

Variational Cluster Approach to Correlated Electron Systems in Low Dimensions

M. Potthoff,¹ M. Aichhorn,² and C. Dahnken¹

¹*Institut für Theoretische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany*

²*Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria*

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A self-energy-functional approach is applied to construct cluster approximations for correlated lattice models. It turns out that the cluster-perturbation theory [D. Sénéchal *et al.*, Phys. Rev. Lett. **84**, 522 (2000)] and the cellular dynamical mean-field theory [G. Kotliar *et al.*, Phys. Rev. Lett. **87**, 186401 (2001)] are limiting cases of a more general cluster method. The results for the one-dimensional Hubbard model are discussed with regard to boundary conditions, bath degrees of freedom, and cluster size.

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Low-dimensional systems of strongly interacting electrons, such as high-temperature superconductors, cuprate ladder compounds, and organic conductors, currently form a focus of intense experimental and theoretical work. It is generally accepted that many of the fascinating physical properties of these materials arise from different kinds of short-range spatial correlations as well as from different phases with long-range order. On a low energy scale, this can be studied within effective models such as the Hubbard model [1], for example. As these models have to be considered in the intermediate- to strong-coupling regime, weak-coupling perturbational approaches are inapplicable. Cluster methods, which approximate the physics of the infinite system by solving the problem for a corresponding finite cluster, appear to be promising in this context as the interaction part can be treated numerically exact. Currently, there are two different groups of cluster methods which are discussed intensively.

The point of reference for the first one is the direct cluster approach [2]. Using an exact diagonalization or quantum Monte Carlo technique, the effect of short-range correlations can be studied by computing static and dynamic correlation functions for an isolated small cluster. This direct method, however, suffers from the fact that phase transitions and long-range order cannot occur in a system of finite size. Furthermore, the spectral function consists of a comparatively small number of poles. This has caused the recent development of an extension called cluster-perturbation theory (CPT) [3–6]. The CPT procedure to calculate the one-electron Green's function \mathbf{G} [7] is sketched in Fig. 1 for the Hubbard model: (i) The lattice is divided into small clusters, and the intercluster hopping V is switched off. The Green's function \mathbf{G}' for the system of decoupled clusters (Hamiltonian H') is calculated numerically. (ii) The Green's function \mathbf{G} of the lattice model H is then approximated by a random phase approximation (RPA)-like expression $\mathbf{G} = \mathbf{G}'(1 - \mathbf{V}\mathbf{G}')^{-1}$ [7]. It has been pointed out that this corresponds to the first order in a systematic expansion in the intercluster hopping [4].

The point of reference for the second type of cluster methods is the dynamical mean-field theory (DMFT) [8,9]. The lattice model H is mapped onto an impurity model H' consisting of a correlated site coupled to an infinite number of uncorrelated “bath” sites. The bath must be determined self-consistently. As a mean-field theory, the DMFT directly works in the thermodynamic limit and is, thus, able to describe phases with long-range order. Because of the locality of the self-energy [10], however, it fails to incorporate the effects of short-range correlations. This has been the reason for the development of cluster extensions of the DMFT [11–14]. The main idea of the cellular DMFT (C-DMFT) [14] is to replace the correlated impurity site by a finite cluster (see Fig. 1) and to proceed as follows: (i) The self-energy Σ is calculated numerically for the system of decoupled clusters with an uncorrelated bath attached to each of the correlated sites

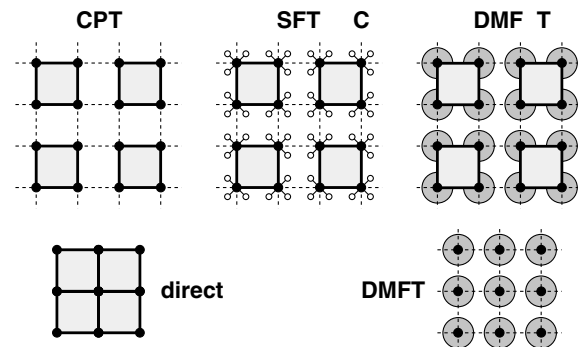


FIG. 1. Reference systems considered within various cluster approximations for the $D = 2$ Hubbard model. Filled circles: On-site interaction. Solid lines: Intracluster hopping. Dashed lines: Intercluster hopping. Open circles: Additional n_b uncorrelated bath sites. Big circles: Bath with $n_b = \infty$. Common to all methods is (i) the numerical solution of the system of decoupled clusters and (ii) the subsequent coupling of the clusters via an RPA-like or Dyson equation. Bath parameters are determined self-consistently. The self-energy-functional theory (SFT) comprises the extreme limits CPT ($n_b = 0$) and C-DMFT ($n_b = \infty$).

(Hamiltonian H'). (ii) The (approximate) Green's function of the lattice model H is then obtained from Σ via the lattice Dyson equation: $G = (G_0^{-1} - \Sigma)^{-1}$. (iii) The parameters of the respective baths have to be recalculated from G and Σ via the C-DMFT self-consistency condition [9,14]. This requires one to repeat the above steps until self-consistency is reached.

The first intention of this Letter is to show that both the CPT and the C-DMFT can be considered as extreme limits of a more general cluster approach which is based on the self-energy-functional theory (SFT) proposed recently [15]. This answers an open question [5] for the relation between the different cluster methods and unifies two approaches which appear to be rather different at first sight. The presented cluster approach based on the SFT not only reproduces the CPT ($n_b = 0$) and the C-DMFT ($n_b = \infty$) but also allows one to construct approximations with an arbitrary number of bath sites n_b . This intermediate approach does not waive any of the general merits such as causality and thermodynamical consistency.

Second, this Letter shows that there is room for new conceptual ideas beyond both the CPT and the C-DMFT: (i) A consistent cluster approach can be constructed, e.g., by attaching uncorrelated baths at the cluster boundary only. (ii) Not only the bath parameters but also the on-site energies of and the hopping between the correlated sites may be determined in a self-consistent (variational) way. (iii) The question of boundary conditions can be answered by the method itself and need not be imposed by hand. To discuss the relevance and advantages or disadvantages of these points, some numerical results will be presented for the one-dimensional ($D = 1$) Hubbard model.

Self-energy-functional theory (SFT).—Consider a system of fermions on an infinite lattice with on-site Coulomb interactions at temperature T and chemical potential μ . Its Hamiltonian $H = H_0(t) + H_1(U)$ consists of a one-particle part which depends on a set of hopping parameters t and an interaction part with Coulomb-interaction parameters U . The grand potential Ω can be obtained from the stationary point of a self-energy functional,

$$\Omega_t[\Sigma] \equiv \text{Tr} \ln[-(G_0^{-1} - \Sigma)^{-1}] + F[\Sigma], \quad (1)$$

as has been discussed in Ref. [15]. Here $G_0 = 1/(\omega + \mu - t)$ and $F[\Sigma]$ is the Legendre transform of the Luttinger-Ward functional $\Phi[G]$. As the latter is constructed as an infinite series of renormalized skeleton diagrams [16], the self-energy functional is not known explicitly. Nevertheless, the exact evaluation of $\Omega_t[\Sigma]$ and the determination of the stationary point is possible [15] on a restricted space S of trial self-energies $\Sigma(t') \in S$. Because of this restriction, the procedure becomes approximative.

Generally, the space S consists of t' representable self-energies. Σ is termed t' representable if there are hopping parameters t' such that $\Sigma = \Sigma(t')$ is the exact self-energy of the model $H' = H_0(t') + H_1(U)$ (“reference system”). Note that both the original system H and the reference system H' must share the same interaction part. For any Σ parametrized as $\Sigma(t')$, we then have [15]:

$$\begin{aligned} \Omega_t[\Sigma(t')] &= \Omega' + \text{Tr} \ln\{-(G_0^{-1} - \Sigma(t'))^{-1}\} \\ &\quad - \text{Tr} \ln(-G'), \end{aligned} \quad (2)$$

where Ω' , G' , and $\Sigma(t')$ are the grand potential, the Green's function, and the self-energy of the reference system H' , while G_0 is the free Green's function of H . For a proper choice of t' (namely, such that certain degrees of freedom in H' , e.g., those in different clusters, are decoupled), a (numerically) exact computation of these quantities is possible. Hence, the self-energy functional (2) can be evaluated exactly for this $\Sigma = \Sigma(t')$. A certain approximation is characterized by a choice for S . As Σ is parametrized by t' , this means to specify a space of variational parameters t' . Any choice leads to a thermodynamically consistent approach since, once the variational procedure is carried out, Eq. (2) provides an explicit expression for a thermodynamical potential. For a further discussion of the general concept of the SFT, see Ref. [15]; a detailed description of its practical application is given in Ref. [17].

Cluster approximations.—Figure 1 illustrates the construction of cluster approximations within the framework of the SFT. To be specific, H is taken to be the Hubbard model with nearest-neighbor hopping. Subdividing the infinite lattice into identical clusters of finite size, H' is obtained from H by switching off the intercluster hopping and by switching on the hopping to new uncorrelated ($U_{\text{bath}} = 0$) bath sites (Fig. 1, middle). Both operations merely change the one-particle part of the Hamiltonian, i.e., $t \rightarrow t'$, while the interaction part (U) remains fixed, as required. To search for a stationary point on this space S of cluster-representable self-energies, one has to proceed as follows: (i) Compute the self-energy $\Sigma(t')$ of the reference system for a given t' . (ii) Use Eq. (2) to evaluate $\Omega_t[\Sigma]$ at $\Sigma = \Sigma(t')$. (iii) Repeat steps (i) and (ii) for different t' to compute the function $\Omega(t') \equiv \Omega_t[\Sigma(t')]$ and the stationary point t'_s given by $\partial \Omega(t'_s)/\partial t' = 0$. As shown in Ref. [17], causality requirements are respected.

The variational adjustment of the intracluster one-particle parameters t' can be looked upon as a (partial) compensation for the error introduced by the finite cluster size. An inclusion of n_b bath sites per original correlated site enlarges the number of variational parameters and thereby the space S . This is expected to (and does) improve the approximation (see results below). In the limit of infinite cluster size (number of correlated sites within a cluster $N_c \rightarrow \infty$), the exact self-energy becomes t' representable and therefore the cluster approximation

itself becomes exact. Since N_c must be finite (small) in any practical calculation, one should focus on local quantities such as the on-site Green's function $G_{ii} = [\mathbf{G}_0^{-1} - \mathbf{\Sigma}(\mathbf{t}')^{-1}]_{ii}^{-1}$, for example.

CPT and C-DMFT.—For a certain cluster approximation, it has to be specified which of the different intracluster one-particle parameters \mathbf{t}' are treated as variational parameters. The simplest idea is to consider the intracluster hopping as fixed at the original values, $t'_{ij} = t_{ij}$ (for i, j in the same cluster), and not to switch on a hopping to bath sites (i.e., not to introduce any bath sites). In this case, there is no variational parameter at all. $\mathbf{\Sigma}(\mathbf{t}')$ is calculated once, and the Green's function \mathbf{G} for the original model is obtained by the (lattice) Dyson equation $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \mathbf{\Sigma}(\mathbf{t}')$. As $\mathbf{\Sigma}(\mathbf{t}')$ is the exact self-energy for H' we also have $\mathbf{\Sigma}(\mathbf{t}') = \mathbf{G}_0^{-1} - \mathbf{G}'^{-1}$ and, consequently, $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \mathbf{G}_0^{-1} + \mathbf{G}'^{-1} = \mathbf{G}'^{-1} - \mathbf{V}$ with \mathbf{V} being the intercluster hopping. As this is equivalent to the RPA-type equation mentioned above, one recovers the CPT.

The C-DMFT is obtained by introducing a hopping t'_{ir} to $n_b = \infty$ bath sites $r = 1, \dots, n_b$ per correlated site $i = 1, \dots, N_c$ and taking this hopping (“hybridization”) and the bath on-site energies $\epsilon'_{i,r}$ as variational parameters, while for the correlated sites $t'_{ij} = t_{ij}$ is still fixed. Assume that bath parameters $\{t'_{ir}, \epsilon'_{i,r}\}$ can be found such that the C-DMFT self-consistency equation is fulfilled. In Ref. [14], this was given in \mathbf{k} -space representation (\mathbf{k} from the reduced Brillouin zone). In the real-space representation, the self-consistency equation reads

$$[\mathbf{G}_0^{-1} - \mathbf{\Sigma}(\{t'_{ir}, \epsilon'_{i,r}\})]_{ij}^{-1} = G'_{ij}, \quad (3)$$

where i, j must belong to the same cluster. This immediately implies that $\mathbf{\Sigma}(\{t'_{ir}, \epsilon'_{i,r}\})$ satisfies the SFT Euler equation $\partial\Omega(\mathbf{t}')/\partial\mathbf{t}' = 0$ or, calculating the derivative,

$$T \sum_{\omega} \sum_{ij} \left(\frac{1}{\mathbf{G}_0^{-1} - \mathbf{\Sigma}(\mathbf{t}')} - \mathbf{G}' \right)_{ji} \frac{\partial \Sigma_{ij}(\mathbf{t}')}{\partial \mathbf{t}'} = 0. \quad (4)$$

This holds since the “projector” $\partial \Sigma_{ij}(\mathbf{t}')/\partial \mathbf{t}' = 0$ if i, j belong to different clusters as these are decoupled in the reference system. We conclude that the self-energy functional is stationary at the C-DMFT self-energy.

In principle, approximations may also be constructed in reciprocal \mathbf{k} space. For the Hubbard model, however, there is no simple reference system as the interaction part is nonlocal in \mathbf{k} space. In particular, it is not possible to recover the dynamical cluster approximation [12] within the SFT.

“Intermediate” approach.—The C-DMFT self-consistency equation can generally be fulfilled for $n_b = \infty$ only. Within a cluster approach based on the SFT there are no formal problems, however, if $n_b < \infty$. A finite n_b yields an approximation inferior as compared to $n_b = \infty$ (C-DMFT) and superior as compared to $n_b = 0$ (CPT) as there are less or more variational pa-

rameters, respectively. For $0 < n_b < \infty$, the parameters must be found to satisfy Eq. (4).

Since the convergence with respect to n_b appears to be rapid for local physical quantities [15], and since the cluster Hilbert-space dimension increases exponentially with n_b , approximations with small n_b (or even $n_b = 0$, CPT) appear advantageous. Anyway, the bath concept must become irrelevant in the limit $N_c \rightarrow \infty$. On the other hand, there are good reasons to introduce bath sites: Depending on the dimensionality of the problem, it can be the description of the local (temporal) correlations that needs to be improved in the first place. Note that, for $N_c = 1$ and $n_b = \infty$, the DMFT is recovered which represents the exact solution for $D = \infty$ [9]. Furthermore, bath sites can serve as particle reservoirs which will be essential for a proper description of filling dependencies. Finally, the presence of bath sites may also facilitate practical calculations to treat the reference system, e.g., by an attenuation of the sign problem in the context of a Hirsch-Fye-like quantum Monte Carlo approach [18].

Intracluster hopping determined variationally.—For both the CPT and the C-DMFT, the hopping between correlated sites is fixed at $t'_{ij} = t_{ij}$ [for the C-DMFT, this is even a necessary condition to satisfy Eq. (3) as can easily be seen from a high-frequency expansion]. Contrary, within the SFT there is *a priori* no reason to fix t'_{ij} . A cluster approximation with t'_{ij} determined variationally represents another intermediate approach as shall be discussed in the following.

Numerical calculations have been performed for the $D = 1$ Hubbard model. Instead of solving the Euler equation (4), we have directly evaluated the self-energy functional according to Eq. (2). The reference system H' is taken to be a set of decoupled Hubbard chains with N_c correlated sites each. For $N_c \leq 10$ (no additional bath

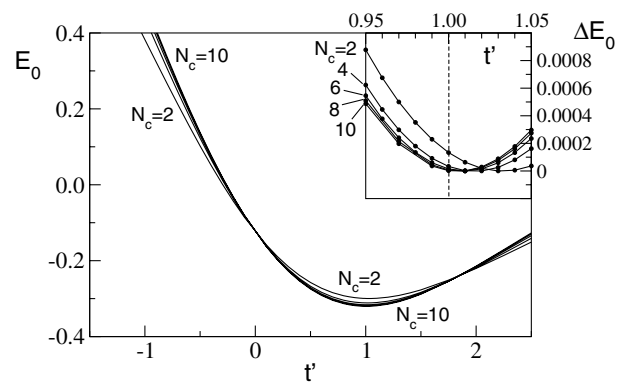


FIG. 2. $E_0 \equiv \Omega + \mu\langle N \rangle$ vs t' as obtained by evaluating the self-energy functional $\Omega = \Omega[\mathbf{\Sigma}(\mathbf{t}')$. Original system H : $D = 1$ Hubbard model with nearest neighbor (NN) hopping $t = 1$ and $U = 8$ for $T = 0$ and $\mu = U/2$ (half filling). Reference system H' : Set of decoupled Hubbard chains with N_c sites each; $N_c = 2, 4, 6, 8, 10$ as indicated. Variational parameter: NN hopping t' of H' . The inset shows $\Delta E_0 = E_0 - E_{0,\min}$ vs t' .

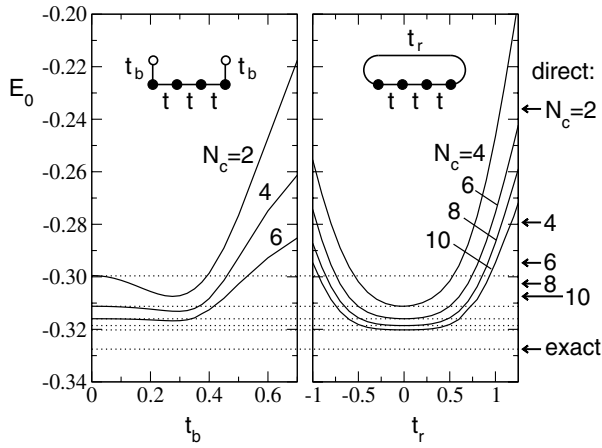


FIG. 3. E_0 as in Fig. 2 but vs different variational parameters: NN hopping t_b to uncorrelated bath sites (left), hopping t_r between the edge sites (right). Dashed lines: E_0 without parameter optimization. Arrows: E_0 calculated for an isolated cluster. Exact result for E_0 from Ref. [20].

sites), the ground-state energy E'_0 (and thereby $\Omega' = E'_0 - \mu\langle N \rangle$ for $T = 0$) and the Green's function \mathbf{G}' are computed using the standard Lanczos algorithm [19]. The self-energy is obtained as $\Sigma(t') = \mathbf{G}'_0^{-1} - \mathbf{G}'^{-1}$. In Eq. (2), the trace “Tr” consists of a sum over a complete set of one-particle quantum numbers and (after analytical continuation to the real ω axis) a frequency integration. To keep the calculations simple, only a single variational parameter is taken into account.

Figure 2 shows $E_0(t') = \Omega(t') + \mu\langle N \rangle$ with $\Omega(t') \equiv \Omega_t[\Sigma(t')]$, where t' is the nearest-neighbor hopping within the cluster. Clearly, E_0 is stationary for t' very close to t but $t' \neq t$. The effect is most obvious for the smallest cluster size $N_c = 2$ (see inset). We conclude that a variational determination of the hopping between the correlated sites in fact improves the approximation. Surprisingly, however, the improvement is almost negligible for reasonable N_c . Similar results are obtained when different selected hopping parameters are varied.

Different variational parameters.—It is possible to construct a consistent cluster approach by attaching uncorrelated bath sites only at the boundaries of the respective cluster. Compared to the C-DMFT, this choice represents a certain restriction of the parameter set which is motivated by the expectation that here bath degrees of freedom compensate for the finite-size errors most efficiently. Figure 3 (left) shows that switching on the hopping t_b to two bath sites in fact lowers the minimal E_0 . With increasing N_c the energy difference $E_0(t_b = t_b^{\min}) - E_0(0)$ decreases, and $E_0(t_b)$ becomes almost flat for small t_b , as expected. Note that the binding energy gain due to inclusion of two bath sites $|E_0(N_c, t_b^{\min}) - E_0(N_c, 0)|$ is always smaller than the gain $|E_0(N_c + 2, 0) - E_0(N_c, 0)|$ due to a larger cluster: Introducing bath sites is less efficient as increasing the cluster size, at least for $D = 1$. Interestingly, the convergence of E_0 with increas-

ing N_c appears to be much faster as compared to the direct cluster method (see arrows in Fig. 3).

Within the CPT, the question of the correct boundary conditions is decided *a posteriori* by inspection of the respective results for the spectral density [5]. Here we introduce a hopping parameter t_r between the edge sites and let the method “decide” by itself. As is seen in Fig. 3 (right), a minimum for E_0 is obtained at $t_r = 0$ (open boundary conditions) while there is no indication for a stationary point at $t_r = t$ (periodic boundary conditions).

The self-energy-functional theory has been shown to provide a consistent and very general framework for the construction of variational cluster approximations including the CPT and the C-DMFT. The extreme flexibility with regard to the choice of variational parameters offers a variety of further methodical developments and applications.

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- [7] A matrix notation is used: Consider, e.g., the Hubbard model. Then \mathbf{G} and \mathbf{V} , for example, have the elements $G_{ij}(\omega)$ and V_{ij} , where i, j refer to sites. Furthermore, $\text{Tr } \mathbf{A} = 2T \sum_{\omega, i} A_{ii}(i\omega)$ for a function \mathbf{A} of the imaginary Matsubara frequencies $i\omega = i(2n + 1)\pi T$ with integer n . The spin index is suppressed.
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