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Non-local effects in the fermion dynamical mean-field framework; application to the two-dimensional Falicov–Kimball model

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Abstract. We propose a new, controlled approximation scheme that explicitly includes the effects of non-local correlations on the $D = \infty$ solution. In contrast to the usual $D = \infty$ case, the self-energy is self-consistently coupled to two-particle correlation functions. The formalism is general, and is applied to the two-dimensional Falicov–Kimball model. Our approach possesses all the strengths of the large- D solution, and allows one to undertake a systematic study of the effects of inclusion of k -dependent effects on the $D = \infty$ picture. Results for the density of states $\rho(\omega)$, and the single-particle spectral density for the 2D Falicov–Kimball model always yield positive definite $\rho(\omega)$, and the spectral function shows striking new features inaccessible for $D = \infty$. Our results are in good agreement with the exact results known from the 2D Falicov–Kimball model.

The effects of strong correlations on the properties of low-dimensional lattice fermion systems is still an open problem, in spite of many efforts spanning over thirty years. Recently, the development of a *dynamical* mean-field theory (DMFT), exact in $D = \infty$ dimensions, has led to a major advance in our understanding of the physics in the local limit [1, 2]. DMFT is a non-perturbative scheme. It has provided a detailed picture of the Mott transition in this limit, and has been fruitfully applied to a large class of models. Moreover, it has proved to be a rather good approximation to actual three-dimensional transition-metal and rare-earth compounds [2]. In spite of its successes, DMFT has its shortcomings: the single-particle self-energy is k -independent, and so is not coupled to k -dependent collective excitations. This is clearly serious, e.g. near a magnetic phase transition where it cannot show any precursor effects. A consequence of the above is that the single-particle spectral function cannot access such effects, and so the approach cannot be employed to describe e.g. angle-resolved photoemission experiments, or to study the changes in Fermi surface topologies driven by interactions for finite D . The above makes it imperative to develop such controlled extensions of DMFT as are able to rectify its unphysical aspects, while preserving its strengths.

The DMFA maps the lattice system onto a self-consistently embedded ‘impurity in a bath’ problem that describes the effects of the coupling to other lattice sites. As in a Weiss mean-field theory, a self-consistency condition is obtained by requiring the averaged Green’s function of the bath G_0 to coincide with the local G at this impurity site. The DMFA becomes exact for $D = \infty$ because one can show that the spatial correlations fall off at least as $1/D^{|i-j|/2}$ with distance $|i - j|$ [5]. This ‘Weiss field’ still has a non-trivial dynamics described by an

effective local action S_{DMF} obtained by integrating out all sites excluding the impurity site. Given S_{DMF} , one can compute the one-particle Green's function at this site, $G_{imp}(\omega)$, which is a functional of $G_0(\omega)$. The self-consistency condition that links G_{imp} back to G_0 is solved iteratively. The main drawback of this method is that Σ is k -independent.

In this paper, we present an extension of the DMFT that allows one to treat effects of non-local spatial correlations. To do so, we exploit the freedom involved in choosing the input bath propagator. We account for non-local correlations via the self-consistent inclusion of the two-particle correlation function in the bath Green's function (GF) $G_0(\omega)$. This is achieved by using the spectral density approximation (SDA) [4]. Thus, our aim is to show that a proper combination of two methods—DMFT and SDA—is eminently suited to describing $1/D$ effects in lattice-correlated fermionic systems. As far as application is concerned, we deal with the FKM, as it was the first model to be solved exactly for $D = \infty$. Attempts at a $1/D$ expansion for the FKM have also been made. Finally, there exist some exact results on the 2D FKM which are of great help in evaluating the quality of our approximation, making it a first choice for testing methods in the context of extensions of the DMFT.

Recently, Hettler *et al* [3] have considered the role of short-range correlations in the Falicov–Kimball model by employing the ‘dynamical cluster approximation’ (DCA). The DCA extends the DMFT by attempting to treat intracluster correlations exactly, and embedding this cluster in a dynamical bath. The influence of non-local correlations on the DOS, as well as on the critical temperature for transition to a checkerboard phase [7], is investigated, and it is found that T_c is depressed by non-local effects, as expected. However, the influence of these correlations on the single-particle spectral function $A(\mathbf{k}, \omega)$ has not been investigated. Given a \mathbf{k} -dependent self-energy, the bandstructure and Fermi surface topology are changed via $E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma(\mathbf{k}, \mu)$ and $E_{\mathbf{k}} = \mu$, where μ is the chemical potential. Furthermore, results available on the 2D FKM clearly reveal the opening up of a gap associated with Fermi surface nesting for any U . This is not the case in the results of Hettler *et al*. We show in this work that the route considered here is consistent with the above statement, and allows one to compute $A(\mathbf{k}, \omega)$ as well. It should be stated that we are not aiming for an *exact* $1/D$ expansion, which would be beset with intractable difficulties. Our aim is rather to devise a scheme that includes non-local correlations while keeping the strengths of the $D = \infty$ approach intact.

We now present this new method. We begin with the formalism for the generic Hubbard model at zero temperature. We then go to the FK to solve the full set of self-consistent equations. We will focus on half-filling; the extension away from $n = 1$ is straightforward. The Hamiltonian is

$$H = - \sum_{\langle ij \rangle, \sigma} t_{\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}$$

on a D -dimensional lattice. The Hubbard model is obtained when $t_{\uparrow} = t_{\downarrow} = t$, and the FKM is given by $t_{\uparrow} = t$ and $t_{\downarrow} = 0$. In the case of half-filling, $\mu = U/2$ by particle–hole symmetry. These models have been extensively studied using the DMFT.

We get a bath propagator which includes $1/D$ effects using the SDA, first pioneered by Roth [4] to describe magnetism in narrow bands. Its basic idea is to compute exactly the first few moments of the spectral density to reconstruct the spectral function $A(\mathbf{k}, \omega)$. With H as above, it is easy to compute the first four moments. They are given by the expectation value of the following n -fold commutator:

$$M_{k\sigma}^{(n)} = \langle [\dots [c_{k,\sigma}^{\dagger}, H], H], \dots, H] \rangle. \quad (1)$$

Using usual scaling arguments [5], one sees that the higher n , the higher will be the powers of $1/D$ involved in the n th moment. In the case of a generic Hubbard model, it turns out that the

$M_{k\sigma}^{(3)}$ contains all the $o(1/D)$ contributions. It can be written as

$$M_{k\sigma}^{(3)} = o\left(\frac{1}{D^0}\right) + U^2 n_{-\sigma}(1 - n_{-\sigma}) B_{k\sigma}$$

with

$$n_{-\sigma}(1 - n_{-\sigma}) B_{k\sigma} = \frac{1}{N} \sum_{(ij)} \{t_{-\sigma} \langle c_{i-\sigma}^\dagger c_{j-\sigma} (1 - 2n_{i\sigma}) \rangle - t_\sigma [\langle n_{i-\sigma} n_{j-\sigma} \rangle - n_{-\sigma}^2 - \langle c_{i\sigma}^\dagger c_{i-\sigma}^\dagger c_{j-\sigma} c_{j\sigma} \rangle - \langle c_{i\sigma}^\dagger c_{j-\sigma}^\dagger c_{j\sigma} c_{i-\sigma} \rangle] e^{-ik \cdot (R_i - R_j)}\}. \quad (2)$$

The SDA then permits one to write an explicit closed-form expression for

$$A_\sigma(\mathbf{k}, \omega) = \delta[\omega - \epsilon_{\mathbf{k}} + \mu - \Sigma_{0,\sigma}(\mathbf{k}, \omega)]$$

where $\Sigma_{0,\sigma}(\mathbf{k}, \omega)$ is given—for the generic Hubbard model—by

$$\Sigma_{0,\sigma}(\mathbf{k}, \omega) = U n_{-\sigma} + U^2 n_{-\sigma}(1 - n_{-\sigma})[\omega + \mu - U(1 - n_{-\sigma}) - B_{k\sigma}]^{-1}.$$

This is the self-energy in the SDA. It is interesting to notice that all the order- $1/D$ correlators enter only through $B_{k\sigma}$, whereby the self-energy acquires a non-trivial \mathbf{k} -dependence. At this stage, this quantity is undetermined, and will have to be obtained self-consistently. The SDA one-particle Green's function can then be computed as $G_{0\sigma}(\mathbf{k}, \omega) = [\omega - \epsilon_{\mathbf{k}} - \Sigma_{0,\sigma}(\mathbf{k}, \omega)]^{-1}$.

We now consider the FKM, ($t_\downarrow = 0$). In this case, the model has a local $U(1)$ symmetry, $[n_{i\downarrow}, H] = 0 \forall i$. It thus follows from Elitzur's theorem that only the second correlator in $B_{k\sigma}$ is non-zero. Considering the conduction electron (\uparrow -spin) Green function, the equation for $B_{k\uparrow}$ shows that the correlation function involving correlated hopping of the \downarrow -spins is zero. This leads to

$$n_\downarrow(1 - n_\downarrow) B_{k\uparrow} = -\frac{t}{N} \sum_{(ij)} e^{-ik \cdot (R_i - R_j)} [\langle n_{i\downarrow} n_{j\downarrow} \rangle - n_\downarrow^2] = -t \chi_\downarrow(\mathbf{k}) \quad (3)$$

where $\chi_\downarrow(\mathbf{k})$ is the order- $1/D$ static structure factor of the down-spin electrons.

It is interesting to notice that the *only* order- $1/D$ contribution to the single-particle self-energy is in fact $\chi_\downarrow(\mathbf{q})$. The above equations are exact in the band as well as in the atomic limit, as can easily be checked. This has important consequences, for it points to a way to achieve further improvement of the formalism. It allows one to formulate a DMFT for the local part, more or less along same lines as for $D = \infty$ [2]. However, in contrast to the case for the regular DMFT where $\Sigma_{0\uparrow} = 0$, G_0 contains information about non-trivial \mathbf{k} -dependent features. Therefore, using this SDA $G_{0\uparrow}$ as the input one-particle bath Green's function in a new DMFT scheme allows one to introduce in a *simple* way the non-local spatial fluctuations at order $1/D$ in the FKM.

We now come to the computation of the dynamical correlations. This results in a dynamically corrected self-energy. To do this beyond the single-site level is a problem that has not been attempted, and here we use the standard DMFT as an approximation to the 2D case. In the case of the half-filled FKM, the method drawn along the lines sketched above can be developed the following way.

As is known [7, 8], the equation-of-motion method (EOMM) gives the exact solution to the FKM for $D = \infty$. We will use the EOMM to get the full (local) impurity Green's function which we denote by $G_{imp,\uparrow}(\omega)$.

The closed set of equations for the on-site Green's function with a bath having $\Sigma_{0,\uparrow}(\mathbf{k}, \omega)$ as a self-energy is given in reference [8], replacing $\epsilon_{\mathbf{k}}$ by $\epsilon_{\mathbf{k}} + \Sigma_{0,\uparrow}(\mathbf{k}, \omega)$.

The local G_{\uparrow} is computed to have the same form as that found in [2], and the local self-energy is computed from Dyson's equation, $\Sigma_{imp,\uparrow}(\omega) = G_{0,imp,\uparrow}^{-1}(\omega) - G_{imp,\uparrow}^{-1}(\omega)$ where $G_{0,imp,\uparrow}(\omega) = [\omega + \mu - \Delta(\omega)]^{-1}$, with

$$\Delta(\omega) = \sum_{\mathbf{k}} \frac{t_{\mathbf{k}}^2}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{0,\uparrow}(\mathbf{k}, \omega)}. \quad (4)$$

One then gets

$$\Sigma_{imp,\uparrow}(\omega) = Un_{\downarrow} + \frac{U^2 n_{\downarrow}(1 - n_{\downarrow})}{\omega + \mu - U(1 - n_{\downarrow}) - \Delta(\omega)}. \quad (5)$$

This local dynamical self-energy is used to correct the local part of the bath self-energy given initially by the SDA, to introduce dynamical effects in the \mathbf{k} -dependent bath GF. This is done using

$$\Sigma_{\uparrow}(\mathbf{k}, \omega) = \Sigma_{imp,\uparrow}(\omega) + \Sigma_{0,\uparrow}(\mathbf{k}, \omega) - \sum_{\mathbf{k}} \Sigma_{0,\uparrow}(\mathbf{k}, \omega) \quad (6)$$

and provides us with a dynamically corrected non-local Green's function

$$G_{\uparrow}(\mathbf{k}, \omega) = [\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\uparrow}(\mathbf{k}, \omega)]^{-1}$$

which is exact in both the atomic and the band limits. The density of states is then obtained by taking the imaginary part of the \mathbf{k} -summed $G(\mathbf{k}, \omega)$. The above procedure in fact gives the exact result for the $D = \infty$ FKM. This is seen easily from the fact that the SDA self-energy becomes \mathbf{k} -independent in this limit, so the last two terms in the above equation for the full self-energy become identical, giving $\Sigma_{\uparrow}(\mathbf{k}, \omega) = \Sigma_{\uparrow}(\omega)$, the $D = \infty$ self-energy for the FKM.

To complete the procedure, one should self-consistently compute the order- $1/D$ correlator which enters the bath Green's function as announced earlier. In the case of the FKM, this means one has to compute the down-spin static susceptibility. To begin with, we compute the vertex function exactly for $D = \infty$. The full $\chi_{\downarrow}(\mathbf{q})$ is then obtained from the Bethe–Salpeter equation in the framework of the EOMM [7]. The result is $\chi_{\downarrow}(\mathbf{q}) = n_{\downarrow}(1 - n_{\downarrow})/D(\mathbf{q})$, where

$$D(\mathbf{q}) = 1 - \sum_{\nu} \frac{dn_{\downarrow}}{dG_{\nu}^{-1}} \frac{\partial \Sigma_{\nu}}{\partial n_{\downarrow}} \Big|_{G_{\nu}} \frac{G_{\nu}^2 + \chi_{\uparrow}^0(\mathbf{q})}{G_{\nu}^2 [\chi_{\uparrow}^0(\mathbf{q}) d\Sigma_{\nu}/dG_{\nu} + 1]} \quad (7)$$

and

$$\chi_{\uparrow}^0(\mathbf{q}) = (-1/N) \sum_{\mathbf{k}} G_{\uparrow}(\mathbf{k} + \mathbf{q}) G_{\uparrow}(\mathbf{k})$$

where the ν -sum is over the Matsubara indices (we take the zero-temperature limit). In the above, the vertex corrections in the equation for the charge susceptibility of the down-spin electrons are approximated by their $D = \infty$ values. To compute the vertex function exactly to order $1/D$ would be a formidable task; this has not been successfully attempted even for the electron gas.

To sum up, the equations (3)–(7) above form a *complete* set of self-consistent equations for the FKM. These include explicit $1/D$ effects through the \mathbf{k} -dependence of $\Sigma_{0,\uparrow}(\mathbf{k}, \omega)$. To solve these equations, we start with an arbitrary $\chi_{\downarrow}(\mathbf{q})$ as an input in our initial $G_{0\uparrow}$. This is used to compute $\Sigma_{0,\uparrow}(\mathbf{k}, \omega)$, and the full $G_{imp,\uparrow}(\omega)$ from the large- D solution along the lines of [8]. At this step, we have a DMF approximation to the FKM that is equivalent to a self-consistent loop, with an external input quantity, the structure factor. The second step of our method is to compute $\chi_{\downarrow}(\mathbf{q})$. For this purpose, we use the DMF approximation to the structure factor equation (7), plugging the $G_{\uparrow}(\mathbf{k}, \omega)$ obtained along with the full *local* vertex

function in the Bethe–Salpeter equation to compute $\chi_{\downarrow}(\mathbf{q})$. This is fed back into the equation for $\Sigma_{0,\uparrow}$ and the whole process is iterated to convergence. The difference between the regular self-consistent DMFT and our method is illustrated in figure 1.

We implemented this new method numerically to study the Falicov–Kimball model on a 2D square lattice at $T = 0$. The up-spin electron dispersion relation is thus $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$, and the corresponding density of states has a Van Hove singularity at $\omega = 0$. The \mathbf{k} -sums are performed on an $L \times L$ mesh, while the ω -integrals are computed using standard integration procedures, using a small broadening η to represent δ -functions. Convergence is obtained when

$$\chi^2 = \sum_{\omega} |G_{new}(\omega) - G_{old}(\omega)|^2 < \varepsilon$$

where ε is a small threshold. At each step of the iterative process, a check on the accuracy of the computation is provided by the Luttinger sum rule

$$\sum_{\mathbf{k}} \int_{-\infty}^{\mu} d\omega A_{\sigma}(\mathbf{k}, \omega) = n_{\sigma}$$

which must be satisfied to high accuracy.

We now describe the results of our computation. Working with a lattice size $L = 64$, and a threshold $\varepsilon = 10^{-9}$, we observe a very fast convergence of the double self-consistent procedure, that needs fewer than ten steps to reach the convergence threshold for $G_{\uparrow}(\omega)$. The Luttinger sum rule is satisfied with an error of less than 10^{-3} .

Figure 2 shows the density of states (DOS) $\rho(\omega)$ obtained by our method for several values of U/t . Firstly, notice that this function is always positive definite, in contrast to the results of reference [9]. This is a positive feature of the present method. We should stress that we are interested in the effect of coupling of the self-energy to $1/D$ fluctuations, which, for the FKM, are completely static. The effect of the interaction is very clear. Starting from the 2D free-fermion value at $U/t = 0$, it opens a gap at $\omega = 0$. The critical $(U/t)_c$ for opening up a gap is very small. As a matter of fact, working with a $L \times L$ lattice we cannot resolve energy details smaller than $2\pi v_F/L \simeq 0.2$ here. However, playing with the parameters of the problem, we see a real gap with U/t as low as 0.1. This result agrees with the exact result on the 2D FKM at weak coupling [12], where the gap and the related checkerboard order arise from the nested FS at $n = 1$. The fact that a gap opens up for arbitrarily small U in our results reflects the fact that

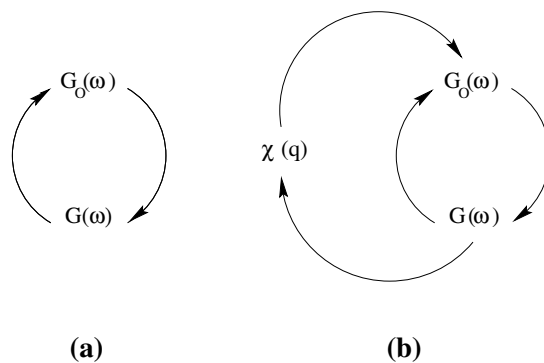


Figure 1. (a) The self-consistency loop in usual DMFT. (b) Our method: \mathbf{k} -dependent features are incorporated via an external input χ_{\downarrow} to the bath Green’s function G_0 , which is computed self-consistently as shown.

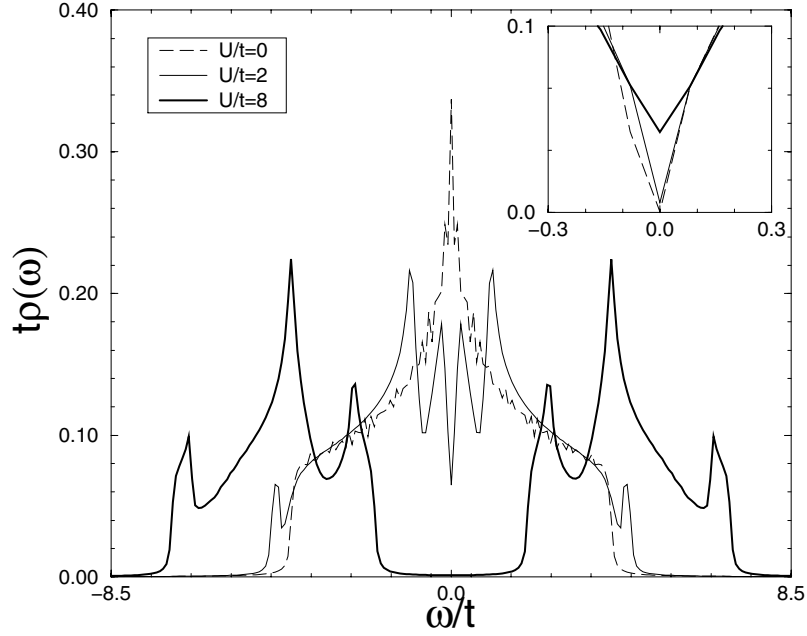


Figure 2. The DOS for the 2D Falicov–Kimball model for several values of U/t at half-filling, with our method. It is always positive definite. The inset shows the behaviour of the $U/t = 2$ gap at $\omega = 0$ when changing the artificial broadening η of the δ -functions: $\eta/t = 5 \times 10^{-2}$, thick line; $\eta/t = 5 \times 10^{-3}$, thin line; and $\eta/t = 2 \times 10^{-4}$, dashed line.

the q -dependence in the non-local susceptibility $\chi_{\downarrow}(\mathbf{q})$ (see below) shows up in the non-local self-energy. In contrast, it is well known from the exact $D = \infty$ solution that a charge gap opens up only when $U \simeq W$, the free bandwidth. Thus, we are able to demonstrate how the effects of coupling the non-local susceptibility to the single-particle self-energy results in conclusions drastically different from those obtained for $D = \infty$. The inset of figure 2 shows the behaviour of the DOS at low frequency for $U/t = 2$, obtained by changing the broadening of the delta functions to get a better precision. The features observed at higher frequencies are related to the unperturbed 2D bandstructure and are absent for infinite D .

The computed $\chi_{\downarrow}(\mathbf{q})$, which contains information about long-range order (LRO), shows interesting behaviour; along the zone diagonal, at the point $\mathbf{k} = [\pi, \pi]$, it is a constant, scaling approximately with lattice size. This is the expected behaviour in the broken-symmetry phase [13], and implies that the $n = 1$ ground state is characterized by checkerboard LRO of the down-spin electrons [10]. In reference [13], the behaviour of $\chi_{\downarrow}(\mathbf{q})$ can be studied only in 1D, because of finite-size restrictions. In contrast, our approach yields unambiguous conclusions in the thermodynamic limit in 2D. Again, this is in clear agreement with the exact result [12].

The greatest advantage of our method, however, is that it allows a detailed study of \mathbf{k} -dependent (at the order of $1/D$) effects in the one-particle spectral function $A(\mathbf{k}, \omega) = -\text{Im} G(\mathbf{k}, \omega)/\pi$. In figure 3, we show $A(\mathbf{k}, \omega)$ for \mathbf{k} along the zone diagonal from $\mathbf{k} = \mathbf{0}$ to $\mathbf{k} = (\pi, \pi)$ for a representative value of $U = 4t$. We notice that $A(\mathbf{k}, \omega)$ satisfies all the symmetry properties consistent with those expected from pure nearest-neighbour hopping on bipartite lattices, and with particle–hole symmetry: $A(\mathbf{k}_0, \omega) = A(\mathbf{k}_0, -\omega)$ for $\mathbf{k}_0 = [\pi/2, \pi/2]$, while along the zone diagonal $A(\mathbf{k}_0 + \delta, \omega) = A(\mathbf{k}_0 - \delta, -\omega)$, $\forall \delta$ along

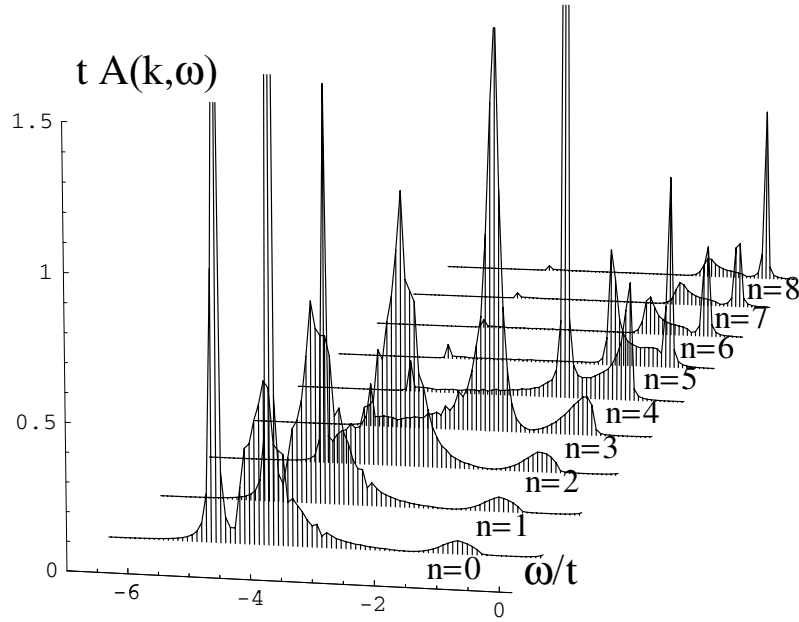


Figure 3. The spectral function $A_{\uparrow}(k, \omega)$ for the 2D Falicov–Kimball model at half-filling, for $U/t = 4$, and \mathbf{k} along the zone diagonal, $\mathbf{k} = (n\pi/8, n\pi/8)$, n going from 0 to 8.

the zone diagonal. We show only the $A(\mathbf{k}, \omega)$ for $\omega < 0$; the $\omega > 0$ part can be obtained from the symmetry property mentioned above. We have checked that our calculations are fully consistent with the above property. Moreover, we see that since $\mathbf{Q} = [\pi, \pi]$ is a nesting vector in 2D, the above property of $A(\mathbf{k}, \omega)$ with $\delta = [\pi/2, \pi/2]$ leads to a natural explanation of the ‘shadow-band’ features observable in ARPES. It would be very interesting to see whether they survive away from $n = 1$.

It is instructive to compare our results to those obtained by Velický *et al* [11] in their pioneering paper on CPA. CPA is equivalent to the exact $D = \infty$ result for the FKM, and so a comparison with [11] allows us to study the effects of $1/D$ effects on $A(\mathbf{k}, \omega)$. A comparison of our data with results for identical parameters from [11] shows that the coupling to $1/D$ fluctuations induces new features in $A(\mathbf{k}, \omega)$ compared to those observed in DMFT. For $D = \infty$, $A(\mathbf{k}, \omega)$ has a two-peak structure with the dispersion controlled solely by the free bandstructure. In our approach, this is modified because of the extra \mathbf{k} -dependence coming through the $B_{\mathbf{k}\downarrow}$. This shows that a formalism capable of explicitly treating intersite correlations permits one to access \mathbf{k} -dependent features in $A(\mathbf{k}, \omega)$, so we suggest that this method can be fruitfully applied to compute ARPES lineshapes in correlated systems. The formalism presented here could also be applied to the computation of effects of short-range order (SRO) in binary alloys, where the \downarrow -spin structure factor would be replaced by the alloy structure factor. A more detailed application to spectroscopy would require the use of the actual bandstructure DOS, and is left for future work. Application to the Hubbard model would require a self-consistent evaluation of *all* the correlation functions, including the spin-flip and pair-hopping correlators in $B_{\mathbf{k}\sigma}$ derived in this paper. To do this is a much harder task, which we plan to attempt in the future.

In conclusion, we have developed a simple, physically appealing way to study the effects of non-local spatial fluctuations on the single-particle spectral properties. We have applied

the formalism to compute the single-particle spectral function and the DOS for the 2D FKM and have obtained results in good accordance with what is known from the exact solution. Extensions of the work to look at the metallic phase in the FKM off $n = 1$, as well as for the Hubbard model, are being studied and will be reported on separately.

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