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Spectral properties and bandstructure of correlated electron systems

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Abstract

We present $\boldsymbol{k}$-dependent one-particle spectra and corresponding effective band structures for the 2D Hubbard model calculated within the dynamical molecular field theory (DMFT). This method has proven to yield highly nontrivial results for a variety of quantities but the question remains open to what extent it is applicable to relevant physical situations. To address this problem we compare our results for spectral functions to those obtained by QMC simulations. The good agreement supports our notion that the DMFT is indeed a sensible ansatz for correlated models even in to $d = 2$.

The observation that the local electron–electron interaction in models of strongly correlated electron systems leads in the limit spatial dimensions $d \to \infty$ to a local one-particle self-energy [1], i.e. the single-particle propagator $G(\boldsymbol{k}, z)$ has the form $G(\boldsymbol{k}, z) = \left[G^{(0)}(\boldsymbol{k}, z)^{-1} - \Sigma(z)\right]^{-1}$ with $G^{(0)}(\boldsymbol{k}, z)$ as the corresponding propagator of the noninteracting system, founded the so-called *dynamical molecular-field theory*: The lattice problem maps onto an impurity system coupled to an effective, self-consistently determined bath [2] and the lattice structure enters only via the free density of states (DOS) $\rho_0(\varepsilon) = \sum_{\boldsymbol{k}} \delta(\varepsilon - \varepsilon_{\boldsymbol{k}})$. The apparent advantages of this approach are that one (i) works in the thermodynamic limit and (ii) treats at least the important local correlations correctly.

This method has been successfully applied to study various physical properties of the one-band Hubbard model (HM) [3] $H_{\mathrm{Hub}} = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + U \sum_l n_{l\uparrow} n_{l\downarrow}$ in the limit $d \to \infty$ [4, 5]. However, the question remains to what extent the dynamical molecular-field theory (DMFT) is applicable to real physical situation, especially to finite dimensions $d = 2, 3$ [6].

A first comparison between magnetic properties of the HM in $d = 3$ and $d = \infty$ [4] already showed that the latter limit seems indeed to provide a quite reliable way to describe at least static quantities of the HM. With respect to e.g. transport properties it is however far more interesting to know how well the DMFT describes the *dynamical* properties of correlated models in finite dimensions. Unfortunately, there are presently no (numerical) exact results for the dynamics of the HM in $d = 3$ since even quantum Monte Carlo methods (QMC) are restricted to far too small system sizes to allow for a reliable evaluation of dynamical quantities like one-particle spectra. Recently, however, significant progress has been made in obtaining one-particle spectra from QMC-data for the HM on a two-dimensional square lattice [7, 8]. This enables the first direct and quantitative comparison between dynamical results from a generalized mean-field theory and numerical exact methods in finite dimensions.

Let us start the discussion of our results obtained by solving the dynamical molecular-field equations with NCA-techniques [9] by noting that the DMFT is relatively insensitive to the actual lattice used. This can be seen from Fig. 1, where we compare calculations for dispersions [1]:

$$\varepsilon_{\boldsymbol{k}} = -\frac{t^*}{\sqrt{d}} \sum_{l=1}^{d} \cos(k_l a) \ , \tag{1}$$

with $d = 2$ (dashed curves) and $d = \infty$ (full curves). As is evident from the inset to Fig. 1(a), the DOS for the noninteracting systems show remarkable differences, namely sharp cut-offs at the band edges $\omega/t^* = \pm\sqrt{2}$ and a van-Hove

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