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Correlated hopping in the Falicov–Kimball model: a dynamical mean-field study

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Abstract

We study the effects of correlated hopping in the two-dimensional (2D) Falicov–Kimball model by means of an extension of the dynamical mean-field approximation (DMFA). The extension is based on the projection technique and the DMFA, in which nonlocal correlations are taken into account through static quantities of a relevant subspace. The effect of the correlated hopping is to introduce nonlocal self-energy components which remain even at $D \to \infty$. We show that the sum rules of the spectral function and its moments are preserved. The spectral function obtained reveals significant nonlocal contributions which are absent in the DMFA.

1. Introduction

Interest in non-perturbative results for strongly correlated electron systems (SCES) has attracted the attention of theorists since the discovery of high- T_c superconductors and heavy fermions. Over the last few years our understanding of SCES has considerably improved, in particular due to the application of the dynamical mean-field approach [1]. One notable example is the Mott–Hubbard metal–insulator transition within the paramagnetic phase of V_2O_3, where the main features of the transition are accounted for within the single-band Hubbard model by the dynamical mean-field approximation (DMFA) [2]. However, this approximation fails to capture the apparent $\boldsymbol{k}$-dependence of the single-particle self-energy close to the transition [3, 4, 5]. This failure indicates that nonlocal correlations are omitted in the DMFA. Indeed, in the DMFA based on the infinite-dimensional limit and a mapping of the lattice problem onto a single impurity model, the self-energy is purely local. In the infinite-dimensional limit the DMFA is exact [1, 6].

However, this is no longer true for models with intersite interactions. Within the DMFA intersite interactions are treated in a Hartree–Fock approximation, hence the DMFA could not fully incorporate the effect of the intersite interactions even at the infinite-dimensional limit. Recently, Schiller [7] showed how to incorporate intersite interactions into the framework of the DMFA. The effect of these interactions is to introduce nonlocal self-energy components which retain full dynamics in the limit of infinite dimensions. However, it is not clear whether or not

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the approximation preserves the sum rules of the spectral function and its moments. At the same time, another extension of the DMFA, which allows inclusion of nonlocal correlations, has been introduced [8, 9, 10, 11] . This extension is based on the projection technique and the DMFA, in which nonlocal correlations are taken into account through static quantities of a relevant subspace. The advantage of this extension is that the sum rules of the spectral function and its moments are preserved. The sum rules of the spectral moments are exact and yield valuable information which helps in judging the reliability of the method.

In this paper we will adopt this approach to study the effect of correlated hopping in the 2D Falicov–Kimball model (FKM) [12]. The effect of correlated hopping has been considered in studying high-T_c superconductivity [13, 14, 15, 16]. Recently, there has been renewed interest in this problem [7, 17]. Correlated hopping results from matrix elements of the Coulomb potential involving neighbouring lattice sites and depends on the occupancy of the opposite spin orientation. It is generally smaller than the onsite Coulomb repulsion, but may not be negligibly small. Typically, correlated hopping is of the order of 0.1–1 eV [18, 19] and is comparable to tight-binding hopping. The model with correlated hopping cannot be solved exactly, and only local mean-field and finite-size diagonalization results are available [13, 14, 15, 16]. Despite this fact and recent work [7, 17] complete understanding has not yet been attained. Thus there is an obvious need for investigation of correlated hopping within the nonperturbation approach, applicable to the entire range of interactions from weak to strong coupling.

The paper is organized as follows. In section 2 we present the general formalism of the extension of the DMFA, and its application to the FKM with correlated hopping. In section 3 we present the numerical results and discussions. The final section contains conclusions and further remarks.

2. Extended dynamical mean-field approximation

The Hamiltonian of the FKM including correlated hopping can be written as follows:

$$H = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j + t'\sum_{\langle i,j\rangle} c_i^\dagger c_j (f_i^\dagger f_i + f_j^\dagger f_j) + U\sum_i f_i^\dagger f_i c_i^\dagger c_i + \varepsilon_f \sum_i f_i^\dagger f_i - \mu\sum_i (c_i^\dagger c_i + f_i^\dagger f_i), \tag{1}$$

where t is the hopping parameter of spinless conduction (c) electrons, t' is the correlated hopping parameter, and ε_f is the energy level of localized f electrons. The onsite Coulomb interaction between c and f electrons is given by U. μ is the chemical potential for both c and f electrons. Here $f_i^\dagger$ (f_i), $c_i^\dagger$ (c_i) are the standard notations for creation (annihilation) operators for f and c electrons at site i. In the limit $D \to \infty$ both parameters t and t' must be scaled as $1/\sqrt{D}$. For $t' = 0$ the Hamiltonian (1) reduces to the standard FKM [12] and the self-energy is due to solely the Coulomb onsite interaction U. The FKM is a simplified Hubbard model with one spin species tied down. Despite the simplification, the FKM contains a rich phase diagram [20, 21], and is a suitable model of the Mott–Hubbard metal–insulator transition. A nonzero t' results in new self-energy terms with full dynamics, which remain even in the absence of the onsite interaction U. To investigate the effect of correlated hopping we employ the extended DMFA [8, 9, 10, 11]. We introduce the retarded Green function for c electrons

$$G_{ij}(t - t') = -\mathrm{i}\theta(t - t')\langle\{c_i(t), c_j^\dagger(t')\}\rangle. \tag{2}$$

where $\theta(t)$ is the step function. The Green function can be written in the form

$$G(\boldsymbol{k}, \omega) = \frac{1}{\omega - \varepsilon_{\boldsymbol{k}} + \mu - \Sigma(\boldsymbol{k}, \omega)} \tag{3}$$

where $\varepsilon_k = -t\gamma_k$, $\gamma_k = 2(\cos k_x + \cos k_y)$. Here, $G(\boldsymbol{k}, \omega)$ is the Fourier transform of the retarded Green function $G_{ij}(t)$ in both time and lattice space and $\Sigma(\boldsymbol{k}, \omega)$ is the self-energy. Using the projection technique, the self- energy can be presented in the form of a continued fraction [22, 23]

$$\Sigma(\boldsymbol{k}, \omega) = \Omega_0(\boldsymbol{k}) - \varepsilon_k + \mu + \cfrac{\chi_1(\boldsymbol{k})}{\omega - \Omega_1(\boldsymbol{k}) - \cfrac{\chi_2(\boldsymbol{k})\ \chi_1^{-1}(\boldsymbol{k})}{\omega - \Omega_2(\boldsymbol{k}) - \ddots - \cfrac{\chi_n(\boldsymbol{k})\ \chi_{n-1}^{-1}(\boldsymbol{k})}{\omega - \Omega_n(\boldsymbol{k}) - M_{n+1}(\boldsymbol{k}, \omega)}}}} \tag{4}$$

where $\chi_i(\boldsymbol{k})$, $\Omega_i(\boldsymbol{k})$, and $M_{n+1}(\boldsymbol{k}, \omega)$ are the susceptibility, frequency and memory functions, respectively, i.e.,

$$\chi_i(\boldsymbol{k}) = \left(A_i \middle| A_i^\dagger\right) \qquad \Omega_i(\boldsymbol{k}) = \left(A_i \middle| \mathcal{L}_i A_i^\dagger\right)\chi_i^{-1}(\boldsymbol{k})$$
$$M_{n+1}(\boldsymbol{k}, \omega) = \left(A_n \middle| \mathcal{L}_n \mathcal{Q}_n \frac{1}{\omega - \mathcal{Q}_n \mathcal{L}_n \mathcal{Q}_n} \mathcal{Q}_n \mathcal{L}_n A_n^\dagger\right)\chi_n^{-1}(\boldsymbol{k})$$

where $i = 0, 1, ..., n$, and operator product $(A|B) = \langle\{A, B\}\rangle$ has been used. Here we have also introduced the dynamical operators A_0, A_1, ..., A_n which are defined as follows:

$$A_i^\dagger = \mathcal{Q}_{i-1}\mathcal{L}_{i-1}A_{i-1}^\dagger \qquad A_0^\dagger = c_{\boldsymbol{k}}^\dagger, \tag{5}$$

where $\mathcal{Q}_i = 1 - \mathcal{P}_i$, and $\mathcal{P}_i = |A_i^\dagger)\frac{1}{\chi_i}(A_i|$ is the projection operator which projects the Liouville space onto the subspace spanned by A_i; $\mathcal{L}_0 = \mathcal{L}$, $\mathcal{L}_i = \mathcal{Q}_{i-1}\mathcal{L}_{i-1}\mathcal{Q}_{i-1}$, where $\mathcal{L}$ is the Liouville operator, i.e., $\mathcal{L}A = [H, A]$. For electrons it is clear that $\chi_0(\boldsymbol{k}) = 1$. So far equation (4) is exact. When the memory function $M_{n+1}(\boldsymbol{k}, \omega)$ is neglected, this approximation is equivalent to restricting the dynamics of the system to a relevant subspace spanned by $\{A_0, A_1...A_n\}$. The memory function $M_{n+1}(\boldsymbol{k}, \omega)$ thus contains all corrections of the remaining subspace. In systems with local interaction, the self-energy $\Sigma(\boldsymbol{k}, \omega)$ depends only on frequency in the limit $D \to \infty$ [6]. Consequently, the lattice model can be mapped onto a single site embedded in a self-consistent medium. In the limit $D \to \infty$ one must also expect that all susceptibility and frequency functions (except for $\Omega_0(\boldsymbol{k})$) are constant in momentum space, and the memory function $M_{n+1}(\boldsymbol{k}, \omega)$ depends only on frequency. However, this no longer happens in systems with nonlocal interactions. In the presence of nonlocal interactions, the susceptibility, frequency and memory functions depend on momentum even at the limit $D \to \infty$. Our approach is to approximate the memory function $M_{n+1}(\boldsymbol{k}, \omega)$ by a local function $M_{n+1}(\omega)$, but to keep the momentum dependence of susceptibility and frequency function $(\chi_i(\boldsymbol{k}), \Omega_i(\boldsymbol{k}))$. This approximation includes nonlocal contributions of the relevant subspace, but neglects those of the remaining subspace. We expect that the nonlocal corrections of the remaining subspace give only negligible effects. Indeed, enlarging the relevant subspace, we are able to include next nonlocal corrections of the remaining subspace. Our approach coincides with the DMFA if the relevant subspace is chosen to be spanned by only A_0. The function $M_{n+1}(\omega)$ together with the susceptibility and frequency functions are then determined by solving a self-consistently embedded cluster. The self-consistently determined medium is constructed in such way that the cluster Green function obtained by solving the effective problem coincides with that of the original lattice. The size of the cluster is chosen according to nonlocal correlation quantities appearing in the problem. If we restrict the consideration to nearest-neighbour interactions then we can choose a self-consistently embedded cluster consisting of two nearest-neighbour sites.

In what follows we will restrict the relevant subspace to $\{A_0, A_1\}$. When the memory function is neglected, the restriction corresponds to the two-pole approximation [24]. Recently, strong-coupling calculations based on an improved two-pole approximation show a quite reasonable agreement with quantum Monte Carlo results [25]. In the homogeneous phase we obtain

$$\begin{aligned}
\chi_0(\boldsymbol{k}) &= 1 \\
\chi_1(\boldsymbol{k}) &= n_f(1-n_f)[(U+t'\gamma_{\boldsymbol{k}})^2 + zt'^2] \\
\Omega_0(\boldsymbol{k}) &= \varepsilon_{\boldsymbol{k}} - \mu + Un_f \\
\Omega_1(\boldsymbol{k}) &= W(\boldsymbol{k}) - \mu + U(1-n_f)
\end{aligned}$$

where $n_f = 1/N\sum_i \langle f_i^\dagger f_i\rangle$, N is the number of lattice sites, z is the lattice number (for a square lattice $z = 2D$), and

$$W(\boldsymbol{k}) = \frac{2zt'(t'-t)(U+t'\gamma_{\boldsymbol{k}}) - z(1-2n_f)Ut'^2}{(U+t'\gamma_{\boldsymbol{k}})^2 + zt'^2}. \tag{6}$$

Here we have neglected all contributions of order $1/D$ and higher. The self-energy in our approach is approximated to

$$\Sigma(\boldsymbol{k},\omega) = Un_f + 2n_f t'\gamma_{\boldsymbol{k}} + \frac{\chi_1(\boldsymbol{k})}{\omega - \Omega_1(\boldsymbol{k}) - M_2(\omega)}. \tag{7}$$

The first two terms in equation (7) are the Hartree terms. Within the Hartree approximation the correlated hopping modifies the single-particle dynamics of the conduction electrons only via the renormalization of the static single-particle hopping amplitude according to $t \to t - 2n_f t'$. Hence in the DMFA, where the correlated hopping is treated in the Hartree approximation, the dynamics of the conduction electrons is basically the same as in the absence of the correlated hopping. The last term in equation (7) is beyond the DMFA. It reflects the dynamical effect of the correlated hopping even in the absence of the onsite interaction U. If we neglect $\Omega_1(\boldsymbol{k})$ then the self-energy (7) basically reduces to that obtained by Schiller [7]. However, $\Omega_1(\boldsymbol{k})$ plays an important role in preserving the sum rules of the spectral function and its moments. It can be proved that the self-energy (7) preserves the sum rules of the first three spectral moments, provided the memory function $M_2(\omega) \sim 1/\omega$ when $\omega \to \infty$. Indeed, since $M_2(\omega) \sim 1/\omega$ as $\omega \to \infty$, one can write the memory function in the form $M_2(\omega) = \sum_{n=0}^{\infty} \alpha_n/\omega^{n+1}$. Expanding the Green function in the powers of $1/\omega$ we obtain

$$G(\boldsymbol{k},\omega) = \frac{1}{\omega} + \frac{m_1(\boldsymbol{k})}{\omega^2} + \frac{m_2(\boldsymbol{k})}{\omega^3} + \frac{m_3(\boldsymbol{k})}{\omega^4} + O\Big(\frac{1}{\omega^5}\Big) \tag{8}$$

where

$$\begin{aligned}
m_1(\boldsymbol{k}) &= \Omega_0(\boldsymbol{k}) \\
m_2(\boldsymbol{k}) &= \Omega_0^2(\boldsymbol{k}) + \chi_1(\boldsymbol{k}) \\
m_3(\boldsymbol{k}) &= \Omega_0^3(\boldsymbol{k}) + 2\Omega_0(\boldsymbol{k})\chi_1(\boldsymbol{k}) + \chi_1(\boldsymbol{k})\Omega_1(\boldsymbol{k}).
\end{aligned}$$

The quantities $m_n(\boldsymbol{k})$ ($n = 1, 2, 3$) above are the first three moments of the spectral functions, i.e.,

$$m_n(\boldsymbol{k}) = \int \mathrm{d}\,\omega\omega^n A(\boldsymbol{k},\omega), \tag{9}$$

where $A(\boldsymbol{k},\omega) = (-1/\pi)\mathrm{Im}G(\boldsymbol{k},\omega + \mathrm{i}0^+)$ is the spectral function. By direct calculations one can show that $m_n(\boldsymbol{k}) = \big(c_{\boldsymbol{k}}\big|\mathcal{L}^n c_{\boldsymbol{k}}^\dagger\big)$. Therefore the sum rules of the first three spectral moments are preserved. Enlarging the relevant subspace, we are able not only to improve the approximation but also to fulfil the sum rule of spectral moments of higher orders. The memory

function $M_2(\omega)$ is determined by solving an effective model of two nearest-neighbour sites embedded in a self-consistently determined medium. This effective model can be constructed by the following action:

$$\begin{aligned} S = & \int_0^\beta \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \widehat{X}^\dagger(\tau)\widehat{\mathcal{G}}^{-1}(\tau-\tau')\widehat{X}(\tau') \\ & + U\int_0^\beta \mathrm{d}\tau c_1^\dagger(\tau)c_1(\tau)f_1^\dagger(\tau)f_1(\tau) + U\int_0^\beta \mathrm{d}\tau c_2^\dagger(\tau)c_2(\tau)f_2^\dagger(\tau)f_2(\tau) \\ & + (\varepsilon_f-\mu)\int_0^\beta \mathrm{d}\tau (f_1^\dagger(\tau)f_1(\tau)+f_2^\dagger(\tau)f_2(\tau)) \\ & + t'\int_0^\beta \mathrm{d}\tau (c_1^\dagger(\tau)c_2(\tau)+c_2^\dagger(\tau)c_1(\tau))(f_1^\dagger(\tau)f_1(\tau)+f_2^\dagger(\tau)f_2(\tau)) \end{aligned} \tag{10}$$

where $\widehat{X}^\dagger=(c_1^\dagger, c_2^\dagger)$. Here $\widehat{\mathcal{G}}(\tau)$ plays the role of the effective medium. It is determined by the self-consistently determined condition which requires that the cluster Green function obtained by (10) coincides with that of the original lattice, i.e.,

$$G_{11}(\omega) = \frac{1}{N}\sum_{\boldsymbol{k}} G(\boldsymbol{k},\omega), \tag{11}$$

$$G_{12}(\omega) = \frac{1}{N}\sum_{\boldsymbol{k}} G(\boldsymbol{k},\omega)\mathrm{e}^{-\mathrm{i}\boldsymbol{k}(\boldsymbol{R}_1-\boldsymbol{R}_2)} \tag{12}$$

(and similarly for other matrix elements of $\widehat{G}(\omega)$). Here $\widehat{G}(\omega) = \langle\langle \widehat{X}|\widehat{X}^\dagger\rangle\rangle_\omega$. The self-consistently determined conditions (11), (12) guarantee that the local and nearest-neighbour-site Green functions are unchanged when the original lattice is replaced by the cluster embedded in the effective medium. The effective model (10) can be solved exactly. Indeed, the four sectors of Hilbert space $\{\widehat{n}_1^f = 0,\ \widehat{n}_2^f = 0\}$, $\{\widehat{n}_1^f = 1,\ \widehat{n}_2^f = 0\}$, $\{\widehat{n}_1^f = 0,\ \widehat{n}_2^f = 1\}$, $\{\widehat{n}_1^f = 1,\ \widehat{n}_2^f = 1\}$ evolve independently under dynamics defined by (10). Therefore we obtain

$$\widehat{G}(\omega) = \frac{w_0}{\widehat{\mathcal{G}}^{-1}(\omega)} + \frac{w_1}{\widehat{\mathcal{G}}^{-1}(\omega)-\widehat{T}_1} + \frac{w_1}{\widehat{\mathcal{G}}^{-1}(\omega)-\widehat{T}_2} + \frac{w_2}{\widehat{\mathcal{G}}^{-1}(\omega)-\widehat{T}_3} \tag{13}$$

where

$$\widehat{T}_1 = \begin{pmatrix} U & t' \\ t' & 0 \end{pmatrix} \qquad \widehat{T}_2 = \begin{pmatrix} 0 & t' \\ t' & U \end{pmatrix} \qquad \widehat{T}_3 = \begin{pmatrix} U & 2t' \\ 2t' & U \end{pmatrix}.$$

Factors w_i $(i = 0, 1, 2)$ are defined by

$$w_i = \frac{\mathcal{Z}_i}{\mathcal{Z}} \tag{14}$$

where

$$\mathcal{Z}_0 = 2\exp\left\{\sum_n \mathrm{Tr}[\ln\widehat{\mathcal{G}}^{-1}(\mathrm{i}\omega_n) - \ln(\mathrm{i}\omega_n)]\mathrm{e}^{\mathrm{i}\omega_n 0^+}\right\}$$

$$\mathcal{Z}_1 = 2\exp\left\{-\beta(\varepsilon_f-\mu) + \sum_n \mathrm{Tr}[\ln\{\widehat{\mathcal{G}}^{-1}(\mathrm{i}\omega_n) - \widehat{T}_1\} - \ln(\mathrm{i}\omega_n)]\mathrm{e}^{\mathrm{i}\omega_n 0^+}\right\}$$

$$\mathcal{Z}_2 = 2\exp\left\{-\beta(\varepsilon_f-\mu) + \sum_n \mathrm{Tr}[\ln\{\widehat{\mathcal{G}}^{-1}(\mathrm{i}\omega_n) - \widehat{T}_3\} - \ln(\mathrm{i}\omega_n)]\mathrm{e}^{\mathrm{i}\omega_n 0^+}\right\}$$

and $\mathcal{Z} = \mathcal{Z}_0 + 2\mathcal{Z}_1 + \mathcal{Z}_2$. The self-energy is then determined as usual through

$$\widehat{\Sigma}(\omega) = \widehat{\mathcal{G}}^{-1}(\omega) - \widehat{G}^{-1}(\omega) \tag{15}$$

where

$$\Sigma_{11}(\omega) = \frac{1}{N}\sum_{\boldsymbol{k}} \Sigma(\boldsymbol{k},\omega)$$

$$\Sigma_{12}(\omega) = \frac{1}{N}\sum_{\boldsymbol{k}} \Sigma(\boldsymbol{k},\omega)\mathrm{e}^{-\mathrm{i}\boldsymbol{k}(\boldsymbol{R}_1-\boldsymbol{R}_2)}.$$

The memory function can thus be expressed via the self-energy. Together with equation (7) we obtain

$$M_2(\omega) = \omega + \mu - U(1-n_f) + \frac{(U^2+8t'^2)n_f(1-n_f)}{\Sigma_{11}(\omega) - Un_f}. \tag{16}$$

Here we have neglected all terms of order $1/D$ and higher. Equations (3), (7), (13)–(16) form the self-consistent system of equations for the Green function. It gives explicitly the nonlocal term to the self-energy. We will solve the system of equations by numerical iterations.

3. Numerical results

In what follows we will use t as the unit of energy. We will consider only the homogeneous phase with $n_f = 1/2$ and $\mu = U/2$ at temperature $T = 1$. We solve the above self-consistent equations by iterations in both real and Matsubara frequencies. The equations for the Matsubara frequencies are easily obtained from those of the real frequency by simply replacing ω by $\mathrm{i}\omega_n$, where $\omega_n = (2n+1)\pi T$.

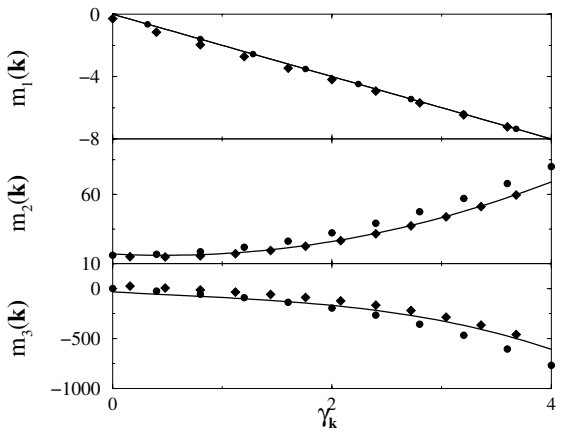

Figure 1. The moments of the spectral function for $U = 8$, $t' = -1$. The filled diamonds are results obtained by the present method, the open circles are those of the DMFA.

The algorithm for solving the self-consistent equations is as follows. (i) Begin with an initial memory function $M_2(\omega)$ (we chose either $M^{\mathrm{init}}(\omega) = 0$ or the Hartree–Fock approximation $M^{\mathrm{init}}(\omega)$). (ii) Next use equation (7) to find $\Sigma(\boldsymbol{k},\omega)$. (iii) Use equation (3) to compute $G(\boldsymbol{k},\omega)$ and together with equations (11) and (12) to compute also the cluster Green function $\widehat{G}(\omega)$. (iv) Determine $\widehat{\mathcal{G}}(\omega)$ from $\widehat{\Sigma}(\omega)$ and $\widehat{G}(\omega)$ by equation (15). (v) Repeat the above steps for Matsubara frequencies and compute the factors w_i by equation (14). (vi) Next, using equation (13) to compute new $\widehat{G}(\omega)$, and using this new $\widehat{G}(\omega)$ and $\widehat{\mathcal{G}}(\omega)$ to determine

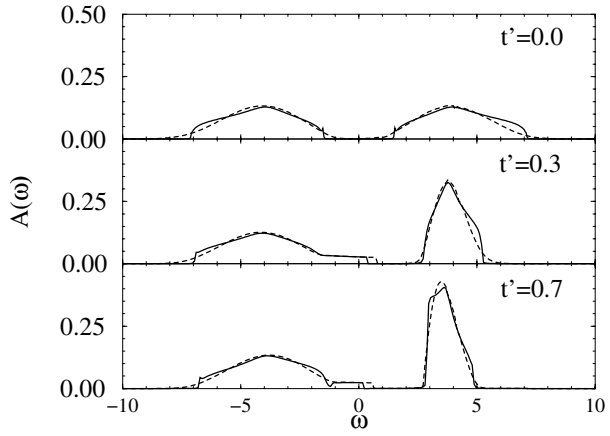

Figure 2. The DOS $A(\omega)$ of the conduction electrons for $U = 8$. The solid lines are the DOS in 2D, while the dashed ones are the DOS in infinite dimensions.

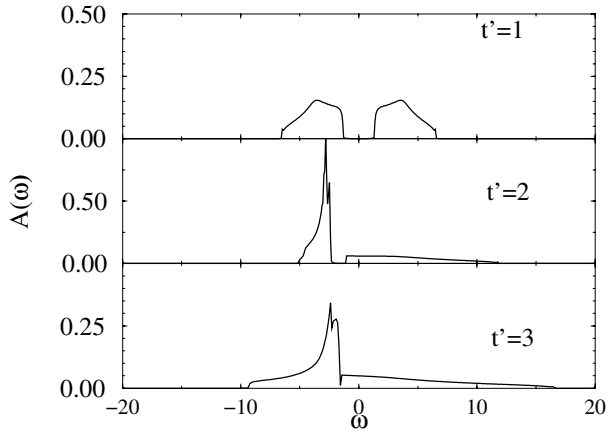

Figure 3. The DOS $A(\omega)$ of the conduction electrons for various positive t' ($U = 8$, $T = 1$).

$\widehat{\Sigma}(\omega)$ by equation (15), determine $M_2(\omega)$ by equation (16). Repeat also this step for Matsubara frequencies. (vii) Go back to step (ii) and repeat the iteration until convergence is reached.

We have obtained a relative error of less than 10^{-4} for the Green function in all our calculations. The sum rule for the spectral function is always fulfilled with error less than 10^{-2}. We compute also the first three moments of the spectral function and check them with their exact values.

In figure 1 we plot the first three moments of the spectral function. It shows that both DMFA and our approach satisfy the sum rule of the first-order moment. However, the DMFA does not satisfy the sum rules of the second- and third-order moments. At the same time in our approach the second- and third-order moments fit very well with their exact values. As noticed by Potthoff *et al* [26], the first three moments provide important information on the spectral function that determine the centres of gravity, the width and weight of the Hubbard

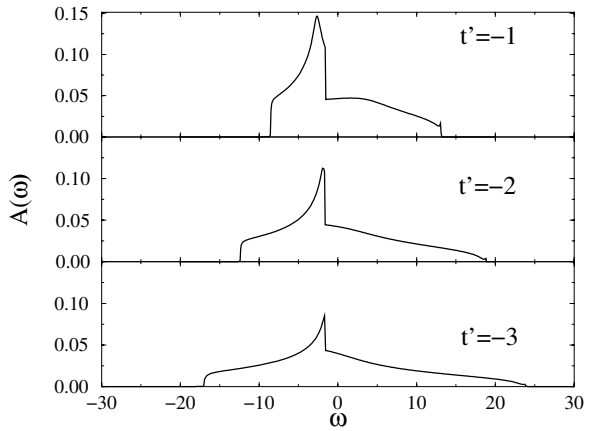

Figure 4. The DOS $A(\omega)$ of the conduction electrons for various negative t' ($U = 8$, $T = 1$).

bands. Therefore our approach is able to include important correlation effects due to the onsite interaction U and correlation hopping. This is an advantage of the present method.

In figures 2–4 we present the evolution of the density of state (DOS) when $|t'|$ increases. We have chosen $U = 8$, such that the system is an insulator when correlated hopping is absent (i.e. $t' = 0$). Since the present approach is justified in the infinite-dimensional limit, we have compared the DOS in 2D and in infinite dimension. In figure 2 we plot the comparison. It shows that the results in the two cases are similar. Indeed, we have neglected all contributions of order $1/D$ and higher to the susceptibility and frequency functions, hence the results should be expected. When $0 < t' < t$ the system becomes metallic as in figure 2 . In this value range of t', the lower band expands toward to the Mott–Hubbard gap, such that the gap is partially filled. As a consequence the chemical potential lies within the lower band, therefore the system is metallic although the Mott–Hubbard gap still exists. When $t' = t$ the system is again an insulator. When $t' > t$ the system becomes metallic again. However, the scenario is different in comparison with the case of $0 < t' < t$. In this case, when $t' > t$, the upper band is widened to the Mott–Hubbard gap, such that the two Hubbard bands merge into one broad band. In figure 4 we plot the DOS for negative t'. When $t' < 0$ the DOS does not split into two bands, hence the system is always in the metallic phase. This feature reflects the increase in the kinetic energy of the conduction electrons. However, this increase of the kinetic energy is not simply absorbing correlated hopping t' into an effective Hartree renormalization of the single-particle hopping within the standard FKM. We also notice that with the presence of correlated hopping the electron–hole symmetry is broken except for $t' = t$. The above behaviours of the DOS show complicated influences of correlated hopping on the spectral properties of the system. Our results qualitatively agree with those of a large-dimensional study [7]. However, we want to emphasize that the present approach has the advantage that the sum rules of first few moments of the spectral function are fulfilled.

In conclusion, we have considered the effect of correlated hopping in the FKM. Within the extended DMFA, correlated hopping introduces nonlocal self-energy components that retain full dynamics even in the absence of the onsite Coulomb interaction. We have shown that the sum rules of the spectral function and its moments are preserved. The spectral function obtained shows a significant nonlocal effect of correlated hopping on the spectral function, which is absent in the DMFA.

Acknowledgments

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