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Slave Boson Approach to Magnetic Order in the Hubbard Model

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Abstract. Using a saddlepoint approximation of a spin-rotation-invariant form of the slave boson representation introduced by Kotliar and Ruckenstein we determine for the Hubbard model on the square lattice the phase diagram when spiral magnetic states are taken into consideration. We display the spiral wave-vector and discuss its temperature dependence.

Introduction

It is fairly well established that there is antiferromagnetic long range order in the ground state of the single band Hubbard model on a two dimensional square lattice at half-filling [1,2]. Relatively little is known about the magnetic state of the model away from half-filling. In this work we report numerical results of a slave boson theory supporting the view that spiral states are good candidates for the ground state of the Hubbard model near half-filling and at intermediate to large interaction strength U.

The method

Our analytical treatment of the Hubbard model is based on the spin-rotation-invariant form [3] of the slave boson representation introduced by Kotliar and Ruckenstein [4]. We consider a saddle-point approximation corresponding to the site-dependent magnetization $\vec{M}_i = M\hat{n}_i$ where $\hat{n}_i = (\cos\vec{Q}\cdot\vec{R}_i, \sin\vec{Q}\cdot\vec{R}_i, 0)$ forms a spiral structure. The free energy takes the form:

$$F = -T\sum_{\vec{k},\sigma} ln(1+e^{\frac{-E_{\vec{k},\sigma}}{T}}) + Ud^2 - 2\beta_0(p_o^2+p^2+d^2) - 4p_0p\beta + \alpha(1-e^2-2p_0^2-2p^2-d^2)$$

with the quasiparticle energies:

$$E_{\vec{k},\sigma} = (z_0^2+z^2)\left(\frac{t_k+t_{k-Q}}{2}\right) + \beta_0 - \mu_0 \pm \left[\left((z_0^2-z^2)\left(\frac{t_k-t_{k-Q}}{2}\right)\right)^2 + (z_0z(t_k+t_{k-Q})+\beta)^2\right]^{\frac{1}{2}}$$

where $e^2, p_0^2+\sigma p^2, d^2$ represent respectively the number of empty, spin σ singly occupied, and doubly occupied sites, and α, β_0 and β the Lagrange multipliers enforcing the constraints; they are determined by minimizing F. For details about this representation we refer to [5,6].

Results

We have solved numerically the saddlepoint equations on a 98x98 lattice. The results are summarized in the (U,δ) phase diagram, fig. 1. At $T=0$ we see that the Antiferromagnetic (AF) state takes place at half-filling only, for any value of U. Upon doping the system immediately enters a spiral phase characterised by $\vec{Q} = (Q_x, Q_x)$ (see below). In this part of the phase diagram the Fermi surface consists of one "hole pocket" centered at $(\pi/2, \pi/2)$. Moreover we obtain that the magnetic gap 2β is severely reduced from $\sim U$ at half-filling (for large U) down to $\sim t$ which implies that the band width is getting close to $8t$, contrary to Hartree-Fock results, but in agreement with exact diagonalisation results, for instance for two holes in the $t-J$ model [7]. When the doping is increased the system undergoes a first-order phase transition towards another spiral phase characterised by $\vec{Q} = (Q_x, \pi)$. In this phase the magnetization is decreasing linearly with the doping up to a second-order phase transition to the Paramagnetic state. Fig. 2 is displaying Q_x in slave boson (SB) and Hartree-Fock (H-F) approaches as functions of the density for $U = 8t$ (the jump indicates the transition from (Q_x, Q_x) to (Q_x, π)). The deviation from π for small doping is given by $\delta U/t$, its large U behaviour for both SB and H-F. In SB Q_x then saturates to ~ 2.2, thus showing no ferromagnetism, in agreement with [4].

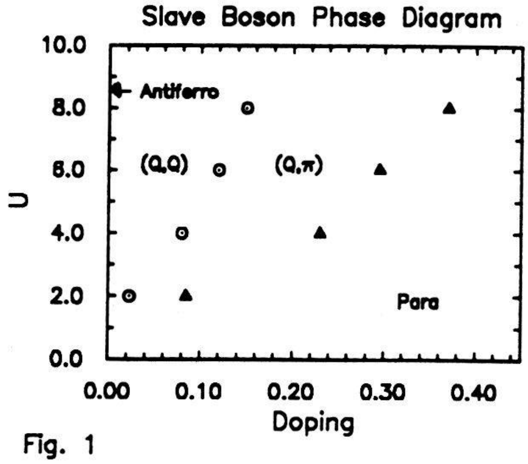

Fig. 1

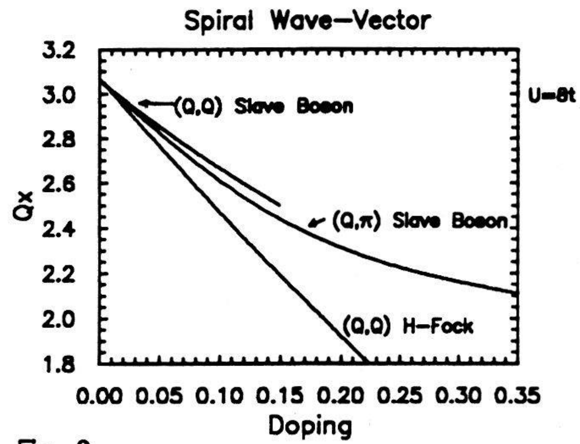

Fig. 2

We also investigated the temperature dependence of $\vec{Q}$ and obtained as ground state the AF state over a finite range of doping given by $\sim 2T/U$.

Conclusion

Within the spin-rotation invariant slave boson mean-field approach [3,4] we showed a phase diagram up to rather large U which exhibits AF, P and 2 different spiral states which extends over a large density domain. We obtain that the temperature is stabilizing the AF state with respect to the spiral one.

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