Semiclassical approximation solved by Monte Carlo as an efficient impurity solver for dynamical mean field theory and its cluster extensions

Hunpyo Lee,1, 2 Yu-Zhong Zhang,3 Hoonkyung Lee,2 Yongkyung Kwon,2 Harald O. Jeschke,1 and Roser Valentí1

1 Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany
2 Division of Quantum Phases and Devices, School of Physics, Konkuk University, Seoul 143-701, Korea
3 Shanghai Key Laboratory of Special Artificial Microstructure Materials and Technology, School of Physics Science and Engineering, Tongji University, Shanghai 200092, P.R. China

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We propose that a combination of the semiclassical approximation with Monte Carlo simulations can be an efficient and reliable impurity solver for dynamical mean field theory equations and their cluster extensions with large cluster sizes. In order to show the reliability of the method, we consider two test cases: (i) the single-band Hubbard model within the dynamical cluster approximation with 4- and 8-site clusters and (ii) the anisotropic two-orbital Hubbard model with orbitals of different band width within the single-site dynamical mean field theory. We compare the critical interaction $U_c/t$ with those obtained from solving the dynamical mean field equations with continuous time and Hirsch-Fye quantum Monte Carlo. In both test cases we observe reasonable values of the metal-insulator critical interaction strength $U_c/t$ and the nature of Mott physics in the self-energy behavior. While some details of the spectral functions cannot be captured by the semiclassical approximation due to the freezing of dynamical fluctuations, the main features are reproduced by the approach.

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I. INTRODUCTION

The single-site dynamical mean field theory (DMFT) approach has been extensively employed to explore the properties of the Hubbard model and, in general, of strongly correlated materials. Though the metal-Mott insulator transition can be successfully accounted for within the DMFT approximation where dynamical fluctuations alone are emphasized, interesting physical phenomena such as spin density waves and superconductivity can not be properly described due to the absence of spatial fluctuations. Cluster-extensions of DMFT like cellular-dynamical mean field theory (CDMFT) and dynamical cluster approximation (DCA) can take into account the inter-site spatial fluctuations within the size of the cluster in addition to the dynamical fluctuations. For example, cluster extensions of DMFT with 4-site clusters in combination with continuous time quantum Monte Carlo (CT-QMC) or exact diagonalization (ED) can partly capture the physics of Fermi liquid (FL), non-FL (or pseudo gap), Mott insulator, and superconductivity on an equal footing.

While it cannot properly account for Fermi-liquid behavior in the weak-coupling limit, it is not adequate at low temperatures due to the freezing of quantum fluctuations in the method, it is especially suited for large interaction strength and multi-sites where the interaction strength $U$, the inverse of the temperature $T$, and the number of cluster sites $N_c$.

The Hirsch-Fye quantum Monte Carlo (HF-QMC) impurity solver shows a computational expense proportional to $N_c^3 L^3$ where $L$ is the number of slices in the imaginary time (temperature). More recently, Khatami et al. proposed the determinant QMC (DQMC) as a new impurity solver where the computational expense has a $(N_c + N_c N_0)^3 L$ dependence with $N_0$ being the number of bath sites connected to each cluster site. This is though a Hamiltonian-based impurity solver that requires an explicit form of a cluster Anderson impurity model to calculate the self-energy. In contrast, CT-QMC, Hirsch-Fye QMC and the method under discussion in the present work, the semiclassical approximation (SCA), are action-based impurity solvers.

The SCA has been proposed as an impurity solver for DMFT and its cluster extensions. (i) This impurity solver is fast since the computational expense depends only on calculation time at each Matsubara frequency of the inverse of a matrix with dimensions $N_c \times N_c$ (for a cluster with $N_c$ sites) or $L_c \times L_c$ (for a single site with $L_c$ orbitals), where $L_c$ is the number of orbitals. (ii) While it cannot properly account for Fermi-liquid behavior in the weak-coupling limit and in general, it is not adequate at low temperatures due to the freezing of quantum fluctuations in the method, it is especially suited for large interaction strength and multi-sites where for example the powerful interaction expansion CT-QMC method is very costly. (iii) It provides self-energy information directly on the real frequency axis. This avoids...
the uncertainty from analytic continuation which has to be done in various QMC approaches\cite{21,22}. The previously used SCA approach\cite{21,22} was limited though to consider small cluster sizes of \(N_c = 4\) due to the difficulty of the multi-dimensional integrations.

In the present work, we propose to combine the SCA approach with the Monte Carlo (MC) method. The latter is used to evaluate the multi-dimensional integrals. We apply our scheme to two test cases: (i) the one-orbital Hubbard model on the square lattice at half-filling within the DCA with cluster sizes \(N_c = 4\) and \(N_c = 8\) and (ii) the anisotropic two-orbital Hubbard model with different band widths on the Bethe lattice at half-filling within single-site DMFT. We present the density of states, momentum dependent spectral functions, and momentum dependent self-energy as a function of real frequency \(\omega\). For case (i) we find that even though the Fermi liquid behavior is not obtained\cite{22}, the critical onsite Coulomb interaction \(U_c/t\) for the metal-insulator transition calculated by our SCA approach for both cluster sizes shows a reasonable agreement with the value obtained from CT-QMC which should be numerically exact. In particular, we find that the behavior of the density of states at the Fermi level in each momentum sector obtained from both SCA and CT-QMC approaches are quantitatively consistent with each other. For case (ii) we also find a reasonable agreement of \(U_c/t\) obtained from SCA and HF-QMC. The orbital-selective phase transition is also correctly detected. However, we observe that if the band-width difference between narrow and wide orbitals is large, a causality problem appears in the SCA results.

The paper is organized as follows. In Sec. II we present the general formalism of the semiclassical approximation and its application to cases (i) and (ii). In Sec. III we discuss our SCA calculations and compare some results with both CT-QMC and HF-QMC and finally, in Sec. IV we summarize our findings.

II. SEMICLASSICAL APPROXIMATION

In this section we will review the formalism of the SCA approach\cite{21,22} adapted to the two test cases considered in this work; the 8-site DCA and two-orbital DMFT systems with paramagnetic solutions.

A. General formalism

The partition function can be written as:

\[
Z = \int D \left[ c^\dagger c \right] e^{-\left(S_0 + S_{\text{int}}\right)},
\]

and

\[
S_0 = -\int_0^\beta d\tau \int_0^\beta d\tau' \psi^\dagger_\sigma(\tau) \hat{a}_\sigma(\tau, \tau') \psi_\sigma(\tau'),
\]

where \(\psi^\dagger_\sigma = (c^\dagger_{1\sigma} \ldots c^\dagger_{N\sigma})\) and \(c^\dagger_{i\sigma} (c_{i\sigma})\) is a Grassmann number corresponding to the Fermionic creation (annihilation) operator at site \(i\) and spin \(\sigma\), and \(\hat{a}_\sigma = \sum_{\xi} a_{\xi\sigma} K_{\xi\sigma}\) where \(a_{\xi\sigma}\) are inverted frequency-dependent Weiss fields and \(K_{\xi\sigma}\) are \(l \times l\) matrices defined according to the chosen cluster. Here, \(l\) denotes the number of sites in the multi-site system (case (i)) or two times the number of orbitals in the multi-orbital system (case (ii)), and \(\xi\) denotes the distance between two sites within the cluster. For example, \(a_{\xi\sigma}^{-1}\) means the local (on-site) Weiss field while \(a_{\xi\sigma}\) is the inter-site Weiss field with the sites located at a distance \(\xi\)-th apart. The orthogonality is imposed by

\[
\text{Tr} \left[ K_{\xi\sigma} K_{\xi'\sigma'} \right] = l \delta_{\xi\xi'} \delta_{\sigma\sigma'}. \tag{4}
\]

\(n_{\uparrow\downarrow}(\tau)n_{\downarrow\uparrow}(\tau)\) in the decoupling scheme can be written as:

\[
n_{\uparrow\downarrow}(\tau)n_{\downarrow\uparrow}(\tau) = \frac{1}{4} (N_i(\tau)^2 - M_i(\tau)^2), \tag{5}
\]

where \(N_i = (n_{\uparrow\downarrow} + n_{\downarrow\uparrow})\) and \(M_i = (n_{\uparrow\uparrow} - n_{\downarrow\downarrow})\) are the particle number and magnetization, respectively. In terms of these definitions and within the SCA approximation, the partition function transforms into

\[
Z = \int D \left[ c^\dagger c \right] e^{\int_0^\beta d\tau \int_0^\beta d\tau' \psi^\dagger_\sigma(\tau) \hat{a}_\sigma(\tau, \tau') \psi_\sigma(\tau') + \frac{Z_\sigma}{4} \sum_{\sigma'} M_{i\sigma'}(\tau)}, \tag{6}
\]

where the \(N_i^2(\tau)\) term, which describes charge fluctuations, is neglected in the SCA approximation. This expression can be rewritten as

\[
Z = \int D \left[ c^\dagger c \right] \prod_{i=1}^k d\phi_i e^S, \tag{7}
\]

with

\[
S = \int_0^\beta d\tau \left( \int_0^\beta d\tau' \psi^\dagger_\sigma(\tau) \hat{a}_\sigma(\tau, \tau') \psi_\sigma(\tau') - \frac{\phi^2_\sigma}{4U} - \frac{\phi_\sigma M_i(\tau)}{2} \right). \tag{8}
\]

Here we assume that the new auxiliary fields \(\phi_i(\tau)\), which are given by a continuous Hubbard-Stratonovich transformation, are \(\tau\)-independent (\(\phi_i(\tau) \equiv \phi_i\)).

We replace \(M_i(\tau)\) by

\[
M_i(\tau) = \int_0^\beta d\tau' \sum_{\sigma\sigma'} c^\dagger_{i\sigma}(\tau) \sigma\sigma' \delta(\tau - \tau') c_{i\sigma'}(\tau'), \tag{9}
\]

where \(\sigma\sigma'\) is the third Pauli matrix. Via a Grassmann integration and Fourier transformation, the partition function (Eq. (6)) is finally given as

\[
Z = \prod_{i=1}^k \int d\phi_i e^{\frac{-\beta\phi^2_\sigma}{4U} + \sum_{\omega_n} \ln \text{Det} \left[ -\beta(\hat{a}_{\sigma}(i\omega_n) + \frac{1}{2} \phi_\sigma \sigma_z) \right]}, \tag{10}
\]
where $\omega_n$ are Fermionic Matsubara frequencies and $k$ is the dimension of integrations. The impurity Green’s function can be obtained as $G_{\sigma}^{\text{imp}}(i\omega_n) = \sum_{\xi} G_{\xi\sigma}(i\omega_n) \hat{K}_{\xi\sigma}$ where $G_{\xi\sigma}(i\omega_n)$ is

$$G_{\xi\sigma}(i\omega_n) = \frac{1}{l} \frac{\partial \ln Z}{\partial a_{\xi\sigma}(i\omega_n)} \quad (11)$$

where $l$ is the normalization factor which is given by Eq. (4). The Green’s function on the real frequency $\omega$ is also calculated by Eq. (11) with replacement of $\omega_n$ into $\omega + i\delta$. In our calculations we consider a broadening factor $\delta = 0.003$. The integration in $i = N_c \times m \times (2m - 1)$ dimensions for classical fields $\phi_i$ is evaluated by the MC approach, where $N_c$ is the number of cluster sites, $m$ is the number of orbitals, and the weight function $W(\phi_i)$ for the MC simulations is given as

$$\ln W(\phi_i) = -\frac{\beta \phi^2}{4U} + \sum_{\omega_n} \ln \det \left[ -\beta (\hat{a}_{\sigma}(i\omega_n) + \frac{1}{2} \phi_i \sigma_k) \right].$$

$$\quad (12)$$

B. 8-site dynamical cluster approximation

The partition function in the SCA approach is described in a real-space basis in Eqs. (13) and (14). The $8 \times 8$ matrices of inversed Weiss fields (Eq. (10) and Eq. (11)) in the 8-site DCA calculations for the Hubbard model on the square lattice are given as

$$\hat{a}(i\omega_n) = \begin{pmatrix}
    a_0 & a_2 & a_3 & a_3 & a_3 & a_3 & a_3 & a_3 \\
    a_2 & a_0 & a_2 & a_3 & a_3 & a_3 & a_3 & a_3 \\
    a_3 & a_2 & a_0 & a_3 & a_3 & a_3 & a_3 & a_3 \\
    a_3 & a_3 & a_3 & a_0 & a_3 & a_3 & a_3 & a_3 \\
    a_3 & a_3 & a_3 & a_3 & a_0 & a_3 & a_3 & a_3 \\
    a_3 & a_3 & a_3 & a_3 & a_3 & a_0 & a_3 & a_3 \\
    a_3 & a_3 & a_3 & a_3 & a_3 & a_3 & a_0 & a_3 \\
    a_3 & a_3 & a_3 & a_3 & a_3 & a_3 & a_3 & a_0
\end{pmatrix},$$

$$\quad (13)$$

where spin indices are omitted for simplicity and the normalization factors $\frac{1}{4}$ and $\frac{1}{\sqrt{2}}$ are introduced in order to fulfill the orthogonality condition Eq. (4). The indices $\xi = 0, 1, 2,$ and 3 indicate on-site, 1st neighbor, 2nd neighbor, and 3rd neighbor, respectively. The cluster we used for constructing the $\hat{a}(i\omega_n)$ matrices with periodic boundary condition is shown in Fig. 1 (a) and the division of BZ for DCA calculations is presented in Fig. 1 (b). The real-space impurity Green’s functions in Eq. (11) are more clearly expressed as

$$G_{\xi}(i\omega_n) = \frac{1}{l} \frac{1}{\det \left[ \hat{A}(a\xi(i\omega_n)) \right]} \frac{\partial}{\partial a\xi(i\omega_n)} \det \left[ \hat{A}(a\xi(i\omega_n)) \right],$$

$$\quad (14)$$

where $\hat{A}(a\xi(i\omega_n)) = -\beta (\hat{a}(i\omega_n) + \phi_i)$ are $8 \times 8$ matrices with spin index $\sigma$. The impurity Green’s function in Eq. (11) is measured by

$$\frac{1}{\det \left[ \hat{A}(a\xi) \right]} \frac{\partial}{\partial a\xi} \det \left[ \hat{A}(a\xi) \right] = \text{tr} \left[ \hat{A}^{-1}(a\xi) \frac{\partial \hat{A}(a\xi)}{\partial a\xi} \right].$$

$$\quad (15)$$

C. 2-orbital dynamical mean field theory

The interaction term of the Hamiltonian for the 2-orbital system (test case (ii)) is given as

$$H_{\text{int}} = U \sum_{\eta} n_{\eta \uparrow} n_{\eta \downarrow} + \sum_{\sigma \sigma'} (U' - \delta_{\sigma \sigma'} J_z) n_{\eta \sigma} n_{\eta 2\sigma'},$$

where $\eta \in \{1, 2\}$ denote orbital indexes. $U$ and $U'$ are, respectively, onsite intra-orbital and inter-orbital Coulomb interaction parameters and $J_z$ is the Ising Hund’s coupling term. We are not considering the spin-flip and pair hopping terms in our calculations. The inversed Weiss field is given as

$$\hat{a}(i\omega_n) = \begin{pmatrix}
    a_{1\uparrow} & 0 & 0 & 0 \\
    0 & a_{1\downarrow} & 0 & 0 \\
    0 & 0 & a_{2\uparrow} & 0 \\
    0 & 0 & 0 & a_{2\downarrow}
\end{pmatrix}.$$

$$\quad (17)$$

FIG. 1: (Color online) Cartoons for (a) the eight-site dynamical cluster approximation in real space and for (b) the division of the Brillouin zone in momentum space we used.
We now decouple the interaction term Eq. [16] using Eq. [8]:

\[ n_{1\uparrow}n_{1\downarrow} = \frac{1}{4}(N_1^2 - M_1^2), \quad n_{2\uparrow}n_{2\downarrow} = \frac{1}{4}(N_2^2 - M_2^2), \]

\[ n_{1\uparrow}n_{2\downarrow} = \frac{1}{4}(N_2^2 - M_3^2), \quad n_{1\downarrow}n_{2\uparrow} = \frac{1}{4}(N_4^2 - M_4^2), \]

\[ n_{1\uparrow}n_{2\downarrow} = \frac{1}{4}(N_2^2 - M_5^2), \quad n_{1\downarrow}n_{2\uparrow} = \frac{1}{4}(N_6^2 - M_6^2). \]

Neglecting charge fluctuations \( N_1^2 \), the partition function can be written as

\[
Z_{\Omega} = e^{\int_{0}^{\beta} \left( \frac{U}{4} (M_1^2 + M_2^2) + \frac{U'}{4} (M_3^2 + M_4^2) + \frac{U''}{4} (M_5^2 + M_6^2) \right)}
\]

where \( U'' = U' - J_z \) and

\[
Z_0 = \int D [c^\dagger] \int_{0}^{\beta} \int_{0}^{\beta} d\tau d\tau' \phi^\dagger (\tau) \phi (\tau') \langle \phi (\tau) \phi (\tau') \rangle.
\]

where \( \phi = (c_{1\uparrow}^\dagger, c_{2\downarrow}^\dagger, c_{2\uparrow}^\dagger, c_{3\downarrow}^\dagger) \) (compare with Eq. [8]). In order to make integration feasible, Eq. [18] is transformed into

\[
S = -\frac{\phi_1^2 + \phi_2^2}{4U} - \frac{\phi_3^2 + \phi_4^2}{4U'} - \frac{\phi_5^2 + \phi_6^2}{4U''} + \int_{0}^{\beta} d\tau \frac{1}{2} \sum_{\xi=1}^{6} \phi_\xi M_\xi (\tau),
\]

where we used the continuous Hubbard-Stratonovich transformation as in Eq. [8]. Next (see Eq. [9]), \( M_\xi (\tau) \) is replaced by

\[
M_\xi (\tau) = \int_{0}^{\beta} d\tau' \phi^\dagger (\tau) \sigma^\dagger \delta (\tau - \tau') \phi (\tau').
\]

Site indices are omitted due to the single-site DMFT calculation and \( \sigma^\dagger \) are 4 x 4 matrices:

\[
\sigma^\dagger_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma^\dagger_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},
\]

\[
\sigma^\dagger_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma^\dagger_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},
\]

\[
\sigma^\dagger_5 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma^\dagger_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.
\]

Finally, the partition function is rewritten as

\[
Z = \int_{-\infty}^{\infty} \prod_{\xi=1}^{6} d\phi_\xi e^{-V(\phi_\xi) + \sum_{\omega_n} \ln \text{Det}[-\beta(\hat{\mathcal{H}}(\omega_n) + \frac{i}{\beta} \phi_\xi \sigma^\dagger_\xi)]},
\]

where \( V(\phi_\xi) = \beta (\frac{\phi_1^2 + \phi_2^2}{4U} + \frac{\phi_3^2 + \phi_4^2}{4U'} + \frac{\phi_5^2 + \phi_6^2}{4U''}) \). The impurity Green’s functions are calculated by Eq. [11].

![Graph](image)

**FIG. 2:** (Color online) The density of states at the Fermi level \( \rho(\omega = 0) \approx \beta G(\frac{\omega}{2}) \) and \( \rho(\omega = 0) \), directly measured in real-frequency space within DCA(SCA), as a function of \( U/t \) for \( N_c = 4 \) and 8 at \( T/t = 1/12 \). From \( \rho(\omega = 0) \) we find the critical metal-insulator interactions \( U_c/t = 4.6 \pm 0.2 \) and \( 5.0 \pm 0.2 \) for \( N_c = 4 \) and 8, respectively. The error bars are smaller than the symbol sizes. The deviations of between \( \beta G(\frac{\omega}{2}) \) and \( \rho(\omega = 0) \) are around ten percent. See the main text for discussion.

**D. Monte Carlo measurement**

The weight functions for MC calculations have been given in Eq. [12]. We employ about 400 Matsubara frequencies for performing the frequency sum in Eq. [12]. The number of classical fields \( \phi_i \) is the same as the number of cluster sites in the DCA calculations (case (i)). For case (ii) the number of classical fields is given by \( (2m - 1) \times m \), where \( m \) is the number of orbitals. In order to avoid a local minimum problem in the MC calculation, we use around forty initial configurations and we perform about \( 4 \times 10^5 \) MC samplings for each different initial configuration. The computational cost for \( 4 \times 10^5 \) MC samplings in the 8-site DCA system is around 90 minutes on a single 4 GHz CPU machine and the error is smaller than \( 5 \times 10^{-4} \).

**III. RESULTS**

**A. The metal-insulator transition in the 8-site dynamical cluster approximation**

In what follows, we will show the reliability of our SCA impurity solver by presenting the results obtained for 4- and 8-site DCA calculations for a two-dimensional Hubbard model on the square lattice at half-filling (case (i)).

First, we compare the critical \( U_c/t \) obtained from DCA(SCA) calculations with that obtained from DCA(CT-QMC) with \( N_c = 4 \) and 8. Within DCA(CT-QMC) \( U_c/t = 4.5 \) (\( N_c = 4 \)) and \( U_c/t = 6.5 \) (\( N_c = 8 \)).
We would like to note that for the two-dimensional Hubbard model on the square lattice at half-filling, previous DCA calculations showed that, at finite temperature, the larger the cluster size is, the smaller the critical value of interaction $U_c/t$. This is due to the fact that DCA calculations account for spatial correlations only within the cluster. This suggests that we should expect a smaller $U_c/t$ for increasing cluster sizes. However, this is not what it is observed above. We think that the reason for this discrepancy lies on the fact that plaquette singlet ordered states become more favorable for $N_c = 4$ than for $N_c = 8$ and artificially stabilize an insulating state in $N_c = 4$. We now check whether this behavior is also observed in the SCA approach. In Fig. 2 we plot the DCA(SCA) density of states at the Fermi level obtained as (1) $\rho(\omega = 0) \approx \beta G(\frac{\omega}{2})$ and (2) directly calculated in real-frequency space $\rho(\omega = 0)$, as a function of $U/t$ for $N_c = 4$ and 8 at $T/t = 1/12$. The imaginary time Green’s function $G(\tau)$ is calculated by the Fourier transformation of $G(i\omega_n)$ in Eq. [11]. We find $U_c/t = 4.4 \pm 0.2$ and $5.0 \pm 0.2$ for $N_c = 4$ and 8 respectively. The trend, i.e., smaller critical interaction $U_c/t$ for $N_c = 4$ than for $N_c = 8$, is the same as in DCA(CT-QMC). We also detect that the critical interactions $U_c/t$ in the SCA method are slightly smaller than those calculated by the CT-QMC method. The reason why the insulating state is overestimated, is due to the fact that the auxiliary field is assumed to be $\tau$ independent in SCA, indicating a freezing of dynamical fluctuations in SCA.

Usually one always employs the relation $\rho(\omega = 0) \approx \beta G(\frac{\omega}{2})$ to determine the critical interaction $U_c/t$ for the metal-insulator transition in DCA(CT-QMC). This is done in order to avoid the performance of an analytical continuation, which will introduce some uncertainties. Therefore, it is interesting to check whether this relation is valid in all cases. Since DCA(SCA) provides results directly in real-frequency space, both definitions can be tested on the same footing. Fig. 2 shows that both definitions are in good agreement in the weak-coupling and strong-coupling regions, but they show deviations of about ten percent close to the critical value due to finite temperature effects. In addition, we find a causality problem in the weak-coupling region (for $U/t$ values smaller than 3.0).

In order to test the reliability of the SCA approximation we present in Fig. 3 a quantitative comparison of $\beta G(\frac{\omega}{2})$ as a function of frequency obtained by the SCA impurity solver and by CT-QMC for $N_c = 4$ and inverse temperatures $\beta = 3/t, 6/t$. We observe a good agreement between both sets of results at high temperature regions.

Next, we would like to analyze the spectral functions in different DCA cluster momentum sectors, i.e., $A(K, \omega)$ at $K = (0, 0), (0, \pi), (\pi, 0), (\pi, \pi)$ and $(\pi, \pi)$ shown in Fig. 4(b) for several values of $U/t$ at $T/t = 1/12$. In Fig. 4(a) we display the non-interacting case ($U/t = 0.0$). While the weights of the spectral functions $A(K, \omega)$ at $K = (0, 0)$ and $(\pi, \pi)$ sectors are well separated from each other, resembling the behavior of band insulators, the spectral functions at $K = (0, \pi)$ and $(\pi, 0)$ sectors cross the Fermi level, showing metallic behavior. The van-Hove singularity is present in the spectral function in the $K = (\pi, 0)/2, (0, \pi)$ sector. The behavior of $A(K, \omega)$ for $N_c = 8$ is comparable to $N_c = 4$ result and can be understood in terms of the non-interacting band structure.

In Fig. 3(b) we show $A(K, \omega)$ for $U/t = 3.2$ (weak-coupling region). $A(K, \omega)$ at $K = (0, 0)$ and $(\pi, \pi)$ intersect with each other due to the band splitting and spectral weight transfer induced by $U$. This is an indication of Mott physics. The insulating behavior still remains in these two sectors and the whole band width is slightly narrowed due to correlation effects. The van-Hove singularity that was present in the $K = (\pi, 0)$ sector in the non-interacting case, is dramatically suppressed with increasing $U/t$. The absence of a strong quasi-particle peak in the weak interaction region is due to the freezing of dynamical fluctuations. This is a shortcoming of the SCA method. As the interaction $U/t$ is increased, a pseudo-gap behavior is present with suppression of the spectral functions at $K = (0, \pi)$ and $(\pi, \pi)$ at $U/t = 4.0$ (Fig. 3(c)), and the Mott insulator appears in the strong-coupling region at $U/t = 6.0$ (Fig. 3(d)).

In order to study the Mott behavior in 8-site DCA in more detail, we present in Fig. 5 the real part of the self-energy $\text{Re}(\Sigma(K, \omega))$ as a function of real frequency $\omega/t$ for $U/t = 4.0$ and $5.2$ at $T/t = 1/12$. The real and imaginary parts of the self-energy give the energy shift and the spectral broadening, respectively, of the one-electron spectrum due to the interaction $U/t$. In Fig. 5(a) for $U/t = 4.0$ where the spectral function shows a pseudo-gap, the real parts of the self-energy $\text{Re}(\Sigma(K, \omega))$ at $K = (0, 0)$ and $(\pi, \pi)$ remain finite below and above the Fermi level, respectively, indicating the shift of the pole positions of the one-electron spec-en.
When the interaction becomes strong, the gap opens and a metallic behavior is seen in the wide band while a metal-insulator transition is observed in narrow band, has been intensively studied in model systems as well as real materials. The behavior at \( K = (0, \pi) \) and \((\pi/2, \pi/2)\) Re(\(\Sigma(K, \omega)\)) shows a positive slope with negative value of quasiparticle weight and the corresponding Im(\(\Sigma(K, \omega)\)) (not shown) exhibits a peak around the Fermi level, indicating the appearance of a non-Fermi liquid. This non-Fermi-liquid behavior is the sign of the Mott gap beginning to form. In Fig. 5, the self-energy has a pole-like structure indicating the Mott insulating state, the pole \(\Sigma(0,0)\) increases until \( U/t = 1 \) and below Fermi level, respectively. The orbital-selective phase transition (OSPT), where metallic behavior is seen in the wide band while a metal-insulator transition is observed in narrow band, has been intensively studied in model systems as well as real materials. The orbital-selective phase transition (OSPT), where metallic behavior is seen in the wide band while a metal-insulator transition is observed in narrow band, has been intensively studied in model systems as well as real materials.

Finally, we compare the results in Fig. 6 to those in Fig. 8 of Ref. [25] calculated within the CT-QMC approach. The behavior at \( K = (0, \pi) \) in both SCA and CT-QMC approaches is qualitatively the same, even though the critical interactions \( U_c/t \) are different. The main difference between these two results is in the \( K = (\pi, \pi) \) sector. The CT-QMC results indicate a first-order transition with a discontinuous behavior of \(\beta G(K, \frac{\pi}{2})\) at the critical interaction \( U_c/t \), while the SCA results show a continuous transition with a smooth decrease of \(\beta G(K, \frac{\pi}{2})\). We think that this discrepancy between the two approaches also comes from the approximation that the dynamical fluctuations are frozen in the SCA method.

**B. Orbital-selective phase transitions in the two-orbital dynamical mean field theory**

The orbital-selective phase transition (OSPT), where metallic behavior is seen in the wide band while a metal-insulator transition is observed in narrow band, has been intensively studied in model systems as well as real materials.
In the following we compare the critical values of the interaction strength obtained from the SCA and HF-QMC approaches. In the case of band widths of $W_1 = 2$ (narrow band) and $W_2 = 4$ (wide band), the critical values in the HF-QMC approach are given as $U_{c1}/t_2 = 2.0$ and $U_{c2}/t_2 = 2.8$ in narrow and wide bands, respectively \cite{13}. Our SCA results show the critical values $U_{c1}/t_2 = 2.0$ and $U_{c2}/t_2 = 3.2$ from the analysis of the Green’s function in the Matsubara frequency space in good agreement with HF-QMC. We encounter though a causality problem if the difference between the band widths of narrow and wide orbitals is large.

IV. SUMMARY

In summary, in this work we propose that the semiclassical approximation in combination with the Monte Carlo method can be used to study large clusters and multi-orbital systems and is easy to embed into DMFT and its cluster extensions. We investigate the single-orbital Hubbard model by the DCA(SCA) method with cluster sizes of $N_c = 4$ and 8 and a two-orbital system by DMFT(SCA). The critical $U_c/t$ as well as $G(I_2)$ as a function of $\omega$ are compared with existing DCA(CT-QMC) results. The critical interactions $U/t$ of SCA and CT-QMC approaches in both cases are in reasonable agreement. In the 8-site DCA cluster calculation, we analyze the spectral functions $A(K, \omega)$ and self-energy at each momentum sector. The only difference between SCA and CT-QMC results is that the CT-QMC shows a discontinuous behavior of the spectral density in the $K = (\pi/2, \pi/2)$ sector around the critical value of interactions, while the SCA exhibits smoothly decreasing behavior. We think that the reason for the discrepancy is that quantum fluctuations are frozen in the SCA approach. In the two-orbital DMFT(SCA) calculation, we observe the orbital selective phase transition as in previous studies performed with DMFT(HF-QMC) \cite{16}. This method is rather powerful since it can be applied for problems where other impurity solvers remain computationally too expensive but one should be aware of possible causality problems in some cases.

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FIG. 7: (Color online) The density of states $\rho(\omega)$ and real part of the self-energy $\text{Re}(\Sigma(\omega))$ for (a) and (d) $U/t_2 = 2.0$, (b) and (e) 2.8, and (c) and (f) 3.6 at $T/t_2 = 1/12$, respectively. The bandwidths for narrow and wide orbitals on the Bethe lattice are $W_1 = 2.56$ ($t_1 = 0.8$) and $W_2 = 4.0$ ($t_2 = 1.0$), respectively. The metal, orbital-selective phase, and Mott insulator are present in (a), (b), and (c), respectively.

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