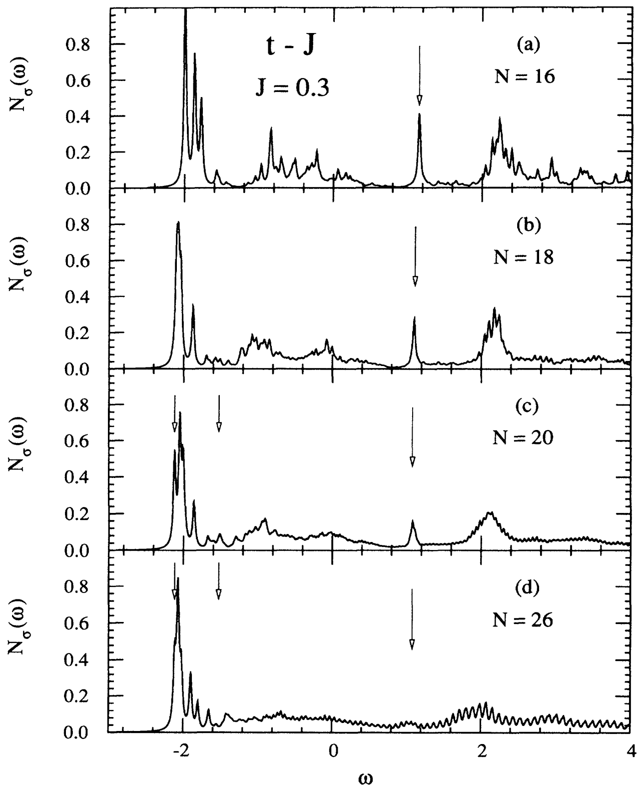


FIG. 2. Density of state of a single hole in the Heisenberg antiferromagnet.

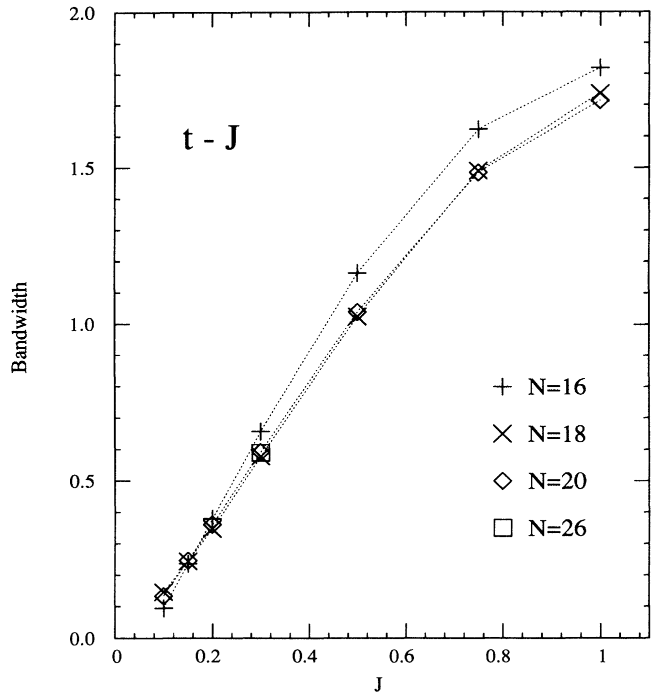


FIG. 3. Coherent bandwidth of the t-J model vs J for various sizes.

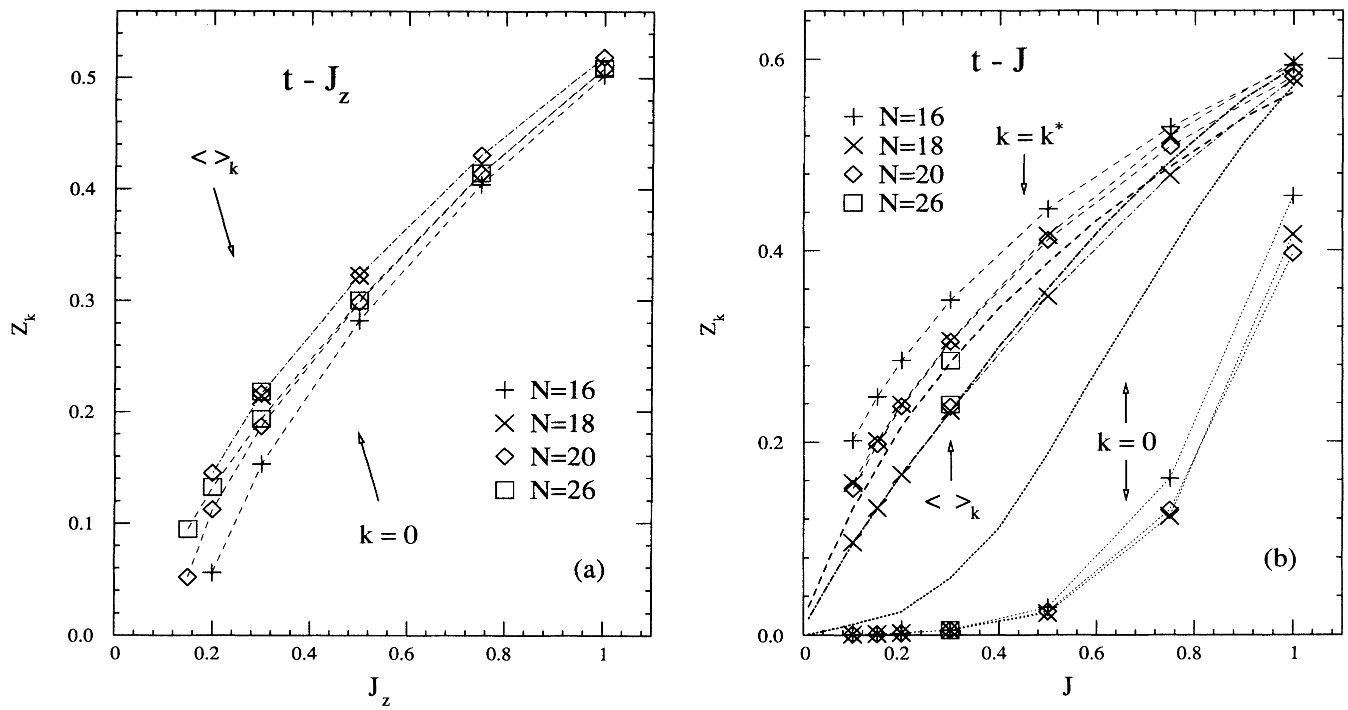
momenta close to $(\pi/2, \pi/2)$.

The bandwidth W is defined by the dispersion of the quasiparticle peaks. This definition only makes sense if $Z_{\mathbf{k}}$ is finite, as our results indicate it to be. The bandwidth versus J is shown in Fig. 3. The data for the largest systems confirm the linear behavior at small J first obtained by perturbative calculations[6] and in early numerical work.[8] An expression like $W \sim 2.275\, J + \alpha$, $\alpha \sim 0.093$, gives a good fit of the $N = 20$ data for $0.1 < J < 0.5$. The linear dependence of the bandwidth on J reflects the large quasiparticle mass enhancement (by a factor $\sim 4t/J$) due to the dressing of the hole propagator by spin fluctuations.

We now discuss the behavior of the QP weight $Z_{\mathbf{k}}$. Generally $Z_{\mathbf{k}}$ has a maximum at $\mathbf{k} \sim (\pi, 0)$ and minimum at $\mathbf{k} = \mathbf{0}$ although the bottom of the band is located at different $\mathbf{k}$ points for $J_\perp = 0$ ($\mathbf{k}^* = \mathbf{0}$ and $\mathbf{Q_0}$) or $J_\perp = J_z$ [$\mathbf{k}^* \sim (\pi/2, \pi/2)$]. Also we observe that weight is transferred from higher energies to the coherent band (i.e., $Z_{\mathbf{k}}$ increases) when J_z increases (independently of $J_\perp$) as shown in Figs. 4(a) and 4(b).

We define now the average weight over the BZ, $\langle Z_{\mathbf{k}} \rangle = \frac{1}{N} \sum_{\mathbf{k}} Z_{\mathbf{k}}$. This quantity is meaningful even in the thermodynamic limit but should not be considered as an approximation to the weight at the FS. This quantity is clearly not very sensitive to the change of grids of reciprocal vectors for increasing size and we expect a smooth behavior with size that allows a precise comparison with the existing theoretical fit.[6] The average weights together with the weights at the bottom of the coherent band versus $1/N$ are shown in Fig. 4(c). In the t-J_z model both $Z_{\mathbf{k=0}}$ and $\langle Z_{\mathbf{k}} \rangle$ versus $1/N$ exhibit very nice scaling behaviors (as for the GS energy[5]) with an inflection point at a characteristic size $N_c \sim 6\, J_z^{-2/3}$,[15] and the beginning of a saturation for $N > N_c$. Clearly, finite size corrections become smaller than (or at most of the order of) $\sim N^{-1}$ for $N >> 1$. The larger J_z, the smaller the size of the hole wave function, and the sooner convergence is found. We believe that the $N = 26$ data that we can fit (for $0.2 < J_z < 0.75$) according to $Z_{\mathbf{k=0}} \sim 0.545 J_z^{0.859}$ [Fig. 4(a)] give accurate estimations (and probably exact lower bounds since $Z_{\mathbf{k}}$ grows with size) of the weights in the thermodynamic limit, apparently down to $J_z = 0.3$. Note that $Z_{\mathbf{k}}$ of the t-J_z model increases when one goes up the band so that $\langle Z_{\mathbf{k}} \rangle < Z_{\mathbf{k=0}}$ [Fig. 4(a)] although the J dependence is very similar over the whole BZ. The scaling behavior of the Z factor of the t-J model [Fig. 4(c)] is not as smooth as for the Ising case since $Z_{\mathbf{k}}$ is no longer a monotonic function of the system size.[19] However, apart from the large change between $N = 16$ and $N = 18$ the data seem to be weakly size dependent for $N \geq 18$.

Our data agree well with the numerical solution[20] of the integral equation for the self-energy within SCBA,[6] as is shown in Fig. 4(b). Indeed, SCBA predicts many features found in our numerical work: (i) the same behavior of $Z_{\mathbf{k}}$ with momentum $\mathbf{k}$ and (ii) the same behavior of the form $a\, J^\nu$ at small J for the relative QP weight $Z_{\mathbf{k}}$. In particular, at the bottom of the band $\mathbf{k} = \mathbf{k}^*$,



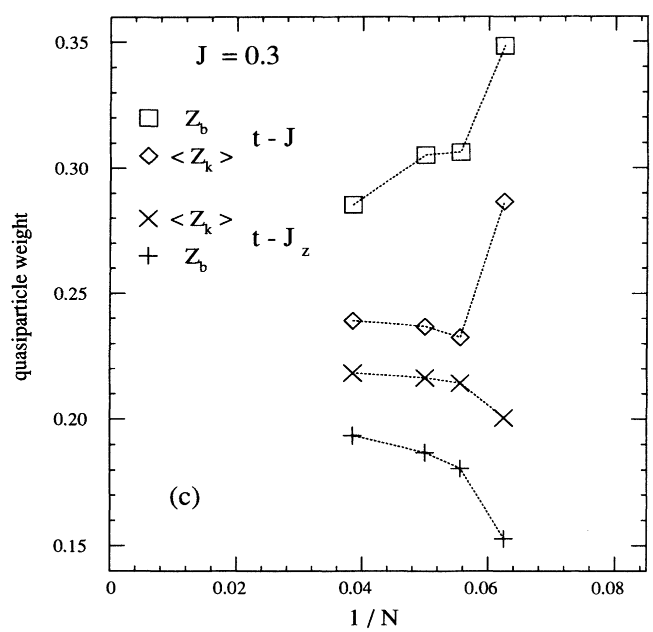


FIG. 4. (a) Quasiparticle weights $Z_{\mathbf{k}}(J)$ at the bottom ($\mathbf{k} = \mathbf{0}$, dashed lines) of the band or averaged over the BZ ($\langle\rangle_{\mathbf{k}}$, dot-dashed lines), as indicated by the arrows, for the t-J_z model. (b) Quasiparticle weights $Z_{\mathbf{k}}(J)$ at the top ($\mathbf{k} = \mathbf{k}^*$, dotted lines) and bottom ($\mathbf{k} = \mathbf{0}$, dashed lines) of the band or averaged over the BZ ($\langle\rangle_{\mathbf{k}}$, dot-dashed lines), as indicated by the arrows, for the t-J model. The symbols corresponding to each size are as indicated in the figure. In each case, thin lines connect the numerical points as a guide to the eye. The thicker lines (dotted, dashed, and dot-dashed) correspond to the self-consistent Born approximation (data taken from Ref. 20) for each case ($\mathbf{k} = \mathbf{k}^*$, $\mathbf{k} = \mathbf{0}$, and $\langle\rangle_{\mathbf{k}}$). (c) $Z_{\mathbf{k}}$ vs $1/N$ in the t-J and t-J_z models.

our fit of the 20-site cluster data [Fig. 4(b)], $a \sim 0.622$ and $\nu \sim 0.598$ is in good agreement with $a \sim 0.63$ and $\nu \sim 0.667$ in the Born approximation.[20] The agreement is even better [see Fig. 4(b)] for the average over the BZ. Also in agreement is the special role played by the center of the zone $\mathbf{k} = \mathbf{0}$ for which $\nu > 2$ (i.e., $Z_{\mathbf{k}}$ vanishes more rapidly with vanishing J at this $\mathbf{k}$ point). Nevertheless, the magnitude of $Z_{\mathbf{k}=\mathbf{0}}$ obtained in the numerical calculation is almost 5 to 10 times smaller as seen in Fig. 4(b).

In a recent paper Sorella[13] reported that quantum Monte Carlo (QMC) data for the Hubbard model suggest that $Z_{\mathbf{k}^*} \rightarrow 0$ when $N \rightarrow \infty$ in disagreement with the present work. We note that Sorella did not really calculate $Z_{\mathbf{k}}$ directly but rather an upper bound of $Z_{\mathbf{k}}$ in a slightly *spin polarized* state. Hence it may well be that the scaling behavior of this quantity with size is not at all characteristic of the scaling behavior of $Z_{\mathbf{k}}$ itself. Also systematic errors in Sorella's extrapolation procedure are likely to be rather large.

Clearly the single-hole problem (vanishing hole concentration for $N \rightarrow \infty$) is a very special case, and the present work does not directly apply to the high-T_c copper oxides[1] at *finite* hole density. Furthermore, it is well established that doping easily destroys the AF order. Exact diagonalizations of the t-J model have indeed shown that for 10% doping the hole pockets at $(\pm\pi/2, \pm\pi/2)$ are already lost.[11] We also note that the peculiar feature $Z_{\mathbf{k}} << 1$ at the top of the band for small J and vanishing hole doping is probably unrelated to any possible breakdown of Fermi liquid behavior, as it occurs at rather high excitation energy.

In conclusion, we have reported here exact cluster calculations of the single-hole spectral density in Ising and Heisenberg antiferromagnets. Special emphasis was put on the finite size scaling behaviors of the spectra, QP weights, etc. In general, a reasonably good convergence is achieved in the largest cluster (26 sites) which gives credibility to exact diagonalization studies. The finite-size analysis is necessary to systematically distinguish between genuine features of the model (like QP peaks) and spurious peaks. Quasiparticle behaviors are found in t-J_z and t-J models. This agrees with a recent spin-wave calculation.[21] Structures that might have to do with string levels are shown to be almost completely wiped out by hole delocalization processes except for large exchange J or J_z *and* for momenta close to the band minimum.

The numerical calculations were done on the CRAY-2 of Centre de Calcul Vectoriel pour la Recherche (CCVR), Palaiseau, France. Support from CCVR is greatly appreciated. Laboratoire de Physique des Solides and Laboratoire de Physique Quantique are laboratoires associés au CNRS.

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