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

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} \hat{z}_{i\sigma} \hat{z}_{j\sigma} f_{i\sigma} f_{j\sigma} + U \sum_i d_{i\uparrow} d_{i\downarrow}.$$  (1)

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

$$f(n, T) = Ud^2 = \sum_{n=\pm} \lambda_n^{(2)} (p_n^2 + d^2) + \mu n$$
$$+ \frac{2}{\beta N} \sum_{\vec{k}\nu=\pm} \ln \left[ 1 - f(E_{\vec{k}\nu} - \mu) \right]$$  (2)

with the quasiparticle tight–binding bands

$$E_{\vec{k}\nu} = \frac{1}{2} \sum_{\eta} \left[ \lambda_\eta^{(2)} + \frac{1}{2} q_\eta (\varepsilon_\vec{k} + \varepsilon_{\vec{k}-(\pi,\pi)}) \right]$$
$$+ \nu \sqrt{A^2 + \frac{1}{4} q_+ q_- (\varepsilon_\vec{k} - \varepsilon_{\vec{k}-(\pi,\pi)})^2},$$  (3)

where the $\vec{k}$–sum runs over the magnetic Brillouin zone, the $\lambda_\eta^{(2)}$ ensure the SB constraints, $A = \frac{1}{2} \sum_{\eta} |\lambda_\eta^{(2)}|$, $q_\eta = |z_\eta|^2$, 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)$\Leftrightarrow$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 reproduces

Fig. 1: $U_c$ vs $t'$ for the PM to AFM transition compared with HF (chain dashed) and QMC ($\times$) 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].
Fig. 2: Band dispersion $E_{k\nu} - \mu$ at $n = 1$ and $t'/t = -0.2$ for $U < U_c$ (a), $U = U_c$ (b), and $U > U_c$ (c).

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 $m_{loc} = \frac{1}{2}(n - 2d^2)$ 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.

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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