Thermodynamics of the planar Hubbard model

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The thermodynamic properties of specific heat, entropy, chemical potential, spin susceptibility χ_s, and charge susceptibility χ_c are studied as functions of temperature and doping within the two-dimensional Hubbard model with various $U/t=4-12$. Quantities are calculated using the finite-temperature Lanczos method with additional phase averaging for a system of 4×4 sites. Results show that the entropy at low T reaches a maximum near half-filling at the electron density $n\sim1\pm0.15$ in the whole regime of studied U/t. The pseudogap in $\chi_s(T)$ becomes clearly pronounced for $U/t\geqslant8$ while χ_c shows a maximum close to half-filling. The relation of results to those within the t-J model and to experiments is discussed.

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I. INTRODUCTION

The Hubbard model is the simplest prototype Hamiltonian for correlated electrons. It has been and still remains the subject of numerous theoretical investigations in connection with the metal-insulator transition,[1] the interplay between the magnetism and the itinerant character of electrons, and possible superconductivity emerging solely from the electronic mechanism. Particular attention has been devoted to the two-dimensional (2D) model on a square lattice, expected to capture the physics of superconducting cuprates. A lot of effort has been put into numerical studies of the ground state properties, using various quantum Monte Carlo (QMC) methods.[2]

On the other hand, there are rather few studies of the 2D Hubbard model at finite $T>0$, in particular away but close to half-filling, i.e., at electron densities $n\neq1$. In the latter regime the minus-sign problem prevents the application of the QMC method at low T in large systems.[2] Gross features of the specific heat $C_V(T)$ have been obtained via the internal energy $E(T)$ using the QMC method.[3] Results reveal the evidence of at least two energy scales at large $U/t\gg1$, the larger one representing the upper Hubbard band. The behavior at low T shows a marked difference between an insulator at half-filling $n=1$ (where more reliable results and methods became recently available[4,5]) with $C_V(T)\propto T^2$, and an anomalous metal at finite hole doping $n_h=1-n>0$ (or analogous electron doping). Within the metallic regime the QMC method was so far not able to reach temperatures below the exchange scale $J\sim4t^2/U$, which sets up an characteristic energy of spin dynamics and is thus essential for establishing the low-T physics at low doping. The uniform spin susceptibility $\chi_s(T)$ has also been calculated[6] using the QMC method, apparently with some unphysical results at $n\neq1$ due to large restrictions. It should be also noted that certain features, e.g., the maximum in $\chi_s(T)$ and two scales in $C_V(T)$, are not specific for the 2D Hubbard model, but are present in the 1D model[7] as well.

On the other hand, low-T properties of the Hubbard model with $U\gg t$ are believed to map well on the properties of the t-J model which is projected on the basis space without doubly occupied sites. Several static and dynamic properties of the planar t-J model were recently calculated and followed well into the regime $T<J$ using the finite temperature Lanczos method (FTLM).[8,9,13,14] Relevant for the present study is the result that the normal-state entropy density $s(T<J)$ (Ref. 10) is maximum at the ''optimum'' hole doping $n_h\sim n_h^*$, where $n_h^*\sim0.15$ at $J/t=0.3$. Also, a pseudogap temperature $T^*(n_h)$, experimentally (among alternatives), defined with the maximum in the uniform spin susceptibility $\chi_s(T)$,[1,13,14] also showed up in the t-J model, where $T^*(n_h)$ decreases with doping and vanishes at the optimum one, again at $n_h\sim n_h^*$.

Our aim is to obtain thermodynamic results within the planar Hubbard model, which is numerically (for an exact diagonalization approach) more demanding relative to the t-J model. We list some relevant questions which we address in the following: (a) Are there any qualitative differences between the thermodynamic properties of the planar t-J model and the Hubbard model at large U/t? (b) How does the entropy optimum doping shift with decreasing U/t, (c) is there a pseudogap scale also at smaller U/t.

We investigate the Hubbard model given by

$$H=-t\sum_{\langle ij\rangle s}(c_{is}^{\dagger}c_{js}+\text{H.c.})+U\sum_i n_{i\uparrow}n_{i\downarrow}, \qquad (1)$$

where $c_{is}^{\dagger}(c_{is})$ and n_{is} are creation (annihilation) and number operators for electrons, respectively, and the sum $\langle ij\rangle$ runs over pairs of nearest-neighbor sites. We limit our calculations to $U/t=4$, 8, and 12, where values range from the modest $U<W$, smaller than the bandwidth $W=8t$, to the strong correlation regime $U>W$. Note that the latter case is usually associated with the physics of cuprates where the spin exchange is $J\sim4t^2/U\sim0.3\ t$.

II. METHOD

We study numerically the Hubbard model on a square lattice using the FTLM,[8,9] based on the Lanczos procedure of exact diagonalization and a random sampling over initial wave functions. The advantage in the case of thermodynamic quantities is that they can be expressed solely in terms of a

grand-canonical average of conserved quantities ($k_B=1$), i.e.,

$$\langle f\rangle = \mathrm{Tr}\, f(N_e,S_z,H)e^{-(H-\mu N_e)/T}/\mathrm{Tr}\, e^{-(H-\mu N_e)/T}, \quad (2)$$

where N_e, S_z, and μ refer to the number of electrons, the z component of the total spin and the chemical potential, respectively. In the case of quantities as in Eq. (2), the FTLM does not require the storage of Lanczos eigenfunctions, but only of Lanczos eigenenergies ϵ_j^n, where $j=0,\ldots,M$ (M represents the number of Lanczos steps) while $n=1,\ldots,R$ runs over random initial Lanczos wave functions. For details of the method we refer to Refs. 9 and 10. Using the FTLM in the above way we are able to investigate the model on the lattice of $N=4\times4=16$ sites with periodic boundary conditions.

The main limitation to the validity of results comes from finite-size effects. The latter can be substantially reduced by employing the boundary condition (flux) averaging.[12] In a system with periodic boundary conditions the latter is achieved by introducing the uniform vector potential $\vec{\theta}$ modifying the hopping elements $t\rightarrow\tilde{t}_{ij}=t\exp(i\vec{\theta}\cdot\vec{r}_{ij})$. We use, further on, N_t uniformly spaced phases $\vec{\theta}$ instead of a fixed $\theta=0$. In this way results are essentially improved at smaller $U<W$. This is particularly evident for noninteracting electrons with $U=0$, where results on small lattices otherwise reveal pronounced finite-size effects. In this case, using $N_t \gg 1$ most properties discussed here become exact even on a finite-size lattice. In the strong-correlation regime results are less sensitive to phase averaging, most evident at half-filling $n=1$ where the Hubbard model maps on the Heisenberg model in which $\vec{\theta}$ becomes irrelevant.

Still the main restriction in the thermodynamic validity of our results comes from finite-size effects which show up at $T<T_{fs}$ where they start to dominate results. As a criterion for T_{fs} we use the thermodynamic sum

$$\overline{Z}(T)=\mathrm{Tr}\exp[-(H-E_0)/T], \quad (3)$$

calculated in a given system at fixed particle number N_e and the requirement $\overline{Z}(T_{fs})=Z^*\gg1$.[9] In the following we use $Z^*\sim30$. In the particular parameter space $U/t=4$–12, the optimum cases are at $n\sim1\pm n_h^*$ with $n_h^*\sim0.15$ (coinciding with largest entropy $s=s_{max}$) where $T_{fs}/t\sim0.1-0.15$. On the other hand, T_{fs} increases toward $n=1$ and even more for $n\rightarrow0,2$, respectively.[9] Since the properties of the Hubbard model [Eq. (1)] on a bipartite lattice are symmetric around half-filling we present results only for the hole-doped regime $n_h=1-n\geqslant0$.

III. ENTROPY AND SPECIFIC HEAT

Within the FTLM and using Eq. (2) we first evaluate the electron density $n=\langle N_e\rangle/N$ and the entropy density s, expressed as

$$s=\ln\Omega/N+(\langle H\rangle-\mu\langle N_e\rangle)/NT, \quad (4)$$

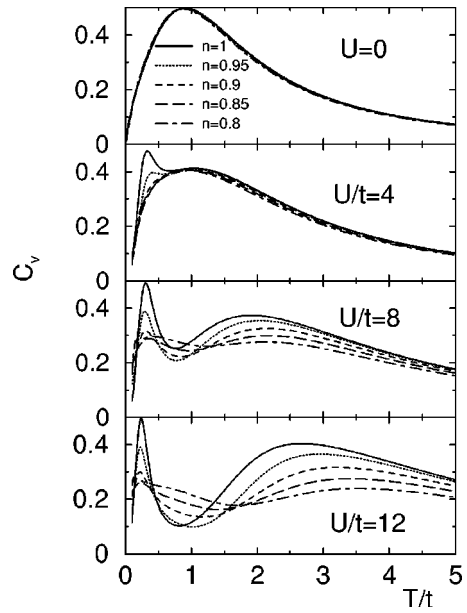

FIG. 1. Specific heat C_V (per unit cell) vs T for various electron densities n near half-filling and different U/t. The $U=0$ result is calculated for an infinite lattice.

both as functions of μ and T. From s we also evaluate the specific heat $C_V=T(\partial s/\partial T)_\mu$. Both s and C_V can be consequently presented as well as in terms of n and T.

Let us first discuss FTLM results for an overall behavior of the specific heat $C_V(T)$ (per unit cell), as shown in Fig. 1 for $U/t=0-12$ in the whole relevant T regime. At *zero doping*, e.g., $n=1$, our results agree with recent QMC calculations,[4] where both methods correctly predict the low- and the high-temperature peak positions seen in $C_V(T)$ and even scaling of those peaks with U. At zero doping the QMC method has an obvious advantage in comparison to the FTLM, since it allows calculations of larger system sizes. On the other hand, the calculation of $C_V(T)$ is less straightforward using the QMC method since it requires calculating finite differences on a finite set of $E(T)$ or performing various fits.

At *finite doping* and high $T>t$ our FTLM results in general agree with those obtained previously with the QMC method.[3] The advantage of the FTLM is that we reach lower $T\sim T_{fs}\sim0.1\ t$, well below the exchange scale $J\sim4t^2/U$. The main message of Fig. 1 is that C_V at finite doping, similarly as at zero doping, reveals the existence of (at least) two energy scales which are well separated for $U>W$, i.e., for $U=12\ t$. Although QMC results[3] were also interpreted in terms of two scales, we should notice that the claimed peak positions at finite doping differ substantially from our result.

The upper maximum is related to excitations within the upper Hubbard band and is well pronounced near half-filling. For a larger doping, i.e., for $n<0.85$, these excitations merge with the lower Hubbard band. At lower $U=4\ t$, the upper maximum is only weakly present even at $n=1$, and disappears at the smallest available doping $n\sim0.95$. Note also that at $U=4\ t$, apart from $n=1$, C_V merges even quantitatively with the noninteracting resultat $U=0$. Here we should point out that properties at $U=0$ in Figs. 1, 2, 4, and 7 are calcu-

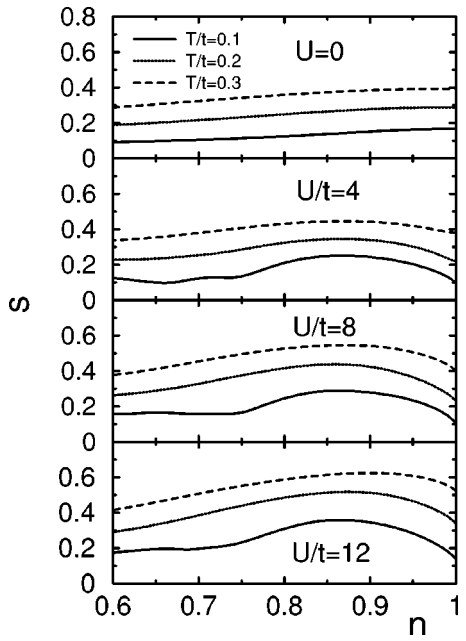

FIG. 2. Entropy density s vs electron density n for low $T/t=0.1$–0.3 and different U/t.

lated for an infinite lattice. When discussing the relation of presented results to those within the t-J model one should take into account that the upper scale (corresponding to the upper Hubbard band) is projected out in the latter; consequently results for C_V typically differ for $T>t$.[10]

In the following we focus on the lower energy scale which is essential for the understanding of quasiparticle and low-T properties. In Fig. 2 we show entropy density s as a function of electron density n for different $U/t=0$–12 and for lowest $T/t=0.1$–0.3. The first observation is that $U>0$ leads to an increase of s, which is largest at an intermediate doping $n=n^*\sim 0.85$. As expected, results for $U=12\,t$ are even quantitatively close to the ones within the t-J model[9,10] with the corresponding $J=0.3t$, where the maximum s has also been observed at $n_h^*=1-n^*\sim 0.15$, and such a doping has been identified as an optimum one.

We should note that such a characterization of ''optimality'' does not seem to be in conflict with the usual one related to highest T_c since experimentally in several cuprates the maximum in T_c and in the entropy[15] appear to be quite close in doping. Plausibly, n^* can be related to the most frustrated case where the kinetic energy of holes (''preferring'' an ferromagnetic ordering) and the effective spin exchange (favoring antiferromagnetism) are competing and therefore one could expect $1-n^*\propto J/t$. Moreover, it is evident from Fig. 2 that the optimal doping $n^*\sim 0.85$ is quite insensitive to U in a broad range $U/t=4-12$.

The position of the entropy maximum n^* is shown in Fig. 3 as a function of T. While it is evident that $n^*=1$ for $U=0$ as well as for $T\gg(t,U)$, it is quite interesting to observe that $n^*(T)$ is quite universal in the regime $4\leqslant U/t\leqslant 12$. That is, it first increases with T quite independent of U. However, for $T>0.5\,t$ and stronger correlations $U\geqslant 8t$ $n^*(T)$ decreases tending towards the $U=\infty$ case where $n^*=2/3$ (as within the t-J model) until finite U becomes irrelevant for large T.

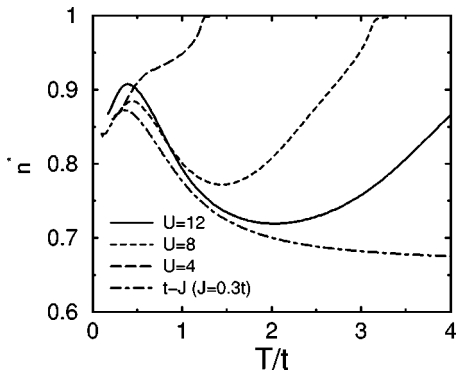

FIG. 3. The density n^* corresponding to maximum s vs T. Results for the t-J model are also shown.

IV. SPIN AND CHARGE SUSCEPTIBILITY

In an analogous way we can evaluate within the FTLM also the the uniform spin susceptibility $\chi_s=\langle(S_z)^2\rangle/NT$, which can also expressed solely in terms of conserved quantitites. In Fig. 4 we present results for $\chi_s(T)$ for various dopings close to half-filling $n=0.8$–1.0 and $U/t=0$–12. We first note that here the phase-averaging method brings about a substantial improvement. This is evident by comparing Fig. 4 with QMC results on the same 4×4 lattice[6] obtained at a fixed phase $\theta=0$, where some unphysical features are evident at $n\neq 1$.

As expected, the onset of $U>0$ leads to an increase of $\chi_s(T)$ at lower $T<t$. It is, however, more interesting to follow the development of pseudogap features with increasing U/t. One of the experimental definitions of the (large)

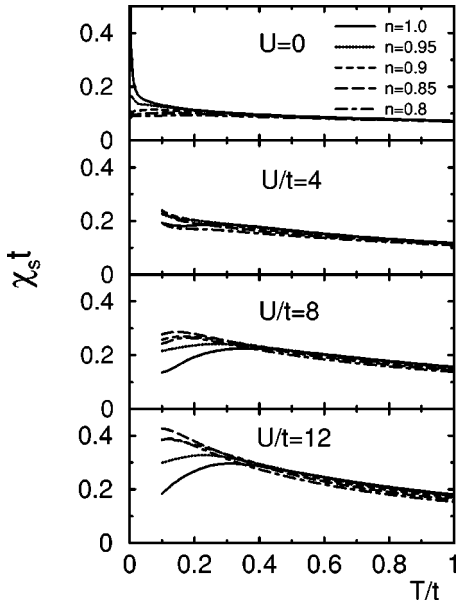

FIG. 4. Spin susceptibility $\chi_s t$ vs T for $n=0.8$-1.0 and different U/t.

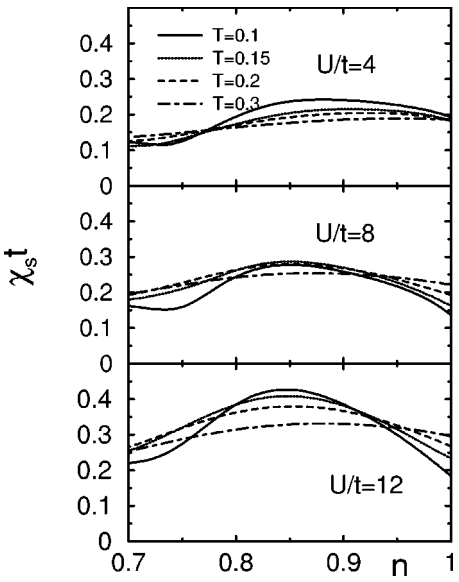

FIG. 5. Spin susceptibility $\chi_s t$ vs n for $T=0.1$–0.3 and different U/t.

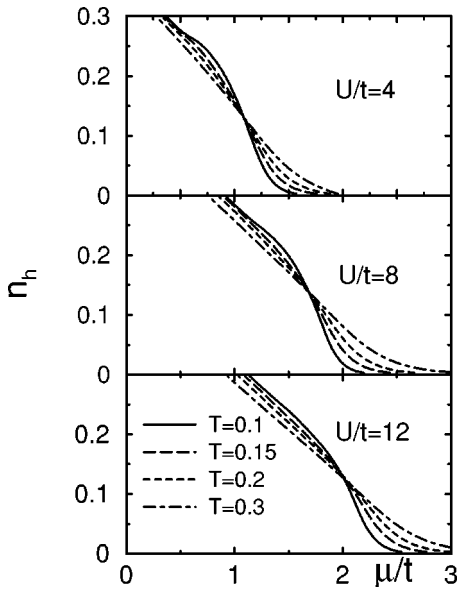

FIG. 6. Hole density n_h vs μ/t for $T/t=0.1$–0.3 and different U/t.

pseudogap temperature is related to the maximum $\chi_s(T=T^*)$.[13] In fact, T^* defined in this way matches well with other experimentally established crossovers.[1,14] It has been found[9,10] that $T^*(n)$ determined in this way within the t-J model matches experiments well. As foreseen from the mapping to the t-J model with $J=0.3\ t$, in Fig. 4 we find essentially the same behavior for the Hubbard model with $U/t=12$. On the other hand, the pseudogap maximum becomes shallower for $U/t=8$, although the location $T^*(n)$ does not shift substantially. The pseudogap features disappear at $U/t=4$.

Analogous is the message in Fig. 5, where we present χ_s as a function of n. At all presented U/t the maximum χ_s appears at an optimum doping $n\sim n^*$. However, this feature is well pronounced only at larger $U/t=8$ and 12, while at $U/t=4$ the maximum is barely visible. The decrease toward half-filling at $U/t=8$ and 12 is a characteristic signature of a strong correlation leading to antiferromagnetic ordering, and has been been observed both in QMC calculations[6] and in experiments on cuprates.[13]

Let us further discuss results for the density $n(\mu,T)$. In Fig. 6 we present the hole density n_h as a function of μ for various T, in order to allow a direct comparison with analogous results for the t-J model[9,10] as well as with experimental results on $La_{2-x}Sr_xCuO_4$.[16] We note that for $n_h>n_h^*=1-n^*$ the dependence $n_h(\mu)$ (apart from a uniform shift) is quite independent of T and U/t. This is consistent with a weaker role of correlations and a rather well defined effective single-electron density of states at the Fermi level $\mathcal{N}_F=dn/d\mu$. The much steeper dependence in the ''underdoped'' regime $n_h<n_h^*$ at low T is a clear manifestation of strong correlations and of the increasing effective $\mathcal{N}_F^c$ on approaching metal-insulator transition. In fact, it has been claimed on the basis of the $T=0$ QMC results[1] that within the Hubbard model $\mathcal{N}_F^c$ diverges approaching half-filling and $T\sim 0$ where $n_h\propto(\mu_0-\mu)^{1/2}$. The latter is qualitatively consistent with the flattening of the chemical potential as a function of doping $\mu(n\to 1)$ in $La_{2-x}Sr_xCuO_4$ observed via the angle-resolved photoemission spectroscopy measurements.[16] Nevertheless, at given lowest $T\sim T_{fs}$ we cannot distinguish a scenario with an enhanced but finite $\mathcal{N}_F^c$ at $T=0$ which would emerge from a picture with holes as well defined quasiparticles in an ordered antiferromagnet[2] from a divergent behavior.[1]

Finally, in Fig. 7 we present results for the related charge susceptibility $\chi_c=dn/d\mu$. For noninteracting electrons at $U=0$, χ_c is essentially T independent (except very close to $n=1$ due to the van Hove singularity), and is given by $\chi_c=\mathcal{N}_F$. Well away from half-filling, i.e., in the ''overdoped''

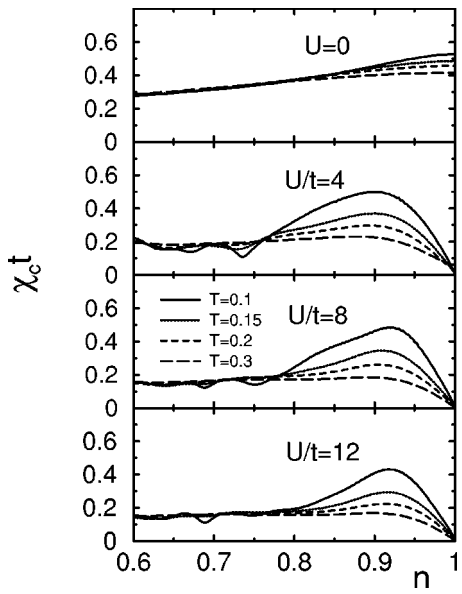

FIG. 7. Charge susceptibility $\chi_c t$ vs n for $T/t=0.1$–0.3 and different U/t.

regime $n<0.8$, the effect of $U>0$ is only quantitative to reduce χ_c. The reduction can be attributed to an overall decrease of the effective $\mathcal{N}_F^c$ due to the transfer of states into the upper Hubbard band. We also note in Fig. 7 that at the same time $U>0$ leads to an even flatter variation of $\chi_c(n)$.

More interesting is the development within the ''underdoped'' regime $n>n^*$, with a pronounced T and doping dependence. Very close to half-filling $n\sim 1$ and for $T>T_{fs}$, we are dealing with chemical potential μ within the charge (Mott-Hubbard) gap. A small density of charge carriers $n_h \ll 1$ in this regime behaves as in a doped nondegenerate semiconductor, (as established within the t-J model at low doping[11]), where

$$n_h \sim P\mathrm{e}^{-(\mu-\epsilon_v)/T}. \tag{5}$$

Consequently, we get $\chi_c \sim n_h/T$. Such a behavior is evident in Fig. 7, quite universally for all $U>0$, and its validity extends at lowest T up to $n_h \sim 0.1$. A large increase in the maximum χ_c at low T, again being rather insensitive to U/t, is again a clear manifestation of strong correlations and of the increasing effective density of states $\mathcal{N}_F^c$ on approaching the metal-insulator transition.

V. CONCLUSIONS

Let us summarize some essential conclusions of the present study of thermodynamic properties of the planar Hubbard model.

(a) As expected, results at large $U/t \geqslant 12$ match, even quantitatively, those of the corresponding t-J model (with $J \sim 4t^2/U$)[9,10] in the low temperature $T<t$ window. Excitations into the upper Hubbard band contribute significantly only at $T>t$. On the other hand, for smaller $U \leqslant 8\ t$ both scales start to merge, and become inseparable for $n \neq 1$.

(b) In the whole span $4 \leqslant U/t \leqslant 12$ our results reveal a coherent picture of low-T properties of the planar Hubbard model. That is, an effective exchange scale $\tilde{J}$ seems to determine both the optimal doping for the entropy $s(n^*)=\max$ with $1-n^* \propto \tilde{J}/t$ as well as the pseudogap scale $T^*(n) \sim \tilde{J}$ in $\chi_s(T)$. It is clear that only at large U we get $\tilde{J} \sim J \sim 4t^2/U$. On the other hand, even for $U<12\ t$ we see that n^* and T^* are quite insensitive to U/t, indicating a quite constant effective $\tilde{J} \lesssim 0.3\ t$ and consequently also $n^* \sim 0.85$. This can be understood in terms of the less localized character of spin degrees, which leads to a reduction of $\tilde{J}$ relative to $J \sim 4t^2/U$ appropriate for $U \gg t$.

(c) The pseudogap feature in $\chi_s(T)$ is very visible at $U=12\ t$. Whereas T^* does not shift much with U/t, the pseudogap intensity is strongly dependent on U/t. That is, the effect is only weakly pronounced at $U/t=8$ and disappears for smaller U/t. This is consistent with the interpretation that the (large) pseudogap T^* is related to an onset of short-range antiferromagnetic correlations, which are only weakly pronounced for $U \lesssim W$ and away from half-filling.

(d) Previous studies of thermodynamic quantities within the t-J model[9] have shown that results (at $J/t=0.3$) are even quantitatively in agreement with the experimental ones in hole-doped cuprates, in particular the doping dependence of the entropy s,[15] the spin susceptibility χ_s,[13] and the chemical potential μ.[16] We have shown that thermodynamic properties of the Hubbard model do not change significantly in a broader range of $U \gtrsim W$, i.e., there is a quantitative similarity of $s(T)$, n^*, $T^*(n)$, etc., so the agreement with experiments also seems to persist in a broader range of U/t.

ACKNOWLEDGMENTS

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