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MAGNETIC PROPERTIES OF THE 2D t–t′–HUBBARD MODEL

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The two-dimensional (2D) t-t'-Hubbard model is studied within the slave-boson (SB) theory. At half-filling, a paramagnetic to antiferromagnetic phase transition of first order at a finite critical interaction strength $U_c(t'/t)$ is found. The dependences on U/t and t'/t of the sublattice magnetization and of the local magnetic moment are calculated. Our results reasonably agree with recent (Projector) Quantum Monte Carlo data. The SB ground-state phase diagram reveals a t'-induced electron-hole asymmetry, and, depending on the ratio t'/t, the antiferromagnetic or ferromagnetic phases are stable down to $U = 0$ at a critical hole doping.

The magnetic behaviour of strongly correlated itinerant electron systems, in particular of high-T_c cuprates, is frequently described on the basis of the one-band Hubbard model with nearest (t) and next-nearest neighbour hopping (t') [1-5]. In this work we explore the ground-state properties of the 2D t-t'-Hubbard model which can be expressed in the four-field SB representation [6] as

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} z_{i\sigma}^{\dagger} z_{j\sigma} f_{i\sigma}^{\dagger} f_{j\sigma} + U \sum_{i} d_i^{\dagger} d_i \, . \qquad (1)$$

Neglecting charge-density-wave states, in the two-sublattice (AB) saddle-point approximation, the free energy per site is given by

$$\begin{aligned} f(n,T) &= Ud^2 - \sum_{\eta=\pm} \lambda_\eta^{(2)}(p_\eta^2 + d^2) + \mu n \\ &\quad + \frac{2}{\beta N} \sum_{\vec{k}\nu=\pm} \ln\left[1 - f(E_{\vec{k}\nu} - \mu)\right] \qquad (2) \end{aligned}$$

with the quasiparticle tight-binding bands

$$\begin{aligned} E_{\vec{k}\nu} &= \tfrac{1}{2}\sum_{\eta}\left[\lambda_\eta^{(2)} + \tfrac{1}{2} q_\eta (\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-(\pi,\pi)})\right] \\ &\quad + \nu\sqrt{A^2 + \tfrac{1}{4} q_+ q_- (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-(\pi,\pi)})^2} \, , \qquad (3) \end{aligned}$$

where the $\vec{k}$–sum runs over the magnetic Brillouin zone, the $\lambda_\eta^{(2)}$ ensure the SB constraints, $A = \frac{1}{2}\sum_\eta \eta[\lambda_\eta^{(2)} + \frac{1}{2} q_\eta (\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}-(\pi,\pi)})]$, $q_\eta = |z_\eta|^2$, and $\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$.

At half-filling and $t' \neq 0$, we obtain a paramagnetic (PM)⇌antiferromagnetic (AFM) phase transition of first order at the critical interaction strength $U_c(t'/t)$ (see Fig. 1) which is accompanied by the opening of the indirect gap in the SB band structure (3) shown in Fig. 2. At $t'/t = -0.2$ we get $U_c/t = 2.63$ which reprodu-

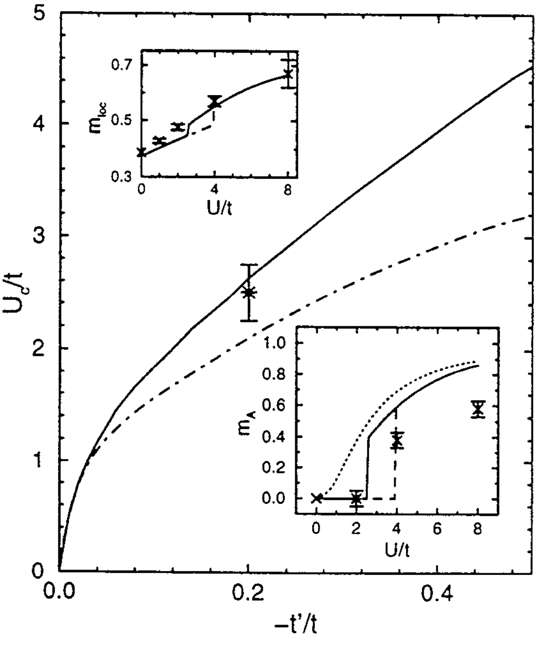

Fig. 1: U_c *vs* t' for the PM to AFM transition compared with HF (chain dashed) and QMC ($*$) results. The insets show m_A and m_{loc} *vs* U at $t'/t = -0.2$ (solid) and -0.4 (dashed) together with the Projector QMC ($\times$) and spin-wave data (dotted) at $t'/t = -0.2$ taken from Ref. [4].

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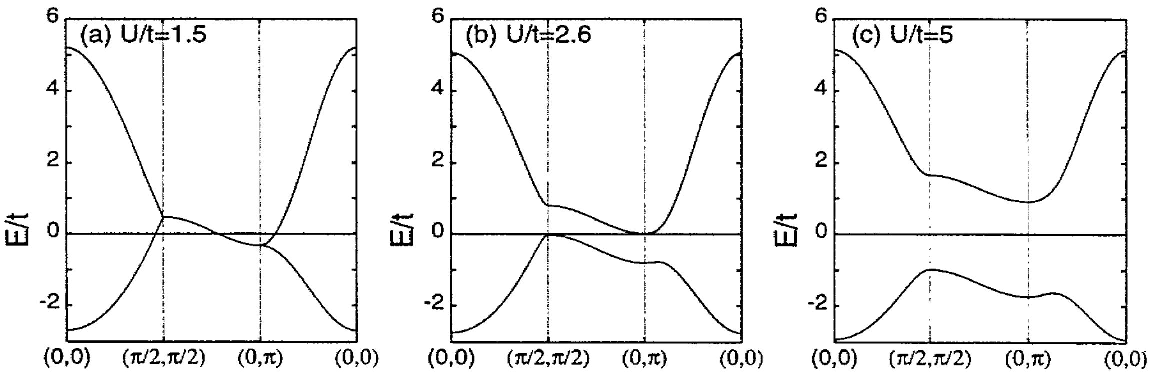

Fig. 2: Band dispersion $E_{\vec{k}\nu} - \mu$ at $n = 1$ and $t'/t = -0.2$ for $U < U_c$ (a), $U = U_c$ (b), and $U > U_c$ (c).

ces the Quantum Monte Carlo (QMC) value [1]. This result may be explained by the shift of the logarithmic van Hove singularity for $t' \neq 0$. Note that in our SB calculation a metallic AFM ground state, as suggested recently in Ref. [3], does not exist. Of course, such a phase may be stabilized introducing additional hopping terms by hand [3]. As seen in Fig. 1, the sublattice magnetization $m_A = p_+^2 - p_-^2$ and the local magnetic moment $m_{loc} = \frac{3}{4}(n - 2d^2)$ reasonably agree with Projector QMC data at $t'/t = -0.2$ [4].

The SB ground-state phase diagram depicted in Fig. 3 reveals a pronounced t'-induced electron-hole asymmetry and the stability of the AFM state (at $t'/t = -0.2$) and of the ferromagnetic (FM) state (at $t'/t = -0.4$) down to $U = 0$ at the critical hole dopings 0.17 and 0.418, respectively. This qualitatively agrees with the Hartree-Fock (HF) calculation of Ref. [1], but contradicts the HF solution obtained in Ref. [5]. Compared with the HF results, the electron correlations incorporated in the SB approach reduce the stability regions of the long-range ordered phases in the favour of the PM phase.

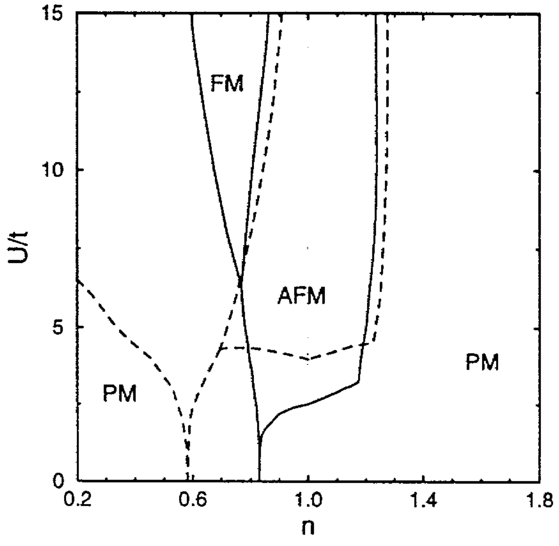

Fig. 3: Phase diagram of the t-t'-Hubbard model at $t'/t = -0.2$ (solid) and $t'/t = -0.4$ (dashed).

In conclusion, the magnetic ground-state properties of the t-t'-Hubbard model are well described by our SB approach, in particular the weak-interaction limit is correctly reproduced.

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