Fictive impurity models: An alternative formulation of the cluster dynamical mean-field method

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''Cluster'' extensions of the dynamical mean-field method to include longer-range correlations are discussed. It is argued that the clusters arising in these methods are naturally interpreted not as actual subunits of a physical lattice but as algorithms for computing coefficients in an orthogonal function expansion of the momentum dependence of the electronic self-energy. The difficulties with causality which have been found to plague cluster dynamical mean-field methods are shown to be related to the ''ringing'' phenomenon familiar from Fourier analysis. The analogy is used to motivate proposals for simple filtering methods to circumvent them. The formalism is tested by comparison to low-order perturbative calculations and self-consistent solutions.

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I. INTRODUCTION

Over the last decade the ''dynamical mean-field'' (DMFT) method[1] has emerged from earlier investigations[2] of the infinite-dimensional limit as a very useful tool for theoretical investigation of correlated electron systems. It provides (within a certain approximation) a nonperturbative means of obtaining the electron self-energy and spectral function, and allows treatment of inelastic and thermal effects on the same footing as ground state energetics. It has revealed new insights into the physics of the Mott transition,[3] of ''colossal'' magnetoresistance manganites,[4] of plutonium,[5] and many other systems, and may be combined with linear muffin-tin orbital (LMTO) band theory (for reviews see Refs. 6,7) to treat correlation effects in realistic models.

As originally formulated[1] the dynamical mean-field method is a *local* approximation. The problem which one actually solves is a single-site model self-consistently embedded in a medium. The results are an exact representation of the physics of lattice models only in a limit of infinite coordination number.[1,2] While the method captures local physics very well, the treatment of intersite correlations is an important open issue. Attempts to formulate a controlled expansion about the infinite coordination limit have not led to useful and tractable expressions. An alternative approach focuses on the self-consistent embedding of a larger cluster in a medium,[8–14] and is closely related to attempts to extend the ''single-site coherent potential approximation (CPA)'' to more than one site.[15,16] Most of the approaches published to date involve choosing a specific cluster (subset of sites of the actual lattice of interest) as well as a specific embedding (geometry of connection of cluster sites to sites of the medium). An alternative E-DMFT method involves using hybrid boson-fermion methods to treat two-particle intersite correlations[17–19] and has had some success.

While these approaches have led to a number of interesting results (for recent examples see, e.g., Refs. 10,20,21), one worries that the choice of specific geometry both of the cluster and its embedding in the medium may bias the physics. Further, the real-space-cluster-based methods sometimes lead to self energies which are noncausal for some momenta and frequencies. This is regarded as a grave defect of the method and its cure is an important open problem.

In this paper we put forward an alternative point of view on the question of extending dynamical mean-field theory to include intersite correlations. Our motivation is as follows. The original local dynamical mean-field method, although often described in terms of a site self-consistently embedded in a medium, may also be described as the ''momentum-independent self-energy approximation.'' It amounts to (i) replacing the general position-dependent self-energy $\Sigma(R,\omega)$ by the on-site value $\Sigma(0,\omega)$ and (ii) providing a prescription for computing $\Sigma(0,\omega)$ from the solution of a single-site quantum impurity model.

Considering the problem more generally, one may write $\Sigma(p,\omega)$ as an expansion in orthogonal functions and truncate the expansion at a finite order, thereby replacing a general function by a small number of frequency-dependent coefficients, which may be determined from the solution of a several site fictive impurity model: ''fictive'' because although the several-site impurity model can be regarded as a cluster self-consistently embedded in a medium, this cluster need not be a subcluster of the physical lattice considered. It should be viewed as merely a device for computing the self-energy functions of interest. The general idea of taking an abstract view of the ''impurity'' or cluster in the dynamical mean-field method is not new. It is mentioned in Ref. 1, and has recently been elegantly exploited by Kotliar and coworkers to link band theory and the dynamical mean-field method.[6] It is also the basis of an approach to the practical solution of the single-site DMFT equations put forward by Potthoff.[22] Here we apply the idea to the study of spatial correlations.

The idea that the cluster model is merely an algorithm for computing coefficients in a low-order orthogonal function expansion of a physical self-energy gives insight into the ''causality violations'' which sometimes occur in dynamical mean-field schemes. In the context of cluster extensions of dynamical mean-field theory, the term ''causality violation'' means that for some momenta and frequencies, the imaginary part of the approximate lattice self-energy computed

from the cluster approximation has the ''wrong'' sign. We shall argue that this is nothing but the ''ringing'' phenomenon familiar from Fourier analysis: if one approximates a non-negative but sharply peaked function by a few low-order terms in an orthogonal function expansion, the approximant will change sign. We shall use the analogy to propose several simple cures. We note that the dynamical cluster approximation (DCA) formalism used, for example, in Refs. 8,9,21 corresponds to a choice of orthogonal functions which are everywhere non-negative but which have no common support. In this sense, ''ringing'' is absent, so the method is plainly causal, but discontinuities in momentum space occur.

The outline of this paper is as follows. In Sec. II we outline the formalism we shall use. In Sec. III we present examples of the use of several-site impurity models to calculate the self-energy of the two-dimensional Hubbard model. Section IV discusses ''causality violations'' and possible cures. Section V is a conclusion.

II. FORMALISM

We study a model of electrons moving on a d-dimensional lattice with short ranged hopping amplitudes (described by a quadratic Hamiltonian H_0) and interactions (described by a Hamiltonian $H_{\rm int}$). Physical properties of the model may be derived from the general ''Luttinger-Ward'' expression for the action, which we may write in terms of the exact Green function $\mathbf{G}$ of the model as

$$S = \mathrm{Tr}\ln(-\mathbf{G}) + \bar{\Phi}_{\rm skel}[\mathbf{G}] \tag{1}$$

with $\bar{\Phi}_{\rm skel}[\mathbf{G}]$ the sum (with appropriate symmetry factors) of all vacuum to vacuum ''skeleton'' diagrams drawn with full Green functions ($\mathbf{G}$) and no self-energy insertions. The electron self-energy $\mathbf{\Sigma}$ may be obtained via

$$\mathbf{\Sigma} = \delta\bar{\Phi}_{\rm skel}/\delta\mathbf{G}. \tag{2}$$

The functional S is defined for any G once the interactions ($H_{\rm int}$) are specified. The correct G for a given ''band structure'' (H_0) is determined from the equation

$$-(\delta_t - H_0)^{-1} \equiv \mathbf{G}_0^{-1} = \frac{\delta S}{\delta \mathbf{G}}. \tag{3}$$

It is convenient for our purposes to eliminate $\mathbf{G}$ in favor of $\mathbf{\Sigma}$ via a Legendre transformation (this transformation is also basic to the work of Potthof[22]) defining

$$\Phi_{\rm skel}[\mathbf{\Sigma}] = \bar{\Phi}_{\rm skel} - \mathrm{Tr}(\mathbf{\Sigma}\mathbf{G}). \tag{4}$$

Note that it follows from Eqs. (2), (4) that

$$\mathbf{G} = -\frac{\delta\Phi_{\rm skel}}{\delta\mathbf{\Sigma}} \tag{5}$$

and that in this representation the theory is fixed by demanding that the $\mathbf{G}[\mathbf{\Sigma}]$ obtained from Eq. (5) is identical to the $\mathbf{G}$ obtained via

$$\mathbf{G}[\mathbf{\Sigma}] = (\mathbf{G}_0^{-1} - \mathbf{\Sigma})^{-1}, \tag{6}$$

i.e., by minimizing with respect to $\mathbf{\Sigma}$ the functional

$$\Omega[\mathbf{\Sigma}] = -\mathrm{Tr}\ln(-\mathbf{G}_0^{-1} + \mathbf{\Sigma}) + \Phi_{\rm skel}[\mathbf{\Sigma}]. \tag{7}$$

The original momentum-independent-self-energy (single-site) dynamical mean-field approximation may be formulated from Eqs. (4),(6) as follows (essentially this derivation is given in Ref. 1): define $\Phi_{\rm loc}$ as the approximation to the exact $\Phi_{\rm skel}[\mathbf{\Sigma}(p,\omega)]$ obtained by replacing the exact momentum dependent self-energy by a local approximant $\mathbf{\Sigma}_{\rm loc}(\omega) = \int (dp)\mathbf{\Sigma}(p,\omega)$ which depends only on frequency. Consistency demands that this be equivalent to replacing $\bar{\Phi}_{\rm skel}[\mathbf{G}]$ in Eq. (4) by the analogous quantity defined with the local Green function. Because $\mathbf{\Sigma}_{\rm loc}(\omega)$ depends only on frequency, the quantity which follows from Eq. (5) is the local Green function $\mathbf{G}_{\rm loc} = \int (dp)\mathbf{G}(p,\omega)$ and Eq. (6) becomes the relation $\mathbf{G}_{\rm loc} = \int (dp)[\mathbf{G}_0^{-1}(p,\omega) - \mathbf{\Sigma}_{\rm loc}(\omega)]^{-1}$.

The crucial observation which makes the single-site dynamical mean-field approximation useful is that because $\Phi_{\rm loc}$ is a functional only of a function of frequency, it may be defined nonperturbatively as the solution of a single-site (quantum-impurity) model which is specified by a frequency-dependent Weiss field and by interaction terms related to the local interactions of the original model. The Weiss field is fixed by demanding that Eq. (6) is satisfied when the left-hand side of this equation is the Green function calculated from the impurity model and the right-hand side is the local Green function calculated from the lattice Hamiltonian, using the impurity model self-energy.

A generalization is now evident. Consider a set of functions $\{\phi_i, \psi_i\}$ such that

$$\delta_{pp'} = \sum_i \phi_i(p)\psi_i(p'), \tag{8}$$

so that

$$\mathbf{\Sigma}(p,\omega) = \sum_i \phi_i(p)\mathbf{\Sigma}_i(\omega) \tag{9}$$

with $\mathbf{\Sigma}_i(\omega) = \int (dp)\psi_i(p)\mathbf{\Sigma}(p,\omega)$. Inserting Eq. (9) into Eq. (4) yields

$$\Phi_{\rm skel}[\{\mathbf{\Sigma}_i\}] = \bar{\Phi}_{\rm skel} - \sum_i \mathrm{Tr}(\mathbf{\Sigma}_i\mathbf{G}_i) \tag{10}$$

with $\mathbf{G}_i = \int (dp)\phi_i(p)\mathbf{G}(p,\omega)$.

Now, construct an approximant for the self-energy as a sum of a small number of terms in the expansion given in Eq. (9)

$$\mathbf{\Sigma}(p,\omega) \approx \mathbf{\Sigma}_{\rm approx}(p,\omega) \equiv \sum_{i=0\cdots n} \phi_i(p)\mathbf{\Sigma}_i(\omega). \tag{11}$$

Define $\Phi_{\rm approx}[\mathbf{\Sigma}_{\rm approx}]$ as the functional obtained from $\Phi_{\rm skel}$ by using the approximate self-energy instead of the exact $\mathbf{\Sigma}$. Equation (5) implies that this construction is equivalent to approximating $\bar{\Phi}_{\rm skel}$ by the set of diagrams drawn using only the $\mathbf{G}$ conjugate [in the sense defined below Eq. (10)] to the retained $\mathbf{\Sigma}_i$. We see that $\Phi_{\rm approx}$ is a functional of $n+1$

frequency dependent fields. It therefore corresponds to the solution to some $(n+1)$-site fictive impurity model involving $n+1$ Weiss fields, and interactions derived (as discussed below) from the original model. The Weiss fields are fixed by the requirement that the impurity-model Green functions $\mathbf{G}_i = -\delta\Phi_{\text{approx}}/\delta\mathbf{\Sigma}_i$ are given by appropriate integrals over the lattice Green function

$$\mathbf{G}_i(\omega) = \int (dp)\,\phi_i(p)[\mathbf{G}_0^{-1}(p,\omega) - \mathbf{\Sigma}_{\text{approx}}(p,\omega)]^{-1}. \tag{12}$$

From this point of view we may interpret the impurity model simply as a mathematical means for calculating, nonperturbatively, an approximation to the self-energy.

The original dynamical mean-field method corresponds to retaining only the $i=0$ term in the self-energy. In the ''DCA'' approach of Jarrell and co-workers,[8] the functions ϕ_i are obtaining by tiling the Brillouin zone into regions $\mathcal{R}_i$ and setting $\phi_i(p)=1$ if p is contained in $\mathcal{R}_i$ and $\phi_i(p)=0$ otherwise. These functions are clearly nonnegative everywhere, and are orthogonal because they have no common support: at any p exactly one ϕ_i is nonzero. This choice of functions leads approximants with discontinuities in momentum space. Other choices are discussed below.

To completely specify the impurity model we must determine the interaction terms. Specifying the interaction terms is a subtle issue in general. One approach is to observe that the skeleton functional, and therefore its approximant Φ_{approx} is defined for any hopping Hamiltonian H_0. We may therefore consider the special case of no hopping (so H_0 is simply the energies of whatever on-site levels are considered). For models (such as the Hubbard model) in which the interaction is local, both the Green function and self-energy are diagonal in the site representation and are easy to compute. Comparison of the exact and approximate expressions then shows (as was already demonstrated for the single-site DMFT in Ref. 1) that the interaction terms in the impurity model are simply the original interaction terms of the lattice model. However, for longer ranged interactions, the situation may become more complicated. Indeed the difficulty with longer-range interactions appears to be common to all schemes. For example, in real space cluster schemes the issue of interactions connecting the cluster to the medium must be addressed[17–19] while in the DCA the Laue-function arguments advanced by Aryanpour *et al.*[14] require a momentum-independent interaction. A separate paper will analyze the issue from the present point of view.[23]

III. EXAMPLE APPROXIMANTS

A. General considerations

A cluster extension of dynamical mean-field theory involves finding an impurity model to represent the frequency-dependent expansion coefficients in Eq. (9). Such a model must involve n fields which have an orthogonality property, so that we may unambiguously determine n independent Green functions and self-energies. One convenient choice is to introduce an $m>n$ component spinor of fermions ψ and write an action of the form

$$S = S^{(2)} + S_{\text{int}} \tag{13}$$

with (we have suppressed the spin indices here)

$$S^{(2)} = \psi^\dagger \left[\sum_{i=0,\ldots,m} b_i \mathbf{M}_i \right] \psi, \tag{14}$$

where b_i are frequency dependent Weiss fields and the $m\times m$ matrices $\mathbf{M}_i$ satisfy

$$\text{Tr}[\mathbf{M}_i \mathbf{M}_j] = m\,\delta_{ij}. \tag{15}$$

A general impurity model Green function is given by

$$\mathbf{G}_{\text{imp}} = g_0\mathbf{M}_0 + g_1\mathbf{M}_1 + g_2\mathbf{M}_2 + \cdots \tag{16}$$

with coefficients $g_i(\omega)$ given by

$$g_i = \frac{1}{m}\frac{\delta \ln Z_{\text{imp}}}{\delta b_i}. \tag{17}$$

The orthogonality relations imply the self-energies

$$\Sigma_{\text{imp},i} = \frac{1}{m}\text{Tr}\left[\mathbf{M}_i \left(\sum_j b_j \mathbf{M}_j - \mathbf{G}_{\text{imp}}^{-1} \right) \right] \tag{18}$$

leading to self-consistency equations of the form (12). The self consistency condition in the local (no-hopping) limit implies $\mathbf{M}_0$ is the unit matrix.

B. Harmonic expansion-second order

Here we write, for a hypercubic lattice in d dimensions

$$\Sigma_{\text{approx}}(p,\omega) = \Sigma_0(\omega) + \sum_a e^{ipa}\Sigma_a(\omega) \tag{19}$$

with $a = \pm x, \pm y, \ldots,$ so that naively there are $2d+1$ mean-field equations

$$G_0 = \int (dp) G_p(\omega), \tag{20}$$

$$G_a = \int (dp) e^{ipa} G_p(\omega), \tag{21}$$

so we should write an impurity model action involving $2d+1$ fields. However, we may argue that in a cubic lattice, all of the components Σ_a are equal, so that the physics may be expressed via an impurity model depending on two fields Σ_0 and Σ_a. There are two self-consistency conditions. The impurity model is then specified by a partition function $Z^{(2)}$ arising from a functional integral over the action

$$S^{(2)} = (\psi_1^\dagger \quad \psi_2^\dagger) \begin{pmatrix} b_0 & b_1 \\ b_1 & b_0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} + S_{\text{int}}^{(2)}. \tag{22}$$

The mean-field equations may be written in symmetrized form as

$$G_{0,\mathrm{imp}}=\frac{\delta \ln Z^{(2)}}{2\,\delta b_0}=\int (dp)G_p(\omega), \tag{23}$$

$$G_{1,\mathrm{imp}}=\frac{\delta \ln Z^{(2)}}{2\,\delta b_1}=\int (dp)\,\gamma_p G_p(\omega), \tag{24}$$

where

$$G_p(\omega)=\frac{1}{\omega-\varepsilon_p-\Sigma_0-2d\,\gamma_p\Sigma_1}. \tag{25}$$

One may consider including longer ranged correlations—for example, in $d>1$ the second neighbor correlation, writing

$$\Sigma_{\mathrm{approx}}(p,\omega)=\Sigma_0(\omega)+\sum_a e^{ipa}\Sigma_1(\omega) + \sum_{a,b\neq a} e^{i(pa+pb)}\Sigma_2(\omega). \tag{26}$$

We must then seek a multisite impurity model which depends upon three Weiss fields b_0,b_1,b_2 and involves three self-energy functions. When written in matrix form the impurity model must thus involve a closed algebra of three orthogonal symmetric matrices $\mathbf{M}_0,\mathbf{M}_1,\mathbf{M}_2$. We have not found a suitable closed algebra of 3×3 matrices; however, a closed algebra of 4×4 matrices exists, with

$$\mathbf{M}_0=1, \tag{27}$$

$$\mathbf{M}_1=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0&1\\1&0&1&0\\0&1&0&1\\1&0&1&0\end{pmatrix}, \tag{28}$$

$$\mathbf{M}_2=\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix}. \tag{29}$$

This choice corresponds to a four-site real-space cluster with the same topology as that considered by Lichtenstein and Katsnelson in a pioneering study of superconductivity and antiferromagnetism in the Hubbard model.[10]

The impurity model action becomes

$$S^{(4)}=\mathrm{Tr}\ln\left[\sum_{\alpha=0,1,2} b_\alpha\mathbf{M}_\alpha\right]+S^{(4)}_{\mathrm{int}} \tag{30}$$

leading to the self-consistency conditions

$$\frac{1}{4}\frac{\delta \ln Z^{((4)}}{\delta b_\alpha}=\int (dp)\,\phi_\alpha(p)G(p,\omega) \tag{31}$$

with (z is the number of nearest neighbors)

$$\phi_0=1, \tag{32}$$

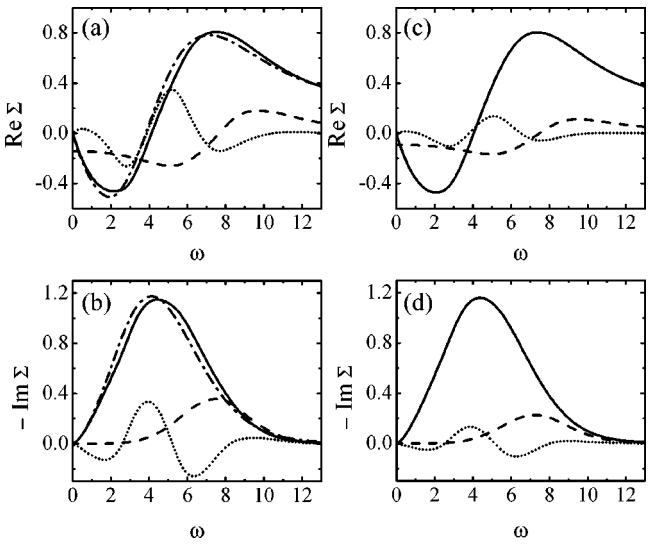

FIG. 1. (a), (b): Real and imaginary part of self-energy obtained from ''iterated perturbation theory'' approximation to half-filled Hubbard model ($U=4$, $T=0$) using one and four-site clusters. Dash-dotted curves are for one-site cluster. Solid, dashed, and dotted curves are Σ_0, Σ_1, and Σ_2 in four-site clusters, respectively. Σ_1 and Σ_2 are multiplied by 4. (c),(d) Self-energies in four-site clusters obtained from simple filtering procedure of Sec. IV, with $f_1=0.85$ and $f_2=f_1^2$.

$$\phi_1=e^{ipa}=\frac{1}{z}\sum_a e^{ipa}, \tag{33}$$

$$\phi_2=e^{i(pa+pb)}=\frac{1}{z(z-1)}\sum_{a,b} e^{i(pa+pb)}. \tag{34}$$

We finally discuss the interaction terms. In models with purely on-site interactions, the $\mathcal{S}^{(n)}_{\mathrm{int}}$ may be fixed by analysis of the local limit, in which $G_\alpha=0$ for $\alpha\neq0$ and G_0 is known. For example, in the Hubbard model, G_0 has poles at $\omega=\pm U/2$. The absence of any intersite correlations ensures that any off-diagonal terms in $S^{(n)}_{\mathrm{int}}=0$ and the identity of the n sites implies the interaction is just

$$S^{(n)}_{\mathrm{int}}=U\sum_{j=1,\ldots,n} n_{j\uparrow}n_{j\downarrow}. \tag{35}$$

When treated perturbatively to order U^2, the two and four impurity models reproduce exactly the appropriate Fourier coefficients of the exact (perturbative) lattice self-energy of the Hubbard model. To gain some idea of effects beyond perturbation theory we show in Figs. 1(a) and 1(b) results for the real and imaginary parts of the self-energy obtained from the iterated perturbation theory (IPT) approximation,[1] in which the impurity model and self-consistency condition are solved by writing the second order perturbation theory expression for the self-energy, but using exact (impurity model) Green functions. We observe that in the IPT approximation to the Hubbard model, non local effects are very small.

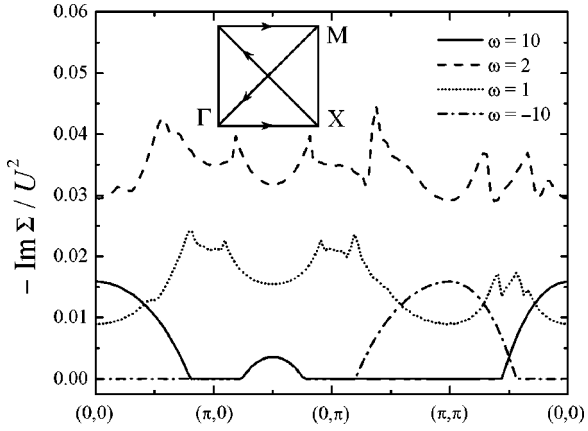

FIG. 2. Momentum dependence of the second-order perturbation theory approximation to the imaginary part of the self-energy of the half-filled two-dimensional Hubbard model at $T=0$. Solid, dashed, dotted, and dash-dotted curves are for $\omega=10$, 2, 1, and -10, respectively.

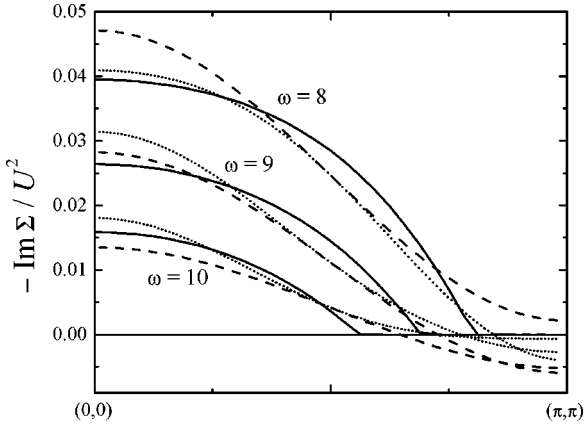

FIG. 3. Comparison of momentum dependence of exact second-order perturbation theory approximation to self-energy of half-filled two-dimensional Hubbard model (solid line) and the approximation using Eq. (36) at $T=0$; dash and dotted curves are the approximation using the first and second, and first three terms in Eq. (36).

IV. CAUSALITY

A. General considerations and a simple example

A key difficulty in cluster extensions of the coherent potential approximation or of dynamical mean-field theory has been causality. Any physical theory must be causal, which implies in particular that $\mathrm{Im}\,\mathbf{\Sigma}(p,\omega)<0$. Many cluster schemes, however, generate functions $\mathbf{\Sigma}_{\mathrm{approx}}(p,\omega)$ with the unfortunate property that for some range of p,ω, $\mathrm{Im}\,\mathbf{\Sigma}_{\mathrm{approx}}(p,\omega)>0$. These violations of causality have apparently never been clearly understood or cured, but are generally viewed a deficiencies of the ''cluster model'' used to calculate the self-energy.

The formal development of the previous section suggests that the causality violations may be thought of as an example of the ''ringing'' phenomenon familiar from Fourier analysis. Any straightforward real-space cluster scheme corresponds to using some set of orthogonal functions to expand the momentum dependence of the exact lattice self-energy $\mathbf{\Sigma}(p,\omega)$ in the sense of Eq. (11). The first term in an orthogonal function expansion is $\phi_0=1$ which is everywhere positive, so the local approximation is guaranteed to be causal, but all of the other orthogonal functions change sign over the Brillouin zone, so an expansion which is truncated at low order is not guaranteed to be positive everywhere in the zone. In particular, if at fixed ω the function $\mathbf{\Sigma}(p,\omega)$ has a strong, narrow peak at some momentum p, then truncating an orthogonal function expansion at a low order will produce a self-energy whose imaginary part changes sign. As noted above, in the DCA approach[8] this problem is avoided, at the expense of introducing discontinuities in the momentum space representations of G and Σ, by choosing the orthogonal functions to be a tiling of the Brillouin zone by rectangular filters. However, the general argument, that acausal behavior found in most schemes arises from ''ringing'' associated with narrow peaks in the momentum dependent self-energy, also suggests that the phenomenon is not of very great significance.

To illustrate the issue we show in Fig. 2 the momentum dependence of the second-order perturbation theory approximation to the imaginary part of the self-energy of the two-dimensional square-lattice Hubbard model, for several different frequencies. At frequencies within the electronic band the momentum dependence of the self-energy is relatively weak, but at frequencies well above the upper band edge or well below the lower band edge, the imaginary part of the self-energy becomes sharply peaked in momentum space. This phenomenon has a simple kinematic origin. At this order of perturbation theory, the imaginary part of the self-energy at $\omega>0$ corresponds to a decay of a particle into two particles and a hole. At $\omega=10$, energy conservation means the allowed final states correspond to two particles near the top of the band [momenta near (π,π)] and a hole near the bottom of the band [momenta near $(0,0)$]. Momentum conservation then restricts the initial momentum to be near $(0,0)$.

We now consider expanding the self-energy in Fourier harmonics. The symmetry of the hypercubic lattice implies that

$$\Sigma(p,\omega)=\Sigma_0(\omega)+2d\,\gamma_p\Sigma_1(\omega)+2d(d-1)\,\gamma_p^{(2)}\Sigma_2(\omega)+\cdots \tag{36}$$

with, for a hypercubic lattice of unit lattice constant in d dimensions,

$$\gamma_p=\frac{1}{d}\sum_{a=1\cdots d}\cos(p_a), \tag{37}$$

$$\gamma_p^{(2)}=\frac{1}{d(d-1)}\sum_{\substack{a=1\cdots d\\ b\neq a}}\cos(p_a)\cos(p_b). \tag{38}$$

The dashed and dotted curves in Fig. 3 show the result of approximating the exactly calculated Σ by the first and second, or first three terms in the series given in Eq. (36). An acausal behavior is observed at frequencies well above the upper band edge or well below the lower band edge, in accordance with the qualitative arguments presented above. At $\omega=8$, we observe the acausal behavior does not occur if

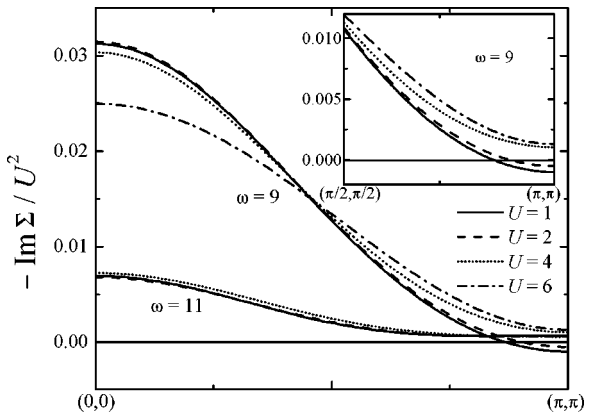

FIG. 4. Main panel: momentum dependence of $\mathrm{Im}\,\Sigma(\omega)$ at $\omega = 9,11$ calculated for $U=1,2,4,6$ by use of the IPT approximation on a four-site cluster. The increase of U is seen to lead to a broadening of the peak, which for the large U values is seen (inset) to eliminate the ''acausal'' behavior entirely.

only the first neighbor term is retained (dashed line) but does occur if both first and second neighbor terms are retained. This is because $\mathrm{Im}\,\Sigma_2(\omega)$ changes sign between $\omega=8$ and 9 to fit the exact $\mathrm{Im}\,\Sigma(p,\omega)$. [One can see this behavior even in Figs. 1(b),1(d).]

As noted above the acausal behavior has (at least in this instance) a simple kinematic origin, which suggest that it may not occur in all circumstances. For example, at larger U, more complicated decay channels (e.g., one particle decaying into three particles and two holes) with fewer kinematic constraints may become important, leading to a broadening of peaks in the momentum dependent self-energy and therefore to a causal self-energy. An example of this phenomenon is shown in Fig. 4, which displays the imaginary part of the self-energy calculated high frequencies in the IPT approximation at several different U values. The broadening of the peak and the destruction of the acausal behavior suggested by the arguments above are clearly observed. We stress that the IPT is an uncontrolled approximation—however, it is a computationally tractable example illustrating a phenomenon which we suspect is of more general significance.

B. Filtering

We have argued that any cluster extension of the dynamical mean field method amounts to a scheme for computing the coefficients in a low-order orthogonal function expansion of the electronic self-energy. This suggests that the reported causality difficulties are generic and inescapable: *no* truncation of an orthogonal function expansion is guaranteed to lead to an everywhere non-negative approximant for an arbitrary test function. We emphasize, however, that the impurity model itself is causal; it is only the resulting lattice self-energy which may have acausal features.

The discussion of the previous subsection suggests that the acausal behavior is ''ringing'' is associated with a relatively large peak near a particular momentum. It is possible that such a peak could be physically important, occurring for example at a fermi surface ''hot spot'' in a system close to a quantum critical point. In such a case, long-ranged interactions are evidently physically crucial, and modeling them with a local model is simply inappropriate. However, as seen in the explicit calculations present above, peaks in $\mathrm{Im}\,\Sigma$ which are both sharp and large relative to typical values of Σ are more often associated with band edges and extremal frequencies. These regions of ω and p are not particularly important for energetics, suggesting that the acausality is simply a minor technical annoyance. In what follows we consider methods of removing it.

We first note that in particular temperature regimes of particular problems (for example, the double exchange model on the simple cubic lattice and at not too low temperatures[16]) the ringing phenomenon might not occur. We also note that a clever choice of expansion functions may mitigate the severity of the problem. For example, we saw in the Hubbard model the difficulties arise from narrow peaks centered near the band edges [$p\approx 0$ and $p\approx(\pi,\pi,\ldots)$]. An expansion based on the functions $1,\gamma_p$ and a function orthogonal to both 1 and γ_p but strongly peaked near 0 and $(\pi,\pi,\ldots)$ might have a wider range of applicability than the straightforward harmonic expansion.

A more general approach is to filter the self-energy, for example by convolving it with a function to smooth out any sharp peaks and then approximating the smoothed function by a low order harmonic expansion. Let us make this approach more precise, writing Eq. (11) as

$$\Sigma_{\mathrm{approx}}(p,\omega)\equiv\sum_{i=0\cdots n} f_i\phi_i(p)\Sigma_i(\omega), \tag{39}$$

where $f_0=1$ and $1>f_{i>0}\geqslant 0$ are the Fourier components of the smoothing function. Carrying through the development of the previous section leads to

$$G_i(\omega)=\frac{\delta\Omega_{\mathrm{approx}}}{\delta\Sigma_i(\omega)}=f_i\int (dp)G_p(\omega)\phi_i(p) \tag{40}$$

so that the quantum impurity model acts to reproduce the smoothed Green's functions of the theory. (We note that sum rules typically constrain the large ω behavior of the local Green function, so that one must choose $f_0=1$ in order to have a consistent representation at least within the simple impurity models of which we have studied.) Figure 5 shows the results obtained using different choices of simple filtering coefficients in the low-order self-energies discussed in the previous section. The result of applying the filtering procedure to a four-site dynamical mean-field calculation is shown in panels (c) and (d) of Fig. 1. Comparison to panels (a) and (b) shows that the main effect (for the parameters studied) is to reduce, by approximately a factor of 2, the magnitude of Σ_1 and Σ_2.

The straightforward filtering approach gives up some fraction of the intersite correlations in order to guarantee a causal theory. A more sophisticated possibility would be a frequency dependent filtering. We saw from the low-order perturbation calculation on the Hubbard model that the self-energy was only very strongly peaked in momentum space for very high- or very low-energy states, where decay kinematics constrained all states involved to be near the band

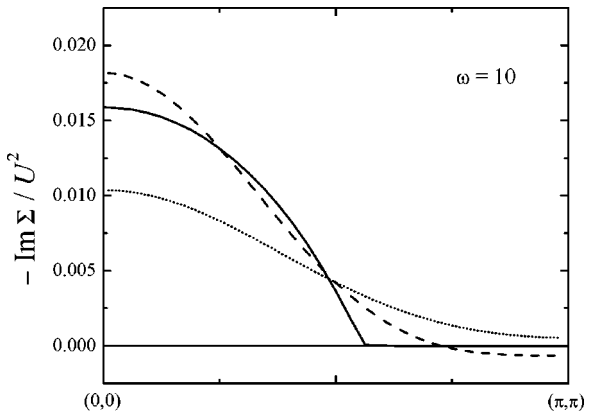

FIG. 5. Comparison of filtered, unfiltered, and exact results for second-order perturbation approximation to self-energy of the half-filled two-dimensional Hubbard model at $\omega=10$. Solid curve is the exact result. Dashed and dotted curves are obtained from four-impurity model with filtering coefficients $f_1=1$ and 0.85, respectively, and $f_2=f_1^2$. Numerical calculation gives the following values for $\mathrm{Im}\,\Sigma_i$: $(\mathrm{Im}\,\Sigma_0,\mathrm{Im}\,\Sigma_1,\mathrm{Im}\,\Sigma_2)=(-0.00418,-0.00234,-0.00114)$ for $f_1=1$ and $(-0.00418,-0.00144,-0.00033)$ for $f_1=0.85$. Calculations are done at $T=0$.

edges. These states are not very important to energetics. One may therefore filter out only these by setting an arbitrary frequency scale ω_f and Δ and writing, e.g., $f_1=1-\overline{f}/[\exp\{(-|\omega|+\omega_f)/\Delta\}+1]$. We note that this filtering may be performed ex post facto: one may solve the impurity model, determine the band-edge regions where filtering is required, and then solve again the impurity model with filtering only in these regions. Figure 6 shows the results obtained using the above frequency-dependent filtering with different choices of parameters. Here, we take $f_2=f_1^2$, and the four-impurity model is self-consistently solved. It is clearly shown that $\Sigma_{1,2}$ are reduced at higher frequency region where acausal behavior has been observed in the second-order perturbation theory approximation (Fig. 5) and IPT (Fig. 4), while there is not much effect in the low frequency region.

A still more sophisticated approach would be to mix different harmonic components, so that low-order terms were modified only if higher-order terms were important (i.e., if filtering were really needed). This approach is most helpful if a priori knowledge of the locations of sharp momentum-space structures is available. Indeed, the calculations presented above of the behavior of the Hubbard model strongly suggest that the singularities are associated with the top and bottom of the band, i.e., with states around $p=(0,0,\ldots)$ or $p=(\pi,\pi,\ldots)$. To define this transformation we begin from the harmonic expansion (11), and then introduce a transformation which mixes the harmonic coefficients, so that

$$\Sigma_{\mathrm{approx}}(p,\omega)\equiv\sum_{i,j=0\cdots n}\phi_i(p)f_{ij}\Sigma_j(\omega), \tag{41}$$

and the self-consistency equation becomes

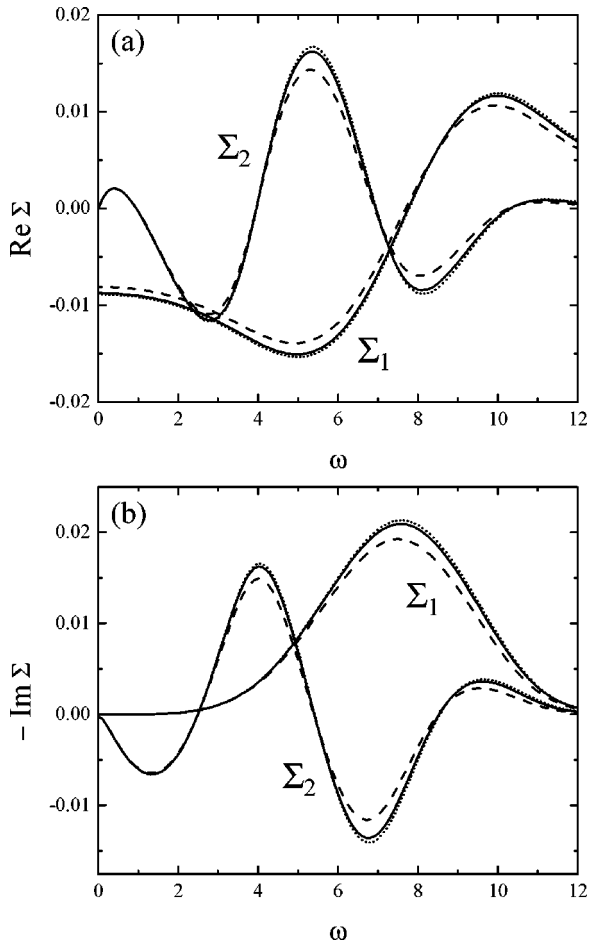

FIG. 6. Real (a) and imaginary (b) part of self-energy, Σ_1 and Σ_2, obtained from iterated perturbation theory approximation to half-filled Hubbard model ($U=2$, $T=0$) using four-site cluster with frequency-dependent filtering. Solid and dashed curves are the results with parameters $(\overline{f},\omega_f,\Delta)=(0.15,6,1)$ and $(0.15,4,1)$, respectively. Dotted curves are the results without filtering.

$$G_i(\omega)=\sum_j f_{ij}\int (dp)G_p(\omega)\phi_j(p). \tag{42}$$

We have, however, not yet explored these more complicated filtering procedures

V. CONCLUSION

In this paper we have argued that one should take a more abstract view of cluster extensions of the dynamical mean-field method; regarding them as algorithms for computing frequency-dependent coefficients in an orthogonal function expansion of the electron self-energy. This approach renders moot the debates about ''correct'' choice of cluster and embedding, and clarifies the meaning of the ''causality violation'' encountered in real-space-cluster extensions of the dynamical mean-field method. We have suggested that the causality violation is in most cases a minor technical problem which can be cured if needed by any of a variety of ''filtering'' procedures.

Several questions arise, for which further research would

be desirable. One is the question of the correct choice of interaction terms in the ''fictive impurity model.'' This issue has been discussed in the context of on-site interactions, especially in connection with the DCA,[14] and, for longer ranged interactions in the context of the E-DMFT approach[18,19] but deserves more attention in the context of the more conventional orthogonal function expansions. A second key issue is the origin of the causality violations. We have shown that in simple perturbative models (chosen because exact expressions for the momentum-dependent self-energy are available) the violations are an example of the familiar ''ringing'' phenomenon, and moreover occur mainly in band edge regions of little kinematical importance. The issue, however, deserves further exploration in less trivial contexts. A third open problem is the question of which approximants to the self-energy are representable by impurity models. We have presented arguments (substantiated by low-order perturbative calculations in different limits) indicating that straightforward orthogonal function expansions, with and without filtering, are representable. However, one might imagine that more complicated approximate representations of the self-energy might be advantageous in some problems. We do not at present have a general framework for determining the circumstances under which a general approximant to Σ is representable in terms of an impurity model. The issue of different choices of filtering function seems also likely to benefit from further research. In particular, it seems likely that one can more efficiently exploit the observation that the acausality is associated mainly with the $p=0$ and $p=(\pi,\pi,\ldots)$. Finally, applying the method to a wider range of models, to explore which choices lead to good representations of the physics of interest, is an urgent task.

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