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Sub-matrix updates for the Continuous-Time Auxiliary Field algorithm

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We present a sub-matrix update algorithm for the continuous-time auxiliary field method that allows the simulation of large lattice and impurity problems. The algorithm takes optimal advantage of modern CPU architectures by consistently using matrix instead of vector operations, resulting in a speedup of a factor of ≈ 8 and thereby allowing access to larger systems and lower temperature. We illustrate the power of our algorithm at the example of a cluster dynamical mean field simulation of the Néel transition in the three-dimensional Hubbard model, where we show momentum dependent self-energies for clusters with up to 100 sites.

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The theoretical investigation of correlated fermionic lattice systems has been one of the most challenging tasks in condensed matter physics. Many of these systems are not tractable with controlled analytic approximations in the regimes of interest, so that numerical simulations need to be employed. Several numerical approaches exist: With exact diagonalization¹ (ED) one calculates the exact eigenstates of a system on a small lattice. Because the Hilbert space grows exponentially with lattice size, ED is limited to comparatively small systems. Variational methods like the density matrix renormalization group theory^{2,3} (DMRG) work well in one dimension, but extensions to two-dimensional systems⁴⁻⁷ are still under development. Standard lattice Monte Carlo methods⁸ are hampered by the fermionic sign problem^{9,10} that limits access to large system size or low temperature away from half filling.

Systems with large coordination number are often studied within the dynamical mean field approximation (DMFT)^{11,12}. Early studies by Metzner and Vollhardt¹³ and Müller-Hartmann¹⁴ showed that the diagrammatics of interacting fermions becomes purely local in the limit of infinite coordination number. In this case the solution of the lattice model may be obtained from the solution of an impurity model and an appropriately chosen self-consistency condition¹⁵.

Later work on cluster extensions of DMFT¹⁶⁻²⁰ took into account non-local correlations in addition to the local correlations already considered within the DMFT by considering “cluster” impurity models with an internal momentum structure²⁰. These cluster approximations are based on a self-energy expansion in momentum space, $\Sigma(k, \omega) \approx \sum_K^{N_c} \Sigma_K(\omega) \phi_K(k)$ ²¹ that becomes exact in the limit of a complete momentum space basis ($N_c \rightarrow \infty$) and can therefore be controlled by increasing the cluster size.

Quantum impurity models are well suited to numerical study. Methods for their solution include

numerical renormalization group approaches²², exact diagonalization²³, and approximate semi-analytical resummation of classes of diagrams^{15,24,25}. However, until a few years ago only the Hirsch-Fye quantum Monte Carlo²⁶ algorithm was able to obtain unbiased and numerically exact solutions of large cluster impurity problems at intermediate interaction strength. This changed with the development of continuous-time methods²⁷⁻³². The vastly better scaling³³ of these methods and the absence of discretization errors allowed access to lower temperatures, larger interactions, and more orbitals.

Large cluster calculations remain computationally challenging as the numerical cost – even in the absence of a sign problem – scales as $O((N_c \beta U)^3)$ in the case of the interaction expansion^{28,31}, and $O(\exp(N_c) \beta^3)$ in the hybridization expansion³⁰ methods (for single orbital cluster Anderson models at inverse temperature β and interaction U for a cluster of size N_c). It is therefore important to develop efficient algorithms to solve cluster impurity models.

Two numerical algorithmic improvements have significantly increased the size of systems accessible by simulations with the Hirsch-Fye algorithm: the “delayed” updates³⁴, and the “sub-matrix” updates³⁵. An important question is therefore if these techniques may be generalized to the continuous-time algorithms and whether similar savings in computer time may be expected, and how these savings translate into newly accessible physics.

Both “delayed” and “sub-matrix” updates are mainly based on efficient memory management; “sub-matrix” updates further reduce the algorithmic complexity of the updating procedure. Modern computer architectures employ a memory hierarchy: Calculations are performed on data loaded into registers. Any data that is not in the registers is stored either in “cache” (currently with a size of a few MB) or in “main memory” (with a size of a few GB). Cache is relatively fast but there is little of it,

while access to main memory is often slow and shared among several compute cores. The bottleneck in many modern scientific applications, including the continuous-time algorithms, is not the speed at which computations are performed but the speed at which data can be loaded from and stored into main memory.

The central object in continuous-time algorithms is a matrix, which for large cluster calculations does not fit into cache. Monte Carlo updates often consist of rank one updates or matrix-vector products. Such updates perform $O(m^2)$ operations on $O(m^2)$ data, where m is the average matrix size, and therefore run at the speed of memory. Matrix-matrix operations (with $O(m^3)$ operations executed on $O(m^2)$ data) could run at the speed of the registers, as more (fast) calculation per (slow) load / store operation are performed. The reason behind the success of both the “sub-matrix” and the “delayed” updates is the combination of several (slow) successive rank-one operations into one fast matrix-matrix operation, at the cost of some minimal overhead. This is illustrated in Fig. 1.

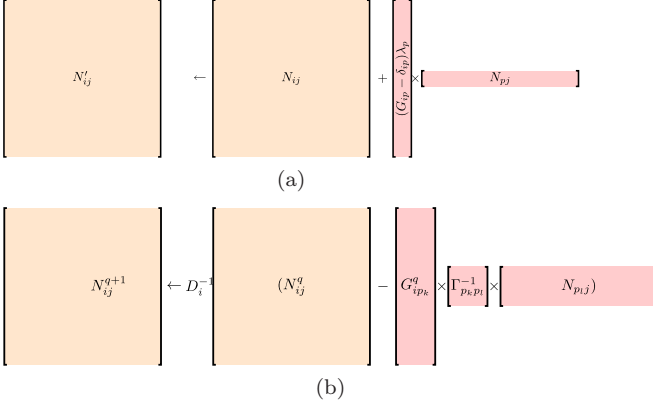


FIG. 1. Illustration of update formulas. 1(a): “rank one” updates of Ref. 31, accessing $O(m^2)$ data points for $O(m^2)$ operations and performing one update. 1(b): sub-matrix updates, accessing $O(m^2)$ values but performing $O(m^2 k)$ operations, for k updates.

The delayed update algorithm can be straightforwardly generalized to (non-ergodic) spin-flip operations in the interaction expansion (CT-INT) and continuous-time auxiliary field algorithms (CT-AUX)³⁶, and an adaptation of the concept of delayed updates to vertex insertion and removals in the interaction expansion was recently proposed by Mikelsons³⁷.

In this article we present a generalization of the “sub-matrix” technique of Ref. 35 to the CT-AUX algorithm, which uses fewer redundant operations than “delayed” updates. We find a speed increase of ≈ 8 for a typical large cluster impurity problem. We demonstrate the scaling both as a function of computational resources and as a function of problem size, and we show results for controlled large scale cluster calculations.

The paper is structured as follows: In Sec. I we reintroduce the CT-AUX algorithm and describe the Monte Carlo random walk procedure. In Sec. II we introduce the sub-matrix updates, and in Sec. III we apply them to CT-AUX. Sec. IV shows physics and benchmarking results for the new algorithm, and Sec. V contains the conclusions.

I. THE CONTINUOUS-TIME AUXILIARY FIELD ALGORITHM

We present the sub-matrix updates for the continuous-time auxiliary field algorithm³¹ (CT-AUX), for which the linear algebra is similar to the well-known Hirsch Fye²⁶ method. To introduce notation and conventions we repeat the important parts of the derivation of Ref. 31, limiting ourselves to the description of the dynamical mean field solution of the single orbital Anderson impurity model. *Lattice* problems, i.e. problems without hybridization terms in the Hamiltonian and with no (cluster) dynamical mean field self-consistency imposed, differ only in the form of the non-interacting Green’s function. Their simulation proceeds along the same lines and will not be treated separately here.

A. Partition Function Expansion

The Hamiltonian of the single orbital Anderson impurity model describes the behavior of an impurity (described by operators $d_\sigma, d_\sigma^\dagger$) with an on-site energy ϵ_0 and on-site interaction U coupled by a hybridization with strength $V_{p\sigma}$ to a bath (described by $a_{p\sigma}, a_{p\sigma}^\dagger$) with dispersion ϵ_p :

$$H = H_0 + V, \quad (1)$$

$$H_0 = -(\epsilon_0 - U/2)(n_\uparrow + n_\downarrow) + \sum_{\sigma,p} (V_{p\sigma} d_\sigma^\dagger a_{p\sigma} + h.c.) + \sum_{\sigma,p} \epsilon_p a_{p\sigma}^\dagger a_{p\sigma}, \quad (2)$$

$$V = U \left[n_\uparrow n_\downarrow - \frac{n_\uparrow + n_\downarrow}{2} \right]. \quad (3)$$

$n_\sigma = d_\sigma^\dagger d_\sigma$ denotes the impurity occupation. Continuous-time algorithms expand expressions for the partition function $Z = \text{Tr} \exp(-\beta H)$ (at inverse temperature β) into a diagrammatic series. In CT-AUX, the series is a perturbation expansion in the interaction:

$$Z = \sum_{n \geq 0} \int_0^\beta d\tau_1 \dots \int_{\tau_{n-1}}^\beta d\tau_n \left(\frac{K}{\beta} \right)^n \text{Tr} \left[e^{-(\beta - \tau_n) H_0} \times \left(1 - \frac{\beta V}{K} \right) \dots e^{-(\tau_2 - \tau_1) H_0} \left(1 - \frac{\beta V}{K} \right) e^{-\tau_1 H_0} \right]. \quad (4)$$

The interaction term V in this expansion can be decoupled with an auxiliary field³⁸

$$1 - \frac{\beta V}{K} = \frac{1}{2} \sum_{s=-1,1} e^{\gamma s(n_\uparrow - n_\downarrow)}, \quad (5a)$$

$$\cosh(\gamma) \equiv 1 + (\beta U)/(2K), \quad (5b)$$

introducing an arbitrary constant K and an auxiliary “spins” s . Hence

$$Z = \sum_{n \geq 0} \sum_{\substack{s_i = \pm 1 \\ 1 \leq i \leq n}} \int_0^\beta d\tau_1 \dots \int_{\tau_{n-1}}^\beta d\tau_n \left(\frac{K}{2\beta}\right)^n Z_n, \quad (6)$$

$$Z_n(\{s_i, \tau_i\}) \equiv \text{Tr} \prod_{i=n}^1 e^{-\Delta \tau_i H_0} e^{s_i \gamma (n_\uparrow - n_\downarrow)}. \quad (7)$$

Note that the insertion of an arbitrary number of “interaction vertices” (auxiliary spin and time pairs) (s_j, τ_j) with $s_j = 0$ into Eq. (6) does not change the value of $Z_n(\{s_i, \tau_i\})$. We will refer to auxiliary spins with value $s_n = 0$ as “non-interacting” spins.

We can express the trace of exponentials of one-body operators in Eq. (6) as a determinant of a $(n \times n)$ matrix N ,

$$\frac{Z_n(\{s_i, \tau_i\})}{Z_0} = \prod_{\sigma=\uparrow, \downarrow} \det N_\sigma^{-1}(\{s_i, \tau_i\}), \quad (8)$$

$$N_\sigma^{-1}(\{s_i, \tau_i\}) \equiv e^{V_\sigma^{\{s_i\}}} - \mathcal{G}_{0\sigma}^{\{\tau_i\}} (e^{V_\sigma^{\{s_i\}}} - 1), \quad (9)$$

$$e^{V_\sigma^{\{s_i\}}} \equiv \text{diag}(e^{\gamma(-1)^\sigma s_1}, \dots, e^{\gamma(-1)^\sigma s_n}). \quad (10)$$

$G_{0\sigma}^{\{\tau_i\}}$ denotes a $(n \times n)$ matrix of bare Green’s functions, $(\mathcal{G}_{0\sigma}^{\{\tau_i\}})_{ij} = \mathcal{G}_{0\sigma}(\tau_i - \tau_j)$. From now on we will omit the spin index σ .

The matrix N is related to the Green’s function matrix G by $G = NG_0$. The matrices G and N for auxiliary spin configurations have the same imaginary time location for all vertices but differ in the value of an auxiliary spin s_p , and are related by a Dyson equation

$$N'_{ij} = N_{ij} + (G_{ip} - \delta_{ip}) \lambda N_{pj}, \quad (11a)$$

$$G'_{ij} = G_{ij} + (G_{ip} - \delta_{ip}) \lambda G_{pj}, \quad (11b)$$

$$\lambda = e^{V'_p - V_p} - 1. \quad (11c)$$

This relation is the basis for Hirsch-Fye spin-flip updates.

B. Random Walk

The infinite sum over expansion orders n and the integral and sum over vertices $\{(s_i, \tau_i)\}$ in Eq. (6) is computed to all orders in a stochastic Monte Carlo process: The algorithm samples time ordered configurations $\{(s_i, \tau_i)\}$ with weight

$$w(\{s_i, \tau_i\}) = \left(\frac{K d\tau}{2\beta}\right)^n \prod_{\sigma=\uparrow, \downarrow} \det N_\sigma^{-1}(\{s_i, \tau_i\}). \quad (12)$$

To guarantee ergodicity of the sampling it is sufficient to insert and remove spins with a random orientation $s_i = \uparrow, \downarrow$ at random times $0 \leq \tau_i < \beta$. Spin insertion updates are balanced by removal updates. For an insertion update we select a random time in the interval $[0, \beta)$ and a random direction for this new spin, leading to a proposal probability $p^{\text{prop}}(n \rightarrow n+1) = (1/2)(d\tau/\beta)$. For removal updates a random spin is selected and proposed to be removed, leading to a proposal probability $p^{\text{prop}}(n+1 \rightarrow n) = 1/(n+1)$. Combination of Eq. (8) with these proposal probabilities leads to the Metropolis acceptance rate $p(n \rightarrow n+1) = \min(1, R)$ with

$$R = \frac{K}{n+1} \prod_{\sigma=\uparrow, \downarrow} \frac{\det[N_\sigma^{(n+1)}]^{-1}}{\det[N_\sigma^{(n)}]^{-1}}, \quad (13)$$

where (n) denotes the dimension of N_σ^{-1} .

In addition to insertion and removal updates we consider spin-flips of auxiliary spins. These updates are self-balancing, and the transition probability from a state $\{(s_1, \tau_1), \dots, (s_i, \tau_i), \dots\}$ to a state $\{(s_1, \tau_1), \dots, (-s_i, \tau_i), \dots\}$ is given by

$$R = \prod_{\sigma=\uparrow, \downarrow} \frac{\det[N_\sigma^{(n)}(\{(s_1, \tau_1), \dots, (-s_i, \tau_i), \dots\})]^{-1}}{\det[N_\sigma^{(n)}(\{(s_1, \tau_1), \dots, (s_i, \tau_i), \dots\})]^{-1}}. \quad (14)$$

In the particle hole symmetric case the parameter K may be chosen such that only even orders in the perturbation series occur and that the average perturbation order is half as large as the one of the algorithm presented here (see Ref. 39 for details in the real-time context, where this scheme allowed propagation to much longer times). As the resulting algorithm is far less general and requires double-vertex insertions it will not be explored here.

Non-interacting auxiliary spins, or auxiliary spins with value 0, do not change the value of Z_n in Eq. 7. We will make use of this fact to precompute a matrix that is equivalent to N but contains non-interacting vertices represented by spin 0 auxiliary spins. Insertion and removal updates then become equivalent to spin flip updates (from 0 to 1 or -1 and vice versa), thus allowing for a similar application of the sub-matrix update algorithm as in the case of the Hirsch-Fye solver³⁵. This procedure is explained in more detail in Sec. III.

II. SUB-MATRIX UPDATES

To derive the sub-matrix updates³⁵ let us consider a typical step k of the algorithm at which the interaction p_k [with spin and time (s_{p_k}, τ_{p_k}) of m interaction vertices] is changed from V_{p_k} to V'_{p_k} . The new matrix G^{k+1} is then given by Eq. (11a),

$$G_{ij}^{k+1} = G_{ij}^k + (G_{ip_k}^k - \delta_{ip_k}) \lambda^k G_{p_k j}^k, \quad (15)$$

$$\lambda^k = e^{V'_{p_k} - V_{p_k}} - 1.$$

λ^k denotes the change of interaction at step k . We proceed by showing how the determinant ratio $\det N^k / \det N^{k+1}$ of Eq. (13) as well as the new matrix N^{k+1} are computed efficiently using the Woodbury formula: We define an inverse matrix A of G , analyze its changes during an update, and show how they can be incorporated in a small $(k \times k)$ matrix Γ that is easily computed by accessing only $k^2 \ll m^2$ matrix elements in each step. The inverse of this matrix is then iteratively computed either by employing an LU decomposition, or a partitioning scheme.

A change to the inverse Green's function matrix $A^k = (G^k)^{-1}$ is of the form⁴⁰

$$\begin{aligned} A_{ij}^{k+1} &= A_{ij}^k + \gamma^k (A_{ip}^k - \delta_{ip}) \delta_{pj} \\ &= A_{ij}^k + \gamma^k A_{ip}^k \delta_{pj} - \gamma^k \delta_{ip} \delta_{pj}, \\ \gamma^k &= e^{-\gamma \sigma(s'_{p_k} - s_{p_k})} - 1. \end{aligned} \quad (16)$$

γ^k , similar to λ^k above, contains the information about the changed interaction at step k . Eq. (16) is commonly known as the Sherman Morrison formula and illustrated in Fig. 1(a). We define $\tilde{A}_{ij}^k = A_{ij}^k + \gamma^k A_{ip}^k \delta_{pj}$, i.e. the matrix A^k where the p -th column is multiplied by $(1 + \gamma^k)$, and therefore $\det \tilde{A}^k = (1 + \gamma^k) \det(A^k)$. We then rewrite Eq. (16) as $A_{ij}^{k+1} = \tilde{A}_{ij}^k - \gamma^k \delta_{ip} \delta_{pj}$, and, using the ‘‘matrix determinant lemma’’ $\det(A_{ij} + u_i v_j) = (1 + v_l (A^{-1})_{lq} u_q) \det A_{ij}$, we have

$$\begin{aligned} \det A^{k+1} &= \det(\tilde{A}^k) \det(1 - \gamma^k [(\tilde{A}^k)^{-1}]_{pp}) \\ &= \det A^k (1 + \gamma^k) \left(1 - \frac{\gamma^k}{1 + \gamma^k} G_{pp}^k\right) \\ &= -\det A^k \gamma^k \left[G_{pp}^k - \frac{1 + \gamma^k}{\gamma^k}\right]. \end{aligned} \quad (17)$$

This formula yields the determinant ratio

$$\frac{\det N^k}{\det N^{k+1}} = -\gamma^k \left[G_{pp}^k - \frac{1 + \gamma^k}{\gamma^k}\right] \quad (18)$$

needed in Eq. (13) for the acceptance or rejection of an update.

We can recursively apply Eq. (17) to obtain an expression for performing multiple interaction changes, as long as they occur for different spins $p_i \neq p_j (i \neq j)$:

$$\begin{aligned} A_{ij}^{k+1} &= A_{ij}^0 + \sum_{l=0}^k \gamma^l (A_{ip_l}^0 - \delta_{ip_l}) \delta_{p_l j} \\ &= \tilde{A}_{ij}^k - \sum_{l=0}^k \gamma^l \delta_{ip_l} \delta_{p_l j} \\ &= \tilde{A}^k - X^k (Y^k)^T, \end{aligned} \quad (19)$$

$$X_{ij}^k = \gamma_j \delta_{ip_j}, \quad (20)$$

$$(Y^k)_{ij}^T = \delta_{p_i j}. \quad (21)$$

The new matrix A^{k+1} is therefore generated from A^0 by successively multiplying columns $p_l, 0 \leq l \leq k$ of A^0 with

γ^l and adding constants to the diagonal. X and Y^T are index matrices that label the changed spins and keep track of a prefactor γ^k .

For measurements we need access to the Green's function G , not its inverse A . It is obtained after k_{\max} steps by applying the Woodbury formula Eq. (22) to Eq. (19): with q denoting a Woodbury step combining k_{\max} vertex update steps:

$$\begin{aligned} G^{q+1} &= (A^{q+1})^{-1} \\ &= \tilde{A}^{-1} + \tilde{A}^{-1} X (1 - Y^T \tilde{A}^{-1} X)^{-1} Y^T \tilde{A}^{-1}, \\ G^{q+1} &= \tilde{G} + \tilde{G} X (1 - Y^T \tilde{G} X)^{-1} Y^T \tilde{G}. \end{aligned} \quad (22) \quad (23)$$

where $\tilde{G} = \tilde{A}^{-1}$. After some simplification, Eq. 23 can be shown to be

$$G_{ij}^{q+1} = D_i^{-1} (G_{ij} - G_{ip_k} \Gamma_{p_k p_l}^{-1} G_{p_l j}). \quad (24)$$

Here we have introduced a $k_{\max} \times k_{\max}$ - matrix Γ , defined as

$$\Gamma_{pq} = G^0(p, q) - \delta_{pq} \frac{1 + \gamma_p}{\gamma_p}, \quad (25)$$

and a vector D that is 1 everywhere but at positions where auxiliary spins are changed:

$$D_{p_k}^{-1} = \frac{1}{1 + \gamma^k}. \quad (26)$$

Note that G^0 is the interacting Green's function at step $k = 0$ and not the bare Green's function \mathcal{G}^0 of the effective action, unless all auxiliary spins are zero.

Translating this Green's function formalism to a formalism for N - matrices is straightforward: writing $G = N \mathcal{G}^0$ and multiplying Eq. (24) from the right with $(\mathcal{G}^0)^{-1}$ yields

$$N_{ij}^{q+1} = D_i^{-1} (N_{ij} - G_{ip_k} \Gamma_{p_k p_l}^{-1} N_{p_l j}), \quad (27)$$

where one G_{ip_k} remains in Eq. (27). This equation is illustrated in Fig. 1(b).

Inserting $G = N G_0$ into Eq. (11a) and setting $V' = 0$ ($N' = 1$) we obtain:

$$1 = N e^V - N G_0 e^V + N G_0 \quad (28)$$

$$(N G_0)_{ij} = (N_{ij} e^{V_j} - \delta_{ij}) / (e^{V_j} - 1) = G_{ij} \quad (29)$$

$$N_{ij} = G_{ij} (1 - e^{-V_j}) + e^{-V_j} \delta_{ij}. \quad (30)$$

The computation of G from N in this manner fails if the interaction V_j is zero. In this case we need to compute $G_{ij} = N_{ik} \mathcal{G}_{kj}^0$ at a cost of $O(N)$ for each i and j .

A. Determinant Ratios and Inverse Matrices

To either accept or reject a configuration change, we need to compute the determinant ratio $\det N^{k+1} / \det N^k$

(Eq. (13)). Following Ref. 35 we write:

$$\det A^{k+1} = (-1)^{k+1} \prod_{j=0}^k \gamma_j \det A^0 \det \Gamma^k. \quad (31)$$

The computation of the determinant $\det \Gamma^k$ is an expensive $O(k^3)$ operation, if Γ^k has to be recomputed from scratch. However, we successively build Γ^k by adding rows and a columns. In the following we present two efficient (and as far as we could see equivalent) methods to iteratively compute determinant ratios of Γ : keeping track of an LU decomposition, and storing the inverse computed using inversion by partitioning.

1. LU decomposition

For each accepted update we keep track of a LU - decomposition of Γ :

$$\Gamma^k = \begin{pmatrix} \Gamma^{k-1} & s \\ w^T & d \end{pmatrix} = \begin{pmatrix} L^{k-1} & 0 \\ x^T & 1 \end{pmatrix} \begin{pmatrix} U^{k-1} & y \\ 0 & \beta \end{pmatrix}, \quad (32)$$

$$Ly = s, \quad (33)$$

$$U^T x = w, \quad (34)$$

$$\beta = G^0(p^k, p^k) - \frac{1 + \gamma^k}{\gamma^k} - x^T y \quad (35)$$

where both x^T and y are computed in $O(k^2)$ by solving a linear equation for a triangular matrix. The determinant ratio needed for the acceptance of an update is

$$\frac{\det A^{k+1}}{\det A^k} = -\beta \gamma^k. \quad (36)$$

These updates have been formulated for spins that have only been updated once. In the case where the same spin is changed twice or more, rows and columns in Γ , or L and U , need to be modified. These changes are of the form $\Gamma \rightarrow \Gamma + uv^T$, and Bennett's algorithm⁴¹ can be used to re-factorize the matrix.

The probability to accept/reject a $(k+1)$ -th spin requires $O(k^2)$ operations (computation of x and y using Eqs. (33) and (34) requires $O(k^2)$ operations, while Eq. (35) requires $O(k)$ operations). On the other hand, the “delayed” algorithm requires $O(km)$ operations to compute the acceptance rate of a $(k+1)$ -th spin flip, for a matrix of size m . In this sense the sub-matrix update methodology not only manages matrix operations efficiently but also improves the computational efficiency of the spin flip acceptance rate.

2. Inversion by Partitioning

Alternatively, we can compute the inverse of Γ by employing the Sherman Morrison formula:

$$\beta = (d - w^T \Gamma_k^{-1} s) \quad (37)$$

$$\Gamma_{k+1}^{-1} = \begin{pmatrix} \Gamma_k^{-1} + (\Gamma_k^{-1} s) \beta^{-1} (w^T \Gamma_k^{-1}) & -\Gamma_k^{-1} s \beta^{-1} \\ -\beta^{-1} w^T \Gamma_k^{-1} & \beta^{-1} \end{pmatrix}, \quad (38)$$

$$\frac{\det \Gamma^{k+1}}{\det \Gamma^k} = \beta, \quad \frac{\det A^{k+1}}{\det A^k} = -\gamma^k \beta. \quad (39)$$

Although both methods obtain the acceptance rates Eq. (36) and (39) in $O(k^2)$ steps, inversion by partitioning requires an additional step of updating the Γ_{k+1}^{-1} , and hence is expected to be slower than the LU decomposition approach. However, the complication of re-orthogonalizing the LU factorized matrix using Bennet's algorithm does not arise.

III. THE RANDOM WALK WITH SUB-MATRIX UPDATES

The sums and integrals of Eq. (6) are computed by a random walk in the space of all expansion orders, auxiliary spins, and time indices. In the cluster case, configurations acquire an additional site index. A configuration c_k at expansion order n contains n interaction vertices with spins, sites, and time indices:

$$c_k = \{(\tau_1, s_1, \sigma_1), \dots, (\tau_n, s_n, \sigma_n)\}. \quad (40)$$

The configuration space \mathcal{C} consists of all integrands / summands in Eq. (6), which we can represent by sets of triplets of numbers, consisting of auxiliary spins, times, and site indices:

$$\mathcal{C} = \{c_0, \dots, c_k((\tau_1, s_1, \sigma_1), \dots, (\tau_k, s_k, \sigma_k)), \dots\}. \quad (41)$$

To efficiently make use of the sub-matrix updates, we add an additional step before insertion and removal updates are performed. In this preparation step, we insert a number k_{\max} of randomly chosen non-interacting vertices with auxiliary spin $s = 0$, which, as discussed in Sec. I, does not change the value of the partition function. Once these vertices are inserted, insertion and removal updates at the locations of the pre-inserted non-interacting vertices become identical to spin-flip updates: an insertion update of a spin $s = 1$ now corresponds to a spin-flip update from spin $s = 0$ to spin $s = 1$, and similar for removal updates. This pre-insertion step of non-interacting vertices then allows for a similar application of sub-matrix updates as in the case of the Hirsch-Fye algorithm.

To accommodate this pre-insertion step, we split our random walk into an inner and an outer loop. In the

outer loop (labeled by q) we perform measurements of observables and run the preparation step discussed above as well as recompute steps. These steps are described in more detail below. In the inner loop (labeled by k) we perform k_{\max} insertion, removal, or spin flip updates at the locations of the pre-inserted non-interacting spins. It is best to choose $\langle m \rangle \gg k_{\max} \gg 1$ so the blocking becomes efficient but matrices of linear size k_{\max} are small enough to fit into cache.

A. Preparation steps

We begin a Monte Carlo sweep with preliminary computations for spins that we will propose to insert or remove. For this, we generate randomly a set of k_{\max}^{ins} pairs of (site, time) indices, where k_{\max}^{ins} denotes the maximum insertions possible. We then compute the additional rows of the matrix N for these noninteracting spins:

$$\tilde{N} = \begin{pmatrix} N & 0 \\ \tilde{R} & 1 \end{pmatrix}, \quad (42)$$

where \tilde{R} is a matrix of size $n \times k_{\max}^{\text{ins}}$ containing the contributions of newly added noninteracting spins,

$$\tilde{R}_{ij} = \mathcal{G}_{ik}^0 (e^{-\gamma \sigma s_k} - 1) N_{kj}, \quad (43)$$

at the cost of $O(n^2 k_{\max}^{\text{ins}})$, as well as the Green's function matrix $G = N \mathcal{G}^0$ for the new spins (cost $n^2 k_{\max}^{\text{ins}}$).

B. Insertion, removal, spinflip of an auxiliary spins

Vertex insertion updates are performed by proposing to flip one of the newly inserted non-interacting spins from value zero to either plus or minus one. The determinant ratio is obtained using Eq. (33), (34), (36), and (35), i.e. by the solution of a linear equation of a triangular matrix. If the update is accepted the auxiliary spin is changed and the matrix Γ is enlarged by a row and a column.

Starting from a configuration $c_k = \{(\tau_1, s_1, \sigma_1), \dots, (\tau_k, s_k, \sigma_k)\}$ we propose to remove the interaction vertex (τ_j, s_j, σ_j) . The ratio of the two determinants (Eq. (35)) is computed by proposing to flip an auxiliary spin from ± 1 to zero. For this we compute s and w as in Eq. (25), and then compute x and y by solving a linear equation for a triangular system [Eq. (33) and Eq. (34)]. Finally Eq. (36) is computed using Eq. (35). If the update is accepted the auxiliary spin is set to zero and Γ is enlarged by a row and a column.

Double vertex updates required for the scheme of Ref. 39 proceed along the same lines and enlarge Γ by two rows and two columns.

To perform a spinflip update we choose a currently interacting spin with value ± 1 and propose to flip it to ∓ 1 using Eq. (33), (34), and (36). If the update is accepted, Γ grows by a row and a column.

C. Recompute step

This scheme of insertion, removal, and spinflip updates is repeated k_{\max} times. With each accepted move the matrix Γ grows by a row and a column. To keep the algorithm efficient we periodically recompute the full N -matrix using the Woodbury formula 27:

$$N_{ij}^{q+1} = D_i^{-1} (G_{ij} - G_{ip_k} \Gamma_{p_k p_l}^{-1} N_{p_l j}), \quad (44)$$

as Γ grows with every accepted update, and the cost of computing determinant ratios is $O(k^2)$. The recompute step consists of two inversions for L and U , which are both $O(k^2)$ operations, and two matrix multiplications, at cost $O(k^2 N)$ and $O(N^2 k)$ respectively. Noninteracting auxiliary spins can then be removed from N_{ij}^{q+1} by deleting the corresponding rows and columns.

D. Measurements

At the end of a sweep, if the system is thermalized, observable averages are computed. As the complete N -matrix is known at this point, the formulas presented in Ref. 31 are employed without change. In most calculations, the computation of the Green's function is the most expensive part of the measurement. In large "dynamical cluster approximation" (DCA)^{16,18,20} calculations it is therefore advantageous to compute directly the Green's functions in cluster momenta, of which there are only N_c , in contrast to the N_c^2 real-space Green's functions. Also, on large clusters, Green's functions are best measured directly in Matsubara frequencies.

IV. RESULTS

We present two types of results. First we examine the performance of sub-matrix updates in practice, using several scaling metrics. We then illustrate a physics application where we test the DCA approximation on large clusters, showing cluster size dependence and extrapolations to the infinite system limit.

A. Scaling of the algorithm

Two types of scaling are commonly analyzed in high performance computing: the so-called "weak" scaling, which defines how the the time to solution varies when the resources are increased commensurately with the problem size, and the "strong" scaling, which is defined as how the time to solution decreases with an increasing amount of resources for fixed problem size.

We begin by analyzing the scaling of the time to solution for fixed resources but varying problem size. As "problem size" we consider the average expansion order

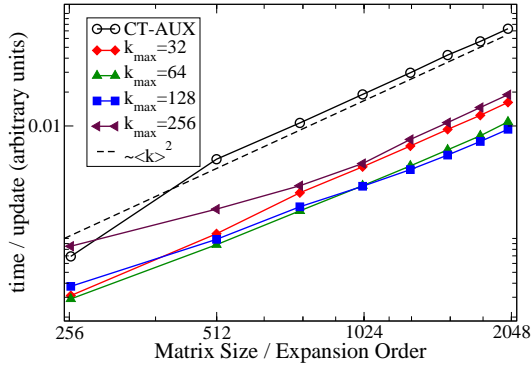


FIG. 2. Time per update (in arbitrary units) for sub-matrix and rank one CT-AUX updates. Open circles (black online): rank one updates. Filled diamonds, triangles, squares, and left triangles: sub-matrix updates for $k_{\max} = 32, 64, 128$, and 256. Dashed line: ideal $O(k^2)$ scaling, arbitrary prefactor.

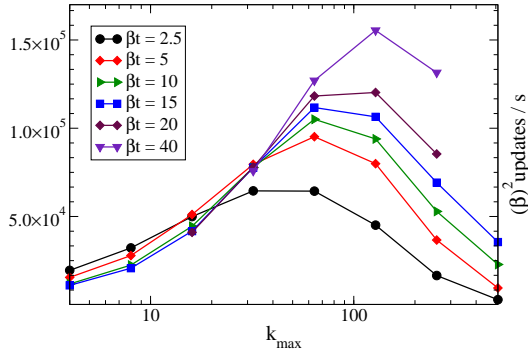


FIG. 3. Updates per time as a function of k_{\max} . 16-site cluster, $U/t = 8$, for temperatures indicated.

or matrix size, $\langle k \rangle$. The average expansion order is related to the potential energy and therefore e.g. extensive in cluster size. For systems with small average expansion orders ($N \lesssim 200$), the entire matrix fits into cache, and therefore there is no advantage in using sub-matrix updates. With increasing average matrix size caching effects become more important.

Fig. 2 shows the strong scaling, as the time per update (in arbitrary units) as a function of expansion order (matrix size), for rank one updates and several k_{\max} . The ideal scaling is $O(k^2)$ per update, or $O(k^3)$ for $\langle k \rangle$ updates needed to decorrelate a configuration.⁴² The scaling per update is indicated by the dashed line.

Submatrix updates are, for problems with expansion orders between 512 and 2048, about a factor of eight faster than straightforward rank one updates.

For small expansion order CT-AUX with and without sub-matrix updates behave similarly. For expansion orders of 256 and larger, the speed increase from sub-matrix updates becomes apparent, and at expansion orders of 512 and larger the difference with and without sub-matrix updates corresponds to the difference of data transfer rates between cache and CPU and main mem-

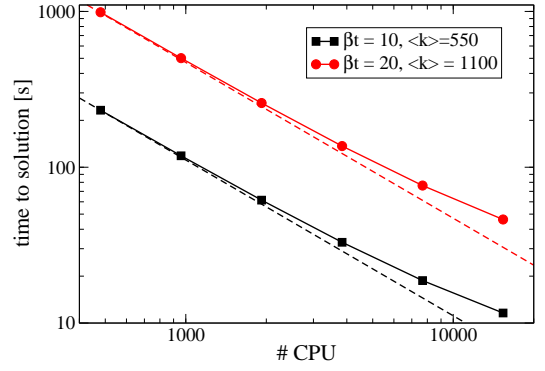


FIG. 4. Time to solution as a function of the number of CPUs, for a 16-site cluster impurity problem. Squares (black online): $U/t = 8$, $\beta t = 10$ ($\langle k \rangle = 550$), half filling. Circles (red online): $\beta t = 20$ ($\langle k \rangle = 1100$). The dashed lines show the ideal scaling.

ory and CPU, or the difference at which memory intensive (Sherman Morrison like vector operations) and CPU intensive (Woodbury like matrix operations) run.

The optimal choice of the expansion parameter k_{\max} for the test architecture lies somewhere between 64 and 128 (performance is relatively insensitive to the exact choice of k_{\max}). This is also illustrated in Fig. 3: for a small choice of k_{\max} the Woodbury matrix-matrix operations do not dominate the calculation and the algorithm is similar to CT-AUX, where much time is spent idling at memory bottlenecks. Caching effects get more advantageous for larger k_{\max} , until for $k_{\max} \gtrsim 128$ most of the time is spent updating and inverting the Γ matrices. Note, however, that the optimal value of k_{\max} is expected to depend on architectural details such as the size of the cache.

In Fig. 4 we present a strong scaling curve by showing the time to solution (in seconds) for two problem sets (symbols), as well as the ideal scaling (dashed lines), as a function of the number of CPUs employed. This time includes communications and thermalization overhead that does not scale with the number of processors. This is the part that according to Amdahl's law⁴³ leads to less than ideal scaling behavior. CT-AUX has a remarkably small thermalization time and is therefore ideally suited for parallelization on large machines. As can be seen, for the chosen problem sizes, the algorithm can be scaled almost ideally to at least 10,000 CPUs. Note, however, that the scaling behavior is expected to depend critically on the number and type of measurements that are performed. This is because the measurements are perfectly parallel, since they are only performed once the calculation is thermalized. Here, we have restricted the measurements to the single-particle Green's function. If, in addition, more complex quantities such as e.g. two-particle observables are measured, the simulation run-time will be dominated by the measurements and the ideal scaling behavior is expected to continue to much larger processor counts.

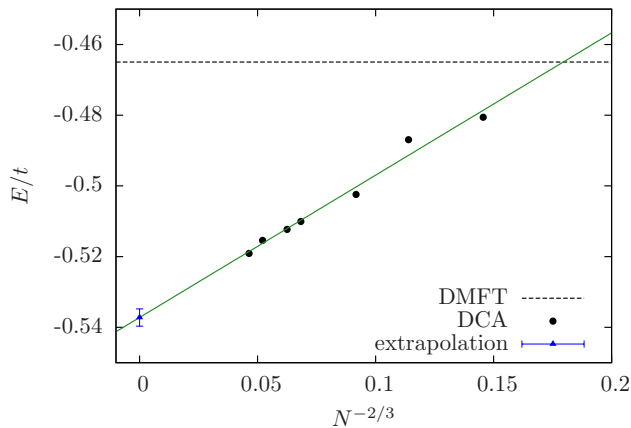


FIG. 5. Extrapolation of the cluster energy as a function of cluster size, at $U/t = 8$, $T/t = 0.5$. Dashed line: DMFT results. Circles (black online) denote DCA results from clusters with size 18, 26, 36, 56, 64, 84, and 100. Solid line (green online): least squares fit. Triangle (blue online): extrapolated result. The error bar denotes the fitting error; statistical (Monte Carlo) errors are smaller than symbol size.

B. Simulations of the 3D Hubbard model

As an illustration of the power of the algorithm we present results from a calculation of the Néel temperature of the three-dimensional Hubbard model at half filling, within the DCA approximation, as a function of cluster size.

A comprehensive study, showing DCA data at and away from half filling, for interaction strengths up to $U \simeq 12$ and clusters of size ≤ 64 , will be published elsewhere⁴⁴. The results we present here are for temperature $T = t$ (far above T_N), for $T = 0.5t$, and for $T = 0.35t$. The lowest temperature is close to the Néel temperature, and long ranged correlations cause a slow convergence. Results were obtained on 128 CPUs in one hour per iteration. In Fig. 5 we show the extrapolation of the energy for several cluster sizes and an extrapolation to the infinite cluster size limit. The plot shows that controlled extrapolations to the thermodynamic limit^{44–47} can be obtained in practice. Monte Carlo errors are much smaller than the symbol size.

Fig. 6 shows self-energy cuts along the main axes in reciprocal space. Plotted are results for single site DMFT and clusters of size 18, 84, and 100, interpolated using Akima splines. While momentum averaged quantities like the energy in Fig. 5 show clear convergence and the possibility for extrapolation, convergence is not uniform in all quantities. The high temperature self-energy plotted in panel 6a is clearly converged as a function of cluster size, the intermediate temperature self-energy plotted in panel 6b shows some cluster size dependence, and the right panel 6c shows a self-energy that even for 100 cluster sites is not yet converged (a sign of the long wavelength physics important near T_N). Reliable extrapolation of the cluster self-energy to the $\Sigma(k, \omega)$ of the infi-

nite system would require even larger clusters. Further insight can be gained from the frequency dependence of the Matsubara self-energy (Fig. 7). Plotted is the frequency dependence at three points in the Brillouin zone. While a significant cluster size dependence is observed at low frequencies, the results converge to the local DMFT limit at high frequencies, as one would expect.

V. CONCLUSIONS

We have presented a variation of the CT-AUX algorithm that, while mathematically equivalent, arranges operations in such a manner that they are ideally suited for modern computational architectures. For large problem sizes, this “sub-matrix” algorithm achieves a significant performance increase relative to the traditional CT-AUX algorithm, by replacing the slow rank-one updates by faster matrix-matrix operations. Our implementation of the sub-matrix updates in the CT-AUX algorithm requires an additional preparation step in which non-interacting vertices with auxiliary spins $s = 0$ are introduced. After this step, the CT-AUX vertex insertion and removal updates become equivalent to spin-flip updates. The sub-matrix algorithm then proceeds by manipulating the inverse of the Green’s function matrix, for which changes under auxiliary spin-flips are completely local. This allows for a significantly faster computation of the QMC transition probabilities under a spin-flip update. The algorithm keeps track of a number k of these local changes, similar to the delayed update algorithm, and then performs a Green’s function update as a matrix-matrix multiply.

Because this algorithm requires additional overhead over the traditional CT-AUX implementation, there is an optimal choice for the maximum number of spin-flip updates k_{\max} per Green’s function update which depends on problem size and architectural parameters such as the cache size. For the test architecture we have used, we have found that $k_{\max} \approx 128$ for large problem sizes. For this optimal value, we find a speed increase up to a factor of 8 relative to the traditional CT-AUX algorithm.

We have shown that simulations for large interacting systems, previously requiring access to high performance supercomputers, become feasible for small cluster architectures, and we have demonstrated the scaling on supercomputers that shows that, by using the sub-matrix algorithm, continuous-time quantum Monte Carlo methods are almost ideally adapted to high performance machines.

As an example we have shown how some cluster dynamical mean field theory quantities, like the energy, can be reliably extrapolated to the thermodynamic limit, and how for other quantities, like the self-energy, even large cluster calculations are not sufficient to obtain converged extrapolations.

The algorithm is similarly suited to the solution of lattice problems, i.e. problems where $V_{p\sigma} = 0$ and where

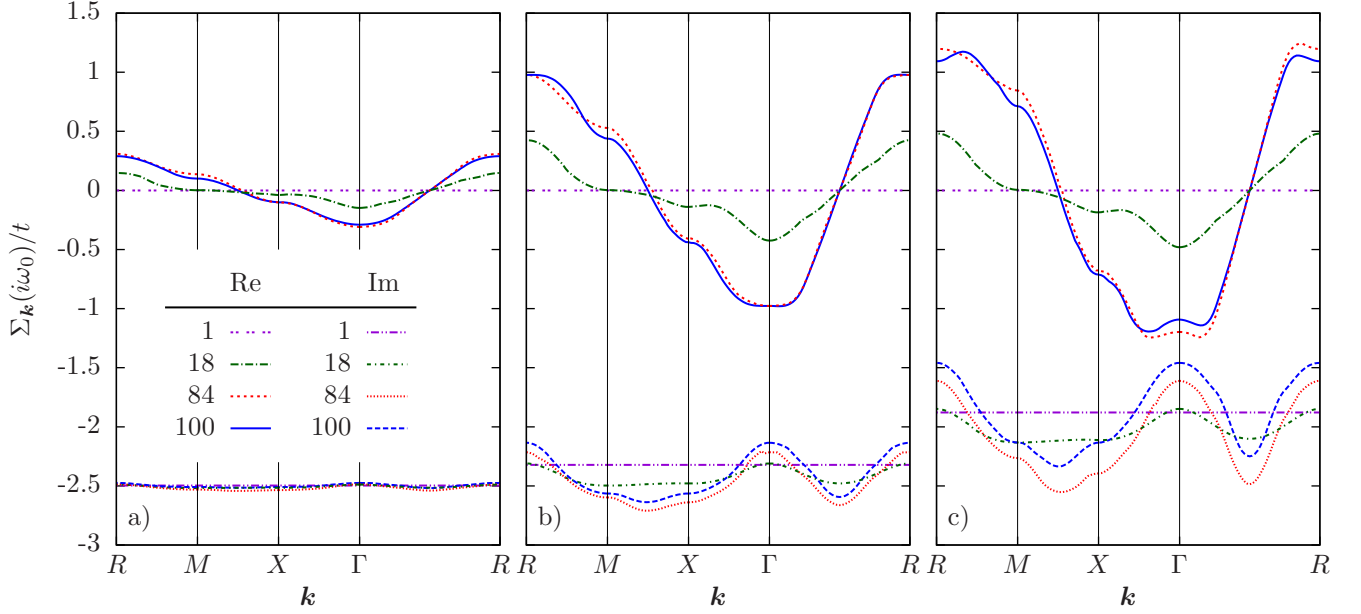


FIG. 6. Real and imaginary parts of the lowest Matsubara frequency of the interpolated DCA cluster self-energy $\Sigma(k, i\omega_0)$ of a 3D Hubbard model above the Néel temperature⁴⁴, for $U/t = 8$, $T/t = 1$ (left panel), $T/t = 0.5$ (middle panel), and $T/t = 0.35$ (right panel), at half filling. The lines denote DMFT results (horizontal straight lines) and results for clusters of size 18, 84, and 100. The interpolation follows a path along the high-symmetry points $\Gamma = (0, 0, 0)$, $X = (\pi, 0, 0)$, $M = (\pi, \pi, 0)$, and $R = (\pi, \pi, \pi)$.

no (cluster) dynamical mean field self-consistency is imposed.

Our results are also readily generalized to the interaction expansion formalism developed in Ref. 27 and 28, offering the possibility to significantly accelerate simulations of multi-orbital systems.

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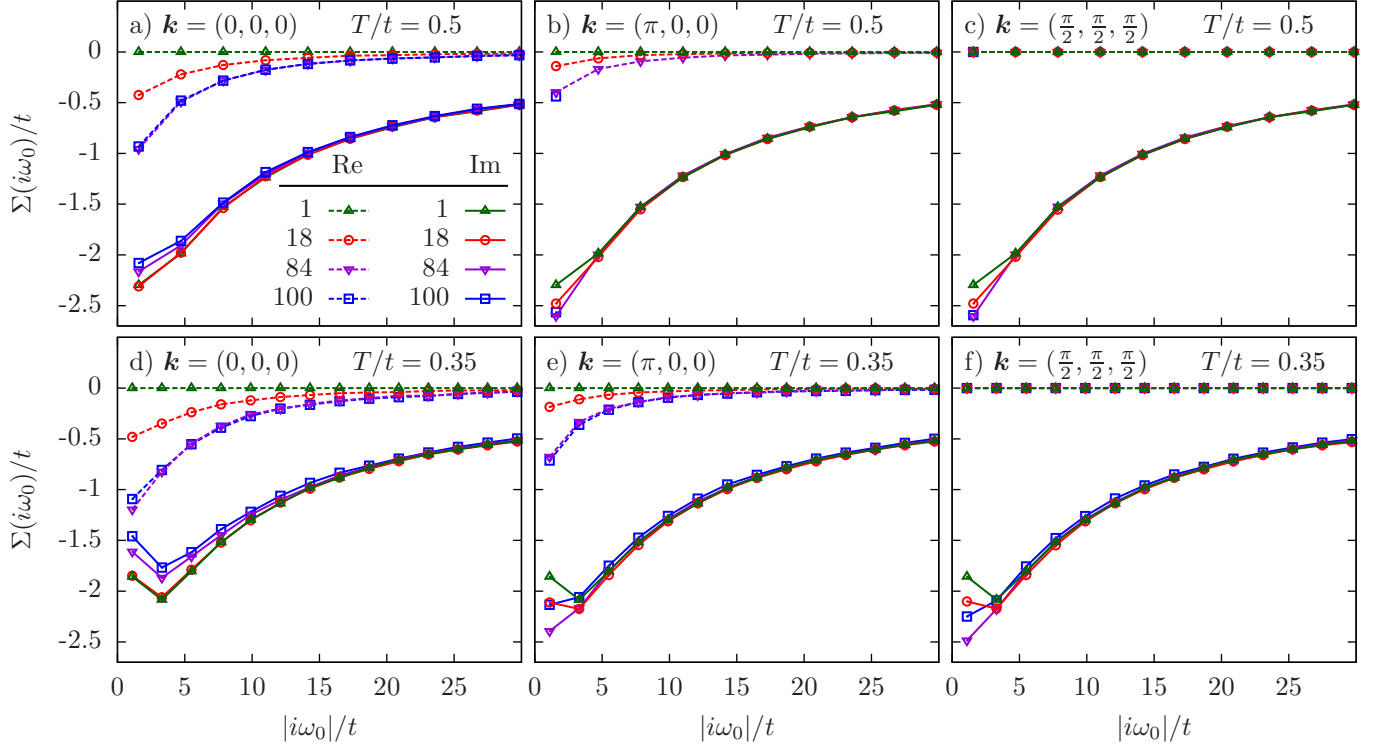


FIG. 7. Real and imaginary parts of the frequency dependence of the interpolated DCA cluster self-energy $\Sigma(k, i\omega_0)$ at selected k -points $(0,0,0)$, $(\pi,0,0)$, and $(\pi/2, \pi/2, \pi/2)$. 3D Hubbard model above the Néel temperature⁴⁴, for $U/t = 8$, $T/t = 0.5$ (upper row), and $T/t = 0.35$ (lower row), at half filling. The lines denote DMFT results (horizontal straight lines) and results for clusters of size 18, 84, and 100.

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