Quasiparticle Dispersion of the 2D Hubbard Model: From an Insulator to a Metal

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On the basis of quantum Monte Carlo results the evolution of the spectral weight $A(\mathbf{k}, \omega)$ of the two-dimensional Hubbard model is studied from insulating to metallic behavior. As observed in recent photoemission experiments for cuprates, the electronic excitations display essentially doping-independent features; a quasiparticlelike dispersive narrow band of width of the order of the exchange interaction J and a broad valence- and conduction-band background. The continuous evolution is traced back to one and the same many-body origin: the doping-dependent antiferromagnetic spin-spin correlation.

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Recent results of angle resolved photoemission spectroscopy (ARPES) [1] revealed strong similarities in the low-energy excitations of a prototype insulating copper oxide, i.e., $Sr_2CuO_2Cl_2$ [2], and metallic cuprates like Bi 2212, Bi 2201, etc.: In both cases the quasiparticle (QP) band has rather small dispersion of typically 1 eV width, it is separated from a broad main valence-band "background" (of about 6 eV width) in much the same way; the $\mathbf{k}$ dispersion is similar and also the intensity modulation as a function of energy is comparable. Thus it appears that the dispersive metallic band evolves continuously from the insulating limit and has a similar physical origin as the undoped valence band in the cuprates. This has important consequences for the copper oxides: The excitation spectrum in the insulating case is decisively determined by many-body effects, documented by the known difficulties of one-electron band-structure calculations for the insulating limit [1], which then strongly suggests a many-body origin of the QP dispersion also in the metallic case.

In this work quantum Monte Carlo (QMC) results for the angular resolved photoemission spectral weight $A(\mathbf{k}, \omega)$ for the two-dimensional (2D) Hubbard model are reported which demonstrate for this "generic" model the above strong similarities between undoped insulating and doped metallic situations: In particular, we find in both cases a very similar small dispersive low-energy band, for which the bandwidth is set by the exchange interaction $J \sim 4t^2/U$ when the Coulomb correlation U is of order of the noninteracting bandwidth $8t$. This new feature is shown in the metallic case to be essentially unrenormalized (for electronically filled, i.e., $\omega < \mu$ states) from the insulating band, while above the chemical potential μ additional states with again an energy scale set by J are filled in. $A(\mathbf{k}, \omega)$ is inferred from the QMC data by applying Bayesian probability theory in the framework of "quantified maximum entropy" [3,4]. A consistent treatment of hyperparameters and error covariances along with high-quality QMC data allows us to reveal details of the low-lying excitations which have not been seen before in QMC simulations. On the basis of these QMC results and the strong similarities to ARPES data in both insulators and metals, we argue that the continuous evolution of the QP dispersion relation observed in the high-T_c cuprates arises from a common many-body origin, namely, from the continuous change of the spin-spin correlation length ξ and the related changes in the hole-spin correlations [5]. Similarities to a phenomenology by Kampf and Schrieffer [6], where the magnetic correlation length ξ is an input parameter, are pointed out.

Our results confirm, but also extend, QMC simulation results by Bulut and co-workers [7–9]: As stated in this previous work the available resolution was such that when $\mathbf{k}$ moved below the Fermi surface only the $6t$ to $8t$ broad lower Hubbard band (LHB) could be resolved for both the insulating [7] and metallic [8] cases. However, it was already suspected there that a narrow QP band exists, since such a band of width J has been found for one hole doped in an antiferromagnetic (AF) insulating t-J model [10,11]. Narrow QP bands were also observed for finite dopings in exact-diagonalization calculations of the one-band Hubbard [12–15] and t-J [16] models, as well as in QMC results for the three-band Hubbard model [17].

The single-band 2D Hubbard model has the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{H.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

on a square lattice, where t is the near-neighbor hopping, $c_{i,\sigma}$ destroys an electron of spin σ on site i, and $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$. The chemical potential μ sets the filling $\langle n \rangle = \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle$. Here we focus on results obtained for both half filling $\langle n \rangle = 1$ and other fillings in order to develop a systematic picture of the low-lying electronic excitations as a function of doping. Two different Coulomb

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correlation values were chosen: $U = 8t$ (which is equal to the bandwidth) and $U = 12t$.

In order to obtain from the QMC data for the single-particle finite-temperature propagator $G(\mathbf{k}, \tau)$ the corresponding spectral weight $A(\mathbf{k}, \omega)$ for real frequencies ω, the following Laplace transform has to be inverted:

$$G(\mathbf{k}, \tau) = -\int_{-\infty}^{\infty} A(\mathbf{k}, \omega) \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} d\omega . \quad (2)$$

It is by now well established [18–22] that the maximum-entropy method [3,4] provides a controlled way to infer the most reliable $A(\mathbf{k}, \omega)$ in light of the QMC data. The results presented in this Letter are based on QMC data with good statistics; i.e., averages over 10^5 updates of all the Hubbard-Stratanovich variables result in $G(\mathbf{k}, \tau)$'s with statistical error less than 0.5%. The quality of our QMC data, as far as mean and variance are concerned, is comparable to those data analyzed in earlier publications for the 2D Hubbard model [7–9]. There, however, the correlation of the errors of the imaginary-time data, measured by the covariance matrix, has been neglected. However, to achieve the desired resolution, it is important to use a likelihood function which takes the error-covariance matrix [18,23] of the QMC data and its statistical inaccuracy consistently into account [24]. As suggested in previous work by White [19], various moments of the spectral weight were also incorporated in extracting $A(\mathbf{k}, \omega)$. In order to check on this analytical-continuation procedure, detailed comparisons with 4×4 exact diagonalizations [13–15] have been performed.

The results presented here are for lattices 8×8 in size and for temperatures ranging from $\beta t = 3$ ($T = 0.33t$) to $\beta t = 10$ ($T = 0.1t$). Covering this temperature range allows us, in effect, to study (at half filling) a situation where the spin-spin correlation length ξ is larger (for $\beta t = 10$) than the lattice size. In this case the system behaves as if it were at $T = 0$ and develops an AF gap. For $\beta t = 3$, on the other hand, the spin-spin correlation length is shorter than our finite lattice and, consequently, the gap is diminished and metallic fluctuations exist [20]. As we will see, the latter situation is especially useful in interpreting the QMC data in the metallic (doped) regime and relating them to those of the insulating (half-filled) case.

We start in Fig. 1 by examining the single-particle spectral weight for $U = 8t$, $\beta t = 10$, at half filling, i.e., $\langle n \rangle = 1$. Figure 1(a) gives a 3D plot of $A(\mathbf{k}, \omega)$ vs ω for $\mathbf{k}$ values out of the Brillouin zone, whereas Fig. 1(b) summarizes these results in the usual "band structure" ω vs $\mathbf{k}$ plot. Here dark (white) areas correspond to a large (small) spectral weight.

We observe in all spectra (also in the $U = 12t$, half-filled case, presented in Fig. 3 two general features: One is that $A(\mathbf{k}, \omega)$ contains a rather dispersionless "incoherent background," extending for both electronically occupied ($\omega < \mu$) states and unoccupied ($\omega > \mu$) states over $\sim 6t$ (~ 6 eV) in the $U = 8t$ case. The new structure, which

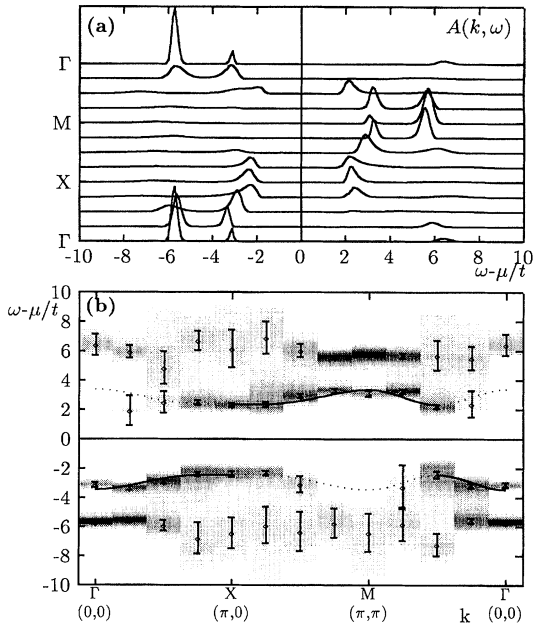

FIG. 1. Single-particle excitation for the 8×8 Hubbard model at half filling, $U = 8t$, $\beta t = 10$: (a) The single-particle spectral weight $A(\mathbf{k}, \omega)$ vs ω and $\mathbf{k}$; (b) ω vs $\mathbf{k}$ "band structure," where sizable structure in $A(\mathbf{k}, \omega)$ is represented by strongly shaded areas and peaks by error bars.

was not previously resolved in QMC work, is a dispersing structure at low energies with a small width of the order of J, which defines the gap Δ and which (at least for $U = 12t$) is well separated from the higher-energy background.

The splitting in the low-energy "band" and the higher-energy background is especially pronounced near Γ (for $\omega < \mu$) and M (for $\omega > \mu$) points due to a relative weight shift from negative to positive energies as $\mathbf{k}$ moves through X or equally through $(\pi/2, \pi/2)$, the midpoint between Γ and M. The overall weight distribution in $A(\mathbf{k}, \omega)$ follows roughly the spin density wave (SDW) prediction as found in the QMC calculation by Bulut, Scalapino, and White [7]: The total integrated weight in the SDW approximation, $\langle n_{\mathbf{k}}^{\mathrm{SDW}} \rangle = \int_{-\infty}^{0} A^{\mathrm{SDW}}(\mathbf{k}, \omega) d\omega$, is in good accord with the QMC momentum distribution [7].

However, the dispersion of the structure near the gap does not follow the SDW prediction: Its dispersion has a significant (about a factor of 2 for $U = 8t$) smaller width set by the value of J. This result is in good accord with the dispersion and width found for the low-energy "foot" in recent ARPES data [2] and t-J model results (there $t \approx 0.4$ eV) [10]. This is illustrated in Fig. 1(b), where the low-energy peaks in $A(\mathbf{k}, \omega)$ are fitted by (full and dotted lines) $E_{\mathbf{k}} = \Delta + J/2(\cos k_x + \cos k_y)^2$, with $\Delta = 2.4t$, rather than by the SDW (strong-coupling) result, i.e., $E_{\mathbf{k}} = \sqrt{\epsilon_k^2 + \Delta^2} \cong \Delta + J(\cos k_x + \cos k_y)^2$. The overall agreement between the ARPES width and the Hubbard model data (for $t \approx 1$ eV) is significant because it shows, in fact, that the energy scale of the low-

lying insulating band is controlled by many-body effects beyond the mean-field SDW result.

Our findings for the spectral-weight dispersion $\omega(\mathbf{k})$ are schematically summarized in Fig. 2(a), which emphasizes again the different energy scales (J, U, SDW [25]) involved. These energy scales become particularly pronounced in the $U = 12t$ case in Fig. 3.

Before moving to the doped situation, we note that the $\beta t = 3$, $U = 12t$ result in Fig. 3 does have the valence-band maximum at the M point and not at the X or $(\pi/2, \pi/2)$ points, in contrast to the $\beta t = 10$ results for both $U = 8t$ and $U = 12t$ (not shown). This at first puzzling "high-temperature" result reflects the fact that at $\beta t = 3$ the spin-spin correlation length ξ is about a factor of 2.5 smaller than the QMC lattice extension. The system then shows precursor effects of a metal, which move the spectral weight (valence-band) maximum—in agreement with the metallic situation in Fig. 4—to the M point. Otherwise, the low-energy band is found to be essentially unaffected by changing temperature from $T = 0.1t$ to $T = 0.33t$.

Keeping this in mind, we consider in Fig. 4 the low-energy electronic structure in the metallic regime for doping $\langle n \rangle = 0.95$. Figure 4(a) shows again the 3D plot of $A(\mathbf{k}, \omega)$ and 4(b) the dispersion relation with the degree of shading representing the intensity of $A(\mathbf{k}, \omega)$, as in Fig. 1(b). As in the half-filled case, we observe two general features, which are both seen in recent photoemission experiments [1]: an incoherent background of $\approx 4t - 6t$ and a pronounced low-energy foot of significantly smaller width, which is clearly resolved between $\Gamma \rightarrow X$ and $\Gamma \rightarrow$

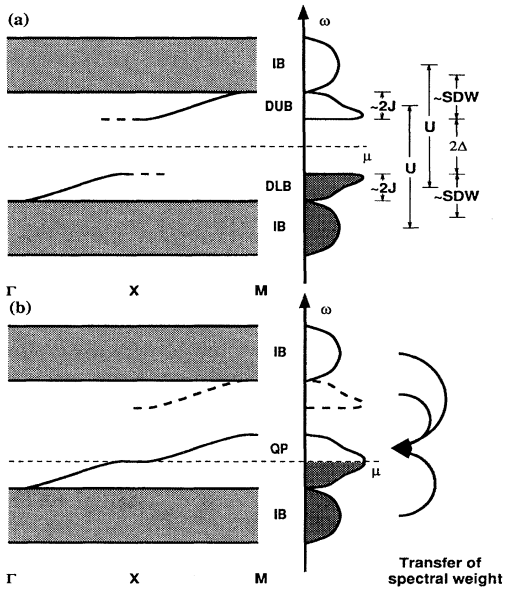

FIG. 2. Schematic plot of the band structure: (a) the insulator and the different energy scales (see text) involved; (b) for the metallic situation. Terminology: "DUB" ("DLB") dispersive upper (lower) band, "IB" incoherent background, "QP" quasiparticle band.

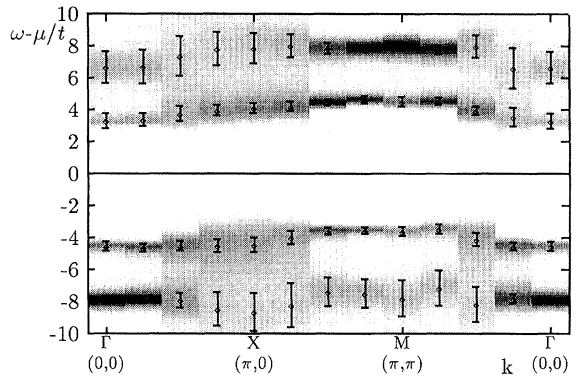

FIG. 3. Single "band structure" ω vs $\mathbf{k}$ for $U = 12t$, $\beta t = 3$. Again strongly shaded areas correspond to maxima of $A(\mathbf{k}, \omega)$.

$(\pi/2, \pi/2)$. The situation is depicted schematically in Fig. 2(b). The width and dispersion of the low-energy band are also in good accord with exact diagonalization results of 4×4 clusters [13,15].

The results for the doped case have several important implications: First, they reveal that the lowest-energy band in the insulator and the band that crosses the chemical potential $\omega = \mu$ in the hole-doped metal are rather similar: The low-energy band is separated from the broad valence-band background ("IB" in Fig. 2) in the same way; it has similar dispersion and it has a similar intensity modulation as a function of energy. Thus the lowest-energy metallic band appears to be effected by similar many-body physics as in the insulating regime,

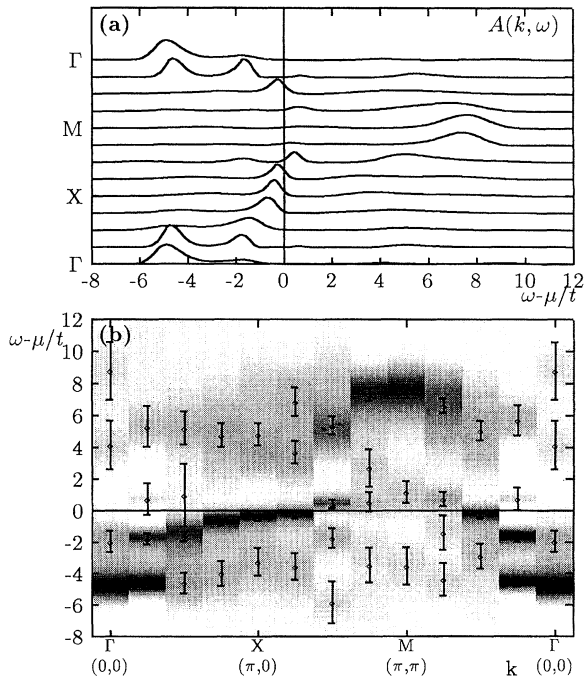

FIG. 4. The same as Fig. 1, but now for doping $\langle n \rangle = 0.95$ and $\beta t = 3$, $U = 8t$: (a) $A(\mathbf{k}, \omega)$; (b) ω vs $\mathbf{k}$ "band structure."

namely, magnetic correlations connected with the (now) short-range AF order. This is not in contradiction but instead substantiated by the fact that the metallic band develops its maximum at the M point: As pointed out above, this happens as soon as the spin-spin correlation length ξ is smaller than the length ($L = 8$), a situation obtained for the filling $\langle n \rangle = 0.95$.

Furthermore, our QMC data display similarities to results derived by Kampf and Schrieffer [6]. There a phenomenological model for the spin susceptibility was used to extract the leading-order contribution to the self-energy from AF fluctuations. The spin-spin correlation length ξ was an input parameter to the model, and by varying this correlation length the model evolved continuously from the insulating AF to the Fermi-liquid regime. For decreasing correlation length, weight was transferred into the QP peak from incoherent backgrounds, which (for ξ large) developed into the upper and lower Hubbard bands [analogously to the spectral weight transfer from our upper and lower structures IB into the QP band, see Fig. 2(b)].

Another noteworthy feature of the doped, metallic situation is that the intensity change (but not the width) as a function of $\mathbf{k}$ for the higher-energy background in $A(\mathbf{k}, \omega)$ still follows essentially the AF SDW picture with, in particular, "shadow bands" resulting from the AF short-range order being clearly visible at Γ ($\omega - \mu \sim -5t$) and M ($\omega - \mu \sim +7t$) points. Even remnants can be detected of folded back shadow bands near the M point for $\omega < \mu$, which in the SDW picture have much less oscillator strength and spectral intensity than the original band (between $\Gamma \rightarrow X$) [26]. Finally, we would like to mention that an important detail of the QMC data, the rather extended flatness of the energy band near the $X(\pi, 0)$ point, which is in good agreement with the ARPES experiments of Dessau and co-workers [1] for Bi 2212, has previously been resolved in QMC work for both the one-band [8] and three-band [17,27] Hubbard models. This rather extended flatness, extending like the ARPES data not only into $X \rightarrow \Gamma$, but also into the $X \rightarrow M$ regions (as displayed in Fig. 3), is already inherent in the undoped low-energy structure near X, a fact which has recently also been found in 2D t-J model studies by Dagotto, Nazarenko, and Boninsegni [10]. Its extension, in particular, into $X \rightarrow M$ direction, is not consistent with available one-electron band calculations [1]. It can be explained by a conventional self-energy diagrammatic analysis summing over the leading spin-fluctuation diagrams [27]. It is thus a many-body effect related to magnetic correlations consistent with the arguments given in this work.

In summary, we have studied the evolution of the 2D Hubbard model from insulator to metal in terms of the electronic spectral weight, obtained from the maximum-entropy analytic continuation of QMC data. These results, combined with recent ARPES data, can be taken as strong indications that the QP dispersion of the high-T_c compounds, not only in the insulating limit but—particularly—in the metallic situation, has a many-body origin: the coupling of the quasiparticles to antiferromagnetic correlations.

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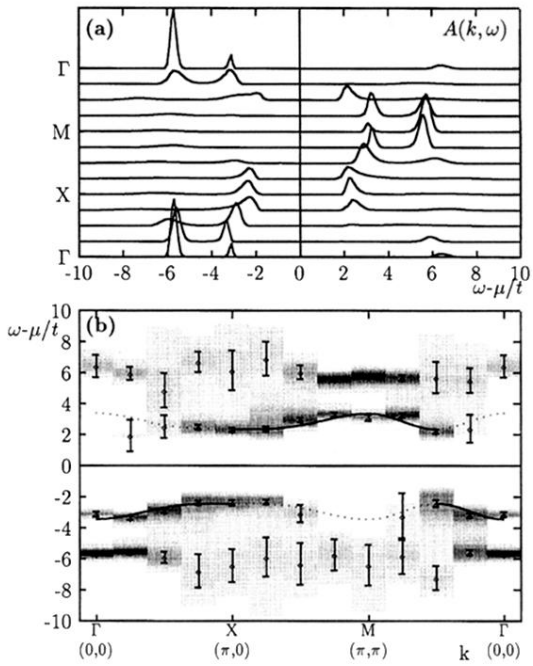
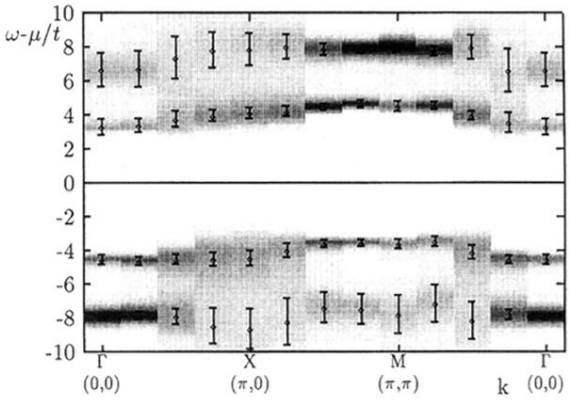


FIG. 1. Single-particle excitation for the 8×8 Hubbard model at half filling, $U = 8t$, $\beta t = 10$: (a) The single-particle spectral weight $A(\mathbf{k}, \omega)$ vs ω and $\mathbf{k}$; (b) ω vs $\mathbf{k}$ "band structure," where sizable structure in $A(\mathbf{k}, \omega)$ is represented by strongly shaded areas and peaks by error bars.



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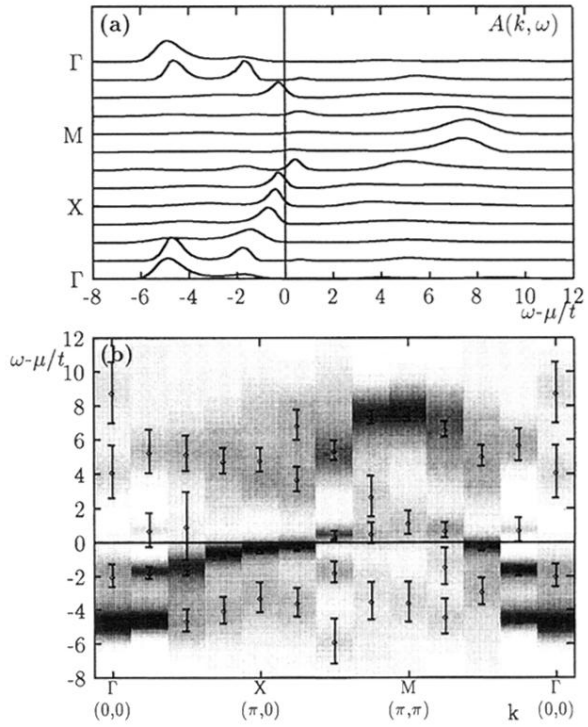

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