International Journal of Modern Physics B
Vol. 17, Nos. 18, 19 & 20 (2003) 3377–3380

World Scientific
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THERMODYNAMICS OF THE PLANAR HUBBARD MODEL

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Received 23 June 2003

The thermodynamic properties: specific heat and entropy are studied as a function 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 $n \sim 1 \pm 0.15$ in the whole regime of studied U/t.

Keywords: Hubbard model; thermodynamic properties.

The Hubbard model, a prototype Hamiltonian for correlated electrons, remains the subject of numerous theoretical investigations connecting magnetism, the itinerant character of electrons, and superconductivity, possibly emerging solely from the electronic mechanism.[1]

There are rather few studies of the 2D Hubbard model at finite temperature, $T > 0$, and away from the half filling, where the minus-sign problem complicates the application of the QMC method at low T.[2] The studies that do exist obtained the specific heat $C_V(T)$ via the internal energy $E(T)$ using the QMC.[3] Results reveal the evidence of at least two energy scales at large $U/t \gg 1$, 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 also more reliable results and methods are recently available)[4,5] with $C_V(T) \propto T^2$, and an anomalous metal at finite hole doping $n_h = 1 - n > 0$.

Low-T properties of the Hubbard model with $U \gg t$ are believed to map well on the properties of the t–J model. The finite temperature Lanczos method (FTLM)[6,7] was used recently to calculate several static and dynamic properties of the planar t–J model well into the regime $T < J$. Jaklič and Prelovšek demonstrated that the normal-state entropy density $s(T < J)$[8] is maximum at the 'optimum' hole doping $n_h \sim n_h^*$ where $n_h^* \sim 0.15$ at $J/t = 0.3$, a result relevant to the recent study.

Our aim is to obtain thermodynamic results within the planar Hubbard model, which is numerically more demanding than the t–J model.

The Hubbard model is given by

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

where $c^{\dagger}_{is}(c_{is})$ and n_{is} are electron creation (annihilation) and number operators respectively, and the sum $\langle ij \rangle$ runs over pairs of nearest-neighbor sites. We limit our calculations to $U/t = 4, 8, 12$, 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 $J \sim 4t^2/U \sim 0.3\ t$.

Using the FTLM,[6,7,9] based on the Lanczos procedure of exact diagonalization and a random sampling over initial wavefunctions, we study the Hubbard model on a 4×4 lattice. The main limitation to the validity of results comes from finite-size effects, which we reduced by employing boundary condition (flux) averaging.[9,10] In a system with periodic boundary conditions the averaging is achieved by introducing the uniform vector potential $\boldsymbol{\theta}$, modifying the hopping elements

$$t \to \tilde{t}_{ij} = t \exp(i\boldsymbol{\theta} \cdot \mathbf{r}_{ij}) \,.$$

This improves results at smaller $U < W$, which is particularly evident for noninteracting electrons with $U = 0$. Otherwise, results on small lattices reveal pronounced finite-size effects. Using phase averaging techniques most properties discussed here become exact even on finite-size lattices.

Within FTLM, we first evaluate the entropy density s, expressed as

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

as a function of μ and T. Knowing s we evaluate the specific heat, $C_V = T(\partial s/\partial T)_{\mu}$. Both s and C_V can also be expressed in terms of n and T.

Figure 1(a) shows FTLM results for an overall behavior of the specific heat $C_V(T)$ (per unit cell). Our calculations were performed over the range of relevant temperatures T, for $U/t = 0 - 12$. At *zero doping*, e.g. $n = 1$, our results agree with recent QMC calculations.[4] In this case both methods correctly predict the position of the low- and high-temperature peaks in $C_V(T)$ and the scaling of these peaks with U.

At *finite doping* and high temperatures, $T > t$, our FTLM results generally agree with those obtained previously using the QMC method.[3] The advantage of FTLM is that we reach lower temperatures well below the exchange scale $J \sim 4t^2/U$, $T \sim T_{fs} \sim 0.1\ t$. Based on C_V, as shown in Fig. 1(a), we find the existence of at least two well separated energy scales, when $U > W$, i.e. for $U = 12\ t$, for both finite and zero doping. Although QMC results[3] were also interpreted in terms of two scales, we note that the claimed peak positions at finite doping differ substantially from our result.

Excitations within the upper Hubbard band produce the upper maximum which is well pronounced near half-filling. For a larger doping, i.e. for $n < 0.85$, these

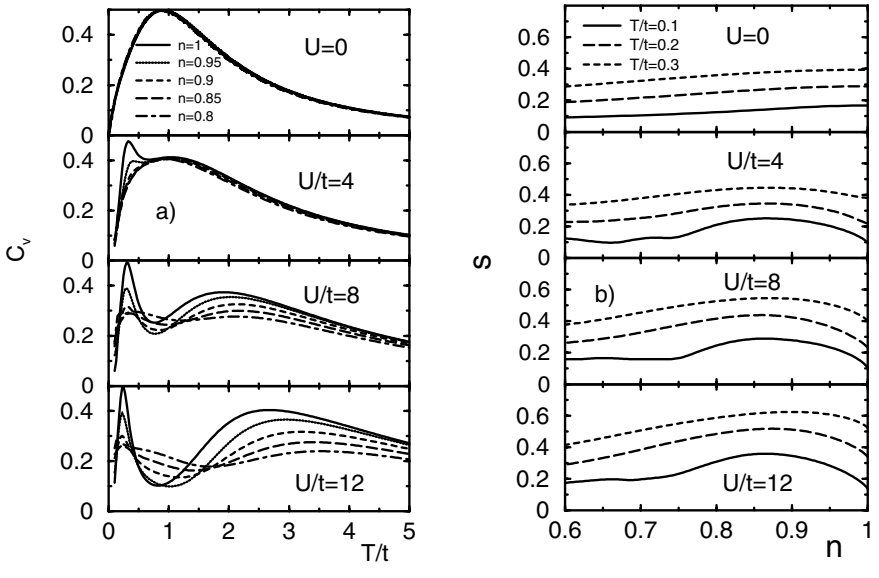

Fig. 1. (a) Specific heat C_V (per unit cell) versus T for various electron densities n near half-filling and different U/t; (b) Entropy density s versus electron density n for low $T/t = 0.1 - 0.3$ and different U/t. $U = 0$ results are calculated for an infinite lattice.

excitations merge with the lower Hubbard band. At lower $U = 4\ t$, the upper maximum is only weakly present even at $n = 1$, and it disappears at smallest available doping, $n \sim 0.95$. Also note that at $U = 4\ t$, except for $n = 1$, C_V merges quantitatively with the noninteracting result at $U = 0$. Here, we need to point out that properties at $U = 0$, in Fig. 1, are calculated for an infinite lattice.

In Fig. 1(b) we show entropy density s as a function of electron density n for values of U/t between zero and 12 and for lowest $T/t = 0.1 - 0.3$. Our 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 we expected, results for $U = 12\ t$ are quantitatively close to predictions of the t–J model,[7,8,9] with $J = 0.3\ t$. In these calculations the maximum s is also observed at $n_h^* = 1 - n^* \sim 0.15$ and this doping has been identified as 'optimum'.

We should point out that our characterization of 'optimality' is not in conflict with the classic definition related to highest T_c because others observed experimentally that in several cuprates the maximum in T_c and in the entropy[11] are 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. In this case we expect $1 - n^* \propto J/t$. Moreover, Fig. 1(b) shows that the 'optimal' doping $n^* \sim 0.85$ is quite insensitive to U over a broad range of U/t between 4 and 12.

Our thermodynamic study of the plannar Hubbard model leads to the conclusions that:

(a) As expected, results at large $U/t \geq 12$ match quantitatively predictions from the corresponding t–J model (with $J \sim 4t^2/U$)[7,8,9] in the low temperature, $T < t$, window. Excitations into the upper Hubbard band contribute significantly only when $T > t$. On the other hand, for smaller $U \leq 8\ t$ both scales start to merge, and become inseparable for $n \neq 1$.

(b) Over the complete range $4 \leq U/t \leq 12$, our results reveal a coherent picture of the low-T properties of the planar Hubbard model. Namely, an effective exchange scale $\tilde{J}$ apparently determines the 'optimal' doping for the entropy, $s(n^*) = \max$ with $1 - n^* \propto \tilde{J}/t$. It is clear that we get $\tilde{J} \sim J \sim 4t^2/U$ only at large U. On the other hand, n^* is quite insensitive to U/t, even for $U < 12\ t$, indicating a nearly constant effective $\tilde{J} \lesssim 0.3\ t$ and consequently $n^* \sim 0.85$. This can be understood in terms of the electron's spin degrees, that deviate slightly from the localized state. This in turn leads to an reduction of $\tilde{J}$ relative to $J \sim 4t^2/U$, which is appropriate for $U \gg t$.

(c) Previous studies of the thermodynamic quantities appearing within the t–J model (at $J/t = 0.3$)[7] have shown that they are in quantitative in agreement with the experimental measurements on hole-doped cuprates. In particular, the calculated doping dependence of the entropy s,[11] the spin susceptibility, and the chemical potential[9] (not discussed in this work) match experimental results. We have shown that thermodynamic properties of the Hubbard model do not change significantly over the broad range of $U \gtrsim W$. This is most prominently reflected in a quantitative similarity of $s(T)$, so the agreement with experiments also seems to persist over a broader range of U/t.

Acknowledgments

Authors acknowledge the support of the Ministry of Education, Science and Sport of Slovenia.

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