Fierz Convergence Criterion: A Controlled Approach to Strongly Interacting Systems with Small Embedded Clusters

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We present an embedded-cluster method, based on the triply irreducible local expansion formalism. It turns the Fierz ambiguity, inherent to approaches based on a bosonic decoupling of local fermionic interactions, into a convergence criterion. It is based on the approximation of the three-leg vertex by a coarse-grained vertex computed from a self-consistently determined cluster impurity model. The computed self-energies are, by construction, continuous functions of momentum. We show that, in three interaction and doping regimes of the two-dimensional Hubbard model, self-energies obtained with clusters of size four only are very close to numerically exact benchmark results. We show that the Fierz parameter, which parametrizes the freedom in the Hubbard-Stratonovich decoupling, can be used as a quality control parameter. By contrast, the GW + extended dynamical mean field theory approximation with four cluster sites is shown to yield good results only in the weak-coupling regime and for a particular decoupling. Finally, we show that the vertex has spatially nonlocal components only at low Matsubara frequencies.

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Two major approaches have been put forth to fathom the nature of high-temperature superconductivity. Spin fluctuation theory [1–8], inspired by the early experiments on cuprate compounds, is based on the introduction of phenomenological bosonic fluctuations coupled to the electrons. It belongs to a larger class of methods, including the fluctuation-exchange (FLEX) [9] and GW approximations [10,11], or the Eliashberg theory of superconductivity [12]. In the Hubbard model, these methods can formally be obtained by decoupling the electronic interactions with Hubbard-Stratonovich (HS) bosons carrying charge, spin, or pairing fluctuations. They are particularly well suited for describing long-range modes. However, they suffer from two main drawbacks: without an analog of Migdal's theorem for spin fluctuations they are quantitatively uncontrolled; worse, the results depend on the precise form of the bosonic fluctuations used to decouple the interaction term, an issue dubbed the "Fierz ambiguity" [13–18].

A second class of methods, following Anderson [19], puts primary emphasis on the fact that the undoped compounds are Mott insulators, where local physics plays a central role. Approaches like dynamical mean field theory (DMFT) [20] and its cluster extensions [21–25], which self-consistently map the lattice problem onto an effective problem describing a cluster of interacting atoms embedded in a noninteracting host, are tools of choice to examine Anderson's idea. Cluster DMFT has indeed been shown to give a consistent qualitative picture of cuprate physics, including pseudogap and superconducting phases [26–54]. Compared to fluctuation theories, it *a priori* comes with a control parameter, the size N_c of the embedded cluster. However, this is of limited practical use, since the convergence with N_c is nonmonotonic for small N_c [33], requiring large N_cs, which cannot be reached in interesting physical regimes due to the Monte Carlo negative sign problem. Thus, converged cluster DMFT results can only be obtained at high temperatures [55]. There, detailed studies [56–58] point to the importance of (possibly long-ranged) spin fluctuations, calling for a unification of both approaches. First steps in this direction have been accomplished by diagrammatic extensions of DMFT [59–80], and by the single-site triply irreducible local expansion (TRILEX) formalism [81,82], which interpolates between long-range and Mott physics and describes aspects of pseudogap physics and the d-wave superconducting dome [83].

In this Letter, we turn the Fierz ambiguity into a convergence criterion in the cluster extension of TRILEX. Like fluctuation approaches, cluster TRILEX is based on the introduction of bosonic degrees of freedom. Like cluster DMFT, it maps the corresponding electron-boson problem onto a cluster impurity problem. The latter is solved for its three-leg vertex, which is used as a cluster vertex correction to the self-energies. This approach improves on fluctuation approaches by endowing them with a control parameter, thus curing the absence of a Migdal theorem. In some parameter regimes, it can solve the cluster DMFT large-N_c stalemate by instead requiring minimal sensitivity to the Fierz parameter as a convergence criterion of the solution.

To illustrate the method, we focus on the two-dimensional Hubbard model, the simplest model to describe high-temperature superconductors. Its Hamiltonian reads

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) an electron of spin σ at Bravais site $\mathbf{r}_i$, t_{ij} is the hopping matrix [with (next-)nearest-neighbor hopping t (t')], and U the local electronic repulsion. We set $t = -0.25$ and use $D \equiv 4|t|$ as the energy unit.

The first step of the TRILEX method consists in decoupling the interaction term with HS fields. There are several possible such decouplings. Here, we choose [84] to express the interaction in the charge and longitudinal spin channel ("Ising decoupling"), i.e, up to a density term

$$U n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} U^{\mathrm{ch}} n_i n_i + \frac{1}{2} U^{\mathrm{sp}} s^z_i s^z_i, \tag{2}$$

with $n \equiv n_\uparrow + n_\downarrow$ and $s^z \equiv n_\uparrow - n_\downarrow$. This holds provided $U^{\mathrm{ch}} - U^{\mathrm{sp}} = U$, or, equivalently,

$$U^{\mathrm{ch}} = \alpha U, \qquad U^{\mathrm{sp}} = (\alpha - 1) U. \tag{3}$$

The Fierz parameter α materializes the freedom in choosing the charge-to-spin fluctuation ratio. The right-hand side of Eq. (2) is decoupled with a charge and a spin boson, resulting in an electron-boson coupling problem [81,82]. Its fermionic and bosonic interacting Green's functions are given by the Dyson equations:

$$G(\mathbf{k}, i\omega) = \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(\mathbf{k}, i\omega)}, \tag{4a}$$

$$W^\eta(\mathbf{q}, i\Omega) = \frac{U^\eta}{1 - U^\eta P^\eta(\mathbf{q}, i\Omega)}. \tag{4b}$$

$\varepsilon(\mathbf{k})$ is the Fourier transform of t_{ij} $\varepsilon(\mathbf{k}) = 2t[\cos(k_x) + \cos(k_y)] + 4t' \cos(k_x)\cos(k_y)$, μ the chemical potential, $\eta = \mathrm{ch}$, sp, and $i\omega$ ($i\Omega$) the fermionic (bosonic) Matsubara frequencies. The self-energy $\Sigma(\mathbf{k}, i\omega)$ and polarization $P^\eta(\mathbf{q}, i\Omega)$ are given by the exact Hedin expressions

$$\Sigma(\mathbf{k}, i\omega) = -\sum_\eta \sum_{\mathbf{q}, i\Omega} G(\mathbf{k} + \mathbf{q}, i\omega + i\Omega) \times W^\eta(\mathbf{q}, i\Omega) \Lambda^\eta_{\mathbf{kq}}(i\omega, i\Omega), \tag{5a}$$

$$P^\eta(\mathbf{q}, i\Omega) = 2 \sum_{\mathbf{k}, i\omega} G(\mathbf{k} + \mathbf{q}, i\omega + i\Omega) G(\mathbf{k}, i\omega) \Lambda^\eta_{\mathbf{kq}}(i\omega, i\Omega). \tag{5b}$$

$\Lambda^\eta_{\mathbf{kq}}(i\omega, i\Omega)$ is the interacting electron-boson vertex. TRILEX approximates it with a vertex computed from a self-consistent impurity model. In previous works [81,82], this impurity model contained a single site.

There are several ways to extend the TRILEX method to cluster impurity problems, like in DMFT. Here, we consider the analog of the dynamical cluster approximation (DCA [21,22,25]), and use periodic clusters so as not to break the lattice translational symmetry, at the price of discontinuities in the momentum dependence of the *vertex function*. Other cluster variants such as a real-space version, inspired from cellular DMFT [23,24], are also possible, but break translation invariance and require arbitrary reperiodization procedures.

We straighforwardly generalize the single-site impurity model of TRILEX to a cluster impurity model defined by the action

$$S_{\mathrm{imp}} \equiv \iint_{\tau\tau'} \sum_{ij\sigma} c^*_{i\sigma\tau} \{-[\mathcal{G}^{-1}]_{ij}(\tau - \tau')\} c_{j\sigma\tau'} + \frac{1}{2} \iint_{\tau\tau'} \sum_{ij} \{ n_{i\tau} \mathcal{U}^{\mathrm{ch}}_{ij}(\tau - \tau') n_{j\tau'} + s^z_{i\tau} \mathcal{U}^{\mathrm{sp}}_{ij}(\tau - \tau') s^z_{j\tau'} \}. \tag{6}$$

The indices $i, j = 1, \ldots, N_c$ stand for the cluster positions $\mathbf{R}_i$, $\mathbf{R}_j$ (shown in Fig. 1 along with the cluster momenta $\{\mathbf{K}_i\}_{i=1\ldots N_c}$). $c^*_{i\sigma\tau}$ and $c_{i\sigma\tau}$ are conjugate Grassmann fields, τ denotes imaginary time. Since we have introduced a charge and a spin bosonic mode, the impurity action contains interactions in both channels [$\mathcal{U}^{\mathrm{ch}}(\tau)$ and $\mathcal{U}^{\mathrm{sp}}(\tau)$]. They are *a priori* retarded due to the nonlocal character of $P^\eta(\mathbf{q}, i\Omega)$

This impurity model is used to compute the cluster impurity vertex $\Lambda^\eta_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega)$ with a continuous-time quantum Monte Carlo algorithm with a hybridization (interaction) expansion for $N_c = 1$ ($N_c = 2$, 4) (as described in Supplemental Material II.C [84]). Next, in the spirit of DCA, we want to use $\Lambda^\eta_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega)$ to approximate the momentum dependence of the lattice vertex $\Lambda^\eta_{\mathbf{kq}}(i\omega, i\Omega)$ by a coarse-graining procedure. We recall that DCA consists in coarse-graining the cluster

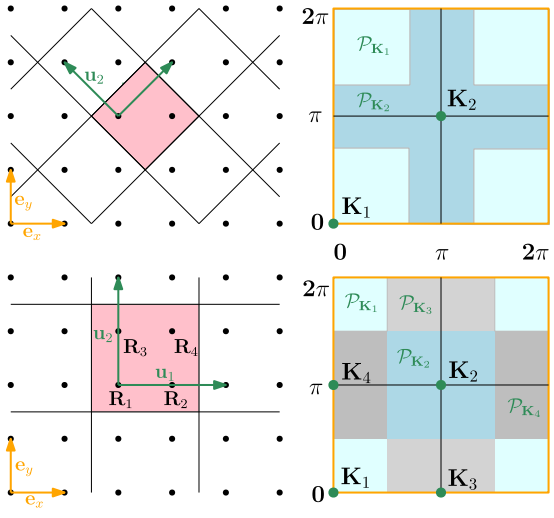

FIG. 1. Cluster geometry: real (left) and reciprocal (right) space, for $N_c = 2$ (top) and $N_c = 4$ (bottom). $\mathbf{e}_x$ and $\mathbf{e}_y$ ($\mathbf{u}_1$ and $\mathbf{u}_2$) are the unit vectors of the Bravais (super)lattice. The colored patches $\mathcal{P}_{\mathbf{K}_i}$ are of equal area.

self-energy as $\Sigma(\mathbf{k}, i\omega) \approx \sum_{\mathbf{K}} \theta_{\mathbf{K}}(\mathbf{k}) \Sigma_{\mathrm{imp}}(\mathbf{K}, i\omega)$, where $\Sigma_{\mathrm{imp}}(\mathbf{K}, i\omega)$ is the cluster impurity self-energy, and $\theta_{\mathbf{K}}(\mathbf{k}) = 1$ if $\mathbf{k}$ belongs to Brillouin-zone patch $\mathcal{P}_{\mathbf{K}}$, and vanishes otherwise. For the vertex function, the passage from $\Lambda^{\eta}_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega)$ to an approximate lattice vertex $\Lambda^{\eta}_{\mathbf{k},\mathbf{q}}(i\omega, i\Omega)$ is not as straightforward. There are several possible coarse grainings for the vertex that reduce to single-site TRILEX for $N_c = 1$ and are exact in the $N_c = \infty$ limit, e.g.,

$$\Lambda^{\eta}_{\mathbf{kq}}(i\omega, i\Omega) \approx \sum_{\mathbf{K},\mathbf{Q}} \theta_{\mathbf{K}+\mathbf{Q}}(\mathbf{k}+\mathbf{q}) \theta_{\mathbf{Q}}(\mathbf{q}) \Lambda^{\eta}_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega), \tag{7a}$$

$$\Lambda^{\eta}_{\mathbf{kq}}(i\omega, i\Omega) \approx \sum_{\mathbf{K},\mathbf{Q}} \theta_{\mathbf{K}}(\mathbf{k}) \theta_{\mathbf{K}+\mathbf{Q}}(\mathbf{k}+\mathbf{q}) \Lambda^{\eta}_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega). \tag{7b}$$

We use a different coarse graining for Σ and for P: we substitute (7a) in (5a) [(7b) in (5b)] to compute $\Sigma(\mathbf{k}, i\omega)$ [$P^{\eta}(\mathbf{q}, i\Omega)$], whence

$$\Sigma(\mathbf{k}, i\omega) = -\sum_{\eta,\mathbf{K},\mathbf{Q}} \sum_{\mathbf{q},i\Omega} G^{\mathbf{K}+\mathbf{Q}}_{\mathbf{k}+\mathbf{q}}(i\omega + i\Omega) W^{\eta,\mathbf{Q}}_{\mathbf{q}}(i\Omega) \times \Lambda^{\eta}_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega), \tag{8a}$$

$$P^{\eta}(\mathbf{q}, i\Omega) = 2\sum_{\mathbf{K},\mathbf{Q}} \sum_{\mathbf{k},i\omega} G^{\mathbf{K}+\mathbf{Q}}_{\mathbf{k}+\mathbf{q}}(i\omega + i\Omega) G^{\mathbf{K}}_{\mathbf{k}}(i\omega) \times \Lambda^{\eta}_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega, i\Omega), \tag{8b}$$

with $X^{\mathbf{K}}_{\mathbf{k}}(i\omega) \equiv \theta_{\mathbf{K}}(\mathbf{k}) X(\mathbf{k}, i\omega)$ (for $X = G$ and W). As convolutions of continuous functions of $\mathbf{k}$ (G and W) with a piecewise-constant function (Λ), Σ and P are continuous in $\mathbf{k}$ by construction.

Finally, the cluster dynamical mean fields $\mathcal{G}_{ij}(\tau)$ and $\mathcal{U}^{\eta}_{ij}(\tau)$ are determined by imposing the following self-consistency conditions,

$$G_{\mathrm{imp}}(\mathbf{K}, i\omega)[\mathcal{G}, \mathcal{U}] = G_{\mathbf{K}}(i\omega), \tag{9a}$$

$$W^{\eta}_{\mathrm{imp}}(\mathbf{Q}, i\Omega)[\mathcal{G}, \mathcal{U}] = W^{\eta}_{\mathbf{Q}}(i\Omega). \tag{9b}$$

The left-hand sides are computed by solving the impurity model. The right-hand sides are the patch-averaged lattice Green's functions $G_{\mathbf{K}}(i\omega) \equiv \sum_{\mathbf{k}\in\mathcal{P}_{\mathbf{K}}} G(\mathbf{k}, i\omega)$ and $W^{\eta}_{\mathbf{Q}}(i\Omega) \equiv \sum_{\mathbf{q}\in\mathcal{P}_{\mathbf{Q}}} W^{\eta}(\mathbf{q}, i\Omega)$. The determination of $\mathcal{G}$ and $\mathcal{U}^{\eta}$ satisfying Eqs. (9a), (9b) is done by forward recursion (see Supplemental Material II.B, [84])

We have implemented this method and studied it in three physically distinct parameter regimes: (A) Weak-coupling regime at half-filling ($U/D = 0.5$, $\delta = 0\%$, $\beta D = 16$, $t' = 0$) at half-filling, (B) Intermediate-coupling regime at large doping ($U/D = 1$, $\delta = 20\%$, $\beta D = 16$, $t' = 0$) at large doping, (C) Strong-coupling regime at small doping ($U/D = 1.4$, $\delta = 4\%$, $\beta D = 8$, $t'/t = -0.3$) at small doping (the Mott transition occurs at $U_c/D \approx 1.5$ within plaquette cellular DMFT [89]). We solve at point A, B, C for different values of α.

In the absence of any approximation, every HS decoupling, hence every value of α, yields the same result: the exact solution does not depend on α. The cluster TRILEX approximation *a priori* breaks this property, but as N_c increases, we expect the α dependence to become weaker. We propose to use the weak α dependence for a given N_c, i.e., the existence of a plateau for at least a range α, as a (Fierz) convergence criterion. That this criterion is *sufficient* to establish convergence is an assumption, which we test here using exact benchmarks for points A, B, and C. Indeed, in these regimes, determinant quantum Monte Carlo (QMC) calculations and/or DCA can be converged and give a numerically exact solution of the Hubbard model, albeit at a significant numerical cost.

We start with point A. In Fig. 2, we show the self-energy $\Sigma(\mathbf{k}, i\omega_0)$ for cluster sizes of $N_c = 1$ (single-site), 2 (dimer), and 4 (plaquette) and for three different values of α. As expected, the dependence on α decreases with N_c. At $N_c = 4$, the self-energy is almost independent on α. The α dependence for $N_c = 1$, 2, 4 is further illustrated in Fig. 3: the $N_c = 4$ results show an extended plateau that is narrower or nonexistent for $N_c = 1$, 2.

The benchmarks, using numerically exact determinant QMC [90] computed with $N_c = 16 \times 16$ sites, are also presented on Figs. 2 and 3. We observe a very good

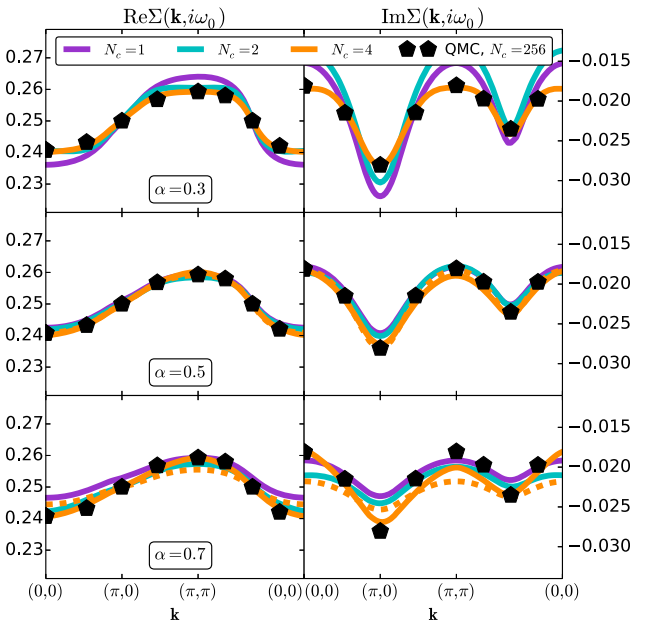

FIG. 2. Point A ($U/D = 0.5$, $\delta = 0\%$, $\beta D = 16$, $t' = 0$). $\mathrm{Re}\Sigma(\mathbf{k}, i\omega_0)$ (left) and $\mathrm{Im}\Sigma(\mathbf{k}, i\omega_0)$ (right) for $N_c = 1$, 2, 4 for various values of α (from top to bottom), along the path $(0,0) - (\pi,0) - (\pi,\pi) - (0,0)$. Solid lines: TRILEX. Dashed lines: GW + EDMFT ($N_c = 4$). Pentagons: determinant QMC (only a subset of $\mathbf{K}$ points is shown for better visibility).

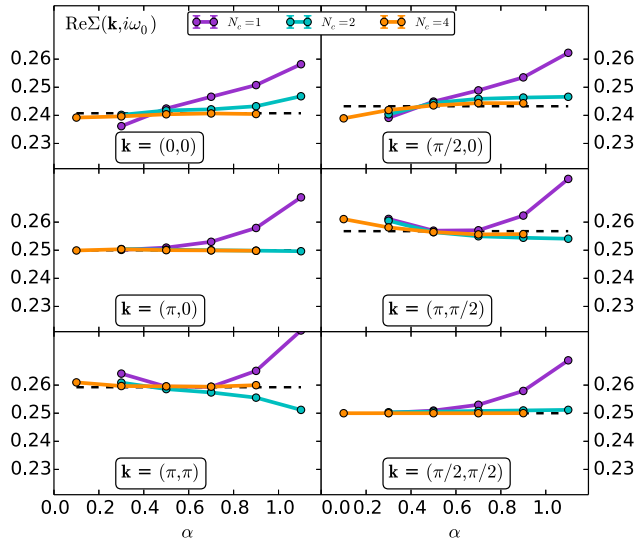

FIG. 3. Dependence of $\mathrm{Re}\Sigma(\mathbf{k}, i\omega_0)$ on α for different momenta (Point A: $U/D = 0.5$, $\delta = 0\%$, $\beta D = 16$, $t' = 0$). Black dashed lines: QMC.

agreement between $N_c = 4$ and the benchmark data, both for the real and imaginary parts of the self-energy, which validates the Fierz criterion in this regime. We also observe that for $\alpha = 0.5$, the results are in agreement with the converged values regardless of N_c. This can be understood by noticing that $\alpha = 0.5$ corresponds to the values of U^η used in the random phase approximation (RPA), which is correct to second order in U.

Moreover, we compare our results with the self-energy obtained by the $GW + \mathrm{EDMFT}$ [60–66] method for $N_c = 4$. $GW + \mathrm{EDMFT}$ can be regarded as a simplification of TRILEX where the vertex corrections are neglected in the nonlocal self-energy contribution. This explains why the $GW + \mathrm{EDMFT}$ results are, independently of α, quite close to the single-site TRILEX results: the vertex frequency and momentum dependences are weak in the low-U limit. Besides, they are different from the cluster TRILEX results and from the exact solution, except for the RPA value of α ($\alpha = 0.5$) where both methods give results close to the exact solution.

At point B (Fig. 4), the agreement between the benchmarks and the real and imaginary parts of the self-energy, for all values of α (with more important deviations for $\alpha = 0.3$), is very good for $N_c = 4$. Contrary to the weak-coupling limit, no value of α in the single-site case matches the exact solution. This points to the importance of nonlocal corrections to the three-leg vertex. This observation is further corroborated by looking at the $GW + \mathrm{EDMFT}$ curve. There, the agreement with the exact result is quite poor, while being similar to the single-site result, like in the weak-coupling limit (for $\alpha = 0.3$, a spin instability precludes convergence of $GW + \mathrm{EDMFT}$ and cluster TRILEX for $N_c = 2$). This discrepancy shows that as interactions are increased, the vertex frequency and momentum dependence play a more and more important role in the nonlocal self-energy, as discussed below. These conclusions are also valid for local observables (see Supplemental Material III.C [84]).

At the strong-coupling point C (Fig. 5), similarly to the previous regimes, the $N_c = 4$ self-energy is almost independent of α, and in good agreement with the converged

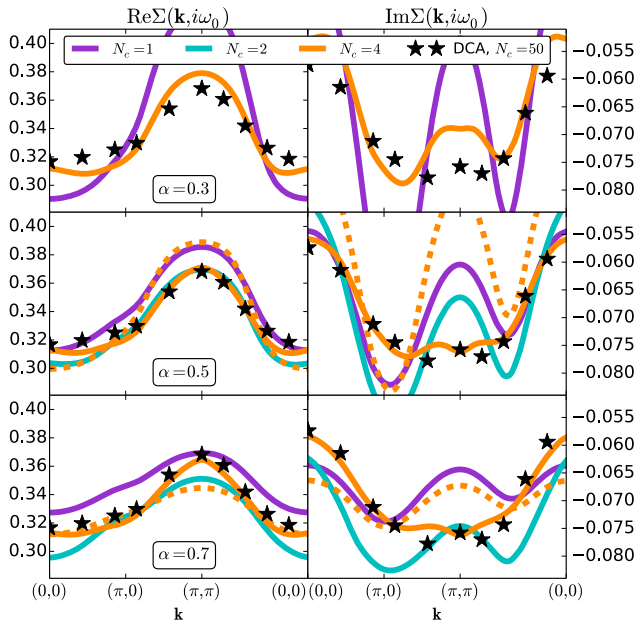

FIG. 4. $\Sigma(\mathbf{k}, i\omega_0)$ at point B ($U/D = 1$, $\delta = 20\%$, $\beta D = 16$, $t' = 0$). Same conventions as Fig. 2. Dashed lines: GW+EDMFT. Stars: DCA from Ref. [55].

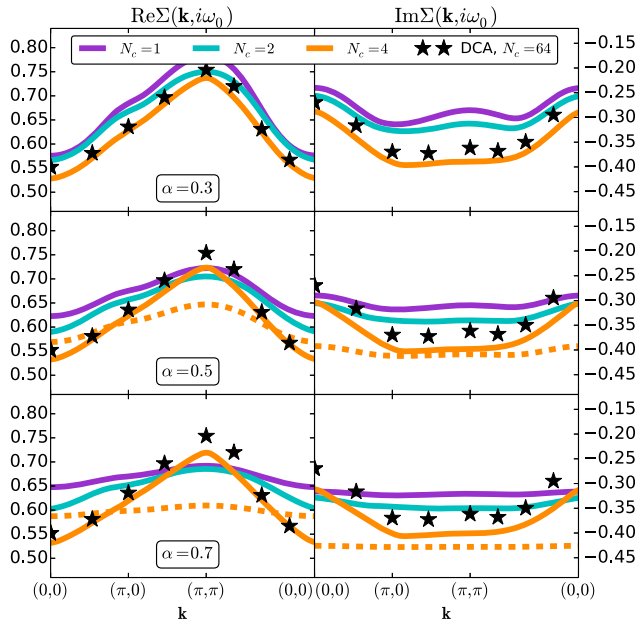

FIG. 5. $\Sigma(\mathbf{k}, i\omega_0)$ at point C ($U/D = 1.4$, $\delta = 4\%$, $\beta D = 8$, $t'/t = -0.3$). Same conventions as Fig. 2. Dashed lines: GW+EDMFT. Stars: DCA.

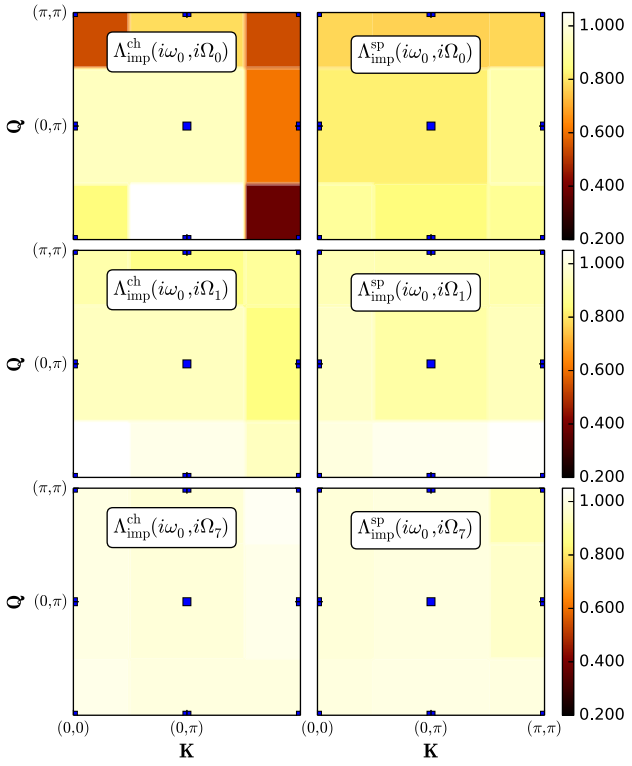

FIG. 6. Point B ($U/D = 1$, $\delta = 20\%$, $\beta D = 16$, $t' = 0$), $\alpha = 0.5$. Impurity vertex $\Lambda^{\eta}_{\mathrm{imp}}(\mathbf{K}, \mathbf{Q}; i\omega_0, i\Omega)$ at $\mathbf{K}, \mathbf{Q} \in [(0,0), (0,\pi), (\pi,\pi)]^2$ (the value is color coded in the square area surrounding each blue point) in the charge (left) and spin (right) channels, for increasing bosonic Matsubara frequency (from top to bottom).

(DCA) solution (especially for its real part). $GW +$ EDMFT at $N_c = 4$ is quite far from the exact result, as can be expected from the previous discussion.

Finally, we analyze the momentum and frequency dependence of the vertex, illustrated in Fig. 6. At low Matsubara frequencies, the vertex acquires a momentum dependence (especially in the charge channel), while it is essentially local at high frequencies. In other words, the largest deviations to locality occur at small frequencies only (see also Supplemental Material III.D [84]). The nonlocal components are smaller or much smaller than the local component, especially for large Matsubara frequencies. This gives an *a posteriori* explanation of the qualitatively good results of the single-site TRILEX approximation. More importantly, the fact that the momentum dependence is confined to low frequencies suggests optimizations for the vertex parametrization and computation.

In conclusion, we have presented a first implementation of the cluster extension of the TRILEX method. For a broad interaction and doping range of the two-dimensional Hubbard model, we obtain, for an embedded cluster with only four impurity sites, continuous self-energies in close agreement with the exact result obtained with comparatively expensive large-cluster lattice QMC and DCA calculations.

Cluster TRILEX is based on the computation and momentum coarse graining of the three-leg vertex function: it thus comes at a cost lower than cluster methods based on four-leg vertices [78,79], but it *a priori* suffers from the Fierz ambiguity. We have shown that this ambiguity can be turned into a practical advantage in two ways: First and foremost, we have shown that proximity to the exact solution coincides with stability with respect to the Fierz parameter α [91]. With this necessary condition, one can assess, at a given (possibly small) cluster size, the accuracy of the solution. Second, in some regimes, there exists a value of α for which accurate results can be reached for smaller cluster sizes. By allowing us to extract more information from smaller embedded TRILEX clusters, the Fierz convergence criterion paves the way to a controlled exploration of low-temperature phases such as superconducting phases, where cluster DMFT cannot be converged in practice.

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