

Cluster-dynamical mean-field theory of the density-driven Mott transition in the one-dimensional Hubbard model

M. Capone,¹ M. Civelli,² S. S. Kancharla,^{2,3} C. Castellani,⁴ and G. Kotliar²¹*Enrico Fermi Center, Rome, Italy*²*Physics Department and Center for Materials Theory, Rutgers University, Piscataway, New Jersey, USA*³*Département de physique and Regroupement québécois sur les matériaux de pointe, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1*⁴*Physics Department, University of Rome "La Sapienza," and INFM Center for Statistical Mechanics and Complexity, Piazzale A. Moro 5, I-00185 Rome, Italy*

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The one-dimensional Hubbard model is investigated by means of two different cluster schemes suited to introduce short-range spatial correlations beyond the single-site dynamical mean-field theory, namely, the cellular dynamical mean-field theory, which does not impose the lattice symmetries, and its periodized version in which translational symmetry is recovered. It is shown that both cluster schemes are able to describe with extreme accuracy the evolution of the density as a function of the chemical potential from the Mott insulator to the metallic state. Using exact diagonalization to solve the cluster-impurity model, we discuss the role of the truncation of the Hilbert space of the bath, and propose an algorithm that gives higher weights to the low-frequency hybridization matrix elements and improves the speed of the convergence of the algorithm.

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I. INTRODUCTION

Strongly correlated electronic systems and the models describing them represent a formidable challenge for theorists. An important advance in this field has been achieved through the development of the dynamical mean-field theory (DMFT),¹ in its single-site version. DMFT is a nonperturbative approach which fully retains local quantum dynamics, but simplifies the spatial dependence of the correlation functions to make the problem tractable. The lattice problem is therefore mapped onto a dynamical local problem, and consequently onto an impurity model subject to a self-consistency relation. The DMFT proved its power by providing the first unified scenario for the longstanding problem of the Mott transition in the Hubbard model, and completely characterizing the peculiar criticality associated with this transition. Numerous theoretical predictions of this approach have been verified experimentally.² The combination of single-site DMFT with electronic structure methods has given new insights into the physical properties of many correlated materials. The main limitation of DMFT is the neglect of spatial correlation in the one-electron spectra, which makes it impossible to treat phases with definite spatial ordering such as *d*-wave superconductivity. Nonlocal effects, such as short-range order, can also be very important in describing the metal-insulator transition in materials such as Ti₂O₃.³

There is therefore a strong motivation for developing extensions of single-site DMFT. Several schemes have been proposed, and they introduce short-range correlations by replacing the single impurity model with a cluster-impurity, containing N_c sites with a given spatial arrangement. The dynamical cluster approximation⁴ consists in a systematic inclusion of a few lattice momenta, which would correspond to the lattice momenta of an N_c -site cluster. From the impu-

urity models point of view, this approach requires periodic boundary conditions on the cluster.⁴ A different approach uses a continuous interpolation of the self-energy in momentum space in the self consistency condition.⁵ An alternative cluster method, the cellular dynamical mean-field theory (CDMFT), has been proposed in Refs. 6 and 7, closely following the spirit of the DMFT. In this approach, the cluster has open boundary conditions, and a "local" theory for the cluster degrees of freedom is obtained through the cavity method. The basic approximation is to assume that the dynamical field experienced by the cluster is Gaussian. A modification of the CDMFT scheme, the periodized-CDMFT (PCDMFT),⁸ enforces the lattice periodicity at every iteration. Both PCDMFT and CDMFT have been proved to give causal spectral functions.⁸

In this work we focus on the CDMFT and PCDMFT and study their performance in the one-dimensional Hubbard model, which is the worst case scenario for every mean-field theory. The ability of CDMFT to capture the physics of the Mott insulating state in one dimension has been already demonstrated in Ref. 9, where the half-filled Hubbard chain was correctly found to be an insulator for every value of U , with a Mott-Hubbard gap which closely follows the Bethe Ansatz (BA) exact solution.¹⁰ Here we extend the analysis of Ref. 9 to the doped metallic state, and compare CDMFT and PCDMFT to the BA results for the whole density range and different values of the interaction strength. This is a much more stringent test of the method, since metallic states, with gapless excitations, are more difficult to describe with a reduced number of sites than insulators. One goal of the investigation is to compare the performance of CDMFT and PCDMFT, with an eye to future applications. As in Ref. 9, we use exact diagonalization to solve the cluster-impurity model. A nontrivial issue is how to discretize the bath to implement the solution of the cluster-impurity model by exact diagonalization. This problem was considered in Refs. 11 and 12 in

the context of single-site DMFT, and, more recently, by Potthoff in the context of cluster methods using a functional technique.¹³ Here we find that a simple modification of the notion of distance in the algorithm of Ref. 11 improves dramatically the quality and the convergence of the results. The paper is organized as follows: Sec. II introduces the model and our theoretical tools, Sec. III presents our results, and Sec. IV is dedicated to the conclusions.

II. MODEL AND METHOD

We consider the one-dimensional Hubbard model

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i, \quad (1)$$

where $c_{i,\sigma}$ ($c_{i,\sigma}^\dagger$) are destruction (creation) operators for electrons of spin σ , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the density of σ -spin electrons, t is the hopping amplitude, U is the on-site repulsion, and μ denotes the chemical potential.

Within cluster DMFT methods an effective action for the cluster degrees of freedom is defined as

$$S^{eff} = \int_{-\beta}^{\beta} d\tau d\tau' \sum_{\mu\nu\sigma} c_{\mu\sigma}^\dagger(\tau) \mathcal{G}_{\mu\nu\sigma}^{-1}(\tau - \tau') c_{\nu\sigma}(\tau') + \int_{-\beta}^{\beta} d\tau \sum_{\mu=1}^{N_c} U n_{\mu\uparrow}(\tau) n_{\mu\downarrow}(\tau), \quad (2)$$

where $\mathcal{G}_{\mu\nu\sigma}^{-1}$ is a Weiss dynamical field and $\mu, \nu = 1, \dots, N_c$ are indices of sites in the cluster. The action for the cluster degrees of freedom can be derived, in close analogy with DMFT, by means of the cavity construction, i.e., by integrating out the degrees of freedom of all the fermions except the ones in the cluster, and assuming that the dynamical field due to the other sites is Gaussian.⁶ The cluster has therefore naturally open boundary conditions, as opposed to the periodic boundary conditions of the dynamical cluster approximation,⁴ and breaks the translational symmetry. In practical implementations of this approach, the initial dynamical Weiss field is specified by the choice of a given $\mathcal{G}_{\mu\nu\sigma}^{-1}$. The effective action is then solved with some technique, providing the cluster Green's function $G_{\mu\nu\sigma}(\tau) = -\langle T_\tau c_{\mu\sigma}(\tau) c_{\nu\sigma}^\dagger \rangle$. Consequently, the cluster self-energy is obtained (dropping the spin index to simplify the notations) as

$$\Sigma_{\mu\nu}^c(i\omega_n) = \mathcal{G}_{\mu\nu}^{-1}(i\omega_n) - G_{\mu\nu}^{-1}(i\omega_n). \quad (3)$$

Just like the single-site DMFT, a cluster-DMFT scheme is completed by self-consistence relation which allows to determine a new Weiss field through the knowledge of the Green's function. The two methods we compare in this paper differ in the way this self-consistency is implemented.

A. CDMFT method

Within CDMFT the cluster self-energy (3) is used to compute the $N_c \times N_c$ matrix of local Green's function for the cluster, given by

$$\hat{G}^{loc}(i\omega_n) = \int_{-\pi/N_c}^{\pi/N_c} \frac{1}{-\pi/N_c(i\omega_n + \mu) \hat{\mathbf{1}} - \hat{t}_k - \hat{\Sigma}^c(i\omega_n)} \frac{dk}{2\pi/N_c}, \quad (4)$$

where the hat labels $N_c \times N_c$ matrices, the momentum integral extends on the reduced Brillouin zone associated to the N_c -site cluster, \hat{t}_k is the Fourier transform of the cluster hopping term,⁹ and $\hat{\mathbf{1}}$ is the $N_c \times N_c$ unit matrix. $G_{loc}(i\omega_n)$ and $\Sigma^c(i\omega_n)$ are then used to obtain a new Weiss field

$$(\mathcal{G}^{new})_{\mu\nu}^{-1}(i\omega_n) = \Sigma_{\mu\nu}^c(i\omega_n) + (G^{loc})_{\mu\nu}^{-1}(i\omega_n), \quad (5)$$

which determines the new effective action (2), from which a new cluster Green's function $G_{\mu\nu}(i\omega_n)$ is obtained and the procedure is iterated until convergence. As noticed above, in this approach the cluster is naturally taken with open boundary conditions, and breaks the full lattice translational invariance. As a consequence, the different sites in the cluster are not equivalent, and the local Green's functions on different sites may be different.

B. PCDMFT method

The lack of translational invariance of the CDMFT may be seen as a limitation of this method. The main idea of the PCDMFT approach is therefore to reintroduce the translational invariance in the CDMFT scheme without imposing periodic boundary conditions on the cluster, as it is done within the dynamical cluster approximation.⁴ The first step of PCDMFT is to compute a lattice self-energy with full lattice translational invariance by *periodizing* the cluster self-energy defined in Eq. (3),

$$\Sigma(k, i\omega_n) = \frac{1}{N_c} \sum_{\mu\nu} e^{ikR_\mu} \Sigma_{\mu\nu}^c(i\omega_n) e^{-ikR_\nu}, \quad (6)$$

where R_μ is the position vector of site μ . Note that the derivation of the lattice self-energy is not unique, and alternative estimators have been proposed in Ref. 7. The lattice self-energy naturally defines a translationally invariant lattice Green's function

$$G(k, i\omega_n) = \frac{1}{i\omega_n + \mu - t_k - \Sigma(k, i\omega_n)}, \quad (7)$$

where t_k is the Fourier transform of the hopping part of the Hamiltonian. The key of PCDMFT is to compute the local Green's function for the cluster degrees of freedom by *projecting* back the translationally invariant Green's function (7) onto the cluster sites. The PCDMFT approximation for the local Green's function of the cluster is therefore given by

$$G_{\mu\nu}^{loc}(i\omega_n) = \int_{-\pi}^{\pi} e^{-ikR_\mu} G(k, i\omega_n) e^{ikR_\nu} \frac{dk}{2\pi}. \quad (8)$$

Finally, exactly as in CDMFT, Eq. (5) is used to obtain a new Weiss field and continue the iterative procedure. We emphasize again that the only difference between CDMFT and PCDMFT is in the way the local Green's function is computed from the cluster self-energy, i.e., in the difference between Eq. (4) and Eq. (8). The latter equation partially reintroduces the full lattice symmetry at each iteration. Finally, it must be noted that, as shown in Ref. 8, both the CDMFT and PCDMFT methods are causal, i.e., they produce self-energies with a negative imaginary part.

C. Exact Diagonalization

Besides the self-consistency defined by the above equations, the CDMFT requires a solution of the cluster action (2) and the evaluation of the Green's function. For practical purposes, it is useful to resort to a Hamiltonian formulation, where the quantum fluctuations on the lattice are realized by hybridization with a conduction bath. This leads to a cluster-impurity Hamiltonian of the form

$$\mathbf{H}_{ACI} = \sum_{\mu\nu\sigma} E_{\mu\nu} c_{\mu\sigma}^{\dagger} c_{\nu\sigma} + U \sum_{\mu} n_{\mu\uparrow} n_{\mu\downarrow} + \sum_{k\sigma} \varepsilon_k a_{k\sigma}^{\dagger} a_{k\sigma} + \sum_{k\mu\sigma} (V_{k,\mu} a_{k\sigma}^{\dagger} c_{\mu\sigma} + \text{H.c.}), \quad (9)$$

where the indices $\mu, \nu = 1, \dots, N_c$ label the cluster sites, $E_{\mu\nu}$ contains the hopping matrix elements inside the cluster and the chemical-potential term. The auxiliary fermionic degrees of freedom $a_{k\sigma}$ describe the bath. Integrating out the bath degrees of freedom $a_{k\sigma}$ we obtain an action of the form (2) with

$$\mathcal{G}_{\mu\nu}^{-1}(i\omega_n) = i\omega_n \delta_{\mu\nu} - E_{\mu\nu} - \sum_k \frac{V_{k,\mu}^* V_{k,\nu}}{i\omega_n - \varepsilon_k}, \quad (10)$$

$\delta_{\mu\nu}$ being the Kronecker delta.

As discussed in Refs. 11 and 12 and more recently in Ref. 13, to implement the DMFT equations using an exact diagonalization solver, it is necessary to discretize the problem by parametrizing the hybridization function in terms of a finite number of poles. Hence the hybridization function [last term in Eq. (10)] is approximated by

$$\sum_{k_i} \frac{V_{k_i,\mu}^* V_{k_i,\nu}}{i\omega_n - \varepsilon_{k_i}}. \quad (11)$$

Here the sums run over a discrete set of $k_i = 1, \dots, N_b$. Note that in general several ε_{k_i} can be identical, i.e., the eigenvalues of the bath can be degenerate. Our numerical study shows that the self-consistency loop tends to create degenerate levels. In particular, we have found that each energy level is typically twofold degenerate for the two-site cluster $N_c = 2$. This result suggested us to simplify the parametrization assuming that each level in the bath has such a degeneracy. This simplified parametrization of the bath, which involves fewer parameters, typically makes the convergence of (P)CDMFT much faster (in terms of the number of iterations needed to reach a given threshold) and allows to easily reach

extremely accurate solution which respect the symmetries of the problem. This observation also suggests that some values of N_b should provide worse results than others for the only reason that they could not allow for the desired degeneracy. As an example, odd number of bath sites are not the best choice for the two-site cluster. For the $N_c = 3$ case, we still find that doubly degenerate energy levels spontaneously develop in the iterative process, even if the practical advantage of the degeneracy is much smaller than for $N_c = 2$. Further investigation of larger N_c clusters is needed to fully understand the origin of the degeneracy.

We emphasize that the above discussed truncation of the bath is the only approximation introduced in the exact diagonalization approach to (C)DMFT. At each iteration, the Weiss field given by Eq. (5) must be projected on the functional space defined by Eq. (10). In practice, the parameters ε_k and V_{k_i} which minimize a difference Δ between Eq. (5) and Eq. (10) are used in the next iterations. What is the optimal criteria for the choice of these poles has been discussed in the literature, where different criterias have been used. In this work we describe a simple modification of the criteria proposed in Ref. 11 which substantially improves the convergence of the algorithm. We see that a proper definition of the difference is crucial as far as the convergence with increasing bath size is concerned. The substantial independence of the results on N_b (beyond a minimum value) observed in Ref. 9 is in fact attributed to a definition of functional distance which weighted too heavily the high-frequency region, and we propose an alternative definition of distance that eliminates this problem.

III. RESULTS

The one-dimensional Hubbard model represents an ideal benchmark for our cluster methods. On the one side we can compare with an exact solution, while on the other, we know that the single-site DMFT is not able to reproduce the Mott insulating state for arbitrarily small value of U and the divergence of the compressibility $\kappa = \partial n / \partial \mu$ approaching the Mott transition.¹⁴ In Ref. 9 the ability of CDMFT to reproduce the insulating state and the dependence of the Mott-Hubbard gap on U have been proven. Here we focus on the behavior of the density n as a function of the chemical potential μ and on the density-driven Mott transition.

The n - μ curves for $U/t=1$ and $U/t=4$ are reported in Figs. 1 and 2, respectively. The BA results are compared with single-site DMFT and (P)CDMFT for $N_c=2$ and $N_b=8$. In the weakly correlated case ($U/t=1$) the difference between the different methods is hardly noticeable in the plots, but it must be noted that the DMFT gives a metallic solution at half filling as opposed to the insulating exact solution which both CDMFT and PCDMFT correctly reproduce already for $N_c=2$. The more correlated $U/t=4$ case emphasizes the great improvement on DMFT brought by CDMFT. Besides the overall extremely good agreement with BA, CDMFT is in fact able to closely follow the compressibility divergence close to the Mott transition, which is missed by DMFT (upper-left inset of Fig. 2). PCDMFT is instead unable to capture this divergence, and gives a finite

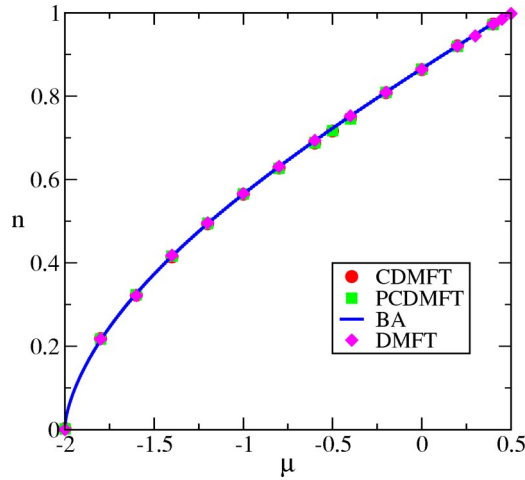


FIG. 1. Density n as a function of μ for $U/t=1$, $N_c=2$, $N_b=8$ within single-site DMFT, CDMFT, and PCDMFT compared with the exact solution.

compressibility, but it becomes more and more accurate in the extremely doped region ($n \leq 0.5$) due to the explicit reinforcement of lattice periodicity (lower-right inset of Fig. 2). The comparison between the two methods, as well as the dependence of the results on the number of bath sites, is made more quantitative in Fig. 3, where the deviation from the exact density is shown for different methods and bath sizes for $U/t=4$. Not surprisingly, for both techniques, the results improve as N_b is increased. In the region close to the Mott-Hubbard transition the CDMFT results nicely approach the exact solution with $\kappa \rightarrow \infty$ as N_b is increased, while for the PCDMFT the improvement with bath size is not able to reproduce this feature. Deep in the metallic phase both techniques become extremely accurate, but the PCDMFT is typically better for $n \leq 0.5$. As an example for $N_c=2$ and $N_b=8$, the PCDMFT error on the density for $\mu = -0.5$ ($n \approx 0.555$) is 6×10^{-4} , while for CDMFT it is 1×10^{-3} (see the lower-right inset of Fig. 2). In both cases N_b is small as

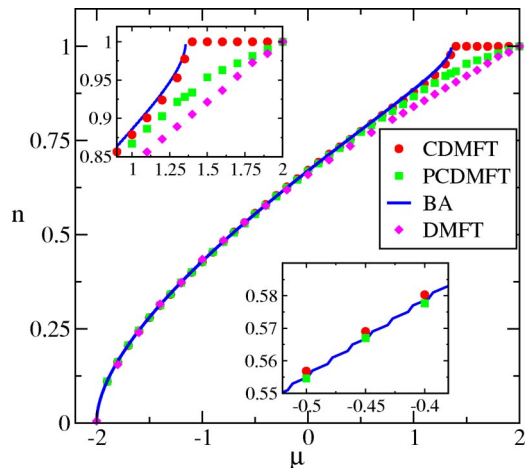


FIG. 2. Density n as a function of μ for $U/t=4$, $N_c=2$, $N_b=8$. The upper-left inset shows a closeup of the region close to half filling, and the lower-right inset shows a region deep in the metallic regime.

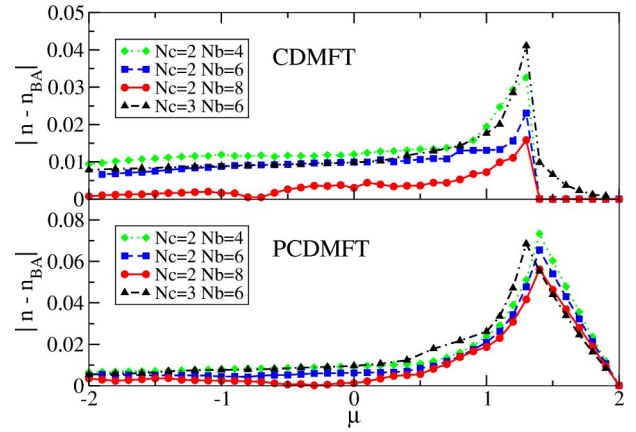


FIG. 3. Deviations between the CDMFT and PCDMFT densities n with respect to the exact solution (BA) for $U/t=4$. In the upper/lower panel we show CDMFT/PCDMFT for different bath and cluster sizes (see legend).

6 or 8 is sufficient to achieve remarkable accuracy. We also show results for $N_c=3$ and $N_b=6$. In this case, even if the cluster size is increased with respect to $N_c=2$, the method has some slight problems due to the odd number of sites, which results in a final critical value of U/t for the Mott transition (even if extremely reduced with respect to DMFT) and a worse agreement with exact results close to the Mott transition. However, moving to the metallic state, the results rapidly approach the exact solution as well as the $N_c=2$ ones.

We note that the expected improvement of results with bath size that we have found was not observed in Ref. 9. We attribute this difference to the more efficient way to discretize the bath we use in this work. More precisely, we use a different definition of distance between the continuous and the discretized Weiss fields that gives more weight to the low Matsubara frequencies which are important to determine low-energy physics, namely, $\Delta = \sum_\nu |\mathcal{G}^{n_s} - \mathcal{G}| / \omega_\nu$. We have checked that, using nonweighted differences and a large number of frequencies, as it was done in Ref. 9, the low-energy part of the spectrum has extremely small weight, and it is therefore almost irrelevant. In this case the inclusion of further bath sites, which would improve the low-energy part of the spectrum, is therefore basically irrelevant. We note in passing that the use of the weighted distance also favored an easier convergence of the iterations.

These considerations are also supported by the analysis of dynamical quantities. As in Ref. 9, we consider the imaginary part of the on-site Green's function G_{11} and the real part of the nearest-neighbor Green's function G_{12} on the Matsubara axis, which are plotted for $U/t=1$ and 7 and for $n=1$ (Fig. 4). Single-site DMFT, CDMFT, and the PCDMFT for $N_c=2$ and $N_b=8$ are compared with the results of density-matrix renormalization group (DMRG), a numerical approach which is known to provide basically exact results for one-dimensional systems (for more details on our calculation of dynamical properties with DMRG, see Ref. 9). The agreement of both CDMFT and PCDMFT with the virtually exact DMRG results is extremely good for $U/t=1$, where the previous CDMFT results of Ref. 9 were quite inaccurate. Inter-

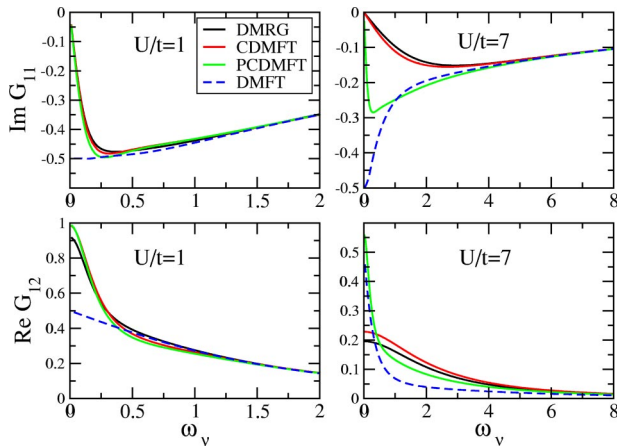


FIG. 4. Imaginary part of the local Green's function G_{11} and real part of nearest-neighbor Green's functions G_{12} for $n=1$. Single-site DMFT and two-site CDMFT and PCDMFT are compared with DMRG for $U/t=1$ (left) and $U/t=7$ (right).

estingly, the single-site DMFT completely fails in the description of dynamical properties even if the $n-\mu$ curve shown in Fig. 1 is close to the exact solution. In the strong coupling case $U/t=7$, CDMFT closely follows the DMRG, while PCDMFT is a poorer approximation, but still substantially better than the single-site DMFT. We also experienced some problem in obtaining converged PCDMFT solutions for $U/t>7$.

IV. CONCLUSIONS

We have tested the ability of CDMFT and PCDMFT to capture the physics of the one-dimensional Hubbard model both in the metallic and the insulating phase. While we expected cluster methods to give reasonable results for short-distance high-energy physical quantities, we found that both

methods are remarkably accurate for basically all the metallic densities, where the low-energy physics is important. The CDMFT method naturally generalizes DMFT to include short-range dynamical correlations within an open cluster of N_c sites, which breaks the full lattice translational symmetry. PCDMFT partially restores the translational symmetry without imposing periodic boundary conditions to the cluster. The CDMFT, already for $N_c=2$, is able to reproduce the divergent compressibility of the one-dimensional system when the Mott transition is approached, providing a qualitative change with respect to single-site DMFT. The PCDMFT, due to the restored translational invariance, gives slightly better results than CDMFT deep in the metallic regime (far from the Mott transition), where correlation effects are smaller, but fails in reproducing correctly the physics close to the Mott transition. The remarkably good results of CDMFT (either from the metallic to the insulating state) and of PCDMFT (in the metallic state only) are also due to a technical improvement in the truncation procedure of the bath hybridization function of the impurity problem. A systematic improvement of the accuracy of the results by increasing the bath size is observed. We also find that some degeneracy of the bath energy levels automatically develops if not explicitly imposed. Explicit enforcement of degenerate levels with the correct degeneracy strongly favors convergence and accuracy of the solutions. These methodological advances will be useful in further studies of more complex systems.

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