Dynamical Variational Principles for Strongly Correlated Electron Systems

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Abstract. The self-energy-functional approach (SFA) is discussed in the context of different variational principles for strongly correlated electron systems. Formal analogies between static and dynamical variational approaches, different types of approximation strategies and the relations to density-functional and dynamical mean-field theory are emphasized. The discussion elucidates the strengths of the SFA in the construction of new non-perturbative approximations but also the limitations of the approach and thereby opens up future perspectives.

Variational approaches have a long and successful tradition in the theory of condensed-matter systems as they offer a smart, controlled and systematic way to treat the problem of electron-electron interaction. A well-known variational approach is Hartree-Fock (HF) theory. It is based on the Rayleigh-Ritz principle and provides a practicable and consistent mean-field description of an interacting electron system. As quantum fluctuations are neglected completely, HF theory must be classified as a static mean-field approximation. This may be contrasted with dynamical mean-field theory (DMFT) [1,2] which includes temporal fluctuations in the mean-field picture. The DMFT, however, cannot be derived from the Ritz principle. It must be constructed from some dynamical variational principle which involves a dynamical (i.e. time- or frequency-dependent) quantity as the basic object. Dynamical variational principles have already been suggested in the sixties [3,4] but, compared to the Ritz principle, were employed with rather limited success only. This brings up the following questions: What are the similarities and the differences between different variational principles and approximation strategies? How can the DMFT be considered as an approximation within a variational concept? Can dynamical variational principles be used for constructing practicable and non-perturbative approximations different from the DMFT? An attempt to answer these questions straightforwardly leads to the self-energy-functional approach (SFA) [5] suggested recently. The purpose of this paper is to discuss different variational approaches and to place the SFA into this context with the objective to explore possible future developments.

1 Variational Principles and Approximation Strategies

Consider a many-electron system in the volume $V$, at temperature $T$ and with chemical potential $\mu$. It is characterized by a Hamiltonian $H_{LV}=$
\[ H_{t,U} = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta, \]  

(1)

where an index (e.g. \( \alpha \)) refers to the states of a one-particle basis.

The characteristic of a variational approach is a certain physical quantity \( X \) to be varied, as e.g. the statistical operator, the electron density, the (local) Green’s function, the self-energy etc. Clearly, at equilibrium this quantity will depend on the model parameters: \( X_{t,U} \) (and on \( V, T \) and \( \mu \)).

In a variational approach, the quantity is considered to be a variable. The first task is to express a thermodynamical potential \( \Omega \) (the grand potential, for example) as a function(al) of this variable: \( \Omega_{t,U}[X] \). As this functional is characteristic for the model system, it will depend on the model parameters. At the equilibrium or “physical” value, i.e. at \( X = X_{t,U} \), one must have \( \partial \Omega_{t,U}[X_{t,U}] = \partial \Omega_{t,U} \) where \( \Omega_{t,U} = -T \ln \text{tr} \exp(-H_0(t) + H_1(U) - \mu N)/T \).

Furthermore, the functional \( \Omega_{t,U}[X] \) should be constructed such that it becomes stationary at the physical value: \( \delta \Omega_{t,U}[X = X_{t,U}] = 0 \). This *variational principle* determines \( X_{t,U} \) once the functional is known. Note that the domain of the functional must be specified in addition since in most cases \( X_{t,U} \) must satisfy some constraint or sum rule or normalization condition.

Even if the functional is known, however, it is usually impossible to evaluate \( \Omega_{t,U}[X] \) for a given \( X \), and one has to resort to approximations. One may distinguish between three types of approximation strategies:

- **Type-I approximation** one derives the Euler equation \( \delta \Omega_{t,U}[X]/\delta X = 0 \) first and then chooses (a physically motivated) simplification of the equation afterwards to render the determination of \( X_{t,U} \) possible. This is the most general but worst type, as normally the approximated Euler equation no longer derives from some approximate functional. This may result in thermodynamical inconsistencies.

- **Type-II approximation** modifies the form of the functional dependence, \( \Omega_{t,U}[\cdots] \rightarrow \tilde{\Omega}_{t,U}[\cdots] \), to get a simpler one that allows for a solution of the resulting Euler equation \( \delta \tilde{\Omega}_{t,U}[X]/\delta X = 0 \). This type is more particular but yields a thermodynamical potential consistent with \( X_{t,U} \). Generally, however, it is not easy to find a sensible approximation of a functional form.

- **Type-III approximation** one restricts the domain of the functional. The restriction comes in addition to those conditions that are physically necessary anyway (e.g. normalizations) and requires a precise definition of the domain. This type is most specific and, from a conceptual point of view, should be preferred as compared to type-I or type-II approximations as the exact functional form is retained. In addition to conceptual clarity and thermodynamical consistency, type-III approximations are truly systematic since improvements can be obtained by an according extension of the domain.
2 Various Variational Approaches

In the following different variational principles and possible approximations shall be discussed according to this scheme, starting with Hartree-Fock and density-functional theory as illuminating examples.

2.1 Ritz Variational Approach

In the Ritz variational approach the ground-state energy is considered as a functional of the quantum state $|\Psi\rangle$. There is a generalization of the Ritz principle to arbitrary temperatures by Mermin [6]. Here the basic variable is the statistical operator $\rho$ characterizing the system’s (mixed) state, and the grand potential as a functional of $\rho$ reads:

$$\Omega_{t,U}[\rho] = \text{tr}(\rho(H_{t,U} - \mu N + T \ln \rho)).$$  \ (2)

Following the classical calculation of Gibbs, it can easily be shown [6] that on the set of normalized and positive definite operators, stationarity of the functional (2) is achieved for $\rho = \rho_{t,U} = e^{-\left(H_{t,U} - \mu N\right)/T}/\text{tr}(e^{-\left(H_{t,U} - \mu N\right)/T})$.

One also has $\Omega_{t,U}[\rho_{t,U}] = \Omega_{t,U}[\rho_{t,U}]$. An additional feature of the functional (2) consists in the fact that $\Omega_{t,U}[\rho] \geq \Omega_{t,U}[\rho_{t,U}]$ for any $\rho$. This “upper-bound property” is extremely helpful but specific to the Ritz principle.

For a many-electron system and an arbitrary $\rho$, the computation of the trace in Eq. (2) is an exponentially hard problem. A nice type-III approximation is the HF approach: Here the variational search is restricted to the subclass of disentangled statistical operators, i.e. statistical operators corresponding to independent-electron states. This can be made precise by introducing the important concept of a reference system:

A reference system is a system with a different (microscopic) Hamiltonian $H_{t',U'}$ ($t' \neq t$, $U' \neq U$) but with a macroscopic state characterized by the same values of the thermodynamic state variables as the original system $H_{t,U}$: $V' = V$, $T' = T$ and $\mu' = \mu$. The sole purpose of the reference system is to specify the domain of the functional (2): Trial statistical operators are taken from the reference system, $\rho = \rho_{t',U'}$, and are varied by varying the parameters $t'$ and $U'$ within a certain subspace. Hence, the choice of the reference system (and the parameter subspace) defines the approximation.

The HF approximation is given by the choice $U' = 0$ and $t'$ arbitrary, i.e. by trial states $\rho_{t',0} = e^{-\left(H_{t',0} - \mu N\right)/T}/Z_{t',0}$. Inserting into Eq. (2) yields

$$\Omega_{t,U}[\rho_{t',0}] = \Omega_{t',0} + \text{tr}(\rho_{t',0}(H_0(t) + H_1(U) - H_0(t'))) \ .$$ \ (3)

The remaining trace can be computed easily using Wick’s theorem as $\rho_{t',0}$ derives from a non-interacting Hamiltonian. The variational parameters $t'$ are
fixed by the conditions \( \delta \Omega_{t,U}[\rho_{t',0}] / \delta t' = 0 \). These are exactly the well-known HF equations as can be seen by some straightforward manipulations.

One learns that type-III approximations can be constructed conveniently by the concept of a reference system. On the one hand, the reference system should comprise a large space of parameters \( t' \) and \( U' \) to generate a powerful approximation. On the other hand, the parameter space must be restricted strongly to keep the calculations feasible.

### 2.2 Density-Functional Approach

For a many-electron system the statistical operator or, at \( T = 0 \), the ground-state wave function actually is an object that is by far too complex. The relevant information is much more efficiently stored in integral quantities, such as the electron density. This is the starting point of density-functional theory (DFT) [7,8,9]. The density, i.e. the quantum-statistical average of the one-particle density operator \( n(r) = \text{tr}(\rho c_\alpha c_\beta) \), represents the basic variable. Normally DFT aims at the inhomogeneous electron gas at \( T = 0 \) but can also be applied to discrete lattice models [10] and finite temperatures [6].

The grand potential \( \Omega_{t,U} \) obviously depends on the model parameters. Due to the Hohenberg-Kohn theorem [7], however, it can also be considered as a functional of the density \( n \) which is stationary at the physical density: \( \delta \Omega_{t,U}[n] = 0 \) for \( n = n_{t,U} \). Furthermore, if evaluated at \( n = n_{t,U} \), it yields the exact grand potential: \( \Omega_{t,U}[n_{t,U}] = \Omega_{t,U} \). Keeping the notations introduced above, \( n \) is a matrix with \( n_{\alpha\beta} = \text{tr}(\rho c_\alpha c_\beta) \), and the functional reads (cf. Refs. [6,10]):

\[
\Omega_{t,U}[n] = \text{tr}(t n) + F_U[n].
\] (4)

Here the trace refers to the one-particle orbitals \( \alpha \), and \( F_U[n] \) is a universal functional, i.e. it depends on the interaction parameters only. Using the Kohn-Sham idea [8,10], the resulting Euler equation has the form of a one-particle Schrödinger equation.

The variational principle \( \delta \Omega_{t,U}[n] = 0 \) is rigorous but cannot be evaluated as \( F_U[n] \) is generally unknown (after separating the Hartree and a kinetic-energy term, the remaining exchange-correlation functional is not explicit). Due to the universality of \( F_U[n] \), however, the density-functional for a reference system with modified one-particle parameters \( t' \) reads \( \Omega_{t',U}[n] = \text{tr}(t' n) + F_U[n] \), and thus \( \Omega_{t,U}[n_{t',U}] = \Omega_{t',U} + \text{tr}((t - t')n_{t',U}) \) which can be exploited for a type-III approximation. Choosing as a reference system \( H_{t',U} \) the homogeneous electron gas, however, turns out to be too restrictive, as this implies a spatially constant density. The local density approximation (LDA) [7,8], on the other hand, has proven to be very successful [9]. At least for systems with weakly varying density it is well justified. The LDA, however, is no longer a type-III approximation but a type-II one as the form of the (exchange-correlation part of the) functional \( F_U[n] \) is approximated to have a local dependence on the density only.
As the proof of the Hohenberg-Kohn theorem is based on the Ritz principle, the upper-bound property is transferred to the exact functional, i.e. \( \Omega_{t,U}[\mathbf{n}] \geq \Omega_{t,U} \) for any \( \mathbf{n} \), but is lost within the LDA due to the type-II character of the approximation.

### 2.3 Time-Dependent DFT

The weak point of the DFT consists in its inability to describe excitations (see, however, Ref. [11]). This is due to the fact that the Hohenberg-Kohn variational principle is built on the static electron density. Information on excitation properties is contained in dynamic response functions which are accessible in principle via time-dependent density-functional theory (TD-DFT) [12]. In TD-DFT one considers a situation with a time-dependent Hamiltonian and focuses on the time-dependent density \( n(r,t) = \langle \Psi(t)|\hat{n}(r)|\Psi(t) \rangle \) resulting from a solution \( |\Psi(t)\rangle \) of the time-dependent Schrödinger equation as the basic variable. Here the action \( A_t = \int dt \langle \Psi(t)|i\partial/\partial t - H(t)|\Psi(t) \rangle \) can be understood as a functional of \( n(r,t) \),

\[
A_{t,U}[\mathbf{n}] = -\int_{t_0}^{t_1} dt \text{tr}(n(t)t(t)) + B_U[\mathbf{n}],
\]

where \( t(t) \) are explicitly time-dependent one-particle parameters. Contrary to usual DFT, the variational principle \( \delta A_{t,U}[\mathbf{n}] = 0 \) does not derive from the Ritz principle, and consequently there is no upper-bound property available. Type-II approximations can be constructed by approximating the universal but unknown part \( B_U[\mathbf{n}] \) of the functional to make it explicit. Far from equilibrium, however, there is no general recipe.

### 2.4 Dynamical Variational Principle

In the linear-response regime close to equilibrium, excitations are described by Green’s functions. The one-electron Green’s function \( G_{\alpha\beta}(\omega) = \langle \{c_{\alpha}; c_{\beta}^\dagger\} \rangle_\omega \) is the basic quantity in the dynamical variational approach of Luttinger, Ward, Baym and Kadanoff [3,4]. Employing a coupling-constant integration [3], the grand potential can be understood as a functional of \( G \):

\[
\Omega_{t,U}[G] = \text{Tr} \ln G - \text{Tr}((G_{t,0}^{-1} - G^{-1})G) + \Phi_U[G],
\]

where \( \text{Tr} = T \sum_n e^{i\omega_n t} \text{tr} \) and \( \omega_n = (2n + 1)\pi T \) are fermion Matsubara frequencies. Furthermore, \( G_{t,0} = (\omega + \mu - t)^{-1} \) is the \( U = 0 \) (free) Green’s function and \( \Phi_U[G] \) the (universal) Luttinger-Ward (LW) functional defined as the sum of all dressed closed skeleton diagrams [3]. By construction, \( \Omega_{t,U}[G_{t,U}] = \Omega_{t,U} \). In arbitrary order in perturbation theory one has \( \delta \Phi_U[G]/\delta G = T \Sigma_U[G] \). Therewith, the Euler equation \( \delta \Omega_{t,U}[G]/\delta G = 0 \) is given by \( G^{-1} - G_{t,0}^{-1} + \Sigma_U[G] = 0 \) which is Dyson’s equation. This shows that \( \Omega_{t,U}[G] \) is stationary at the physical Green’s function \( G = G_{t,U} \).
The LW functional is formally given by a diagrammatic sum that cannot be carried out in practice. A self-evident type-II strategy is to sum up a suitable subclass of diagrams to obtain an approximate but explicit expression for $\Phi_U[G]$. In this way the HF approximation can be recovered but there are also new approximations like the fluctuation-exchange approximation [13,14].

These “conserving approximations”, however, are necessarily restricted to the weak-coupling regime.

A type-III approximation, on the other hand, would be non-perturbative by construction. Consider a reference system with modified one-particle parameters: $H_{t',U} = H_0(t') + H_1(U)$. This defines the domain of the functional $\Omega$ to consist of Green’s functions $G_{t',U}$ with arbitrary $t'$. The interaction is kept fixed ($U' = U$). To evaluate the functional $\Omega$ at $G_{t',U}$ requires the evaluation of $\Phi_U[G_{t',U}]$, in particular. Due to the universality of $\Phi_U[\cdot \cdot \cdot]$ (no $t$ dependence) and due to the choice $U' = U$, one has $\Phi_U[G_{t',U}] = \Omega_{t',U} - \text{Tr} \ln G_{t',U} + \text{Tr}((G_{t',0}^{-1} - G_{t',U}^{-1})G_{t',U})$. Thus,

$$\Omega_{t,U}[G_{t',U}] = \Omega_{t',U} - \text{Tr}(G_{t,0}^{-1}G_{t',U}) + \text{Tr}(G_{t,0}^{-1}G_{t',U}).$$

Hence, on any domain specified by a suitable subspace of one-particle parameters $t'$ which renders the solution of the reference system possible (for fixed $U$), the functional $\Omega$ can be evaluated exactly. A possible (but oversimplified) example is the choice $t' = 0$. It reduces the reference model to the atomic limit where the computation of $G_{t',U}$ and $\Omega_{t',U}$ in (7) is easy. Cluster approximations represent straightforward generalizations of this example. Unfortunately, this type-III approach for Eq. (6) yields nothing new: Since $\text{Tr}(G_{t,0}^{-1} - G_{t',0}^{-1})G_{t',U} = \text{tr}(t - t')n_{t',U}$ with the one-electron density of the reference system $n_{t',U} = T \sum_n e^{i\omega_n t'} G_{t',U}(i\omega_n)$, one gets $\Omega_{t,U}[G_{t',U}] = \Omega_{t,U}[\rho_{t',U}]$ with $\Omega_{t,U}[\rho]$ given by Eq. (2), i.e. the same as in the Ritz variational approach. Interestingly, this implies that upper bounds for the grand potential can be obtained, i.e. $\Omega_{t,U}[G_{t',U}] \geq \Omega_{t,U}$ for arbitrary $t'$.

### 2.5 Dynamical Mean-Field Approach

Equipped with these insights, one can address the question of deriving the DMFT from a variational principle. Originally, the DMFT was introduced as the exact theory of lattice models with local (Hubbard-type) interactions in infinite spatial dimensions $D = \infty$ [2]. Later on, it was recognized [15,16] that in $D = \infty$ the lattice model $H_{t,U}$ can be self-consistently mapped onto an impurity model $H_{t',U}$ with the same interaction $U$. Using this self-consistent mapping procedure as an approximation (“dynamical mean-field approximation”), one can treat lattice models for any finite $D$.

Instead of considering Dyson’s equation in the form, $\mathcal{G} = (G_{t,0}^{-1} - \Sigma_U[G])^{-1}$ (with $\Sigma_U[G] = (1/T) \delta \Phi_U[G]/\delta G$), which is solved by the exact $G_{t',U}$, the DMFT considers the following simplified equation between local quantities at lattice site $i$:

$$\langle G \rangle_{ii} = (G_{t,0}^{-1} - \hat{\Sigma}_U[G])_{ii}^{-1}.$$  

(8)
Here $\Sigma_U[G]$ is the derivative of the LW functional but with \textit{local} vertices only as it is the case for an impurity model. Clearly, this is a type-I approximation. Eq. (5) is often called the DMFT self-consistency condition. This is because its solution is achieved by an iterative procedure in practice: Starting with a guess for $\Sigma$, one computes the local lattice Green’s function as $(G)_{ii} = (G^{-1}_{t,0} - \Sigma^{-1})_{ii}$ at first. This is not yet a solution of Eq. (5) since in general $\Sigma \neq \Sigma_U[G]$ for this $G$. For the necessary update of $\Sigma$ define $(G_{t',0})_{ii} = 1/(1/(G)_{ii} + (\Sigma)_{ii})$. Assuming that $G_{t',0}$ can be understood as the free impurity Green’s function of an impurity model $H_{t',U}$ for some $t'$, the (numerical) solution of the impurity problem yields a new $\Sigma = \Sigma_U[(G)_{ii}] = \Sigma_U[G]$. Iteration of this cycle until self-consistency yields a solution $G$ of Eq. (5). Note that the resulting DMFT self-energy is local.

Here, the question is whether Eq. (5) can be interpreted as an Euler equation of some variational principle. Starting with the functional (6), one can try a type-II approximation by replacing $\Phi_U[G]$ with the LW functional of the impurity model $\tilde{\Phi}_U[G]$. This implies $(1/T)\delta\tilde{\Phi}_U[G]/\delta G = \tilde{\Sigma}_U[G]$, and the resulting Euler equation reads: $G^{-1} = G^{-1}_{t,0} - \Sigma_U[G]$. This equation is easily seen to be equivalent with Eq. (5) since $\Sigma_U[(G)_{ii}] = \Sigma_U[G]$ by definition. Hence, DMFT can be understood as a type-II approximation.

Another functional has been suggested recently [17]:

$$
\Omega_{t,U}[G] = \text{Tr} \ln \frac{1}{G^{-1}_{t,0} - \Sigma_U[G]} - \text{Tr}(\Sigma_U[G]G) + \Phi_U[G].
$$

(9)

Clearly, $\Omega_{t,U}[G_{t,U}] = \Omega_{t,U}$, and furthermore the corresponding Euler equation, $((G^{-1}_{t,0} - \Sigma_U[G])^{-1} - G) \cdot (\delta \Sigma_U[G]/\delta G) = 0$, is equivalent with Dyson’s equation, $G = (G^{-1}_{t,0} - \Sigma_U[G])^{-1}$ (assuming local invertibility of the functional $\Sigma_U[G]$). The functional (9) therefore yields a valid variational principle. As a type-II approximation, one may replace $\Phi_U[G] \rightarrow \tilde{\Phi}_U[G]$ and $\Sigma_U[G] \rightarrow \Sigma_{U'}[G'] = (1/T)\delta\tilde{\Phi}_U[G]/\delta G$ in the functional (6). The resulting Euler equation is equivalent with the DMFT self-consistency equation (5) which implies that DMFT can also be understood as a type-II approximation to the functional (6).

Attempts to prove that a stationary point of the type-II approximated functionals (6) or (9) must be an extremum have failed [17]. Furthermore, while (as shown above) a type-III approximation to the principle based on Eq. (6) with $U$ fixed yields upper bounds to the grand potential, the DMFT cannot be obtained as a type-III approximation starting from Eqs. (5) or (9): Choosing an impurity model $H_{t',U}$ as a reference system to generate trial Green’s functions and to define a restricted domain of the functional (6) or (9), respectively, concurrently means that the optimal Green’s function will be local. This is obviously a very poor approximation for the Green’s function of a lattice model and differs from the DMFT result. The discussion shows that the question whether or not the DMFT grand potential is an upper bound to the true grand potential is still open.
2.6 Functionals of the Local Green’s Function

It is also possible [18,19] to focus on the local Green’s function $G^{(\text{loc})} = (G)_{ii}$ (instead of the full $G$) and to set up a variational principle of the form

$$\delta \Omega_{t,U}[G^{(\text{loc})}] = 0.$$  \hspace{1cm} (10)

A functional which is stationary at the physical $G^{(\text{loc})} = G_{t,U}^{(\text{loc})}$ and which yields $\Omega_{t,U}[G_{t,U}^{(\text{loc})}] = \Omega_{t,U}$ can be constructed order by order in the interaction strength [18]. Unfortunately, the diagrammatic formalism is much more cumbersome as compared to the construction of the LW functional. As is shown in Ref. [19], the dynamical mean-field approximation is equivalent with a simple ($U$-independent) approximation to the kinetic-energy part of the functional. So the DMFT appears as a type-II approximation again.

2.7 Self-Energy-Functional Approach

The motivation to characterize the DMFT as a type-III approximation is the following: If it is possible to recover the DMFT merely by restricting the domain of the functional corresponding to an exact variational principle, different choices of the domain will place the DMFT in a systematic series of different and possibly new approximations which, as the DMFT, are all non-perturbative and thermodynamically consistent.

For this purpose it is helpful to focus on the self-energy. Within the self-energy-functional approach (SFA) [5], the self-energy functional

$$\Omega_{t,U}[\Sigma] = \text{Tr} \ln \frac{1}{G_{t,0}^{-1} - \Sigma} + F_U[\Sigma]$$  \hspace{1cm} (11)

is considered. Here, $F_U[\Sigma] = \phi_U[G|\Sigma] - \text{Tr}(\Sigma G_U[\Sigma])$ is the Legendre transform of the Luttinger-Ward functional which is well defined provided that the functional $\Sigma_U[G]$ is invertible locally. $F_U[\Sigma]$ is universal (independent of $t$) by construction and $-(1/T)\delta F_U[\Sigma]/\delta \Sigma = G_U[\Sigma]$ which is the inverse of the functional $\Sigma_U[G]$. Obviously, $\Omega_{t,U}[\Sigma_{t,U}] = \Omega_{t,U}$. The Euler equation $\delta \Omega_{t,U}[\Sigma]/\delta \Sigma = 0$ is given by $(G_{t,0}^{-1} - \Sigma)^{-1} = G[\Sigma]$ and equivalent with Dyson’s equation.

To construct a type-III approximation, a reference system $H'_{t',U} = H_0(t') + H_1(U)$ with unchanged interaction part is considered. The one-particle parameters $t'$ are taken such that the different “correlated” sites (non-zero on-site interaction) are decoupled. Instead, $t'$ shall include an arbitrary hopping to “bath” sites (zero on-site interaction) with arbitrary one-particle energies. In case of the Hubbard model on a lattice with $L$ sites, the corresponding reference system constructed in this way is a set of $L$ decoupled single-impurity Anderson models (which in case of translational symmetry are equivalent).
Dynamical Variational Principles

Trial self-energies $\Sigma_{t',U}$ are local by construction. The Euler equation resulting from this type-III approach reads $\partial \Omega_{t,U}[\Sigma_{t',U}]/\partial t' = 0$, i.e.:

$$\left( (G^{-1}_{t,0} - \Sigma_{t',U})^{-1} - G_{U}[\Sigma_{t',U}] \right) \cdot \frac{\partial \Sigma_{t',U}}{\partial t'} = 0. \quad (12)$$

Now let $t'$ (the bath parameters) be such that $G_{t',U}$ solves the DMFT self-consistency condition (8). Since $\tilde{\Sigma}_{U}[\Sigma_{t',U}] = \Sigma_{t',U}$, one has $(G_{t',U})_{ii} = (G^{-1}_{t,0} - \Sigma_{t',U})_{ii}^{-1}$. Hence, this $t'$ solves Eq. (12). (Note that $\partial \Sigma_{t',U}/\partial t'$ is local). So by a restriction of the domain of the self-energy functional (11) to local self-energies, the DMFT is characterized as a type-III approximation.

Interestingly, a type-II approximation does not work: A replacement of the form $F_{U}[\Sigma] \rightarrow \tilde{F}_{U}[\Sigma]$ in Eq. (11) yields the Euler equation $\tilde{G}_{U}[\Sigma] = (G^{-1}_{t,0} - \Sigma_{t',U})^{-1}$ where $\tilde{G}_{U}[\Sigma] = -(1/T)\delta \tilde{F}_{U}[\Sigma]/\delta \Sigma$. If this was equivalent with the DMFT self-consistency condition, a local self-energy would be a solution. This would imply, however, that $\tilde{G}_{U}[\Sigma]$ is non-local for a local $\Sigma$. Hence, $\tilde{F}_{U}[\Sigma]$ cannot be the Legendre transform of $\tilde{\Phi}_{U}[G]$ where $\tilde{\Phi}_{U}[G]$ (as above) is the Luttinger-Ward functional with vertices restricted to a single site. An alternative choice for $\tilde{F}_{U}[\Sigma]$, however, does not suggest itself.

One can conclude that a functional of the self-energy is necessary and sufficient to obtain the DMFT as a type-III approximation while a functional of the Green’s function is necessary and sufficient to get the DMFT as a type-II approximation. The decisive point is that rather a local self-energy can be tolerated as an approximation than a local Green’s function.

3 New Approximations

The immediate return of these considerations is a number of non-perturbative and thermodynamically consistent type-III approximations as shown in Fig. 1. These differ from the DMFT by a different restriction of the domain for the self-energy functional (11), i.e. by a different reference system with a different subspace of variational parameters $t'$ but the same interaction ($U' = U$). The evaluation of a type-III approximation requires the repeated computation of the grand potential and the Green’s function or self-energy of the reference system to get $\Omega_{t,U}[\Sigma_{t',U}]$ which must be optimized with respect to $t'$ subsequently.

The class of possible reference systems is essentially spanned by two parameters, namely $n_s - 1$ which is the number of additional bath sites per correlated site and $N_c$ which is the number of correlated sites in a cluster that is decoupled from the rest of the correlated sites (Fig. 1). The DMFT is obtained for $N_c = 1$ and $n_s = \infty$ since a continuous bath ($n_s = \infty$) is necessary to represent an arbitrary local free Green’s function.

The choice $N_c = 1$ but $n_s < \infty$ yields new approximations (“dynamical impurity approximations”, DIA) which are inferior as compared to the full DMFT but allow for much simpler and faster calculations when $n_s$ is small.
Fig. 1. Different possible approximations within the SFA (see text).

The most simple but non-trivial approximation \((n_s = 2\text{-DIA})\) has been shown \([5,20]\) to already cover the essence of the DMFT scenario \([1]\) for the Mott metal-insulator transition in the Hubbard model. At the critical point for \(T = 0\) the calculations can be done even analytically \([20]\), and with increasing \(n_s\) the grand potential, static quantities and the entire phase diagram rapidly converge to the full DMFT results \([5,21]\). The DIA is similar but superior as compared to the exact-diagonalization approach \([1]\). Even for small \(n_s\) the approach is thermodynamically consistent and, off half-filling, respects the Luttinger sum rule, for example. The DIA has also been employed successfully to study the influence of phonons on metal-insulator transitions in the Holstein-Hubbard model \([22,23]\).

Nothing new is obtained for \(n_s = \infty\) and \(N_c > 1\): Here the SFA recovers the cellular DMFT \([24]\). (Note that the dynamical cluster approximation \([25]\) is a type-II approximation). More interesting is the case \(n_s = 1\) and \(N_c > 1\) which turns out \([26]\) to represent a variational generalization of the cluster-perturbation theory \([27]\). This V-CPT is well suited to describe phases with spontaneously broken symmetry and has been employed to study one-particle excitations and antiferromagnetic order in the \(D = 2\) and \(D = 1\) Hubbard model at half-filling \([28]\) and charge ordering in the extended Hubbard model \([29]\). A further application concerns antiferromagnetism in quarter-filled ladder systems \([30]\). An impressing example of the power of the V-CPT approach has been given recently in a study of the competition between antiferromagnetism and d-wave superconductivity in the hole- and electron-doped Hubbard model \([31]\). The question of phase separation is addressed in Ref. \([32]\).

Summing up, the SFA is able to unify different cluster theories and local approximations within a single and consistent framework which offers a large flexibility in the use of bath sites, ficticious fields, boundary conditions and particle reservoirs \([20]\). The formalism provides a controlled compromise between the demands for a non-perturbative and systematic theory working in the thermodynamic limit on the one hand, and the limited computational capabilities to diagonalize finite-size systems on the other.
4 Open Problems

The self-energy-functional approach allows to construct a series of consistent approximations which improve systematically as $N_c \to \infty$. It is by no means clear, however, whether bath sites $n_s > 1$ help to speed up the convergence with respect to $N_c$ and whether a cluster extension of DMFT or the V-CPT is more efficient. This can be clarified only empirically by considering different lattice models in different dimensions. As a few bath sites have turned out to be sufficient for reproducing the essential mean-field ($N_c = 1$) physics in a number of studies of the single-band Hubbard model, further applications of the DIA are worthwhile to explore e.g. the mean-field phase diagrams of more complex (multi-orbital) models. Furthermore, one may also envisage the application of a simplified DMFT where a single (but continuous, $n_s = \infty$) bath is optimized for a multi-orbital model. This might be well justified for not too low temperatures.

On the technical side, there are two main future tasks: The full diagonalization and the Lanczos method which have been used so far, should be supplemented by a “reference system solver” based on stochastic techniques to improve the scaling of the numerical effort with the system size. Secondly, it would be advantageous to have an iterative technique at hand that directly yields a solution of the SFA Euler equation without the need for numerical differentiation. First results using full diagonalization [21] are encouraging.

On the conceptual side, the question for the possibility to give strict upper bounds to the grand potential is still open. Probably, a positive answer requires to establish a link to the Ritz variational principle. On the other hand, no example is known yet where the SFA grand potential at a stationary point is lower than the exact one.

There are different directions into which the formalism may be extended. As the coherent-potential approximation for the disorder Anderson model has the same (mean-field) status as the DMFT for the Hubbard model, it suggests itself that a self-energy-functional approach can also be constructed for systems with disorder (and interaction). First applications [33] demonstrate that such a theory is feasible. A challenge consists in the extension of the theory to include two-particle Green’s functions in a generalized variational principle. Here the recently proposed functional-integral formulation of the SFA [35] can be helpful. Two-particle correlation functions are interesting by themselves and may furthermore facilitate an even greater flexibility in the choice of reference systems. At the same time such an approach could provide a conceptual clear way to treat models with non-local interactions. Currently, this problem is circumvented by a more pragmatic decoupling procedure [29].

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