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Conserving Approximation for the Multi-Band Hubbard Model

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We study the multi-band Hubbard model within a diagrammatic expansion which is conserving in the sense of the Baym/Kadanoff formalism. One- and two-particle properties are computed in Hartree-Fock and in the Fluctuation Exchange (FLEX) approximation, a technique recently proposed by Bickers and Scalapino. The results are checked in direct comparison with exact Quantum-Monte-Carlo results. For finite hole doping the magnetic structure factor $S(\vec{q})$ exhibits a maximum away from $\vec{q} = 0$. This behavior signals the formation of an incommensurate spin ordering of the system which is observed in experimental studies of the cuprate $La_{2-x}Sr_xCuO_4$. The hypothesis of Varma which states a marginal Fermi liquid for the high temperature superconductors is object of our following investigations. We find indications for an anomalous frequency behavior of the polarisation even at $\vec{q} = 0$ near the charge transfer instability, a result which is important to describe Raman scattering experiments in high-T_c oxides.

I. Introduction

It is commonly established that CuO_2-layers are the most relevant structure elements of high temperature superconducters and that they are responsible for the remarkable properties in the normal and superconducting state. The neighborhood of antiferromagnetism and superconductivity, and the appearence of a Mott-isolator transition, indicate that electronic correlations play an important role in these materials.

II. Model

The starting point of our calculations is the multi-band Hubbard model, which includes both O-2p and Cu-3d-orbitals:

$$H = H_0 + H_1,$$

with

$$\begin{aligned} H_0 &= \sum_{i,\sigma}(E_d-\mu)d^\dagger_{i\sigma}d_{i\sigma} + \sum_{\substack{j,\sigma\\ \alpha=x,y}}(E_p-\mu)c^{(\alpha)\dagger}_{j\sigma}c^{(\alpha)}_{j\sigma} \\ &\quad -t_{ij}\sum_{\substack{<i,j>,\sigma\\ \alpha=x,y}}(-1)^{p_{ij}}(d^\dagger_{i\sigma}c^{(\alpha)}_{j\sigma}+h.c.) \\ H_1 &= U_d\sum_i n_{di\uparrow}n_{di\downarrow} + U_p\sum_j n_{pj\uparrow}n_{pj\downarrow} \\ &\quad +\frac{U_{pd}}{2}\sum_{\substack{<i,j>\\ \sigma\sigma'}} n_{di\sigma}n_{pj\sigma'}. \end{aligned}$$

Here $d^\dagger_{i\sigma}$ and $c^{(\alpha)\dagger}_{j\sigma}$ denote the electron creation operators for Cu d and O p orbitals at sites i and j. The one-electron part H_0 is determined by the on-site energies E_d (Cu) and E_p (O) with the charge-transfer energy $\Delta = E_p - E_d$, and a Cu-O hopping $t_{ij} = \pm t$ between nearest-neighbor sites $< i,j >$. The chemical potential μ allows to adjust the doping. The interaction part H_1 includes the on-site Coulomb energies U_d (Cu) and U_p (O) and the nearest-neighbor repulsion U_{pd}.

III. Conserving Approximation

We perform a perturbation expansion up to intermediate values of the correlation parameters. While a simple Random-Phase-Approximation (RPA) is far away from agreement with exact QMC-results, Bickers and Scalapino developed a perturbation expansion in the Fluctuation Exchange (FLEX) approximation [1], that leads to good results for the one-band Hubbard model. This method is based on the Conserving-Approximation (CA) formalism of Baym and Kadanoff [2], which obeys the macroscopic conservation laws even in an infinite order approximation. We have extended this CA-FLEX formalism to the multi-band Hubbard model described in the preceding section [3].

IV. Numerical Results

The magnetic susceptibilties are given by

$$\chi_{SDW/CDW}(\vec{q}, i\omega_m) = \frac{1}{N}\sum_{ij} e^{i\vec{q}\cdot(\vec{x}-\vec{x}')} \cdot\int_0^\beta d\tau\, d\tau'\, e^{-i\omega_m(\tau-\tau')}\langle(n_{i\uparrow}\mp n_{i\downarrow})(n_{j\uparrow}\mp n_{j\downarrow})\rangle,$$

where i,j refer to copper places only. The upper signs correspond to the spin density wave (SDW), the lower to the charge density wave (CDW) susceptibility. These expressions are identical to the QMC definitions [4] and can therefore be compared directly. In Fig. 1 the static SDW-susceptibility is shown as function of the system temperature T. The point-dashed curve refers to the simplest CA: The one-particle propagator is computed in Hartree-Fock (HF) approximation and the susceptibility is calculated by ladder and bubble summation. These HF-CA results

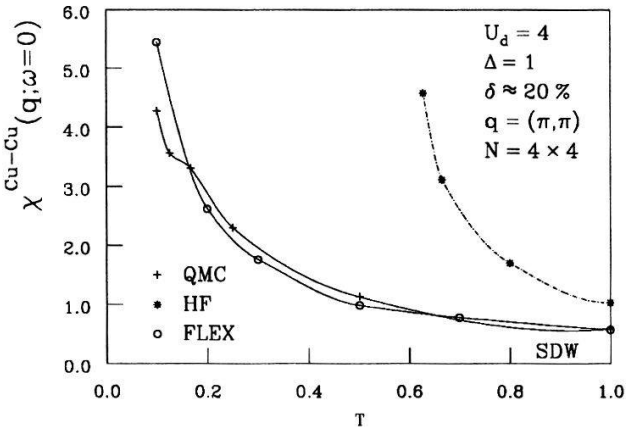

Figure 1: The SDW susceptibility as function of temperature versus QMC results. The approximations are explained in the text.

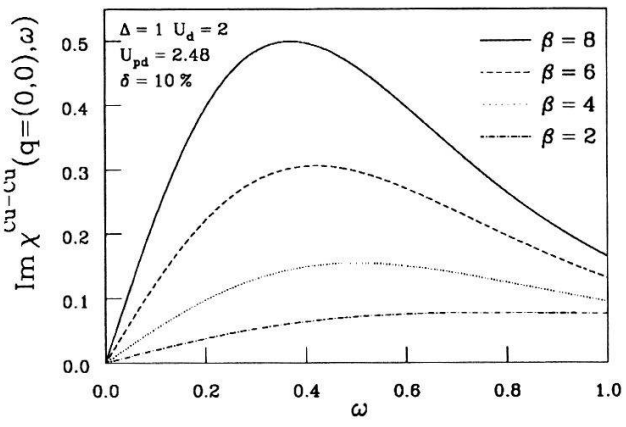

Figure 3: The CDW susceptibility in the neighborhood of the charge transfer instability.

are far away from agreement with the QMC data. We also calculated a time-dependent HF-approximation with selfconsistent one-particle FLEX propagators. Although this approximation is not conserving, we get in Fig. 1 an excellent agreement with the QMC-results for the SDW-susceptibility, which is one of the most sensitive two particle functions in our system. We extract the magnetic structure form factor $S(\vec{q})$ which delivers information about the spin ordering of the system:

$$S(\vec{q}) = \frac{1}{\beta} \sum_{\omega_m} \chi_{SDW}(\vec{q}; i\omega_m).$$

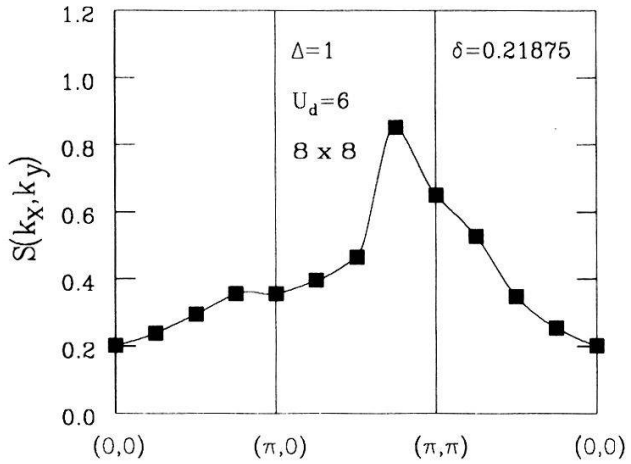

Figure 2: The magnetic structure form factor for finite hole doping.

In the undoped case ($\delta = 0$) $S(\vec{q})$ is sharply peaked at $\vec{q} = (\pi, \pi)$ which indicates the antiferromagnetic order of the system. For finite hole doping the maximum of $S(\vec{q})$ moves away from $\vec{q} = (\pi, \pi)$ as shown in Fig. 2 for $\delta \approx 20\%$. This shift signals the formation of an incommensurate spin ordering of the system, which was observed in experimental studies [5].
The developed perturbation expansion for the multi-band Hubbard model can also be used to study the low energy behaviour of the system. Varma's hypothesis [6] for the frequency dependence of the spin and charge polarisation should be valid for a wide range of wave vectors, especially for $\vec{q} = (0,0)$ in order to describe Raman scattering experiments. Whereas $Im\chi_{SDW}$ decreases to zero for $\vec{q} \to (0,0)$ the imaginary part of the charge density wave suceptibility χ_{CDW} shows the desired Varma behaviour (Fig. 3) near the charge-transfer instability which is a special feature of the multi-band Hubbard model.

Acknowledgments

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