# Reply to "Comment on 'Cluster methods for strongly correlated electron systems' "

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We reply to the Comment by Aryanpour, Maier, and Jarrell [Phys. Rev. B **71**, 037101 (2005)] on our paper [Phys. Rev. B **65**, 155112 (2002)]. We demonstrate, using general arguments and explicit examples, that whenever the correlation length is finite, local observables converge exponentially fast in the cluster size $L_c$ within cellular dynamical mean field theory. This is a faster rate of convergence than the $1/L_c^2$ behavior of the dynamical cluster approximation, thus refuting the central assertion of their Comment.

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The development of cluster extensions of dynamical mean field theory is an active area of research. Cluster dynamical mean field theories construct approximations to the solution of model Hamiltonians on the lattice in terms of the solution of a cluster impurity model. Different cluster schemes should be viewed as different truncations of the full quantum many-body problem. As the size of the cluster tends to infinite, all cluster schemes approach the exact solution of the lattice model. A relevant question is, for a given computational power (which only allows the investigation of small cluster sizes), which truncation is closer to the result in the thermodynamic limit.

Our previous publication[1] investigated and extended two cluster schemes, the cellular dynamical mean field theory[2] (CDMFT) and the dynamical cluster approximation[3] (DCA), by applying them to an exact solvable model and concluded that CDMFT converges faster than DCA to the exact solution of that model. In their Comment,[4] Aryanpour *et al.* introduce a generalization of the original DCA equations that take into account better the nonlocal interaction, and they argue that their method converges faster than CDMFT to the exact solution of the model as the size of the cluster increases. They also comment that our findings of rapid convergence of CMDFT are surprising, in light of an earlier publication[5] in which they concluded that CDMFT converges to the infinite cluster size limit with corrections of order $O(1/L_c)$, where $L_c$ is the size of the cluster while DCA converges faster, with corrections of order $O(1/L_c^2)$.

In this Reply to their Comment we point out that *local observables* in CDMFT generally converge exponentially at finite temperatures, as long as the relevant correlation length is finite (a situation that excludes a critical point). This statement persists at zero temperature in systems which have an energy gap.

We demonstrate the exponential convergence of CDMFT in three steps. First, we present general arguments in favor of exponential convergence of local observables in CDMFT whenever the relevant correlation length is finite. This is a direct consequence of the cavity construction underlying the method. In the process we explain why the convergence criterion introduced in Ref. 5 and used to conclude that CDMFT converges as $1/L_c$ is not an appropriate measure of convergence of local observables in CDMFT, which instead converge much faster than a power law in $L_c$. Then, we present the numerical results for the SU($N$) spin chain studied in Ref. 1 that agree completely with our general arguments and we display explicitly an example of the exponential convergence in this model. Finally, we discuss another simple case, the semiclassical limit of the Falikov-Kimball model in one dimension. Previous work established[7] that in this limit quantum cluster approximations reduced to classical cluster approximations. This allows us to compare DCA and CDMFT in detail using simple analytical considerations. In particular, we unveil, in an explicit example, that the DCA predictions for local observables converge as $1/L_c^2$ even when the same quantities obtained solving a finite system of size $L_c$ (with for example periodic boundary condition) converge exponentially fast (in $L_c$) to their thermodynamic limit value.

Let us start with some general considerations. If one was able to trace out exactly all the degrees of freedom outside the cluster to get an exact effective action for the degrees of freedom inside the cluster, then the translation invariance of the effective action would be broken (degrees of freedom near the boundary of the cluster are affected by the enviroment more than the bulk degrees of freedom) but observables within the cluster would still be translationally invariant. So, on very general grounds we expect that the Weiss field (or hybridization function $\Delta$), which describes the effects of the degrees of freedom integrated out, is large near the boundary and small (in fact exponentially small if the correlation length is finite) inside the cluster.

CDMFT is an approximate way to realize this cavity construction. It produces a Weiss field which is large at the boundary and small in the bulk, but because of its approximate character it produces nontranslation invariant observables. However, whenever the correlation length is finite: (1) bulk quantities for a free system of size $L$ with, for example, free boundary conditions converge exponentially fast in $L$ to their thermodynamic limit and (2) the CDMFT approximation should improve the convergence of bulk quantities, which as a consequence should be at least as fast as the one of the system with free boundary conditions. Note that this is not the case of DCA that still converges as $1/L_c^2$ worse than the results for a finite system with, for example, free boundary conditions which would converge exponentially fast in

 

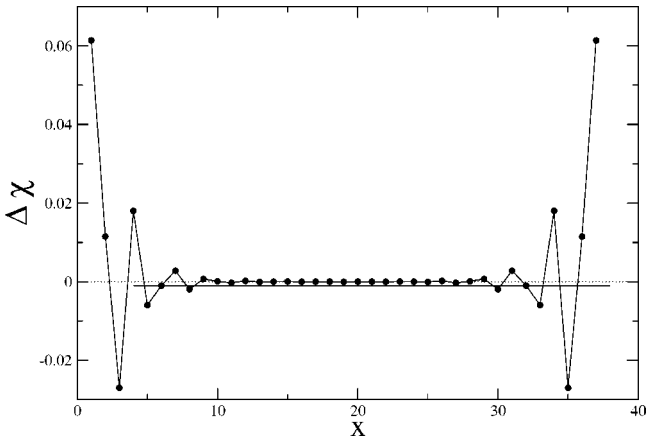


FIG. 1. $\Delta\chi=(\chi_x-\chi)/\chi$ as a function of $x$, for $\beta$, the inverse temperature, equal to 4, $L_c=38$, and $t=\mu=1$. The continuous line is the relative error of the DCA prediction on $\chi$. The dotted line is a guide for the eye.

$L_c$. We will discuss an explicit example of this behavior below.

Because CDMFT breaks the translation invariance inside the cluster it is important to extract properly the value of local observables. These are well represented in the center of the cluster (see Fig. 1), and will have more deviations near the boundary. The role of the cavity field is to try to reduce these deviations, but in approximate treatments there will always be errors of order 1 near the boundary. Aryanpour *et al.*[4] concluded the $1/L_c$ convergence by estimating the value of a local observable of interest by doing a flat average (of the value of the local observable) over the cluster. Since the error is of the order 1 on the boundary, one obtains an error that dies out as the ratio surface over volume of the cluster, i.e., $1/L_c$. On the other hand, if we extract this value from the center of the cluster, which is the natural prescription dictated by the approximate CDMFT cavity construction, we obtain exponential convergence as we show below.

We now turn to the simple one-dimensional SU($N$) chain studied in Ref. 1 whose Hamiltonian is

$$H=-t\sum_{i,\sigma}(f^{\dagger}_{i,\sigma}f_{i+1,\sigma}+f^{\dagger}_{i+1,\sigma}f_{i,\sigma}) + \frac{J}{2N}\sum_{i,\sigma,\sigma'}(f^{\dagger}_{i,\sigma}f_{i,\sigma'}f^{\dagger}_{i+1,\sigma'}f_{i+1,\sigma}+f^{\dagger}_{i+1,\sigma}f_{i+1,\sigma'}f^{\dagger}_{i,\sigma'}f_{i,\sigma}), \quad (1)$$

where $f$ are fermion operators, $i=1,\ldots,L$ and $\sigma=1,\ldots,N$, and we take the large $L$ and $N$ limits. This model is a generalization introduced by Affleck and Marston[6] of the Hubbard-Heisenberg model where the SU(2) spins are replaced by SU($N$) spins, the on-site repulsion is scaled as $1/N$, and the large $N$ limit is taken.

One can apply CDMFT and DCA to this model. Note, however, that because the interaction is nonlocal, there are different possible extensions of usual cluster methods to this case. We extended DCA in a way based on the real-space perspective,[1] Aryanpour *et al.* introduced a different generalization of DCA which takes into account better the nonlocal interactions. Our procedure is therefore not an incorrect application of DCA, as claimed by Aryanpour *et al.*, but only a different generalization of DCA to the case of nonlocal interaction. The results of the two different generalizations are discussed in Refs. 1 and 4, and in the following we shall focus on the generalization of Aryanpour *et al.*, which has been shown to converge to the thermodynamic limit with an error of the order of $1/L_c^2$ where $L_c$ is the size of the cluster. This rate of convergence is a general property of DCA,[5] at least far from critical points.

In the following we will use $J$ as the unit of temperature and therefore we put $J=1$ and we rescale the hopping term $t\to t/J$. The thermodynamics of this model can be solved exactly since in the large $N$ limit the quantity $\chi=1/N\Sigma_{\sigma}f^{\dagger}_{i,\sigma}(t)f_{i+1,\sigma}(t)$ does not fluctuate. Indeed (1) reduces to a free-fermions Hamiltonian with a "renormalized" hopping term $t\to t+\chi$ and a self-consistent condition on $\chi$,

$$\chi=\frac{1}{L}\sum_{k}f(\beta E_k)\cos k, \quad E_k=-2(t+\chi)\cos k+\mu, \quad (2)$$

where $\mu$ is the chemical potential, $f(\beta E_k)$ is the Fermi function, and $\beta$ is the inverse temperature.[1]

DCA and CDMFT result in self-consistent equations for $\chi_x=1/N\Sigma_{\sigma}<f^{\dagger}_{x,\sigma}f_{x+1,\sigma}>$.[1,4] Because of the translation invariance of DCA the $\chi_x^{DCA}$ are independent of $x$ inside the cluster. Once self-consistency is achieved one can use the cluster quantity to obtain the DCA lattice prediction $\chi_{latt}^{DCA}$ as explained in Ref. 4. This quantity converges to the exact $\chi$ with corrections of $O(1/L_c^2)$.[4,5] Contrary to DCA, the self-consistent CDMFT equations break the translation invariance inside the cluster.

In Fig. 1 we plot the relative error of the CDMFT prediction on $\chi$, $\chi_x-\chi$, as a function of $x$, where $\chi_x$ is the CDMFT solution for $\beta$, the inverse temperature, equal to 4, $t=\mu=1$, and $L_c=38$. For comparison we also we also plot (continuous line) the relative error of the DCA prediction on $\chi$ obtained by solving the the DCA self-consistent equations presented in Ref. 4.

Figure 1 clearly shows the behavior discussed previously, namely translation invariance inside the cluster is broken: errors are smaller in the bulk while they remain of the order 1 at the boundary. Aryanpour *et al.*[4] concluded, by carrying out a flat average $\Sigma_x\chi_x/(L_c-1)$ over the cluster, that the error within CDMFT is expected to be of the order $1/L_c$ (more generically is surface over volume, hence, $1/L_c$ also in dimension larger than 1). As discussed above, it is better to extract the CDMFT estimators weighting bulk values more than boundary values. The easiest thing to do is to just take the value of $\chi_x$ at the center of the cluster. In Fig. 2 we compare the error obtained doing the flat average (square, dotted line) to the one obtained focusing on the bulk values (circle, solid line). This figure conveys two important pieces of information: First, the $\Delta\chi_{bulk}=|\chi_{L_c/2}-\chi|$ is much smaller than the flat average one $\Delta\chi_{fa}=|\Sigma_x\chi_x/(L_c-1)-\chi|$ for large values of $L_c$. Second, as shown in the inset, the error $\Delta\chi_{bulk}$ multiplied by $L_c^2$ is still decreasing fast as a function of $L_c$, i.e., $\Delta\chi_{bulk}$ decreases much faster than $1/L_c^2$. Instead, the er-

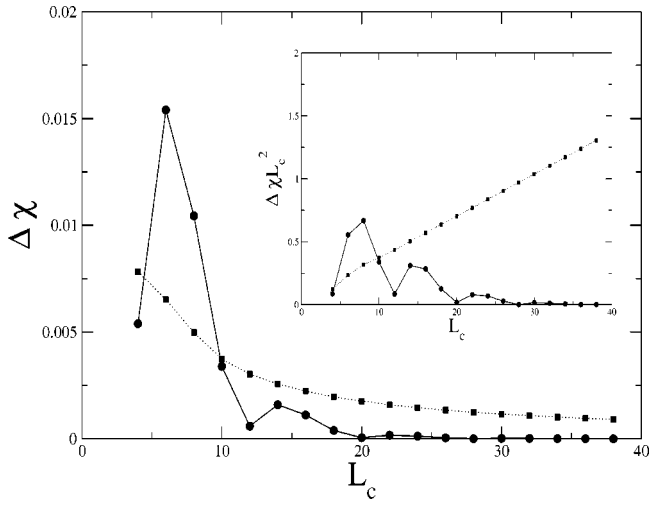


FIG. 2. $\Delta\chi_{bulk}$ (circles, solid line) and $\Delta\chi_{fa}$ (squares, dotted line) as a function of $L_c$. Inset: $\Delta\chi_{bulk}L_c^2$ (circles, solid line) and $\Delta\chi_{fa}L_c^2$ (squares, dotted line) as a function of $L_c$.

ror corresponding to the flat average leads to a straight line corresponding to the $1/L^c$ behavior discussed above and in Ref. 4. Note that in this plot the DCA prediction would lead to a function approaching a constant when $L_c \to \infty$. Finally, in Fig. 3 we plot $\Delta\chi_{bulk}$ in a logarithmic scale as a function of $L_c$. The exponential convergence is manifest (the straight line is a guide for the eye) and in complete agreement with our general discussion above. For comparison we also plot the DCA counterpart. It is clear that the convergence of DCA is much slower than the CDMFT one (indeed it goes[4] as $1/L_c^2$ compared to the exponential convergence of CDMFT). Another simple example that sheds light on the convergence properties of CDMFT and DCA is the Falikov-Kimball model in the large $U$ limit. In this limit the system becomes a classical Ising model and the quantum cluster schemes map on classical cluster schemes.[7] In the following we will focus on the easy one-dimensional case in the paramagnetic phase. In this case, since the Weiss field is zero, doing CDMFT on a cluster of size $L_c$ corresponds only to solving a finite system of size $L_c$ with free boundary conditions. Instead DCA

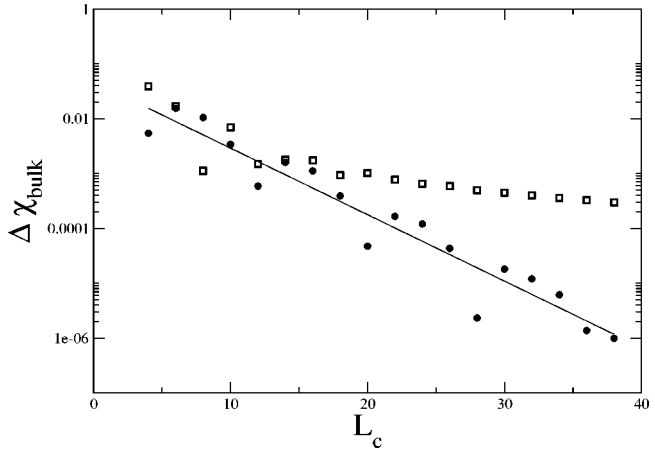


FIG. 3. $\Delta\chi_{bulk}$ as a function of $L_c$ in a logarithmic scale (circles) compared to its DCA counterpart (squares).

corresponds to solving a finite system of size $L_c$ with periodic boundary conditions and a coupling[7]

$$J_{DCA} = J\left(\frac{\sin\frac{\pi}{2L_c}}{\frac{\pi}{2L_c}}\right)^2,$$

where $J$ is the original spin-spin coupling. So, DCA and CDMFT differ in the different boundary conditions but *also* in the fact that for DCA the internal spin-spin coupling is modified from its original value whereas for CDMFT is not. This leads to very different convergence properties. Let us focus for example on the prediction for the spin-spin correlation $C=\langle S_i S_{i+1}\rangle$. The CDMFT and DCA results read

$$C_{CDMFT} = \tanh\beta J,$$

$$C_{DCA} = \frac{\tanh\beta J_{DCA} + (\tanh\beta J_{DCA})^{L_c-1}}{1 + (\tanh\beta J_{DCA})^{L_c}}.$$

In this case the CDMFT prediction is exact because tracing out the spins outside the cluster indeed leads to a zero magnetic field on the boundary but this is of course a peculiarity of this simple case. Instead, there are two types of corrections to DCA [note that $J_{DCA}=J+O(1/L_c{}^2)$]. There are corrections which die out exponentially fast as $\propto(\tanh\beta J)^{L_c}$. These are the same types of corrections that one obtains using periodic boundary conditions or other types of boundary conditions for a free system. However, there is a much larger correction coming from the first term in the numerator of $C_{DCA}$ which leads to

$$C_{DCA} = \tanh\beta J - \frac{\beta J\pi^2}{3(\cosh\beta J)^2(2L_c)^2} + O(L_c^{-4}).$$

Thus applying DCA to this problem one obtains a convergence as $1/L_c^2$, which is much worse than the exponential one corresponding to solving the free model with periodic boundary conditions. The origin of this behavior can be traced to the fact that as DCA forces translation invariance inside the cluster the couplings are changed everywhere in the system by an amount of the order $1/L_c^2$. So, even if the correlation length is finite this error dominates the convergence.

While we stress the obvious advantages of CDMFT, it is also worthwhile to point out the aspects of the CDMFT method (and cluster methods in general) that still require development. The lack of translation invariance of CDMFT, which in the toy model manifests itself in the site dependence of the bond expectation value $\chi_x$, is certainly one of them. For example, CDMFT predicts a finite temperature phase transition for the one dimensional Falikov-Kimball model in the semiclassical limit.[5,7] This is due to the fact that the value of the Weiss field on the boundary is strongly coupled to the value of the propagator on the other boundary and, unfortunately, as discussed previously, the error is much larger at the boundary than in the bulk. This may not be a serious problem for phases with broken symmetry, but certainly is in translationally invariant phases. One possible so-

lution of this problem would be to modify the self-consistent equations that express the Weiss field as a function of the propagator so as to use more heavily bulk values of the propagator, which have a reduced error relative to the boundary. Clearly, further investigations are needed to optimize CDMFT in light of this point. A related issue, stressed in Refs. 1 and 2, is that the lattice self-energy in CDMFT is a derived quantity, obtained from the cluster self-energy entering the CDMFT equations. The lattice self-energy is obtained using a matrix $w$, via the formula (10) in Ref. 1. If $w$ is positive definite, then the lattice self-energy is causal, but one can sometimes obtain better estimates by using other matrices. For the toy model, the matrix $w$ is not restricted since the self-energy is real. The positive definitiveness of $w$ is a sufficient, but not necessary condition to maintain causality. A general constructive way to find the best estimator of the lattice self-energy (preserving causality) for an arbitrary model Hamiltonian is lacking. However, an important criterion to follow is trying to extract the prediction on the lattice self-energy from the bulk values of the cluster self-energy in order to minimize the error as discussed previously.

None of these issues, however, affect the basic fact that expectation values of physical observables which are *local* (namely defined on a restricted neighborhood in physical space) converge as $1/L_c^2$ for DCA as shown in Ref. 4, while for CMDFT they converge exponentially in situations like the one outlined for the toy model, when the correlation length is finite, and not as $1/L_c$ as claimed by Aryanpour *et al.*[4] (note that it has been proved recently that the correlation function of any two fermionic operators decays exponentially with a correlation length which is in the worst case of the order of the inverse temperature.[8]) By exploiting the freedom in the choice of basis, which is inherent to the original CMDFT formulation, one can improve convergence of observables which become local when the approximation is formulated in a different basis set. The problem of convergence as a function of cluster size at zero temperature or at a quantum critical point, or for quantities that are dominated by massless excitations, remains an open question. However, these problems could be better addressed by techniques other than quantum cluster methods.

Finally, most studies can only be done for small clusters, and it is important to understand whether the results obtained in small clusters are representative of the thermodynamical limit. Recent CDMFT studies of the Hubbard model, in one dimension, show that while even-odd effects are important, even clusters of small size can give very accurate results[9] as compared with exact Bethe ansatz results in the thermodynamical limit.

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[1] G. Biroli and G. Kotliar, Phys. Rev. B **65**, 155112 (2002).
[2] G. Kotliar, S. Y. Savrasov, G. Palsson, and G. Biroli, Phys. Rev. Lett. **87**, 186401 (2001).
[3] M. Jarrell, Th. Maier, C. Huscroft and S. Moukouri, Phys. Rev. B **64**, 195130 (2001).
[4] K. Aryanpour, Th. A. Maier, and M. Jarrell, preceding Comment, Phys. Rev. B **71**, 037101 (2005).
[5] Th. Maier and M. Jarrell, Phys. Rev. B **65**, 041104 (2002).
[6] I. Affleck and B. Marston, Phys. Rev. B **37**, 3774 (1988).
[7] G. Biroli, O. Parcollet, and G. Kotliar, Phys. Rev. B **69**, 205108 (2004).
[8] M. B. Hastings, cond-mat/0406348 (unpublished).
[9] M. Capone, M. Civelli, V. Kancharla, C. Castellani, and G. Kotliar, cond-mat/0401060 (unpublished).