Upper Hubbard Band of the 2-D Hubbard Model

Walter Zimmermann[1], Raymond Frésard[2], and Peter Wölfle[1]

[1]Institut für TKM, Postfach 6980, Universität Karlsruhe, D-76128 Karlsruhe
[2] Institut de Physique, A-L Breguet 1, CH-2000 Neuchâtel

We calculate the one-electron Green's function of the Hubbard model on the square lattice using a spin-rotation invariant six-slave boson representation. In the strong coupling regime its spectrum splits off into a quasi-particle peak, and a lower and an upper incoherent branch, which we focus on, using a functional integral formulation. By including Gaussian fluctuations around a paramagnetic saddle-point, we obtain the main contributions to G as the graphs which are of lowest order in the fluctuations, in the strong coupling regime. The k-dependence of the weight of the upper band shows the physically expected behavior. We also find that its total weight quickly decreases away from half-filling under an increase of the hole doping.

The calculation of the spectral function of the 2-d Hubbard Model remains a serious challenge despite of decades of work. Its relevance to the understanding of the High T_c-superconductors has been repeatedly emphasized in the literature. The strong correlation effects have so far been elucidated in various limits, such as the large space dimensionality limit [1], or in one dimension, but the 2-d and 3-d systems keep on escaping our understanding. In these systems even highly sophisticated self-consistent schemes, such as FLEX fail to even qualitatively reproduce the splitting of the non-interacting band into lower and upper bands [2]. In this work we resort to the Spin-Rotation-Invariant slave-boson approach [3], which naturally splits off the low energy and high energy incoherent excitations, on top of the quasi-particle peak.

In this approach the creation operator of a physical electron $c^+_{i,\sigma}$ is written in terms of auxiliary bosons e, p_μ, d and fermions $f^+_{i,\sigma}$ as: $c^+_{i,\sigma} = \frac{1}{2}\sum_{\mu,\sigma'}\left(e_i p^+_{i,\mu}\tau^\mu_{\sigma,\sigma'} + d^+_i \sigma\sigma' p_{i,\mu}\tau^\mu_{-\sigma',-\sigma}\right) f^+_{i,\sigma}$. In order to evaluate the Green's function $G_{i,j,\sigma}(\tau) = -T < c_{i,\sigma}(\tau)c^+_{j,\sigma}(0) >$ we expand the slave-bosons around their mean-field amplitudes. Doing that to quadratic order in the action yields the propagators of the slave-bosons and constraints fields, which can be gathered from [4]. We now concentrate on the high energy excitations. In the strong coupling regime they are described by the d-boson. The lowest order contributions to the Green's function are given by:

$$G(\vec{k},\omega)_{High} = \frac{\Pi(\vec{k},\omega) + \Pi_{p_z}(\vec{k},\omega) + \Pi_{p_0}(\vec{k},\omega)}{1 - t_{\vec{k}}(\Pi(\vec{k},\omega) + \Pi_{p_z}(\vec{k},\omega) + \Pi_{p_0}(\vec{k},\omega))} \tag{1}$$

where $t_{\vec{k}}$ is the dispersion of the non-interaction band and the various $\Pi's$ are defined in Fig. 1. Please note that they also contain the appropriate vertices.

We now discuss the numerical results. The calculations have been performed for $U = 25t$ and $\beta t = 2.5$, where the paramagnetic phase does not show any kind of instability. We postpone the detailed discussion of the spectral function and density of states to a separate publication. In short the spectral function exhibits a strong $\vec{k}$-dependence. It is typically

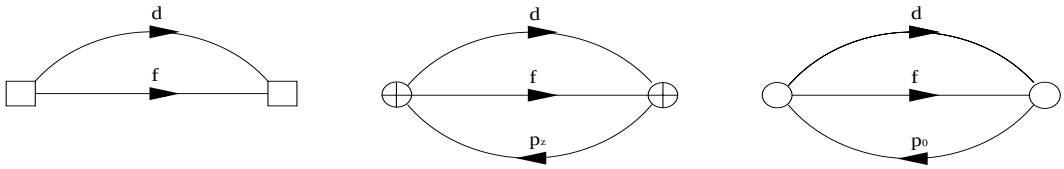

Figure 1: From left to right: $\Pi(\vec{k},\omega)$, $\Pi_{p_z}(\vec{k},\omega)$ and $\Pi_{p_0}(\vec{k},\omega)$

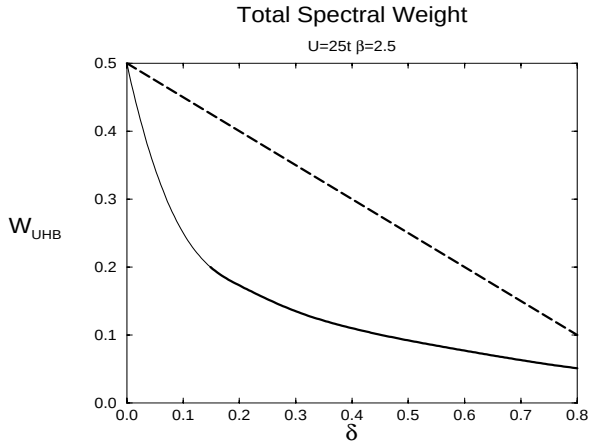

Figure 2: Total weight, SB calculation(full line) and $t-J$ model sum rule(dashed line).

large for wave-vectors in the vicinity of the Fermi surface, and small otherwise. It is smallest at the band center. This is expected since the states are occupied. Its width in frequency is mostly k-independent, and close to the bare band-width. All the main features of the exact diagonalization results are reproduced by our approximation [5]. The doping dependence of the total weight of the upper Hubbard band W_{UHB} is shown on Fig. 2. It is seen to fall off quickly under a decrease of the density. The decay is substantially larger than what one may expect from the sum-rule of the $t-J$ model. This is in agreement with the numerical data of Eskes and Olès [6]. In summary we applied for the first time the SRI slave-boson formulation of the Hubbard model to the calculation of the Green's function away from half-filling. Our results are in good agreement with known numerical data. This work has been supported by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 195. One of us (RF) is grateful to the Fonds National Suisse de la Recherche Scientifique for financial support under Grant 8220-0284525.

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