Self-energy-functional theory for systems of interacting electrons with disorder

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Based on a functional-integral formalism, a generalization of the self-energy-functional theory (SFT) is proposed which is applicable to systems of interacting electrons with disorder. Similar to the pure case without disorder, a variational principle is set up which gives the physical (disorder) self-energy as a stationary point of the (averaged) grand potential. Although the resulting self-energy functional turns out to be more complicated, the formal structure of the theory can be retained since the unknown part of the functional is universal. This allows one to construct nonperturbative and thermodynamically consistent approximations via searching for a stationary point on a restricted domain of the functional. The theory and the possible approximations are worked out for models with local interactions and local disorder. This results in a derivation of different mean-field approaches and various cluster extensions, including well-known concepts such as the statistical dynamical mean-field theory, the molecular coherent-potential approximation, and the dynamical cluster approximation. Due to the common formal framework provided by the SFT, one achieves a general systematization of dynamical approaches, i.e., approaches based on the spectrum of one-particle excitations. Different mean-field and different cluster schemes naturally appear in this framework and complement the existing ones. Their prospects for future applications are discussed.

I. INTRODUCTION

The combined influence of electron-electron interaction and of disorder on material properties represents a central question of solid-state theory. In diluted magnetic semiconductors[1] like $Ga_{1-x}Mn_xAs$ or $Zn_{1-x}Mn_xSe$, the magnetic properties, such as the Curie temperature, sensitively depend on the (random) distribution of the Mn ions as well as on the type and the strength of their effective magnetic interaction which results from strong Coulomb interaction among the Mn $3d$ valence electrons. Several transition-metal oxides[2] with partially filled metal $3d$ shells (e.g., manganites or cuprates) are antiferromagnetic Mott or charge-transfer insulators and exhibit a rich phase diagram upon doping with charge carriers. The disorder potential introduced due to the substitution process considerably affects their magnetic, charge, and orbital ordering.

While these examples show the need for a comprehensive theory of interacting and disordered electron systems, they also demonstrate the immense complexity one faces in any theoretical approach. Even strongly simplified (Anderson-Hubbard-type) models with local interactions and local disorder only are highly nontrivial if studied in a regime which excludes a simple perturbative treatment.[3–7]

For three (and higher) dimensions, one may, in the first place, focus on the *local* charge and spin dynamics of the electrons and, complementary to scaling theories,[3] disregard the long-wavelength modes which govern the immediate vicinity of a phase transition. In this context, mean-field approaches and cluster extensions are well justified. The mean-field concept is formally valid in the limit of high dimensions. Subsequent cluster extensions are suited to reincorporate short-range correlations which are neglected in the purely local mean-field approach. Clearly, a mean-field treatment excludes important effects such as the destruction of long-range order due to thermal order-parameter

fluctuations[8] or Anderson localization,[9] for example. Nevertheless, tractable mean-field theories can be valuable tools for an understanding of interacting and disordered systems with different competing orders and complex phase diagrams.

A mean-field theory can be formulated on the level of Hamiltonians and electronic states. This yields simple approaches such as the Hartree-Fock appoximation to treat the interaction part and the virtual-crystal approximation to treat the disorder part of the problem.[10,11] These are completely static theories which, in addition to spatial fluctuation, also neglect temporal fluctuations.

Temporal degrees of freedom can be taken into account in a mean-field theory when this is based on the spectrum of excitations. Placing the one-particle Green's function in the center of interest results in a mean-field theory which is distinguished by the fact that it yields the *exact* result in the limit of infinite spatial dimensions. With a proper scaling of the model parameters, this limit preserves a highly nontrivial dynamics.[12,13] This distinguished mean-field theory, for the interaction part of the problem, is the dynamical mean-field theory (DMFT).[14–17] It gives the exact (local) interaction self-energy of the prototypical Hubbard model[18–20] in the $D=\infty$ limit. For the disorder part, the coherent-potential approximation[21–24] (CPA) gives the exact (local) disorder self-energy of the disorder Anderson model[9] in the $D=\infty$ limit.

Phenomena depending on dimension are missed in a local mean-field approach but can be restored step by step using cluster expansions.[11,25] Using a single-site mean-field theory as a starting point for a systematic expansion is surely an inadequate approach to include long-wavelength modes and their effects. The main motivation for the subsequent inclusion of spatial correlations in cluster theories is rather the expected rapid convergence of local observables.

The purpose of the present paper is to contribute to a systematization of mean-field approaches and their cluster

extensions in the combined case of interactions and disorder and to explore different approximation schemes. The strategy is to seek for a proper generalization of the self-energy-functional theory (SFT) developed recently.[26,27] For the pure (disorder-free) case, it has been shown that well-known mean-field and cluster approaches are recovered, and different approximations can be constructed in a systematic way which guarantees thermodynamical consistency.[28,29] Here, we describe a different derivation of the SFT which is nonperturbative, i.e., a formulation which does not refer to formal sums of skeleton diagrams. This formulation is well suited for an extension of the theory to disordered (and interacting) systems. The generalized SFT is worked out in detail. It is shown that it makes contact with (i.e., rederives) a number of previous approaches:

(i) the DMFT+CPA put forward by Janiš and Vollhardt[30] and by Dobrosavljević and Kotliar,[31,32] which has recently been used to study metal-insulator transitions[33] at noninteger filling and the effects of disorder on magnetism;[34–36]

(ii) the local distribution approach of Abou-Chacra *et al.*[37] which has recently been evaluated numerically by Alvermann and Fehske[38] and which is the conceptual basis for:

(iii) the statistical DMFT proposed by Dobrosavljević and Kotliar[39,40] with several recent applications,[41] e.g., to strongly coupled disordered electron-phonon systems;

(iv) the molecular CPA (Ref. 11) and its combination with the cellular[42,43] DMFT (C-DMFT) of Kotliar *et al.* and Lichtenstein and Katsnelson;

(v) the dynamical cluster approximation (DCA) for disordered systems as introduced by Jarrell and co-workers;[44,45]

(vi) the disorder analog of a simplified DCA recently introduced by Tran[46]

as well as with several variants of these approaches such as the typical medium theory[47] (TMT) involving the geometrical averaging of the local density of states which has been suggested by Dobrosavljević *et al.* and applied in combination with DMFT by Byczuk *et al.*[48,49]

The construction of a generalized SFT provides *a unified theoretical framework* which is able to rederive and thereby to classify the above-mentioned approximations (i)–(iv). This procedure automatically discloses the view on other approximations: Generalizations of the periodized cellular DMFT (PC-DMFT) (Ref. 50) and of the cluster-perturbation theory[51,52] (CPT) as well as the variational cluster approach[28,53,54] (VCA) are suggested for disordered (and interacting) systems.

The main intention of the paper is to work out the formal concepts. The benchmarking and application of the different approaches require a numerical implementation which is beyond the present scope but intended for the future.

The paper is organized as follows: Section II introduces a number of basic quantities needed for the subsequent construction of the self-energy functionals. In Sec. III the self-energy functional for pure systems is derived nonperturbatively within the functional-integral formalism. A brief *general* discussion of approximations follows in Sec. IV for the case of a fixed disorder configuration. This provides the basis for the statistical SFT in Sec. V and for the statistical

DMFT, in particular. The main ideas for the construction of the generalized self-energy functional of configuration independent self-energies are provided in Sec. VI, while Sec. VII shows how to generate consistent approximations. The specialization to limiting cases, in particular to the disordered but noninteracting electron system, is given in Sec. VIII. This concludes the general buildup of the theory. The case of disorder in the interaction part is briefly sketched in Appendix A. In the rest of the paper, several concrete approximations are derived and classified. This includes well-known but also different approximation schemes. Mean-field approximations are disussed in Sec. IX, cluster approximations in Sec. X. A summary and a discussion of general topics in Sec. XI conclude the paper.

II. HAMILTONIAN AND DYNAMIC QUANTITIES

We consider a system of fermions in equilibrium at temperature T and chemical potential μ. In the grand-canonical ensemble, the macrostate of the system is given by the density operator

$$\rho = \frac{\exp[-(H - \mu N)/T]}{\mathrm{Tr}\, \exp[-(H - \mu N)/T]}, \tag{1}$$

where N is the total particle-number operator and H is the Hamiltonian. H is assumed to consist of a free (bilinear) part H_0 which exhibits the (discrete) translational symmetries of an underlying D-dimensional lattice, a disorder potential H_{dis}, and an interaction part H_{int}:

$$H = H(t, \eta, U) = H_0(t) + H_{\mathrm{dis}}(\eta) + H_{\mathrm{int}}(U). \tag{2}$$

The free part

$$H_0(t) = \sum_{\alpha\beta} t_{\alpha\beta} c_\alpha^\dagger c_\beta \tag{3}$$

is characterized by a set of hopping parameters $t_{\alpha\beta}$, where an index α labels the states of an orthonormal one-particle basis $\{|\alpha\rangle\}$. Typically, α refers to the sites x of the lattice as well as to some local degrees of freedom (e.g., spin projection $\sigma = \uparrow, \downarrow$), i.e., $\alpha = (x, \sigma)$. The full hopping matrix with elements $t_{\alpha\beta}$ is denoted by t.

The interaction part

$$H_{\mathrm{int}}(U) = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \tag{4}$$

is a four-fermion point interaction and is specified by the (Coulomb) interaction parameters $U_{\alpha\beta\delta\gamma}$. The full set of interaction parameters is written as U for short.

The disorder potential

$$H_{\mathrm{dis}}(\eta) = \sum_{\alpha\beta} \eta_{\alpha\beta} c_\alpha^\dagger c_\beta \tag{5}$$

is bilinear and given in terms of parameters $\eta_{\alpha\beta}$, which are random numbers with a joint probability distribution $P(\eta)$ with $P(\eta) \geq 0$ and $\int d\eta P(\eta) = 1$. The configurational average for any quantity A_η depending on η is

$$\langle A \rangle_P = \int d\boldsymbol{\eta} P(\boldsymbol{\eta}) A_{\boldsymbol{\eta}}. \tag{6}$$

For the theoretical setup, $H_{\text{dis}}(\boldsymbol{\eta})$ and $H_{\text{int}}(U)$ are taken to be completely general. The construction of mean-field approximations will be most convenient for a local (Hubbard-type) interaction U and a diagonal (local) disorder potential, $\eta_{\alpha\beta} = \delta_{\alpha\beta}\eta_\alpha$, with independent energies: $P(\boldsymbol{\eta}) = \prod_\alpha p(\eta_\alpha)$.

Using the functional-integral formalism,[55] the grand potential,

$$\Omega_{t,\boldsymbol{\eta},U} = -T \ln Z_{t,\boldsymbol{\eta},U}, \tag{7}$$

and the partition function for a given configuration $\boldsymbol{\eta}$,

$$Z_{t,\boldsymbol{\eta},U} = \text{Tr} \exp\{-[H(t,\boldsymbol{\eta},U) - \mu N]/T\}$$
$$= \int D\xi D\xi^* \exp(A_{t,\boldsymbol{\eta},U,\xi\xi^*}), \tag{8}$$

depend on the model parameters via the action

$$A_{t,\boldsymbol{\eta},U,\xi\xi^*} = \sum_{n,\alpha\beta} \xi_\alpha^*(i\omega_n)[(i\omega_n + \mu)\delta_{\alpha\beta} - t_{\alpha\beta} - \eta_{\alpha\beta}]\xi_\beta(i\omega_n)$$
$$- \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \int_0^{1/T} d\tau \, \xi_\alpha^*(\tau)\xi_\beta^*(\tau)\xi_\gamma(\tau)\xi_\delta(\tau). \tag{9}$$

Here $\xi_\alpha(i\omega_n) = T^{1/2}\int_0^{1/T} d\tau e^{i\omega_n\tau}\xi_\alpha(\tau)$ $[\xi_\alpha^*(i\omega_n) = T^{1/2}\int_0^{1/T} d\tau e^{-i\omega_n\tau}\xi_\alpha^*(\tau)]$ are Grassmann fields at the fermionic Matsubara frequencies $i\omega_n = i(2n+1)\pi T$ (with $n = 0, \pm 1, \ldots$). The configurational average of the grand potential is given by

$$\Omega_{t,P,U} = \int d\boldsymbol{\eta} P(\boldsymbol{\eta})\Omega_{t,\boldsymbol{\eta},U} = \langle \Omega_{t,\boldsymbol{\eta},U} \rangle_P. \tag{10}$$

The subscript P indicates the dependence on the probability distribution.

For later purposes, we need the free one-particle Green's function,

$$G_{t,0,0} = \frac{1}{i\omega_n + \mu - t}, \tag{11}$$

which is a matrix with the elements $G_{t,0,0,\alpha\beta}(i\omega_n)$. The dependence of $G_{t,0,0}$ on t is indicated by the subscript. Dependencies on the chemical potential μ and the temperature T will not be indicated; μ and T are assumed to be fixed. Similarly,

$$G_{t,\boldsymbol{\eta},0} = \frac{1}{i\omega_n + \mu - t - \boldsymbol{\eta}} \tag{12}$$

denotes the free Green's function in the presence of the disorder potential. The action determines the full Green's function $G_{t,\boldsymbol{\eta},U}$, the elements of which read

$$G_{t,\boldsymbol{\eta},U,\alpha\beta}(i\omega_n)$$
$$= \frac{-1}{Z_{t,\boldsymbol{\eta},U}} \int D\xi D\xi^* \xi_\alpha(i\omega_n)\xi_\beta^*(i\omega_n)\exp(A_{t,\boldsymbol{\eta},U,\xi\xi^*}). \tag{13}$$

Finally, we introduce the (interaction) self-energy

$$\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U} = G_{t,0,0}^{-1} - \boldsymbol{\eta} - G_{t,\boldsymbol{\eta},U}^{-1} = G_{t,\boldsymbol{\eta},0}^{-1} - G_{t,\boldsymbol{\eta},U}^{-1}. \tag{14}$$

$\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}$ depends on the configuration $\boldsymbol{\eta}$. The configuration independent (full) self-energy

$$S_{t,P,U} = G_{t,0,0}^{-1} - \boldsymbol{\Gamma}_{t,P,U}^{-1} \tag{15}$$

is defined with the help of the averaged Green's function

$$\boldsymbol{\Gamma}_{t,P,U} = \langle G_{t,\boldsymbol{\eta},U} \rangle_P. \tag{16}$$

III. CONFIGURATION-DEPENDENT SELF-ENERGY FUNCTIONAL

The main idea of the SFT is to express a thermodynamical potential as a functional of the (interaction) self-energy, which is stationary at the physical self-energy of the system. Variation of the self-energy is achieved by taking trial self-energies from a (exactly solvable) reference system and varying its parameters. To be able to evaluate the self-energy functional (which, in most cases, is defined only formally), it is of crucial importance that the reference system shares with the original system the nontrivial part of the functional so that this can be eliminated. Details of the SFT are described in Refs. 26–29. In the following, we present a construction of the self-energy functional for a fixed configuration $\boldsymbol{\eta}$. The construction is nonperturbative (i.e., does not refer to formal sums of skeleton diagrams) and allows for a generalization in the case of disorder (see Sec. VI).

To start with, we note that the action can be considered as a functional of the (inverse) free Green's function [Eq. (12)]:

$$\hat{A}_{U,\xi\xi^*}[G_0^{-1}] = \sum_{n,\alpha\beta} \xi_\alpha^*(i\omega_n)G_{0,\alpha\beta}^{-1}(i\omega_n)\xi_\beta(i\omega_n)$$
$$- \frac{1}{2} \sum_{\alpha\beta\gamma\delta} U_{\alpha\beta\delta\gamma} \int_0^{1/T} d\tau \, \xi_\alpha^*(\tau)\xi_\beta^*(\tau)\xi_\gamma(\tau)\xi_\delta(\tau). \tag{17}$$

Here G_0^{-1} is considered to be a free "variable." The physical action $A_{t,\boldsymbol{\eta},U,\xi\xi^*}$ [Eq. (9)] is obtained by evaluating the functional $\hat{A}_{U,\xi\xi^*}[\ldots]$ at the physical inverse free Green's function $G_0^{-1} = G_{t,\boldsymbol{\eta},0}^{-1}$ [Eq. (12)], i.e.,

$$A_{t,\boldsymbol{\eta},U,\xi\xi^*} = \hat{A}_{U,\xi\xi^*}[G_{t,\boldsymbol{\eta},0}^{-1}]. \tag{18}$$

Note that a hat is used to distinguish functionals from physical quantities. Additional dependencies of a functional (parameters) are indicated by subscripts.

In the same way, via Eqs. (7) and (8), the grand potential can be considered as a functional of G_0^{-1}, and one has

$$\Omega_{t,\boldsymbol{\eta},U} = \hat{\Omega}_U[G_{t,\boldsymbol{\eta},0}^{-1}], \quad \Omega_{t,0,U} = \hat{\Omega}_U[G_{t,0,0}^{-1}]. \tag{19}$$

Again, one has to distinguish clearly, e.g., between $\Omega_{t,\boldsymbol{\eta},U}$, the exact grand potential of the model $H(t,\boldsymbol{\eta},U)$ on the one hand, and $\hat{\Omega}_U[G_0^{-1}]$, a functional of the variable G_0^{-1} on the other. The latter only acquires the value $\Omega_{t,\boldsymbol{\eta},U}$ if evaluated at $G_0^{-1} = G_{t,\boldsymbol{\eta},0}^{-1}$.

The functional derivative

$$\frac{1}{T}\frac{\delta\hat{\Omega}_U[G_0^{-1}]}{\delta G_0^{-1}} = -\frac{1}{\hat{Z}_U[G_0^{-1}]}\frac{\delta\hat{Z}_U[G_0^{-1}]}{\delta G_0^{-1}} = -\hat{\mathcal{G}}_U[G_0^{-1}] \tag{20}$$

defines a functional $\hat{\mathcal{G}}_U$ as

$$\hat{\mathcal{G}}_{U,\alpha\beta}[G_0^{-1}] = -\frac{1}{\hat{Z}_U[G_0^{-1}]}\int D\xi D\xi^* \, \xi_\alpha(i\omega_n)$$
$$\times \xi_\beta^*(i\omega_n)e^{\hat{A}_{U,\xi\xi^*}[G_0^{-1}]}, \tag{21}$$

which has the property

$$\hat{\mathcal{G}}_U[G_{t,\boldsymbol{\eta},0}^{-1}] = G_{t,\boldsymbol{\eta},U}, \quad \hat{\mathcal{G}}_U[G_{t,0,0}^{-1}] = G_{t,0,U}. \tag{22}$$

Namely, at the physical inverse free Green's function, the functional integral in Eq. (20) defines the physical interacting Green's function, see Eq. (13).

Up to this point, the derivations are standard. The decisive point in the construction of the self-energy functional is the following equation:

$$\hat{\mathcal{G}}_U[G^{-1} + \boldsymbol{\Sigma}] = G. \tag{23}$$

The only purpose of this is to constitute a relation between the variables G and $\boldsymbol{\Sigma}$ which may formally be solved for G. This formal solution $G = \hat{G}_U[\boldsymbol{\Sigma}]$ then defines a functional $\hat{G}_U[\boldsymbol{\Sigma}]$ (which parametrically depends on U), i.e., we have

$$\hat{\mathcal{G}}_U[\hat{G}_U[\boldsymbol{\Sigma}]^{-1} + \boldsymbol{\Sigma}] = \hat{G}_U[\boldsymbol{\Sigma}] \tag{24}$$

for any $\boldsymbol{\Sigma}$ by construction. It is important to note that the functional $\hat{G}_U[\boldsymbol{\Sigma}]$ is universal, i.e., it neither depends on t nor on $\boldsymbol{\eta}$. If evaluated at the physical self-energy, the functional yields the exact Green's function

$$\hat{G}_U[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}] = G_{t,\boldsymbol{\eta},U} \tag{25}$$

since, by definition, $\hat{G}_U[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}]$ solves Eq. (24) if $\hat{G}_U[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}]^{-1} = G_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}$.

The final step is to use the (universal, i.e., t and $\boldsymbol{\eta}$ independent) functionals $\hat{\Omega}_U[G_0^{-1}]$ and $\hat{G}_U[\boldsymbol{\Sigma}]$ to express the grand potential as a functional of the self-energy. We define the functional $\hat{F}_U[\boldsymbol{\Sigma}]$ as

$$\hat{F}_U[\boldsymbol{\Sigma}] = \hat{\Omega}_U[\hat{G}_U[\boldsymbol{\Sigma}]^{-1} + \boldsymbol{\Sigma}] - \text{Tr} \ln \hat{G}_U[\boldsymbol{\Sigma}], \tag{26}$$

where $\text{Tr}\, A \equiv T\sum_n\sum_\alpha e^{i\omega_n 0^+}A_{\alpha\alpha}(i\omega_n)$. Equations (20) and (24) imply

$$\frac{1}{T}\frac{\delta\hat{F}_U[\boldsymbol{\Sigma}]}{\delta\boldsymbol{\Sigma}} = -\hat{G}_U[\boldsymbol{\Sigma}]. \tag{27}$$

Hence, $\hat{G}_U[\boldsymbol{\Sigma}]$ is a "gradient" of the "scalar" self-energy functional $\hat{F}_U[\boldsymbol{\Sigma}]$. The physical meaning of $\hat{F}_U[\boldsymbol{\Sigma}]$ is obvious when comparing with the original derivation of the SFT (cf. Ref. 26): $\hat{F}_U[\boldsymbol{\Sigma}]$ is the Legendre transform of the Luttinger-Ward functional.[56]

Now, the grand potential can be considered as a functional of the self-energy:

$$\hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}] = \text{Tr} \ln \frac{1}{G_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}} + \hat{F}_U[\boldsymbol{\Sigma}]. \tag{28}$$

Two properties of this functional are very useful.

First, at the exact self-energy $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}$, the self-energy functional yields the exact grand potential:

$$\hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}] = \Omega_{t,\boldsymbol{\eta},U} \tag{29}$$

since

$$\hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}] = \text{Tr} \ln G_{t,\boldsymbol{\eta},U} + \hat{F}_U[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}] \tag{30}$$

from Eqs. (28) and (14) and

$$\hat{F}_U[\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}] = \hat{\Omega}_U[G_{t,\boldsymbol{\eta},0}^{-1}] - \text{Tr} \ln G_{t,\boldsymbol{\eta},U} \tag{31}$$

from Eqs. (26) and (25). Hence, Eq. (29) follows from Eq. (19).

Second, consider the derivative

$$\frac{1}{T}\frac{\delta\hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}]}{\delta\boldsymbol{\Sigma}} = \frac{1}{G_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}} - \hat{G}_U[\boldsymbol{\Sigma}]. \tag{32}$$

The equation

$$\hat{G}_U[\boldsymbol{\Sigma}] = \frac{1}{G_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}} \tag{33}$$

is a (highly nonlinear) conditional equation in the variable $\boldsymbol{\Sigma}$ with parameters t, $\boldsymbol{\eta}$, and U which is solved by the physical self-energy $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U}$. It is by no means straightforward to find a solution, however, since the functional $\hat{G}_U[\boldsymbol{\Sigma}]$ is not known explicitly but was constructed in a formal way only. Obviously, this is equivalent to a search for the stationary point of the grand potential as a functional of the self-energy:

$$\frac{\delta\hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}]}{\delta\boldsymbol{\Sigma}} = 0. \tag{34}$$

This establishes a very general variational principle without the need for an expansion in powers of the interaction strength, i.e., the construction is nonperturbative.

IV. APPROXIMATIONS FOR A FIXED CONFIGURATION

For the discussion of possible approximations, we first consider a fixed configuration $\boldsymbol{\eta}$. Then $t + \boldsymbol{\eta}$ is a fixed matrix of hopping parameters but without translational symmetries. The idea of the SFT is to construct approximations by

searching for the stationary point of the functional Eq. (28) on a *restricted* domain of trial self-energies. Trial self-energies are chosen from a reference system which shares with the original system the same interaction part $H_{int}(U)$. In the Hamiltonian of the reference system,

$$H' = H_0(t') + H_{int}(U), \qquad (35)$$

the bilinear part $H_0(t')$ is varied arbitrarily. We have set $\boldsymbol{\eta}' = 0$ for the reference system. However, no translational symmetry is assumed for the hopping t'.

Since the interaction part is the same and due to the universality of the functional $\hat{F}_U[\boldsymbol{\Sigma}]$, only the first term of the self-energy functional of the reference system,

$$\hat{\Omega}_{t',0,U}[\boldsymbol{\Sigma}] = \text{Tr} \ln \frac{1}{\boldsymbol{G}_{t',0,0}^{-1} - \boldsymbol{\Sigma}} + \hat{F}_U[\boldsymbol{\Sigma}], \qquad (36)$$

differs from the functional of the original system Eq. (28). A combination of the functionals Eqs. (28) and (36) therefore gives

$$\hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}] = \hat{\Omega}_{t',0,U}[\boldsymbol{\Sigma}] + \text{Tr} \ln \frac{1}{\boldsymbol{G}_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}} - \text{Tr} \ln \frac{1}{\boldsymbol{G}_{t',0,0}^{-1} - \boldsymbol{\Sigma}}. \qquad (37)$$

The unknown functional $\hat{F}_U[\boldsymbol{\Sigma}]$ cancels out.

To search for the stationary point of the self-energy functional of the original system, we insert as trial self-energies the exact self-energies of the reference system: $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_{t',0,U}$. This yields a function of t',

$$\Omega_{t,\boldsymbol{\eta},U}(t') \equiv \hat{\Omega}_{t,\boldsymbol{\eta},U}[\boldsymbol{\Sigma}_{t',0,U}]. \qquad (38)$$

Searching for the stationary point of $\Omega_{t,\boldsymbol{\eta},U}(t')$ as a function of t' means to search for the stationary point of the exact self-energy functional Eq. (28) on the restricted set of trial self-energies generated by the reference system with parameters t'. From Eqs. (29) and (14) for the reference system, we have

$$\Omega_{t,\boldsymbol{\eta},U}(t') = \Omega_{t',0,U} + \text{Tr} \ln \frac{1}{\boldsymbol{G}_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}_{t',0,U}} - \text{Tr} \ln \boldsymbol{G}_{t',0,U}. \qquad (39)$$

The important point is that the right-hand side (rhs) can be computed exactly if the reference system is an exactly solvable model. Specifying a certain reference system means to generate a particular approximation. Typically, a suitable reference system can be found for lattice models by tiling the original lattice into clusters of finite size and by neglecting the intercluster hopping.

V. STATISTICAL SFT

To make contact with the statistical DMFT,[39,40] we consider a system with local interaction and local (and uncorrelated) disorder. The statistical DMFT treats the disorder part of the problem exactly, while the (dynamical) mean-field approximation is used for the interaction part. Within the
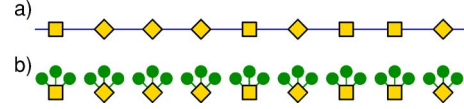

FIG. 1. (Color online) (a) Representation of the Anderson-Hubbard model in one dimension. Squares/diamonds: fixed configuration of sites with local (Hubbard) interaction and local binary-alloy disorder. Lines: nearest-neighbor hopping. (b) Reference system generating a mean-field approximation ($n_s = 4$). Circles: bath sites (no interaction) with on-site energies and hybridizations to original sites (square, diamonds) to be treated as independent variational parameters.

framework of the SFT, a mean-field approximation is generated by a reference system in which all sites are decoupled. This implies that spatial correlations are neglected altogether in the computation of the self-energy. The local (temporal) dynamics, however, can be optimized by introducing additional local degrees of freedom in the reference system. For the Hamiltonian of the reference system, this means introducing additional uncorrelated sites ("bath sites"), the on-site energies of which, as well as their hybridizations with the original correlated sites, are treated as variational parameters.

To be explicit, the discussion is restricted to the Anderson-Hubbard model

$$H = \sum_{xx'\sigma} t_{xx'} c_{x\sigma}^\dagger c_{x'\sigma} + \sum_{x\sigma} \eta_x n_{x\sigma} + U \sum_x n_{x\uparrow} n_{x\downarrow}. \qquad (40)$$

Here, x refers to the sites of a lattice, $n_{x\sigma} = c_{x\sigma}^\dagger c_{x\sigma}$, and η_x are independent random numbers distributed according to

$$P(\boldsymbol{\eta}) = \prod_x p(\eta_x) \qquad (41)$$

with some density $p(\eta_x)$. A reference system generating a mean-field approximation is $H' = \sum_x H'_x$ with (see Fig. 1)

$$H'_x = \sum_\sigma t'_{xx} c_{x\sigma}^\dagger c_{x\sigma} + U \sum_x n_{x\uparrow} n_{x\downarrow} + \sum_\sigma \sum_{i=2}^{n_s} \varepsilon_i^{(x)} a_{xi\sigma}^\dagger a_{xi\sigma}$$
$$+ \sum_\sigma \sum_{i=2}^{n_s} V_i^{(x)} (a_{xi\sigma}^\dagger c_{x\sigma} + c_{x\sigma}^\dagger a_{xi\sigma}). \qquad (42)$$

It consists of effective impurity models with n_s sites each: the correlated site x (with $U \neq 0$) and $n_s - 1$ bath sites (with $U = 0$) labeled by i. The effective impurity models can be solved independently to get a trial self-energy.

There is an indirect coupling, however, via the optimization of the variational parameters $t' = (t'_{xx}, \varepsilon_i^{(x)}, V_i^{(x)})$: The Euler equation,

$$\frac{\partial}{\partial t'} \Omega_{t,\boldsymbol{\eta},U}(t') = 0, \qquad (43)$$

simplifies due to the fact that the trial self-energy (and its derivative with respect to t', see Ref. 57) is necessarily local. Using Eq. (39) and carrying out the derivative, Eq. (43) can be written as
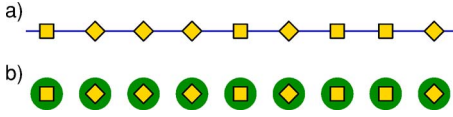
FIG. 2. (Color online) The same as Fig. 1 but for a continuum of bath sites ($n_s \rightarrow \infty$), represented by big circles. The reference system generates the generalized or statistical DMFT (see text).

$$\sum_{n,x} \left(\frac{1}{\mathbf{G}_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}_{t',0,U}} - \mathbf{G}_{t',0,U} \right)_{n,xx} \frac{\partial \Sigma_{xx}(i\omega_n)}{\partial t'} = 0. \quad (44)$$

Now, the variation of the one-particle parameters of the impurity model at site x does not affect the self-energy of the impurity model at site x' ($x' \neq x$). Therefore, the Euler equation simplifies to

$$\sum_{n} \left(\frac{1}{\mathbf{G}_{t,\boldsymbol{\eta},0}^{-1} - \boldsymbol{\Sigma}_{t',0,U}} - \mathbf{G}_{t',0,U} \right)_{n,xx} \frac{\partial \Sigma_{xx}(i\omega_n)}{\partial t'_{xx}} = 0, \quad (45)$$

where t'_{xx} denotes the variational parameters at the correlated site x. This is a set of equations labeled by the site index x. Due to the matrix inversion in Eq. (45), however, the equations are coupled. This implies that for a generic configuration, the individual self-energies of the effective impurity models are different at the stationary point as the sites of the original lattice model are inequivalent.

For $n_s \rightarrow \infty$, i.e., for a continuous bath (see Fig. 2), an additional formal simplification is possible: As is obvious from Eq. (45), a solution t' of the coupled equations

$$\left(\frac{1}{\mathbf{G}_{t,\boldsymbol{\eta},0}^{-1}(i\omega_n) - \boldsymbol{\Sigma}_{t',0,U}(i\omega_n)} \right)_{xx} = (\mathbf{G}_{t',0,U}(i\omega_n))_{xx}, \quad (46)$$

yields a stationary point of the self-energy functional. Note that for any *finite* $n_s < \infty$ there is no solution: The rhs of Eq. (46) is the Green's function of a finite system which exhibits a finite set of poles on the real frequency axis (after analytical continuation). Contrary, the left-hand side represents an approximate lattice Green's function, which in the thermodynamic limit $L \rightarrow \infty$ has branch cuts on the real axis induced by the branch cut of the free Green's function.

In the case of systems with a few inequivalent sites, i.e., for inhomogeneous systems with a somewhat reduced translational symmetry, Eq. (46) exactly recovers a generalization of the DMFT, which has been put forward to describe correlation effects at surfaces and in thin films.[58] They are just the self-consistency equations of this generalized DMFT. Typically, only a few effective impurity models have to be considered in this approach.[59,60]

For disordered systems without any translational symmetry, the self-consistency equation (46) constitutes the statistical DMFT as introduced by Dobrosavljević and Kotliar.[39,40] In principle, Eq. (46) can be solved iteratively. For any iteration in the self-consistency cycle, one then needs the local Green's function at each site of the system, which in each case requires the solution of an interacting impurity problem. Equation (46) and the absence of translational symmetry also imply the need for an inversion of matrices, with dimension

given by the system size. For these reasons, the statistical DMFT is a numerically extremely expensive method.

Choosing a reference system consisting of decoupled effective impurity models with finite (and actually small) n_s could thus be an interesting alternative. Calculations based on such a statistical dynamical impurity approximation (stat-DIA), however, have not yet been performed. Since all physical quantities derive from an explicit though approximate expression for a thermodynamical potential, the stat-DIA is a thermodynamically consistent approximation. This can be seen as an advantage compared to statistical DMFT approaches which employ additional approximations to render practical calculations possible.

The self-consistency equation (46) allows for a stochastic reinterpretation: For a given configuration of on-site energies $\{\eta_x\}$, the local Green's function G_{xx} will be site dependent. The *distribution* of the local Green's function at a site x (generated by all configurations), however, will be the same as the distribution at a site $x' \neq x$ since the on-site energies η_x have been assumed to be independent random numbers distributed according to the *same* density $p(\eta_x)$ for each x. Moreover, the distribution of the local Green's function at a site x, generated by all configurations $\{\eta_x\}$, is identical to the distribution of the local Green's function on all lattice sites for one fixed typical configuration of on-site energies. Hence, the index x in the self-consistency equation (46) can be viewed as a label for a particular realization of the random variable G_{xx}.

For a Bethe lattice, Eq. (46) can be reinterpreted as a stochastic recursion equation. Starting from an arbitrary initial sample for the local Green's function, $\{G_{xx}\}$, the equation recursively generates a sequence of samples which converges to a sample which is representative of the distribution of the local Green's function. The practical advantage of this reinterpretation consists in the fact that a Gibbs-sampling Monte Carlo algorithm for the calculation of marginal distributions can be applied (see Ref. 41, for an example). The iterative solution of the self-consistency equation (46) for a given typical configuration of on-site energies is then equivalent to the recursive update of a sample of local Green's functions. Furthermore, the matrix inversion required in Eq. (46) can be avoided in the case of a Bethe lattice. For a general (e.g., cubic) lattice, however, the stochastic scheme breaks down, and one has to return to the site interpretation again.

VI. CONFIGURATION-INDEPENDENT SELF-ENERGY FUNCTIONAL

The above discussion has shown the practical needs to construct more simple approximations. An intuitive strategy involves considering quantities involving configurational averages and searching for sensible approximations of the averaged quantities instead of considering full distributions. The simplest and most natural average is the arithmetical average $\langle \cdots \rangle_P$, which has been introduced in Sec. II. It shall be understood that one has to be extremely careful when discussing *transport properties* in terms of the averaged one-particle Green's function $\boldsymbol{\Gamma}_{t,P,U}$: Close to Anderson localiza-

tion, the distribution of the local Green's function (at $\omega=0$) can exhibit an extreme asymmetry and a long tail such that the average is of no physical meaning and can by no means serve as an order parameter for a metal-insulator transition.[38]

Here our goal is to construct nonperturbative and thermodynamically consistent approximations for averaged quantities which give information on thermodynamic properties and one-particle excitations. Within the framework of the self-energy-functional approach, this can be achieved by introducing functionals that involve quantities averaged according to the given probability distribution P. In particular, we consider functionals of the configuration-independent (full) self-energy S and the configuration-dependent (interaction) self-energy Σ_{η} as defined at the end of Sec. II.

Analogous to Eq. (23), the equation

$$\left\langle \frac{1}{\Gamma^{-1} + S - \eta - \Sigma_{\eta}} \right\rangle_P = \Gamma \qquad (47)$$

constitutes a relation between the averaged Green's function Γ on the one hand and S and Σ_{η} on the other. The functional $\hat{\mathcal{G}}_U[\cdots]$ in Eq. (23) is replaced by the functional $\langle 1/(\cdots - \eta)\rangle_P$, and the probability distribution P, instead of the interaction parameters U, plays the role of the external parameter. Contrary to Eq. (23), the above relation is diagonal in the frequency $i\omega_n$ (which is suppressed in notations).

Assume that S and (for any configuration η) Σ_{η} are given. Then, the equation can formally be solved for Γ. This defines a functional $\hat{\Gamma}_P[\cdots,\cdots]$, which assigns the averaged Green's function $\Gamma=\hat{\Gamma}_P[S,\{\Sigma_{\eta}\}]$ to any S and Σ_{η}. This functional plays a role analogous to the functional $\hat{G}_U[\Sigma]$ in Sec. III.

Analogous to Eq. (25), we have

$$\hat{\Gamma}_P[S_{t,P,U},\{\Sigma_{t,\eta,U}\}] = \Gamma_{t,P,U} \qquad (48)$$

since Eq. (47) holds when evaluated for $S=S_{t,P,U}$, $\Sigma_{\eta}=\Sigma_{t,\eta,U}$, and $\Gamma=\Gamma_{t,P,U}$ as is obvious from Eqs. (14)–(16). From Eq. (33) we have

$$\hat{G}_U[\Sigma_{\eta}] = \frac{1}{G_{t,0,0}^{-1} - \eta - \Sigma_{\eta}} \qquad (49)$$

for any η. This equation and

$$\hat{\Gamma}_P[S,\{\Sigma_{\eta}\}] = \frac{1}{G_{t,0,0}^{-1} - S} \qquad (50)$$

form a (highly nonlinear) system of conditional equations for the variables $S(i\omega_n)$ and $\Sigma_{\eta}(i\omega_n)$. The external parameters t, P, and U specify the model under consideration. Equations (49) and (50) are satisfied for the exact self-energies $S(i\omega_n) = S_{t,P,U}(i\omega_n)$ and $\Sigma_{\eta}(i\omega_n) = \Sigma_{t,\eta,U}(i\omega_n)$.

In the following, we show that the conditional equations Eqs. (49) and (50) can be considered as stationarity conditions of the averaged grand potential as a functional of the self-energies. We define the self-energy functional

$$\hat{\Omega}_{t,P,U}[S,\{\Sigma_{\eta}\}] = \text{Tr} \ln \frac{1}{G_{t,0,0}^{-1} - S}$$
$$+ \left\langle \text{Tr} \ln \frac{1}{\hat{\Gamma}_P[S,\{\Sigma_{\eta}\}]^{-1} + S - \eta - \Sigma_{\eta}} \right\rangle_P$$
$$- \text{Tr} \ln \hat{\Gamma}_P[S,\{\Sigma_{\eta}\}] + \langle \hat{F}_U[\Sigma_{\eta}] \rangle_P. \qquad (51)$$

The sum of the second and third terms on the rhs is a functional which is universal, i.e., it is independent of t [note that the terms do not cancel each other as the operations $\ln(\cdots)$ and $\langle\cdots\rangle_P$ do not commute]. With Eqs. (14)–(16), (47), and (48), the evaluation of the functional at the exact self-energies yields

$$\hat{\Omega}_{t,P,U}[S_{t,P,U},\{\Sigma_{t,\eta,U}\}] = \langle \text{Tr} \ln G_{t,\eta,U} \rangle_P + \langle \hat{F}_U[\Sigma_{t,\eta,U}] \rangle_P$$
$$= \langle \Omega_{t,\eta,U} \rangle_P = \Omega_{t,P,U}, \qquad (52)$$

i.e., the exact averaged grand potential. The functional derivatives are readily calculated:

$$\frac{1}{T} \frac{\delta\hat{\Omega}_{t,P,U}[S,\{\Sigma_{\eta}\}]}{\delta S} = \frac{1}{G_{t,0,0}^{-1} - S} - \hat{\Gamma}_P[S,\{\Sigma_{\eta}\}] \qquad (53)$$

and

$$\frac{1}{T} \frac{\delta\hat{\Omega}_{t,P,U}[S,\{\Sigma_{\eta}\}]}{\delta\Sigma_{\eta}} = \left(\frac{1}{\hat{\Gamma}_P[S,\{\Sigma_{\eta}\}]^{-1} + S - \eta - \Sigma_{\eta}} \right.$$
$$\left. - \hat{G}_U[\Sigma_{\eta}] \right) P(\eta). \qquad (54)$$

Hence, setting the functional derivatives to zero yields two equations equivalent to Eqs. (49) and (50). Therefore, the functional is stationary at the exact self-energies:

$$\frac{\delta\hat{\Omega}_{t,P,U}[S_{t,P,U},\{\Sigma_{t,\eta,U}\}]}{\delta S} = 0,$$

$$\frac{\delta\hat{\Omega}_{t,P,U}[S_{t,P,U},\{\Sigma_{t,\eta,U}\}]}{\delta\Sigma_{\eta}} = 0. \qquad (55)$$

The self-energy functional Eq. (51) represents a generalization of the self-energy functional Eq. (28) for interacting systems with disorder. It is completely general and provides an exact variational principle.

VII. CONSISTENT APPROXIMATIONS

In the spirit of the SFT for pure systems, approximations shall be constructed by restricting the domain of self-energies in the functional Eq. (51) while retaining the exact functional dependence. We consider both the full as well as the interaction self-energy. Trial self-energies are taken from a reference system, which is a system in the same macroscopic state, i.e., with the same temperature T and the same chemical potential μ as the original system, but has different one-particle parameters t'. The Hamiltonian of the reference system reads

$$H' = H(t', \boldsymbol{\eta}, U) = H_0(t') + H_{\text{dis}}(\boldsymbol{\eta}) + H_{\text{int}}(U). \quad (56)$$

H' has the same interaction part as compared to the original system. Likewise, the disorder potential, i.e., the distribution $P(\boldsymbol{\eta})$, is assumed to be unchanged. Hence, the self-energy functional of the reference system is given by

$$\hat{\Omega}_{t',P,U}[S,\{\Sigma_{\boldsymbol{\eta}}\}] = \text{Tr} \ln \frac{1}{G_{t',0,0}^{-1} - S}$$
$$+ \left\langle \text{Tr} \ln \frac{1}{\hat{\Gamma}_P[S,\{\Sigma_{\boldsymbol{\eta}}\}]^{-1} + S - \boldsymbol{\eta} - \Sigma_{\boldsymbol{\eta}}} \right\rangle_P$$
$$- \text{Tr} \ln \hat{\Gamma}_P[S,\{\Sigma_{\boldsymbol{\eta}}\}] + \langle \hat{F}_U[\Sigma_{\boldsymbol{\eta}}]\rangle_P. \quad (57)$$

Only the first term on the rhs is different as compared to the functional for the original system Eq. (51). Combining Eqs. (51) and (57), the last three terms on the respective rhs cancel out, and one is left with

$$\hat{\Omega}_{t,P,U}[S,\{\Sigma_{\boldsymbol{\eta}}\}] = \hat{\Omega}_{t',P,U}[S,\{\Sigma_{\boldsymbol{\eta}}\}] + \text{Tr} \ln \frac{1}{G_{t,0,0}^{-1} - S}$$
$$- \text{Tr} \ln \frac{1}{G_{t',0,0}^{-1} - S}. \quad (58)$$

Note that the full and the interaction self-energies are considered as variables at this point, and that for the cancellation of the functionals it is of crucial importance to choose the reference system to have the same interaction and disorder. The self-energy functional Eq. (58) is still exact.

As trial self-energies we insert the exact self-energies of the reference system: $S = S_{t',P,U}$ and $\Sigma_{\boldsymbol{\eta}} = \Sigma_{t',\boldsymbol{\eta},U}$. Searching for the stationary point of the exact self-energy functional Eq. (51) on the subspace of trial self-energies taken from H' and parametrized by t' means to search for the stationary point of a function of t':

$$\Omega_{t,P,U}(t') \equiv \hat{\Omega}_{t,P,U}[S_{t',P,U},\{\Sigma_{t',\boldsymbol{\eta},U}\}], \quad (59)$$

where t, P, and U are fixed by the original system. From Eqs. (52) and (15) for the reference system, we get the comparatively simple result:

$$\Omega_{t,P,U}(t') = \Omega_{t',P,U} + \text{Tr} \ln \frac{1}{G_{t,0,0}^{-1} - S_{t',P,U}} - \text{Tr} \ln \Gamma_{t',P,U}. \quad (60)$$

This result is formally very similar to Eq. (39) for pure systems. Again, the important point is that the rhs can be computed exactly if the reference system is an exactly solvable model. The only difference consists in the fact that the grand potential, the Green's function, and the self-energy of the reference system on the rhs are replaced by the corresponding averaged quantities and the configuration-independent (full) self-energy.

A certain approximation may be constructed along the following steps: (i) A reference system is specified with P and U fixed as in the original system. The hopping part, i.e., t', however, is fully at one's disposal and should be used to simplify the problem posed by the reference system. (ii) For

a given set of variational parameters t', the reference system's Hamiltonian $H' = H(t', \boldsymbol{\eta}, U)$ is diagonalized for any configuration $\boldsymbol{\eta}$ to get the (many-body) eigenenergies and eigenstates. (iii) The grand potential $\Omega_{t',\boldsymbol{\eta},U}$ and, from the Lehmann representation, the Green's function $G_{t',\boldsymbol{\eta},U}$ are obtained for any $\boldsymbol{\eta}$. (iv) Averaging yields $\Omega_{t',P,U} = \langle \Omega_{t',\boldsymbol{\eta},U}\rangle_P$ and $\Gamma_{t',P,U} = \langle G_{t',\boldsymbol{\eta},U}\rangle_P$. The self-energy is computed via $S_{t',P,U} = G_{t',0,0}^{-1} - \Gamma_{t',P,U}^{-1}$. (v) Inserting these results as well as the free Green's function of the original model into Eq. (60) yields $\Omega_{t,P,U}(t')$. (vi) Steps (ii)–(v) are repeated for different t' to find the stationary point t'_s given by

$$\frac{\partial \Omega_{t,P,U}(t'_s)}{\partial t'} = 0. \quad (61)$$

This approximation strategy shares a number of advantageous features with the corresponding strategy for pure systems: Any approximation constructed in this way is a thermodynamically consistent one since the theromdynamics as well as the (averaged) one-particle excitation properties both derive from an explicit expression for the approximate averaged grand potential $\Omega_{t,P,U}(t'_s)$ at the stationary point (see the discussion in Ref. 61). The only approximation consists in the restriction of the domain of the self-energy functional. The approach is systematic as an enlarged domain leads to an improved approximation (see the discussion in Ref. 57). As the exact functional form is retained, approximations are nonperturbative by construction.

VIII. LIMITING CASES

Equation (51) gives the self-energy functional $\hat{\Omega}_{t,P,U}[S,\{\Sigma_{\boldsymbol{\eta}}\}]$ for a disordered and interacting system. To discuss the limiting cases of the pure, of the noninteracting, and of the pure and noninteracting systems, we first have to specify the domain of this functional. This also applies to the functionals $\hat{\Gamma}_P[S,\{\Sigma_{\boldsymbol{\eta}}\}], \hat{G}_U[\Sigma]$, etc.

For a given set of interaction parameters U and for a given probability distribution P, the domain $\mathcal{D} = \mathcal{D}_S \times \mathcal{D}_{\Sigma}$ of the self-energy functional $\hat{\Omega}_{t,P,U}[S,\{\Sigma_{\boldsymbol{\eta}}\}]$ shall consist of (full) self-energies $S \in \mathcal{D}_S$ and (for any $\boldsymbol{\eta}$) interaction self-energies $\Sigma_{\boldsymbol{\eta}} \in \mathcal{D}_{\Sigma}$ taken from the reference system. Namely, a (full) self-energy S belongs to $\mathcal{D}_S$ if there is some t' such that $S = S_{t',P,U}$, i.e., such that S is the exact self-energy of the problem given by $H' = H(t', \boldsymbol{\eta}, U)$ and P for some t'. Likewise, a set of interaction self-energies $\{\Sigma_{\boldsymbol{\eta}}\}$ (for all possible $\boldsymbol{\eta}$) belongs to $\mathcal{D}_{\Sigma}$ if there is some t' such that $\Sigma_{\boldsymbol{\eta}} = \Sigma_{t',\boldsymbol{\eta},U}$, i.e., such that $\Sigma_{\boldsymbol{\eta}}$ is the exact (interaction) self-energy of the problem given by $H' = H(t', \boldsymbol{\eta}, U)$ for some t'. Hence, the hopping parameters t' *span* the domain of the self-energy functional.

This definition is very convenient as it automatically ensures the correct analytical and causal properties for any self-energy in the domain. It also avoids formal difficulties for pure or noninteracting systems which arise from the fact that conditional equations such as Eq. (47) become tautological in these limits and cannot serve to define a self-energy functional. With the above definition of the domain, however, this

becomes irrelevant as for the cases of pure or noninteracting systems the domain consists of a single element or a null set only.

With these preparations, let us discuss the limits in detail:

(i) The pure and noninteracting case is given by $P(\boldsymbol{\eta}) = \delta(\boldsymbol{\eta} - \boldsymbol{\eta}_0)$ and $U=0$. Note that we can set $\boldsymbol{\eta}_0=0$ for simplicity (in the absence of disorder, a nonzero $\boldsymbol{\eta}_0$ merely implies a redefinition of the hopping: $\boldsymbol{t} + \boldsymbol{\eta}_0$). The domain of the self-energy functional Eq. (51) shrinks to the point $\boldsymbol{S} = \boldsymbol{\Sigma}_{\boldsymbol{\eta}} = 0$. According to Eqs. (26) and (25), this implies

$$\hat{F}_{U=0}[0] = \hat{\Omega}_{U=0}[\boldsymbol{G}_{t,0,0}^{-1}] - \mathrm{Tr}\ln \boldsymbol{G}_{t,0,0} = 0 \qquad (62)$$

as $\mathrm{Tr}\ln \boldsymbol{G}_{t,0,0}$ is the grand potential of a system of noninteracting electrons with hopping $\boldsymbol{t}$. For $\boldsymbol{\eta} = \boldsymbol{\eta}_0 = 0$ and $\boldsymbol{S} = \boldsymbol{\Sigma}_{\boldsymbol{\eta}} = 0$, the second and third terms on the rhs of Eq. (51) cancel, and thus one is left with

$$\hat{\Omega}_{t,P_0,0}[0,0] = \mathrm{Tr}\ln \boldsymbol{G}_{t,0,0}, \qquad (63)$$

which is the correct result.

(ii) In the case of $P(\boldsymbol{\eta}) = \delta(\boldsymbol{\eta})$ but finite interaction $U \neq 0$, one still has $\boldsymbol{\Sigma}_{\boldsymbol{\eta}} = \boldsymbol{\Sigma} = \boldsymbol{S}$ on the domain, and due to the cancellation of the second and third terms on the rhs of Eq. (51), the self-energy functional reduces to Eq. (28), as expected.

(iii) For a system of noninteracting electrons $(U=0)$ moving in a disorder potential with $P(\boldsymbol{\eta}) \neq \delta(\boldsymbol{\eta})$, one has $\boldsymbol{\Sigma}_{\boldsymbol{\eta}} = 0$ on the domain of the self-energy functional and thus $\hat{F}_{U=0}[0]=0$. With $\hat{\Gamma}_P[\boldsymbol{S}] \equiv \hat{\Gamma}_P[\boldsymbol{S}, \boldsymbol{\Sigma}_{\boldsymbol{\eta}}=0]$, this yields the self-energy functional $\hat{\Omega}_{t,P}[\boldsymbol{S}] \equiv \hat{\Omega}_{t,P,U=0}[\boldsymbol{S}, \boldsymbol{\Sigma}_{\boldsymbol{\eta}}=0]$ with

$$\hat{\Omega}_{t,P}[\boldsymbol{S}] = \mathrm{Tr}\ln \frac{1}{\boldsymbol{G}_{t,0,0}^{-1} - \boldsymbol{S}} - \mathrm{Tr}\ln \hat{\Gamma}_P[\boldsymbol{S}]$$
$$+ \left\langle \mathrm{Tr}\ln \frac{1}{\hat{\Gamma}_P[\boldsymbol{S}]^{-1} + \boldsymbol{S} - \boldsymbol{\eta}} \right\rangle_P \qquad (64)$$

for the problem with disorder only. The last two terms play the same role as the functional $\hat{F}_{U,\boldsymbol{\eta}}[\boldsymbol{\Sigma}]$ for the problem with interaction only. This functional is discussed in the next section.

IX. MEAN-FIELD APPROXIMATIONS

Mean-field approximations for systems with local disorder and local interactions represent a simple but instructive class of approximations within the framework of the self-energy-functional approach. It is well known that any mean-field theory of disorder will be deficient in various ways. Issues such as localization cannot be addressed, for example, by means of the famous CPA.[62] Nevertheless, the mean-field concept represents an important benchmark and starting point for improvements and is, in many cases, the best we have at hand for practical calculations.

We start by considering the functional (64) for the noninteracting, disorder-only limit of the model (40). This is the Anderson model
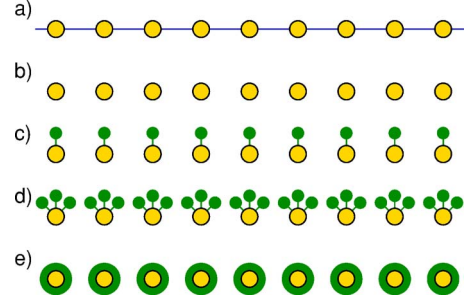

FIG. 3. (Color online) (a) Representation of the (disorder) Anderson model Eq. (65). (b) Reference system generating the atomic approximation (see text). (c) Two-site approximation. (d) Improved mean-field approximation due to atomic reference system with more bath sites ($n_s=4$). (e) The optimum mean-field approximation generated by a continuum of bath sites is the coherent-potential approximation (CPA). If (a) represents the (pure) Hubbard model, (b) yields a Hubbard-I-type atomic approximation, (d) is a typical mean-field approximation, and the optimum mean-field approximation (e) is given by the DMFT. In case that (a) represents the Anderson-Hubbard model Eq. (40), the reference system (d) leads to the DMFT+CPA approach.

$$H = \sum_{xx'} t_{xx'} c_x^\dagger c_{x'} + \sum_x \eta_x c_x^\dagger c_x, \qquad (65)$$

with local disorder given by Eq. (41) and some density $p(\eta_x)$ characterizing, for example, an alloy with R components $(\sum_r p_r = 1)$:

$$p(\eta) = \sum_{r=1}^{R} p_r \delta(\eta - \eta_r). \qquad (66)$$

For simplicity, the spin index is suppressed.

A mean-field or single-site approximation is generated by a reference system consisting of decoupled sites [see Fig. 3(b)], i.e., by switching off the hopping term. For an alloy-type disorder, this reference system is exactly solvable, as one has to compute the Green's function for a finite number of R configurations. Models with a continuous distribution $p(\eta_x)$ have to be simulated by a finite but large R. Adding "bath" sites to the reference system, i.e., sites with fixed, configuration-independent on-site energies, enlarges the space of variational parameters $\boldsymbol{t}'$ and trial self-energies $\boldsymbol{S} = \boldsymbol{S}_{t',P}$ and implies an improved mean-field approximation [see Figs. 3(c) and 3(d)]. Note that the disorder part is still the same as in the original model (65), as it is required to justify Eq. (60).

The Hamiltonian of the reference system reads

$$H' = \sum_x t_{xx}' c_x^\dagger c_x + \sum_x \eta_x c_x^\dagger c_x + \sum_x \sum_i V_i^{(x)} (c_x^\dagger a_{xi} + \mathrm{H.c.})$$
$$+ \sum_x \sum_i \varepsilon_i^{(x)} a_{xi}^\dagger a_{xi}. \qquad (67)$$

It consists of the local part of Eq. (65) and, for each site $\boldsymbol{x}$, includes bath sites with (configuration-independent) energies $\varepsilon_i^{(x)}$ hybridizing with the original sites via $V_i^{(x)}$, where $i = 2, \ldots, n_s$. As the Hamiltonian describes an impurity model

with identical and decoupled replicas at any site x, it is in fact sufficient to focus on one impurity model only. The site index x can be suppressed in this case. This reflects the translational symmetry of averaged quantities in the original model (65).

Due to the decoupling of the original sites, the reference system yields a trial self-energy which is local. Spatial correlations due to nonlocal contributions of the self-energy are neglected. Differences between different mean-field approximations are due to the temporal correlations, i.e., due to additional bath sites. Obviously, the optimum single-site approximation is obtained for a continuum of bath sites $n_s \to \infty$ [Fig. 3(e)].

A. Atomic approximation

The simplest approximation is obtained for $n_s = 1$, i.e., no additional bath sites [Fig. 3(b)]. This case is instructive as it allows for a largely analytical treatment which elucidates some general features of the disorder SFT. The reference-system Hamiltonian consists of the first two terms on the rhs of Eq. (67). We consider the case of a binary alloy ($R = 2$) with on-site energies η_1 and η_2 and corresponding probabilities p_1 and p_2. The only variational parameter left is the (configuration-independent) on-site energy $t_0' \equiv t_{xx}'$.

For $T = 0$ and $\mu = 0$, the averaged grand potential of the reference system $\Omega' \equiv \Omega_{t',P,0}$ is easily calculated:

$$\Omega'/L = p_1(t_0' + \eta_1)\Theta(- t_0' - \eta_1) + p_2(t_0' + \eta_2)\Theta(- t_0' - \eta_2). \quad (68)$$

This is the first term on the rhs of Eq. (60).

The averaged Green's function of the reference system [Eq. (16)] is obtained immediately as $\Gamma_{xx}'(\omega) = \delta_{xx}\Gamma'(\omega)$ with

$$\Gamma'(\omega) = \frac{p_1}{\omega - t_0' - \eta_1} + \frac{p_2}{\omega - t_0' - \eta_2}. \quad (69)$$

Using the considerations of Ref. 27 [see Eq. (20) therein], only the poles $\omega_{1,2}' = t_0' + \eta_{1,2}$ enter the result for the third term on the rhs of Eq. (60):

$$\text{Tr} \ln \frac{\Gamma_{t',P,0}}{L} = \sum_{r=1,2} \omega_r'\Theta(- \omega_r') - \frac{R_S}{L}. \quad (70)$$

The term R_S (see Ref. 27) cancels out later.

With the free Green's function of the reference system, $G_0'(\omega) = 1/(\omega - t_0')$, we get from Eq. (15) the self-energy as $S_{xx'}(\omega) = \delta_{xx'}S(\omega)$, where

$$S(\omega) = \langle\eta\rangle + \frac{\langle\eta^2\rangle - \langle\eta\rangle^2}{\omega - t_0' - \eta_1 - \eta_2 + \langle\eta\rangle}. \quad (71)$$

Let $\varepsilon(\boldsymbol{k})$ be the eigenvalues of the hopping matrix $\boldsymbol{t}$ and let $\Gamma_{xx'}(\omega) = L^{-1}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}(x-x)}\Gamma_{\boldsymbol{k}}(\omega)$, with L the number of lattice sites and $\Gamma_{\boldsymbol{k}}(\omega) = 1/[\omega - \varepsilon(\boldsymbol{k}) - S(\omega)]$ the averaged Green's function of the original system as it appears in Eq. (60). From Eq. (71) we find

$$\Gamma(\omega) = \frac{\alpha_1}{\omega - \omega_1} + \frac{\alpha_2}{\omega - \omega_2}, \quad (72)$$

with poles $\omega_{1,2} = [\varepsilon(\boldsymbol{k}) + t_0' + \eta_1 + \eta_2]/2 \pm \{[\varepsilon(\boldsymbol{k}) + 2\langle\eta\rangle - \eta_1 - \eta_2 - t_0']^2/4 + \langle\eta^2\rangle - \langle\eta\rangle^2\}^{1/2}$ and weights $\alpha_1 = (\omega_1 - \eta_1 - \eta_2 + \langle\eta\rangle - t_0')/(\omega_1 - \omega_2)$ and $\alpha_2 = (\omega_2 - \eta_1 - \eta_2 + \langle\eta\rangle - t_0')/(\omega_2 - \omega_1)$. The $\boldsymbol{k}$ dependence of the poles is only due to $\varepsilon(\boldsymbol{k})$, i.e., $\omega_r = \omega_r(\boldsymbol{k}) = \omega_r(\varepsilon(\boldsymbol{k}))$. Hence, using Eq. (21) of Ref. 27 and the definition of the free density of states $\rho_0(z) = L^{-1}\sum_{\boldsymbol{k}} \delta[z - \varepsilon(\boldsymbol{k})]$, we get

$$\text{Tr} \ln \frac{\Gamma_{t,P,0}}{L} = \sum_{r=1,2} \int_{-\infty}^{\infty} dz\, \rho_0(z)\omega_r(z)\Theta[- \omega_r(z)] - \frac{R_S}{L} \quad (73)$$

for the second term on the rhs of Eq. (60).

Adding the three contributions, one can search for a stationary point numerically. Here, we restrict ourselves to the particle-hole symmetric case, i.e., we assume $\rho_0(z) = \rho_0(-z)$, $\eta_1 = \eta_2$, and $p_1 = p_2 = 1/2$. While the different contributions to the SFT grand potential Eq. (60) are asymmetric, it is straightforward to see that their sum is symmetric with respect to a sign change of the variational parameter: $\Omega_{t,P,0}(t_0') = \Omega_{t,P,0}(-t_0')$. Furthermore, the dependence on t_0' is smooth for $|t_0'| < |\eta_1|$. Hence, the SFT grand potential is stationary at $t_0' = 0$, which had to be expected by virtue of particle-hole symmetry.

The optimum self-energy is given by Eq. (71) with $t_0' = 0$. It consists of the "virtual-crystal" potential $\langle\eta\rangle$ [note that $S(\omega) \equiv \langle\eta\rangle$ is the so-called virtual-crystal approximation[11]] and a frequency-dependent part with one simple pole at $\omega = 0$. Its weight is given by the disorder strength, namely, by the variance $\langle\eta^2\rangle - \langle\eta\rangle^2 = \eta_1^2$. For any finite η_1, this leads to a splitting of the averaged local density of states into a lower and an upper alloy band. In the case of strong disorder, this result is qualitatively correct as could be expected since the high-frequency behavior of $S(\omega)$ is correct up to the order $1/\omega^2$. However, the widths of the alloy bands turn out to be too small.

This atomiclike approximation is very much reminiscent of the Hubbard-I approximation[18] for the pure but interacting system, although the Hubbard-I self-consistency condition is somewhat different from the SFT Euler equation and leads to different results away from the particle-hole symmetric point. The analogy between approximations for disordered but noninteracting and pure but interacting systems relies on the same structure of the reference system. In this analogy, the static part of the disorder self-energy, the virtual-crystal potential $\langle\eta\rangle$, corresponds to the static part of the Hubbard-I self-energy which, for the Hubbard model, is given by $U\langle c_{x\sigma}^\dagger c_{x\sigma}\rangle$, i.e., to the Hartree(-Fock) approximation. A combination of both Hubbard-I-type approximations for the interacting and disordered system is straightfordly set up with an atomiclike reference system including (local) interaction and disorder.

In view of the simplicity of the Hubbard-I-type approach, it is remarkable that the variational optimization of the on-site hopping ensures thermodynamic consistency with re-

spect to the particle number, i.e., the averaged particle number as obtained from the (approximate) disorder-averaged grand potential as a μ derivative is always the same as the averaged particle number calculated by integration of the (approximate) disorder-averaged single-particle Green's function. The proof for this consistency is analogous to that given in Ref. 61, see Appendix B.

It is also interesting that the stationary point $t' = 0$ actually (locally) *maximizes* the SFT grand potential as has been verified by a simple numerical evaluation of Eq. (60) for the particle-hole symmetric case. In general, and for high-dimensional parameter spaces in particular, we expect that stationary points are saddles.

B. Two-site approximation

The two-site approximation [see Fig. 3(c)] is the simplest mean-field approach beyond the atomic approximation. For the case of the pure Hubbard model without disorder, the two-site approximation has proven to be very instructive and successful.[27,63–66] It provides a handy mean-field approach which is able to reproduce qualitatively the DMFT phase diagram for the Mott transition in the single-band model and which has been employed to study more complex two- and multiorbital systems. A recent application[67] to the Anderson-Hubbard model has shown that the approach can straightforwardly be extended to disordered (and interacting) systems along the lines described here. The two-site approximation qualitatively reproduces the results of the DMFT+CPA method but with a minimum computational effort.

C. Coherent-potential approximation

The two-site approach can, of course, be improved by adding more bath sites [Fig. 3(d)]. The best mean-field approach is then obtained for $n_s \to \infty$, i.e., for a continuum of bath sites [Fig. 3(e)]. Varying all parameters, i.e., $t'_0 \equiv t'_{xx}$, $\varepsilon_i = \varepsilon_i^{(x)}$, and $V_i \equiv V_i^{(x)}$, yields the optimum local self-energy as the stationary point

$$0 = \frac{\partial}{\partial t'} \hat{\Omega}_{t,P}[S_{t',P}] = \sum_n \sum_x \frac{\delta \hat{\Omega}_{t,P}[S_{t',P}]}{\delta S_{xx}(i\omega_n)} \frac{\partial S_{xx}(i\omega_n)}{\partial t'} \quad (74)$$

of the function $\Omega_{t,P}(t') \equiv \hat{\Omega}_{t,P}[S_{t',P}]$. Here it has been used that the self-energy (and also its t' derivative) is local and nonzero at the impurity site only. From Eq. (64), we have

$$\Omega_{t,P}(t') = \operatorname{Tr} \ln \frac{1}{G_{t,0,0}^{-1} - S_{t',P}} - \operatorname{Tr} \ln \hat{\Gamma}_P[S_{t',P}]$$

$$+ \left\langle \operatorname{Tr} \ln \frac{1}{\hat{\Gamma}_P[S_{t',P}]^{-1} + S_{t',P} - \boldsymbol{\eta}} \right\rangle_P. \quad (75)$$

Note that the last term on the rhs is just the averaged grand potential of the reference system $\Omega_{t',P}$.

The Euler equation (74) is satisfied if

$$0 = \frac{\delta \hat{\Omega}_{t,P}[S_{t',P}]}{\delta S_{xx}(i\omega_n)} \quad (76)$$

for each site x and for each Matsubara frequency ω_n. Calculating the derivative of the functional Eq. (64), we obtain

$$\frac{1}{T} \frac{\delta \hat{\Omega}_{t,P,0}[S_{t',P}]}{\delta S_{xx}(i\omega_n)} = \left(\frac{1}{i\omega_n + \mu - t - S(i\omega_n)} \right)_{xx}$$

$$- \left(\left\langle \frac{1}{\hat{\Gamma}_P[S_{t',P}]^{-1} + S(i\omega_n) - \boldsymbol{\eta}} \right\rangle_P \right)_{xx}. \quad (77)$$

The first term on the rhs is the local element of the averaged Green's function of the lattice model, $\Gamma_{\text{loc}}(i\omega_n)$, which is calculated with the approximate local self-energy $S(i\omega_n)$ (exploiting translational symmetry, the site index can be suppressed). The second term on the rhs is the averaged Green's function of the reference system at the impurity site $\Gamma'_{\text{loc}}(i\omega_n)$. The optimum local disorder self-energy is thus determined by the condition that the local averaged Green's function equals the averaged impurity Green's function of the reference system:

$$\Gamma_{\text{loc}}(i\omega_n) = \Gamma'_{\text{loc}}(i\omega_n). \quad (78)$$

This is exactly the self-consistency condition of the coherent-potential approximation.

To elucidate this point, we note that, for the reference system Eq. (67), $\Gamma'_{\text{loc}}(i\omega_n)$ is the average of the impurity Green's function for the different on-site energies, i.e.,

$$\Gamma'_{\text{loc}}(i\omega_n) = \sum_r p_r \frac{1}{i\omega_n + \mu - \eta_r - \Delta(i\omega_n)}, \quad (79)$$

where $\Delta(i\omega_n) = \Sigma_i V_i^2 / (i\omega_n + \mu - \varepsilon_i)$ is the hybridization function. On the other hand, from the definition of the disorder self-energy for the reference system, we have

$$\Gamma'_{\text{loc}}(i\omega_n) = \frac{1}{i\omega_n + \mu - \Delta(i\omega_n) - S(i\omega_n)}. \quad (80)$$

Eliminating the hybridization function, we get

$$\Gamma'_{\text{loc}}(i\omega_n) = \sum_r p_r \frac{1}{\dfrac{1}{\Gamma'_{\text{loc}}(i\omega_n)} + S(i\omega_n) - \eta_r}. \quad (81)$$

After a few manipulations, this equation can be cast into the form

$$\sum_r p_r \frac{\eta_r - S(i\omega_n)}{1 - \Gamma'_{\text{loc}}(i\omega_n)[\eta_r - S(i\omega_n)]} = 0, \quad (82)$$

which makes contact with the original derivation of the CPA where the averaged atomic scattering matrix is set to zero.[24] Introducing the free Bloch-band dispersion $\varepsilon(\boldsymbol{k})$ as the Fourier transform of the hopping t and the free Bloch-density of states $\rho_0(z) = (1/L) \Sigma_k \delta[z - \varepsilon(\boldsymbol{k})]$, we have

$$\Gamma_{\text{loc}}(i\omega_n) = \int \frac{\rho_0(z)dz}{i\omega_n + \mu - z - S(i\omega_n)}. \qquad (83)$$

In combination with Eq. (78), this equation can be used to eliminate $\Gamma'_{\text{loc}}(i\omega_n)$ from Eq. (81) to obtain a single conditional equation for $S(i\omega_n)$.

For a practical calculation, one may set up the following self-consistency cycle: Starting from a guess for the hybridization function $\Delta(i\omega_n)$, the averaged impurity Green's function $\Gamma'_{\text{loc}}(i\omega_n)$ can be computed from Eq. (79). With the help of Eq. (80), $S(i\omega_n)$ is determined, which is then used in Eq. (83) to get the CPA Green's function $\Gamma_{\text{loc}}(i\omega_n) = \Gamma'_{\text{loc}}(i\omega_n)$. Using Eq. (80) again, a new hybridization function can be found.

Obviously, the bath sites of the reference system play the role of an "effective medium." The bath parameters or, equivalently, the hybridization function $\Delta(i\omega_n)$ parametrizes the local disorder self-energy in the most general way, consistent with causality requirements. The present rederivation of the CPA therefore very clearly shows the CPA to be the best local approximation.

D. Dynamical mean-field theory

The reference systems shown in Fig. 3 can also be used in the context of a *pure* system without disorder but with local interaction such as the Hubbard model. In this case, the theory reduces to the conventional SFT. The reference system (b) with the hopping between the correlated sites switched off generates an atomic approximation very much the same as the Hubbard-I approximation[18] but with the Hubbard-I self-consistency replaced by the SFT Euler equation for that reference system which is different. The rather crude atomiclike approximation can be improved by adding uncorrelated bath sites. This yields the reference system (d), which is a set of disconnected single-impurity Anderson models with $n_s < \infty$ sites each. Qualitatively, the results of the two-site dynamical-impurity approximation[27,63–66] [Fig. 3(c)] are already close to the $n_s = \infty$ limit. The convergence with increasing n_s is rapid (see Ref. 68, for example).

The most general local trial self-energy compatible with the requirements of causality is generated in the limit $n_s = \infty$. Here, the calculation proceeds in a way analogous to the previous section and yields the Euler (or self-consistency) equation (see Ref. 26):

$$G_{\text{loc}}(i\omega_n) = G'_{\text{loc}}(i\omega_n). \qquad (84)$$

Here $G_{\text{loc}}(i\omega_n)$ is the on-site element of the lattice Green's function [Fig. 3(a)] calculated approximately from the approximate local self-energy via the Dyson equation for the lattice model, and $G'_{\text{loc}}(i\omega_n)$ is the exact Green's function of the reference system [Fig. 3(e)] at the impurity site. Equation (84) is just the self-consistency equation of the dynamical mean-field theory.[12,14–16]

The CPA for a noninteracting system with local disorder has a formal structure which is very similar to the DMFT for a pure system with local interaction. This is apparent when comparing the respective self-consistency conditions (78) and (84) and also the respective self-consistency cycles

which serve to iteratively solve the mean-field equations. As the DMFT, the CPA becomes exact in the limit of high spatial dimensions $D \to \infty$ as has been shown by Vlaming and Vollhardt[13] and Schwartz and Siggia.[69] Both approaches are characterized as approximations that yield the optimum local self-energy. All of these are made very obvious within the framework of the SFT, which discloses the formal analogies between Green's-function-based approaches to disordered or interacting systems.

A self-evident idea that has been pursued in the past is to derive the DMFT (or a different many-body approach to pure interacting systems) by using the formal structure of the CPA. This requires, however, a transformation of a pure system with local interaction to a noninteracting system with local disorder to which the CPA can be applied. Hubbard's alloy analogy[70] and also a refined version[71] represent such transformations. The subsequent application of the CPA to Hubbard's ficticious alloy yields the so-called Hubbard-III approximation. The alloy analogy (the transformation) itself, however, must be seen as a rough approximation which fails to recover Fermi-liquid properties even for weak interactions. The "many-body CPA" by Hirooka and Shimizu,[72] the "generalized CPA" by Janiš,[73] as well as the "dynamical CPA" of Kakehashi[74] go beyond a simple analogy. The ideas of the dynamical CPA are to perform the transformation to an effective one-particle Hamiltonian within the functional-integral formalism by means of a Hubbard-Stratonovich transformation and to recover the DMFT by the subsequent use of the CPA (see Ref. 75 for a discussion).

In this context, it is also worth mentioning the Falicov-Kimball model which can be considered as a variant of the Hubbard model with the hopping of one of the two spin species switched off. The exact solution of the Falicov-Kimball model in the limit $D \to \infty$ has been worked out by Brandt and Mielsch.[76–78] They could show that the local (interaction) self-energy of the mobile carriers is given by the CPA (disorder) self-energy—no alloy analogy is necessary for this simplified model. It is tempting to understand the dynamics of the mobile carriers as the scattering of noninteracting particles from the (local and uncorrelated binary) disorder potential generated by the immobile ones.

E. DMFT + CPA

For a system with Hubbard-type interactions and local disorder, e.g., the prototypical Anderson-Hubbard model Eq. (40), the optimum mean-field theory is generated by the reference system shown in Fig. 3(e). Note that the reference system shares with the original system the same interaction part and the same disorder potential. The continuum of bath sites is uncorrelated and configuration independent.

We start from Eq. (60). For the present case, the Euler equation $\partial\Omega_{t,P,U}(t')/\partial t' = 0$ is satisfied if

$$\frac{1}{T} \frac{\delta\hat{\Omega}_{t,P,U}[S_{t',P,U}, \{\mathbf{\Sigma}_{t',\boldsymbol{\eta},U}\}]}{\delta S_{xx}(i\omega_n)} = 0 \qquad (85)$$

for the local elements of the self-energy. This is the Euler equation which fixes the variational paramters t'. Analogous to Eq. (77), we then obtain

$$\left(\frac{1}{i\omega_n + \mu - t - S_{t',P,U}}\right)_{xx} = \hat{\Gamma}_P[S_{t',P,U}, \{\Sigma_{t',\eta,U}\}]_{xx}, \quad (86)$$

i.e., the local averaged Green's function equals the averaged impurity Green's function of the reference system, $\Gamma_{\text{loc}}(i\omega_n) = \Gamma'_{\text{loc}}(i\omega_n)$, as in the noninteracting case with disorder.

Analogous to the procedure described in Sec. IX C, this self-consistency equation can be solved in an iterative manner: Starting with a guess for the variational parameters t' or, equivalently, for the hybridization function $\Delta(i\omega_n) = \Sigma_i V_i^2/(i\omega_n + \mu - \varepsilon_i)$, the interacting impurity Green's function is calculated for any (local) configuration of the reference single-impurity Anderson model and averaged over the configurations to get $\Gamma'_{\text{loc}}(i\omega_n)$. The self-energy is obtained from Eq. (80), which is the defining equation Eq. (15) for the self-energy also in the case of an interacting impurity model. $S(i\omega_n)$ is then used in Eq. (83) to get the averaged lattice Green's function $\Gamma_{\text{loc}}(i\omega_n)$. Via the self-consistency equation, this gives us $\Gamma'_{\text{loc}}(i\omega_n)$ and, using Eq. (80) again, a new hybridization function. Note that for a continuum of bath sites the optimum on-site element of the hopping t'_0 is always given by $t'_0 = t_{xx}$. This can be shown in essentially the same way as has been done in Ref. 61 for the pure case.

The self-consistency condition Eq. (86) and the cycle described above constitute what is known as the DMFT+CPA approach, which has been put forward by Janiš and Vollhardt[30] and by Dobrosavljević and Kotliar[31,32] in a different context: Originally, the DMFT+CPA has been introduced and characterized as the exact theory in the limit of infinite spatial dimensions which remains nontrivial for a proper scaling of the hopping parameters.[12] The presented rederivation places the DMFT+CPA into the broader framework of the SFT.

The TMT, as suggested recently by Dobrosavljević *et al.*,[47] can be seen as a variant of the DMFT+CPA (see also Refs. 48 and 49). Here a modification of the above-described self-consistency cycle is considered by replacing (*ad hoc*) the usual arithmetical average of the interacting impurity Green's function over the (local) configurations by a *geometrical* one. Actually, this geometrical average is applied to the corresponding (positive definite) spectral density, and the Green's function $\Gamma'_{\text{loc}}(i\omega_n)$ is obtained afterwards from this average as the usual Hilbert transform. A rederivation of this variant within the SFT does not seem to be possible: Any approximation generated within the SFT preserves the elementary sum rule $\int d\omega A_{\text{loc}}(\omega) = 1$ for the local spectral density, while this must be violated when averaging geometrically. Despite this conceptual shortcoming, the TMT can be motivated physically (see Refs. 47 and 48) and clearly improves upon the mean-field concept as it is able to describe aspects of Anderson localization. It should be seen as a pragmatic simplification of the statistical DMFT that allows for practical computations in many cases which are not accessible to the statistical DMFT. As can be shown for a simplified model,[79] the results of TMT qualitatively agree very well with those obtained from a full evaluation of the statistical DMFT for interaction- and disorder-driven metal-insulator transitions.
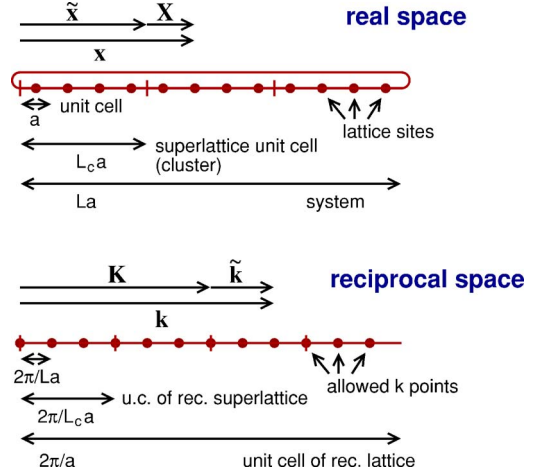

FIG. 4. (Color online) Decomposition of real-space lattice vectors, $x = \tilde{x} + X$, and reciprocal-space wave vectors, $k = \tilde{k} + K$, for a $D=1$ dimensional lattice (lattice constant a) with $L=12$ sites tiled with $L/L_c = 3$ clusters consisting of $L_c = 4$ sites each. x, original lattice; $\tilde{x}$, superlattice; and X, sites in a cluster. Reciprocal space: There are L allowed wave vectors k in the unit cell of the lattice reciprocal to x, and there are L/L_c allowed wave vectors $\tilde{k}$ in the unit cell of the lattice reciprocal to the superlattice $\tilde{x}$. K are the reciprocal superlattice vectors, $\exp(iK\tilde{x}) = 1$.

X. CLUSTER EXTENSIONS

A mean-field approximation neglects spatial correlations by considering an effective *single-site* problem to generate the self-energy. A straightforward idea to improve upon the mean-field concept is therefore to replace the effective single-site model by an effective cluster model consisting of a finite (small) number of sites. This should restore the important short-range correlations and provide a systematic approach with the inverse cluster size as a small parameter. The goal is to construct a cluster approximation which, on the one hand, reduces to the CPA or to a simpler mean-field approach, which, on the other hand, becomes exact in the infinite-cluster limit, and which preserves the translational and point-group symmetries of the lattice, in addition. This, however, is by no means trivial, and naive theories often suffer from causality violations.[11] In contrast, it is easy to see that all approximations that are constructed within the SFT, including the different cluster approximations discussed in the following, are manifestly causal. This is briefly discussed in Appendix C.

Before discussing the different cluster approaches in detail, let us introduce some notations (see Fig. 4): We consider a system on a D-dimensional lattice of L sites with periodic boundary conditions and $L \to \infty$ in the end. The position vector to a site in the lattice is denoted by x. There are L allowed wave vectors in a unit cell of the reciprocal lattice, which are denoted by k. The lattice is tiled with L/L_c clusters consisting of L_c sites each. Let $\tilde{x}$ be the position vector of the cluster origin and X the position vector of a site in a cluster, referring to the cluster origin. We then have the unique decomposition $x = \tilde{x} + X$. The vectors $\tilde{x}$ form a superlattice with a unit-cell volume enlarged by the factor L_c. In a unit cell of the
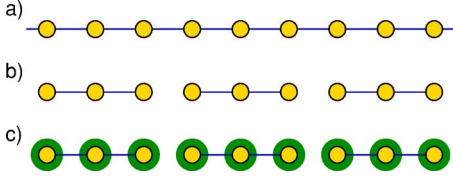
FIG. 5. (Color online) (a) Representation of the Anderson model Eq. (65). (b) Reference system generating the (disorder) variational-cluster approximation (VCA) (without variational optimization: cluster-perturbation theory). (c) Reference system generating the molecular CPA (M-CPA). In the case of an additional local (Hubbard) interaction, (a) represents the Anderson-Hubbard model, (b) yields a generalized VCA, and (c) generates the C-DMFT +M-CPA approximation.

reciprocal superlattice, there are L/L_c allowed wave vectors $\tilde{\boldsymbol{k}}$. Its volume is reduced by the factor L_c as compared to the volume of the reciprocal unit cell of the original lattice. For a given $\boldsymbol{k}$, we have the unique decomposition $\boldsymbol{k}=\tilde{\boldsymbol{k}}+\boldsymbol{K}$, where $\boldsymbol{K}$ are the vectors of the reciprocal superlattice, i.e., $\exp(i\boldsymbol{K}\tilde{\boldsymbol{x}})=1$. In the reciprocal unit cell of the original lattice, there are L_c vectors $\boldsymbol{K}$. These can also be interpreted as the allowed cluster wave vectors when imposing periodic boundary conditions on the individual cluster.

Consider the $L\times L$ matrix $\boldsymbol{U}$ with elements

$$U_{x,k}=\frac{1}{\sqrt{L}}e^{ikx}, \qquad (87)$$

the $L/L_c\times L/L_c$ matrix $\boldsymbol{V}$ with elements

$$V_{\tilde{x},\tilde{k}}=\frac{1}{\sqrt{L/L_c}}e^{i\tilde{k}\tilde{x}}, \qquad (88)$$

and the $L_c\times L_c$ matrix $\boldsymbol{W}$ with elements

$$W_{X,K}=\frac{1}{\sqrt{L_c}}e^{iKX}. \qquad (89)$$

$\boldsymbol{U}$, $\boldsymbol{V}$, and $\boldsymbol{W}$ are unitary and define Fourier transformations between the respective real and reciprocal spaces. Note that $\boldsymbol{U}\neq \boldsymbol{VW}=\boldsymbol{WV}$. A quantity $A_{x,x'}$ which is invariant under lattice translations x_0, i.e., $A_{x+x_0,x'+x_0}=A_{x,x'}$, is diagonalized by $\boldsymbol{U}$: $(\boldsymbol{U}^\dagger \boldsymbol{A}\boldsymbol{U})_{kk'}=A(k)\delta_{k,k'}$. A quantity $A_{x,x'}$ which is invariant under superlattice translations $\tilde{x}_0$ as well as under cluster translations X_0 (i.e., which is cyclic on the cluster), $A_{x+\tilde{x}_0,x'+\tilde{x}_0}=A_{x+X_0,x'+X_0}=A_{x,x'}$, is diagonalized by $\boldsymbol{VW}$: $(\boldsymbol{W}^\dagger \boldsymbol{V}^\dagger \boldsymbol{A}\boldsymbol{VW})_{\tilde{k}K\tilde{k}'K'}=A(\tilde{k},K)\delta_{\tilde{k},\tilde{k}'}\delta_{K,K'}$.

A. Variational cluster approach

A straightforward extension of the single-site atomic approximation (see Sec. IX A) is the (disorder) VCA, which is the analog of the VCA known[28,53,54] for the interacting but pure system. To be definite, consider the Anderson model Eq. (65) again. The model is represented in Fig. 5(a). A suitable reference system to include short-range correlations in the disorder self-energy consists of a set of isolated clusters of L_c sites tiling the original lattice, as shown by Fig. 5(b). Since

within the SFT the (only) approximation is to replace the exact self-energy by the self-energy of the reference system, the VCA must become exact in the limit $L_c\to\infty$, i.e., the VCA is a systematic approach which is controlled by the inverse cluster size as a small parameter.

To calculate the cluster self-energy $S_{t',P}$, the Anderson model must be solved on an individual cluster (by switching off the intercluster hopping) for all configurations. For large cluster size L_c, the computational cost therefore scales exponentially with L_c. This is, of course, characteristic for all cluster approximations.

The intracluster hopping parameters t' including the on-site energies are considered as variational parameters. A nonvariational variant of the VCA is obtained if one sets these parameters to the original (physical) hopping parameters within the cluster: $t'=t_{\text{intra}}$. This constitues the analog of the CPT,[51,52] which is known for the interacting, pure system.

Obviously, the CPT is also systematic and controlled by $1/L_c$. The additional optimization of the variational parameters t' within the VCA is expected to speed up the convergence with increasing L_c as it does for interacting but pure systems.[28] One should note, however, that the variational optimization should become less and less important with increasing L_c as the exact solution is approached for $L_c\to\infty$ with $t'=t_{\text{intra}}$ anyway. It is therefore advisable to restrict the space of variational parameters and to optimize a few parameters only as, for example, those parameters that are close to the cluster boundary.

Parameter optimization is beneficial if (local) interactions are considered, in addition (as, e.g., in the Anderson-Hubbard model). Figure 5(b) defines a generalized VCA for this case. The additional interactions can drive a spontaneous breaking of a continuous symmetry. This is signaled within the VCA by a stationary point of the SFT grand potential at a nonvanishing value of a symmetry-breaking field. Note that the respective field term can be added to the reference-system Hamiltonian if this is given by a one-particle term. This "Weiss" field is a ficticious one, which clearly has to be distinguished from a physical field and which describes spontaneous as opposed to induced symmetry breaking. For pure systems and spontaneous SU(2) and U(1) symmetry breaking, this concept has already been applied successfully.[53,54,61,80]

B. Molecular CPA

The (disorder) VCA is obtained as the cluster generalization of the atomic approximation. Likewise, within the framework of the SFT, the cluster generalization of the CPA leads to the so-called molecular CPA (M-CPA).[81] To be definite, we again consider the Anderson model Eq. (65). The reference system generating the M-CPA is shown in Fig. 5(c). It consists of a set of isolated clusters of L_c sites each and a continuum of bath sites attached to each of the original sites.

As in the case of the CPA, this allows one to derive a simplified Euler equation. Analogous to Eqs. (74) and (77), we can derive the following stationarity condition:

$$0 = T\sum_n \sum_{x,x'} \left(\frac{1}{i\omega_n + \mu - t - S(i\omega_n)} \right.$$

$$\left. - \mathbf{\Gamma}_{t',P}(i\omega_n) \right)_{x'x,11} \frac{\partial S_{xx'}(i\omega_n)}{\partial t'}. \quad (90)$$

x and x' must belong to the same cluster since $S_{xx'}(i\omega_n)=0$ and also the "projector" $\partial S_{xx'}(i\omega_n)/\partial t'=0$ if x and x' belong to different clusters as these are decoupled in the reference system. Note that t' is a matrix labeled as $t'_{xx',ii'}$, where $i=1,\ldots,n_s$ and $i\neq 1$ refers to the additional bath sites attached to each original site x. The same holds for $\mathbf{\Gamma}_{t',P}$ and $S\equiv S_{t',P}$. As the reference system exhibits local disorder on the original sites x, there are nonzero elements of the self-energy for $i=i'=1$ only. We write $S_{xx',11}=S_{xx'}$ for short. Obviously, $S_{xx'}=S^{(\tilde{x})}_{XX'}\delta_{\tilde{x}\tilde{x}'}=S_{XX'}\delta_{\tilde{x}\tilde{x}'}$.

Both the original and reference systems are invariant under translations of the superlattice. Hence, Fourier transformation given by $V_{\tilde{x}\tilde{k}}$ [Eq. (88)] is appropriate. This yields

$$0 = T\sum_n \frac{L_c}{L}\sum_{\tilde{k}}\sum_{XX'} \left(\frac{1}{i\omega_n + \mu - t(\tilde{k}) - S(i\omega_n)} \right.$$

$$\left. - \mathbf{\Gamma}_{t',P}(i\omega_n) \right)_{X'X,11} \frac{\partial S_{XX'}(i\omega_n)}{\partial t'}. \quad (91)$$

Here, $\tilde{k}$ runs over the L/L_c wave vectors in the reduced Brillouin zone. The trial self-energy S as well as $\mathbf{\Gamma}_{t',P}$ are $\tilde{k}$ independent matrices in the intracluster position vectors X,X' while $t(\tilde{k})$ is $\tilde{k}$ dependent.

The M-CPA self-consistency equation reads[11]

$$\frac{L_c}{L}\sum_{\tilde{k}} \left(\frac{1}{i\omega_n + \mu - t(\tilde{k}) - S} \right)_{XX'} = (\mathbf{\Gamma}_{t',P})_{XX'}, \quad (92)$$

where the frequency dependence has been suppressed for convenience. This generalizes the CPA self-consistency equation (78), which is obtained from Eq. (92) for $X=X'$ and cluster size $L_c=1$.

Comparing with the stationarity condition Eq. (91), we note that the SFT grand potential is stationary at the M-CPA self-energy, i.e., at the self-energy $S(i\omega_n)=S_{t',P}$ if variational parameters t' can be found such that Eq. (92) is satisfied for any $i\omega_n$, X, and X'. Hence, the reference system [Fig. 5(c)] generates the M-CPA.

The following self-consistency cycle can be set up: We start with a guess for the one-particle parameters of the reference system, i.e., the parameters for a single cluster $t'_{0,X,X'}\equiv t'_{\tilde{x}+X,\tilde{x}+X',11}, \varepsilon^{(X)}_i$ and $V^{(X)}_i$ $(i=2,\ldots,n_s)$. For a fixed (intracluster) configuration of the disorder potential η_X, the intracluster part of the Green's function $G_{t'_0,\eta}$ is an $L_c \times L_c$ matrix G' with elements $G'_{\tilde{x}+X,\tilde{x}+X'}$. By solving its equation of motion, one easily verifies $G'(i\omega_n)=1/[i\omega_n+\mu-t'_0-\eta-\mathbf{\Delta}(i\omega_n)]$, where the matrix hybridization function $\mathbf{\Delta}(i\omega_n)$ is diagonal with elements $\mathbf{\Delta}_X(i\omega_n)=\sum^\infty_{i=2}V^{(X)2}_i/(i\omega_n+\mu-\varepsilon^{(X)}_i)$. Averaging over the different configurations (e.g., 2^{L_c} for a
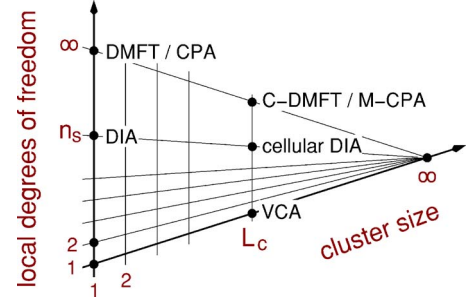

FIG. 6. (Color online) Systematics of different approximations that can be constructed within the SFT framework for pure interacting systems, disorder-free systems, or interacting systems with disorder. The interaction and/or disorder are/is assumed to be local. The axis intercepts L_c and n_s characterize the reference system and thereby the type of approximation. A local approximation ("dynamical impurity approximation," DIA) is obtained for $L_c=1$. The optimum local approximation with $n_s\to\infty$ bath sites is the DMFT, CPA, or DMFT+CPA, respectively. A cluster ("cellular" or "molecular") extension of DMFT/CPA is obtained for $L_c>1$. The variational cluster approximation (VCA) is a cluster approximation without the use of bath sites ($L_c>1$, $n_s=1$). The exact solution would be obtained in the limit $L_c\to\infty$ irrespective of n_s.

binary alloy) yields $\mathbf{\Gamma}_{t',P}(i\omega_n)$ and, by comparison with the free Green's function, the self-energy $S(i\omega_n)$. This fixes the lhs of Eq. (92), i.e., the averaged Green's function of the original model. Equation (92) is then used to get a new $\mathbf{\Gamma}_{t',P}(i\omega_n)$ and thus a new hybridization function via $\mathbf{\Delta}(i\omega_n)=i\omega_n+\mu-t'_0-\eta-G'(i\omega_n)^{-1}$. Parameters $\varepsilon^{(X)}_i$ and $V^{(X)}_i$ are obtained as the poles and weights of $\mathbf{\Delta}(i\omega_n)$. From the above it is obvious, however, that the self-consistency cycle can be set up for $\mathbf{\Delta}$ directly. The variational determination of t'_0 is not a problem: Analogous to the discussion given in Ref. 61, a high-frequency expansion easily shows that, at stationarity, t'_0 must equal the intracluster part of the original hopping t.

Note that for the noninteracting but disordered system, the M-CPA is related to the CPA as is, for the interacting but pure system, the C-DMFT (Refs. 42 and 43) to the DMFT. The M-CPA is a conceptually simple and straightforward generalization of the single-site CPA, which includes short-range correlations in the disorder self-energy but is mean-field-like on a scale beyond the cluster size. Like the VCA, the M-CPA is systematic and controlled by $1/L_c$ as a small parameter, in principle. Practical calculations, however, are restricted to comparatively small clusters due to the exponential growth of the number of local (intracluster) configurations. For systems with local interactions and disorder, the structure of the reference system [Fig. 5(c)] generates a combined C-DMFT+M-CPA approach, which is the straightforward cluster extension of the DMFT+CPA (Sec. IX E). The approximations within the SFT for different n_s and L_c are schematically grouped in Fig. 6.

C. Translation symmetry

There is an apparent problem remaining: Due to the construction of the reference system as a set of decoupled clusters, the trial self-energies do not preserve the translational
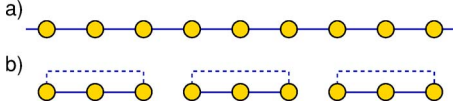
FIG. 7. (Color online) (a) Anderson model. (b) Possible reference system consisting of isolated clusters with periodic boundary conditions generating a variant of the CPT. Within the VCA, the hopping marked as a dashed line may be treated as a variational parameter.

symmetries of the original lattice. This is a self-evident problem for any cluster approximation which is formulated in real space and has initiated the development of several further cluster approximations in the past. It has turned out,[11] however, that the construction of a self-consistent and systematic approach which, on the one hand, recovers (for $L_c = 1$) the CPA and, on the other, approaches ($L_c \rightarrow \infty$) the exact solution, which respects the requirements of causality, and which perserves the lattice translational symmetries at the same time, is not easy to find.

A straightforward idea is to use a reference system as displayed in Fig. 7(b). Here, isolated clusters are considered again but with a hopping t' satisfying periodic boundary conditions. This restores translational invariance within the cluster at least. The idea has been put forward in the context of a pure but interacting system as a modified cluster-perturbation theory (CPT with periodic boundary conditions) by Zacher *et al.*[82] but was recognized[83] to give less convincing results when compared to the usual CPT. Later on, it could be shown[28] within the VCA that periodic boundary conditions are, in fact, unfavorable: One simply has to treat the hopping integral connecting the edges of a cluster as a variational parameter. The SFT grand potential turns out to be stationary if this hopping integral vanishes. This corresponds to open boundary conditions. In any case, however, it is obvious that the full translational symmetry cannot be restored with the reference system of Fig. 7(b).

Another straightforward idea is to formulate the original problem as well as the reference system in reciprocal space by using annihilators c_k instead of c_x. In graphical representations of H and H' like the one in Fig. 7, dots would have to be reinterpreted as referring to one-particle states labeled by k. The advantage is that, by construction, H' always exhibits the full translational symmetry. While there are no principle objections, it appears to be impossible in practice, however, to generate meaningful approximations in this way. The reason is that a local interaction in real space transforms into a delocalized one in reciprocal space: The interaction parameters $U_{kk'k''k'''}$ basically couple any k point to any other. Likewise, a local uncorrelated disorder transforms into a delocalized correlated one. As H and H' must share the same interaction and disorder, it is unlikely to find a t' that permits a (simple) solution of the resulting problem.

A pragmatic way out would be to distinguish formally between the self-energy $S_{t',P}$ that is determined as the stationary point of the SFT grand potential, on the one hand, and the translationally invariant ("physical") self-energy, on the other. The latter is obtained from $S = S_{t',P}$ by some periodization procedure which employs a universal functional $\hat{T}$

"periodizing" the self-energy: $S \rightarrow \hat{T}[S]$. This idea has been suggested in the context of the C-DMFT.[42,50] One possibility is to Fourier transform the optimized self-energy $S_{t',P}$ from real space, $S_{xx'}$, to reciprocal space via $U_{x,k'}$, Eq. (87). This yields the self-energy in the representation $S_{kk'}$. Substituting $S_{kk'} \rightarrow S_{kk'}\delta_{k,k'} \equiv \hat{T}[S]_{kk'}$ gives a translationally invariant (physical) self-energy $\hat{T}[S]$. In real space, this periodization reads

$$\hat{T}[S]_{xx'} \equiv \frac{1}{L}\sum_{yy'} \delta_{x-x',y-y'} S_{yy'}. \qquad (93)$$

$\hat{T}$ could also be applied to the Green's function calculated from S via Dyson's equation. This is the usual procedure within the CPT to generate translationally invariant Green's functions. While the problem of translational symmetries can be fixed in this or in a similar way, the procedure appears to be *ad hoc* as it is placed on top of a variational (or self-consistent) calculation which itself involves S instead of $\hat{T}[S]$.

D. Periodized M-CPA, periodized VCA

Koller and Dupuis[84] have discussed a modified form of the self-energy functional for (pure) systems of interacting bosons to get translationally invariant trial self-energies. This method can be adapted to disordered systems as described below.

Consider the Anderson model Eq. (65) and the following self-energy functional:

$$\hat{\Omega}_{t,P}^{(1)}[S] = \mathrm{Tr}\,\ln \frac{1}{G_{t,0,0}^{-1} - \hat{T}[S]} - \mathrm{Tr}\,\ln \hat{\Gamma}_P[S]$$
$$+ \left\langle \mathrm{Tr}\,\ln \frac{1}{\hat{\Gamma}_P[S]^{-1} + S - \boldsymbol{\eta}} \right\rangle_P. \qquad (94)$$

As compared to the original functional $\hat{\Omega}_{t,P}[S]$ given by Eq. (64), the modified functional $\hat{\Omega}_{t,P}^{(1)}[S]$ differs in the first term as this includes the periodizing functional $\hat{T}$. As usual, the hopping term of the Anderson model is supposed to be translationally invariant, $\hat{T}[t] = t$. The exact self-energy is therefore translationally invariant, too, and satisfies $\hat{T}[S_{t,P}] = S_{t,P}$. Hence, we have

$$\hat{\Omega}_{t,P}^{(1)}[S_{t,P}] = \hat{\Omega}_{t,P}[S_{t,P}]. \qquad (95)$$

Using a one-particle basis of Bloch states labeled by wave vectors k to evaluate the traces, we furthermore have

$$\frac{\delta\hat{\Omega}_{t,P}^{(1)}[S]}{\delta S_{kk'}} = \left(\frac{1}{G_{t,0,0}^{-1} - \hat{T}[S]}\right)_{kk} \delta_{k',k} - \Gamma[S]_{k'k}. \qquad (96)$$

Since $\Gamma[S_{t,P}]_{kk'} = \delta_{k,k'}\Gamma[S_{t,P}]_{kk}$, this shows that the exact (translationally invariant) self-energy is a stationary point of the modified self-energy functional. Concludingly, the functionals $\hat{\Omega}_{t,P}^{(1)}[S]$ and $\hat{\Omega}_{t,P}[S]$ are different, in general, but co-

incide and are stationary at the exact self-energy $S_{t,P}$. They are similarly suited for constructing approximations.

Consider now a trial self-energy $S_{t',P}$ from a reference system with the same disorder (i.e., the same distribution function P) but with hopping parameters t' breaking translational symmetries, as is the case, e.g., for the reference system given by Fig. 5(c). The condition for stationarity of the modified self-energy functional within the restricted set of trial self-energies then reads

$$0 = T\sum_n \sum_{k,k'} \left\{ \left[\frac{1}{i\omega_n + \mu - t - \hat{T}[S](i\omega_n)} \right]_{kk} \delta_{k,k'} \right.$$
$$\left. - [\mathbf{\Gamma}_{t',P}(i\omega_n)]_{k'k} \right\} \frac{\partial S_{kk'}(i\omega_n)}{\partial t'}. \qquad (97)$$

Here, $S \equiv S_{t',P}$ for short. This replaces the condition Eq. (90) characteristic for the M-CPA.

Fourier transformation U [Eq. (87)] yields $S_{kk'} = L^{-1}\sum_{xx'} e^{-ikx} e^{ik'x'} S_{xx'}$ and thus

$$0 = T\sum_n \sum_{x,x'} \left\{ \frac{1}{L}\sum_k e^{-ik(x-x')} \left(\frac{1}{i\omega_n + \mu - t - \hat{T}[S]} \right)_{kk} \right.$$
$$\left. - [\mathbf{\Gamma}_{t',P}(i\omega_n)]_{x'x} \right\} \frac{\partial S_{xx'}(i\omega_n)}{\partial t'}. \qquad (98)$$

For the reference system of Fig. 5(c) with isolated clusters, we have $S_{xx'} = S_{\tilde{x}+X,\tilde{x}'+X'} = S_{\tilde{x}+X,\tilde{x}+X'} \delta_{\tilde{x}\tilde{x}'}$ (and the same for its t' derivative) and thus the Euler equation (98) is satisfied if

$$\frac{1}{L}\sum_k \frac{e^{ik(X-X')}}{i\omega_n + \mu - \varepsilon(k) - \hat{T}[S](k)} = (\mathbf{\Gamma}_{t',P})_{XX'}. \qquad (99)$$

As compared to the self-consistency condition of the M-CPA [Eq. (92)], the main difference consists in the fact that its solution is based on a self-consistency cycle which involves at each step the periodized self-energy $\hat{T}[S]$ instead of S. The Green's function of this periodized M-CPA, $G \equiv (i\omega_n + \mu - t - \hat{T}[S])^{-1}$, is likewise translationally invariant: $\hat{T}[G] = G$.

The analog of the self-consistency equation (99) for the pure but interacting system is the self-consistency equation of the PC-DMFT, see Ref. 50. Hence, the above derivation also shows how the PC-DMFT can be rederived within the SFT framework. Furthermore, the construction of a combined PC-DMFT+periodized M-CPA is straightforward. It is also straightforward to constuct a periodized VCA for disordered or interacting systems along the lines above.

As in the usual VCA (and also in the usual M-CPA) one, in principle, has the choice between open and periodic boundary conditions in the reference system. In the case of the periodized VCA or periodized M-CPA, a translationally invariant self-energy and Green's function are generated by either choice. The value of the SFT grand potential at the stationary point decides which kind of boundary conditions should be preferred.

With a suitably defined functional $\hat{T}$, there are no problems to extend the approach and to restore point-group symmetries of the underlying lattice which could be violated by the choice of the reference system. Essentially the same arguments given for the case of translational symmetries can be repeated.

There is yet another way to modify the original functional and thereby to construct a theory which respects the translational symmetries of the underlying lattice. This shall be mentioned here for the sake of completeness. Consider the functional

$$\hat{\Omega}_{t,P}^{(2)}[S] = \mathrm{Tr}\ln\hat{T}\left[\frac{1}{G_{t,0,0}^{-1} - S} \right] - \mathrm{Tr}\ln\hat{\mathbf{\Gamma}}_P[S]$$
$$+ \left\langle \mathrm{Tr}\ln\frac{1}{\hat{\mathbf{\Gamma}}_P[S]^{-1} + S - \eta} \right\rangle_P. \qquad (100)$$

Again, only the first term on the rhs is modified. Note that this is essential for the construction of approximations: It ensures that the implicitly known but universal functional given by the remaining terms cancels out when comparing with the functional of a suitably defined reference system, as usual. $\hat{\Omega}_{t,P}^{(2)}[S]$ coincides with $\hat{\Omega}_{t,P}[S]$ and $\hat{\Omega}_{t,P}^{(1)}[S]$ at the exact self-energy $S_{t,P}$ and is stationary there. With the reference system of Fig. 5(c), the following self-consistency equation can be derived:

$$\frac{1}{L}\sum_k e^{ik(X-X')} \left(\frac{1}{i\omega_n + \mu - t - S} \right)_{kk} = (\mathbf{\Gamma}_{t',P})_{XX'}. \qquad (101)$$

As compared to the periodized M-CPA, the conceptual disadvantage consists in the fact that only the propagator $\hat{T}[(G_{t,0,0}^{-1} - S)^{-1}]$ but not the self-energy is translationally invariant.

E. Dynamical cluster approximation

Originally, the DCA has been proposed as a cluster extension of the DMFT for interacting systems.[85–87] Essentially the same ideas, however, can also be used to construct a generalization of the single-site CPA for the disorder problem.[44,45] Here, it is shown that the (disorder) DCA can be rederived within the SFT framework by utilizing the real-space perspective on the DCA first discussed by Biroli *et al.*[50]

While the main idea of the periodized M-CPA to restore translational symmetry is to consider a modified but equivalent self-energy functional, one could also keep the exact functional form $\Omega_{t,P}[S]$ but modify the hopping of the original system, i.e., $t \rightarrow \bar{t}$. Approximations are then constructed by starting from $\Omega_{\bar{t},P}[S]$ and using a reference system consisting of isolated clusters again. To ensure that the resulting approximations systematically approach the exact solution for cluster size $L_c \rightarrow \infty$, the replacement $t \rightarrow \bar{t}$ must be controlled by L_c, i.e., it must become exact (up to irrelavant boundary terms) in the infinite-cluster limit.
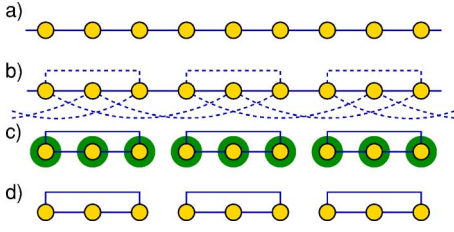
Consider, for example,

FIG. 8. (Color online) (a) Anderson model. (b) The original Anderson model but with a modified one-particle part $t \rightarrow \overline{t}$, which is the starting point for the dynamical cluster approximation (DCA). $\overline{t}$ is invariant under superlattice and cluster translations. (c) Reference system generating the DCA. Note that t' has the same translational symmetries as $\overline{t}$. (d) Reference system generating a simplified DCA (see text).

$$\overline{t} = (VW)U^\dagger t U(VW)^\dagger. \qquad (102)$$

For clusters of finite size L_c, the combined Fourier transformation VW is different from U. For $L_c \rightarrow \infty$, however, this becomes irrelevant. With $\varepsilon(\mathbf{k}) = (U^\dagger t U)(\mathbf{k})$ we have

$$\overline{t}_{xx'} = \frac{1}{L_c} \sum_K e^{iK(X-X')} \frac{L_c}{L} \sum_{\widetilde{k}} e^{i\widetilde{k}(\widetilde{x}-\widetilde{x}')} \varepsilon(\widetilde{k}+K). \qquad (103)$$

Obviously, $\overline{t}$ is invariant under superlattice translations as well as under cluster translations (with periodic cluster boundary conditions). The original system and the modified system with $\overline{H} = H(\overline{t}, \boldsymbol{\eta}, 0)$ are represented by Figs. 8(a) and 8(b). The construction of $\overline{t}$ is such that it exhibits the same translational symmetries as the one-particle parameters t' of a reference system consisting of isolated clusters tiling the original lattice with periodic boundary conditions, see Figs. 8(c) and 8(d). Since both t and $\overline{t}$ are invariant under superlattice translations, we can compare $t_{\mathbf{XX'}}(\widetilde{\mathbf{k}}) = (V^\dagger t V)_{XX'}(\widetilde{\mathbf{k}})$ with $\overline{t}_{XX'}(\widetilde{\mathbf{k}}) = (V^\dagger \overline{t} V)_{XX'}(\widetilde{\mathbf{k}})$. It turns out that they are equal up to a phase factor:

$$\overline{t}_{XX'}(\widetilde{\mathbf{k}}) = \frac{1}{L_c} \sum_K e^{iK(X-X')} \varepsilon(\widetilde{\mathbf{k}}+K)$$

$$= \frac{L_c}{L} \sum_{\widetilde{x}\widetilde{x}'} e^{-i\widetilde{k}(\widetilde{x}+X-\widetilde{x}'-X')} t_{\widetilde{x}+X,\widetilde{x}'+X'} = e^{-i\widetilde{k}(X-X')} t_{XX'}(\widetilde{\mathbf{k}}).$$

$$(104)$$

To rederive the disorder DCA within the framework of the SFT, we use the functional $\Omega_{t,P}[\boldsymbol{S}]$ and the reference system of Fig. 8(c). Therewith, one formally arrives at the M-CPA self-consistency condition, Eq. (92), but with t replaced by $\overline{t}$:

$$\frac{L_c}{L} \sum_{\widetilde{k}} \left(\frac{1}{i\omega_n + \mu - \overline{t}(\widetilde{\mathbf{k}}) - \boldsymbol{S}} \right)_{XX'} = (\boldsymbol{\Gamma}_{t',P})_{XX'}. \qquad (105)$$

The bold symbols are matrices in the cluster variables X, X'. The self-energy and the averaged Green's function of the reference system are independent of $\widetilde{\mathbf{k}}$. The decisive difference as compared to the M-CPA is that the (modified) hopping of the *original* system $\overline{t}$ is invariant under cluster trans-

lations, as is the case for t'. This is important as it allows one to simultaneously diagonalize all matrices in Eq. (105) by the cluster Fourier transformation W. Furthermore, from the definition of $\overline{t}$, the W transformation yields $\overline{t}(\widetilde{\mathbf{k}}) \rightarrow \varepsilon(\widetilde{\mathbf{k}}+\mathbf{k}) = \varepsilon(K)$, i.e., we find

$$\frac{L_c}{L} \sum_{\widetilde{k}} \frac{1}{i\omega_n + \mu - \varepsilon(\widetilde{\mathbf{k}}+K) - (W^\dagger S W)_K} = (W^\dagger \boldsymbol{\Gamma}_{t',P} W)_K. \qquad (106)$$

This, however, is just the self-consistency equation of the disorder DCA.[44]

We can thus state that, analogous to the work of Biroli *et al.*[50] for the usual DCA, it is found that the disorder DCA is equivalent to the M-CPA applied to the system with modified hopping [Eq. (102)]. Hence, it has been shown that the (disorder) DCA (as well as the usual DCA and also the combined theory for interacting systems with disorder) can be recovered within the framework of the SFT when starting from a suitably modified problem. As previously noted,[28] however, a strict rederivation starting from the original system (with t) appears to be impossible.

In this context, an interesting different approximation suggests itself: Starting with the modified hopping $\overline{t}$ and using the reference system shown in Fig. 8(d) generate a simplified (disorder) DCA without bath degrees of freedom. This simplified DCA is a systematic (controlled by $1/L_c$) cluster approximation and gives a translationally invariant self-energy and propagator. The simplified DCA is related to the periodized VCA in the same way as the DCA is related to the periodized M-CPA. The analogous formulation of a simplified DCA for the pure but interacting system represents a variational extension of a non-self-consistent approximation ("periodic CPT") recently introduced by Tran.[46]

XI. SUMMARY AND DISCUSSION

An advantageous feature of the self-energy-functional approach for systems of interacting electrons is that approximations are easily specified by choosing a reference system. The reference system helps to span a space of trial self-energies which are optimized using an appropriate dynamical variational principle. Since a reference system must share with the original system under consideration the same interaction part, the number of possible reference systems is severely limited. This leads to a straightforward classification of approximations which may be called "dynamic" as these are essentially based on an approximation for the self-energy or, equivalently, the Green's function, i.e., quantities characterizing the spectrum of one-particle excitations.

For systems with local interactions, the set of dynamical approximations includes the dynamical mean-field theory, which corresponds to a reference system consisting of decoupled single-impurity models. Modifying this reference system generates DMFT-related dynamical approximations but does not spoil the main attractive properties of the DMFT, in particular, its nonperturbative character and its thermodynamical consistency. This is interesting as it opens up a way

to construct approximations which (i) are based on simpler reference systems that can be solved with less numerical effort or/and (ii) include spatial correlations beyond the local mean-field concept. In fact, the classification of dynamical approximations has led to approximations which have successfully been employed in the past (see Fig. 6 for pure systems): The DIA as well as the VCA.

The main idea of this paper has been to translate this story to the case of disordered (and interacting) systems. The disorder is assumed to be local and uncorrelated between different sites. One possible way is to apply the conventional SFT to treat the interaction part of the problem for any disorder configuration and to average subsequently. This procedure treats the disorder part of the problem exactly. Choosing a decoupled set of effective impurity models as a reference system yields an extension of the DMFT for systems with reduced translational symmetries or, after reinterpretation of the mean-field (Euler) equations as stochastic recursion equations, to the so-called statistical DMFT. This is feasible in the case of a Bethe lattice only. Even then and even with a simpler reference system including a minimum number of bath sites, however, the statistical SFT remains a numerically extremely expensive method.

The alternative consists in an *approximate* treatment of the disorder on the same footing as the interaction. Technically, this requires a reformulation of the SFT for interacting systems within a functional-integral language which, as a by-product, provides an entirely nonperturbative construction of the SFT, i.e., avoids formal summations of skeleton diagrams. The functional-integral framework then allows one to formulate a disorder SFT in essentially the same way as for pure interacting systems; the main corners of the theory are left unchanged: The (averaged) grand potential can be expressed as a functional of the (disorder) self-energy with the physical self-energy being a stationary point. The functional still consists of a simple and explicitly known part depending on the one-particle parameters as well as of a complicated and basically unknown part which, however, is "universal," i.e., depends on the probability distribution only. Choosing a reference system with the same distribution function, the universal part can be eliminated, and an exact evaluation of the self-energy functional becomes possible on the space of trial self-energies generated by the reference system. Restricting the search for the stationary point to this limited subspace generates approximations.

It is conceptually very satisfying that within this generalized SFT, the coherent-potential approximation for the disorder problem takes the place of the DMFT for an interacting system. Similar to the DMFT, the CPA is a dynamical approximation for the self-energy and is distinguished by the fact that it becomes formally exact in the limit of infinite spatial dimensions. "Replacing interaction by disorder," any reference system for the case of an interacting system can also be considered as a reference system for the disorder case. This establishes a one-to-one mapping of the respective approximations, with the DMFT corresponding to the CPA and the cellular DMFT corresponding to the molecular CPA. Via this mapping, a disorder DIA and a disorder VCA appear as different approximations as well as the periodized M-CPA, namely, the disorder pendant of the periodized cel-

lular DMFT, when starting from a different but equivalent functional involving the periodizing functional $\hat{T}$. Starting from the self-energy functional with a suitably modified hopping $t \to \bar{t}$, one also recovers the disorder analog of the dynamical cluster approximation. Finally, a simplified DCA without bath degrees of freedom can be set up.

The case of noninteracting disordered systems could actually be treated by specialization of a more general functional $\hat{\Omega}_{t,P,U}[S, \{\Sigma_{\eta}\}]$ depending on the full *and* configuration-dependent interaction self-energies. This is applicable to interacting *and* disorderd systems. Though formally more complicated, the unknown part of the functional is universal, i.e., depends on U and P only. The classification of dynamical approximations extends accordingly (see Fig. 6).

Summing up, the type of dynamical approximations that can be constructed for systems with local interactions or/and local disorder are mean-field and cluster approximations which differ with respect to the number of local variational degrees of freedom included in the reference system. All approximations fulfill the requirements of causality. They are nonperturbative as, contrary to truncating diagrammatic approximations, the exact functional form is retained. Thermodynamical consistency is ensured by the existence of an approximate but explicit expression for the grand potential, i.e., for a thermodynamical potential, from which the physical quantities are derived. Additional but systematic modifications of the self-energy functional have been shown to generate (cluster) approximations that respect the symmetries of the underlying lattice, particularly the translational symmetries.

Convergence properties of the different quantum-cluster schemes with a continuum of bath sites have been discussed in Refs. 88–91 and apply to the schemes with $n_s = 1$ in an analogous way. For $L_c \to \infty$, local quantities generally converge exponentially fast within the C-DMFT/M-CPA and within the (disorder) VCA. This has to be compared with the $1/l_c^2$ behavior obtained within the DCA and within the simplified DCA (with $L_c = l_c^D$). For practical purposes, however, the quality of a given approximation for *small* L_c is more important and can apparently be estimated *a posteriori* only. It is, for example, an open question whether cluster schemes with or without bath degrees of freedom should be preferred in this respect (see, however, Ref. 28).

The application of the SFT has been restricted to systems with local interactions and local disorder. This is consistent with the spirit of the cluster–mean-field approximations discussed above. One should note, however, that nonlocal or even long-ranged interactions or disordered nearest-neighbor or longer-ranged hopping or spatially correlated disorder in the on-site energies, for example, pose difficulties. While the general self-energy functional can be set up as usual, it appears to be impossible to find a suitable reference system and thereby usable approximations in most cases: As the reference system should have the same interaction and disorder, it is hard to find a decoupling of its degrees of freedom by modifying the hopping part only. This problem could be handled either pragmatically by additional mean-field decouplings of nonlocal terms connecting different clusters[54] or,

more thoroughly, by considering more complex functionals involving two-particle correlation functions.[92]

One should be aware that the various local approximations and their different cluster extensions all neglect long-range correlations beyond the linear scale of the cluster. This is typical for any cluster–mean-field approach. To our knowledge, there is no possibility to systematically restore long-range correlations by a suitable embedding of an isolated cluster in the environment within the presented formalism (apart from simply enlarging the cluster). The same holds for cluster schemes formulated within reciprocal space.

This implies that a proper description of transport properties is hardly possible. Effects like Anderson localization, for example, cannot be captured within a mean-field approach like CPA and are obviously difficult to restore by cluster schemes extending CPA (see Ref. 44, for an example). Anyway, it is basically impossible to access two-particle correlation functions, and the conductivity in particular, within an approach that places one-particle excitations in the center of interest. The statistical DMFT (statistical SFT) represents an exception as here the full distribution of the (one-particle) density of states can be used to discriminate between extended and localized states, for example.

Besides the spectrum of one-particle excitations, however, the SFT derives an approximate but explicit expression for a thermodynamical potential and thus provides a consistent picture of the entire thermodynamics and of static expectation values. This includes spontaneous symmetry breaking, i.e., the determination of order parameters. The formal framework presented here should therefore be ideally suited to study the effects of disorder on different types of long-range order, such as magnetism or superconductivity. For different material classes, such as diluted magnetic semiconductors, cuprate-based high-temperature superconductors, manganites, rare-earth compounds, etc., these are central questions.

ACKNOWLEDGMENT

APPENDIX A: DISORDER IN THE INTERACTION

It is formally straightforward to extend the theory to the case of disorder in the interaction part of the Hamiltonian. The theory can be constructed without major modifications.

Consider a system with Hamiltonian $H = H_0(t) + H_{\text{dis}}(\boldsymbol{\eta}) + H_{\text{int}}(U)$, where $H_0(t)$ and $H_{\text{int}}(U)$ describe the one-particle and the interaction part as before, while

$$H_{\text{dis}}(\boldsymbol{\eta}) = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \eta_{\alpha\beta\delta\gamma} c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \qquad (A1)$$

is an interaction term with random parameters $\boldsymbol{\eta}$ distributed according to some $P(\boldsymbol{\eta})$. The definition of the free Green's function [Eq. (11)], the interacting Green's function [Eq. (13)], and the averaged Green's function [Eq. (16)] is for-

mally unchanged. The self-energies are defined as

$$\boldsymbol{\Sigma}_{t,\boldsymbol{\eta},U} = \boldsymbol{G}_{t,0,0}^{-1} - \boldsymbol{G}_{t,\boldsymbol{\eta},U}^{-1}, \quad \boldsymbol{S}_{t,P,U} = \boldsymbol{G}_{t,0,0}^{-1} - \boldsymbol{\Gamma}_{t,P,U}^{-1}. \quad (A2)$$

The reasoning in Sec. III is unchanged. The functionals $\hat{A}_{U,\boldsymbol{\eta},\xi\xi^*}[\boldsymbol{G}_0^{-1}]$, $\hat{\Omega}_{U,\boldsymbol{\eta}}[\boldsymbol{G}_0^{-1}]$, $\hat{\mathcal{G}}_{U,\boldsymbol{\eta}}[\boldsymbol{G}_0^{-1}]$, $\hat{\mathbf{G}}_{U,\boldsymbol{\eta}}[\boldsymbol{\Sigma}]$, and $\hat{F}_{U,\boldsymbol{\eta}}[\boldsymbol{\Sigma}]$, however, additionally depend on the parameter $\boldsymbol{\eta}$. The same holds for Sec. VI except for Eq. (47), which has to be replaced by

$$\left\langle \frac{1}{\boldsymbol{\Gamma}^{-1} + \boldsymbol{S} - \boldsymbol{\Sigma}_{\boldsymbol{\eta}}} \right\rangle_P = \boldsymbol{\Gamma}. \qquad (A3)$$

The final self-energy functional thus reads

$$\hat{\Omega}_{t,P,U}[\boldsymbol{S}, \boldsymbol{\Sigma}_{\boldsymbol{\eta}}] = \text{Tr} \ln \frac{1}{\boldsymbol{G}_{t,0,0}^{-1} - \boldsymbol{S}} - \text{Tr} \ln \hat{\boldsymbol{\Gamma}}_P[\boldsymbol{S}, \boldsymbol{\Sigma}_{\boldsymbol{\eta}}]$$
$$+ \left\langle \text{Tr} \ln \frac{1}{\hat{\boldsymbol{\Gamma}}_P[\boldsymbol{S}, \boldsymbol{\Sigma}_{\boldsymbol{\eta}}]^{-1} + \boldsymbol{S} - \boldsymbol{\Sigma}_{\boldsymbol{\eta}}} \right\rangle_P$$
$$+ \langle \hat{F}_{U,\boldsymbol{\eta}}[\boldsymbol{\Sigma}_{\boldsymbol{\eta}}] \rangle_P. \qquad (A4)$$

Approximations are constructed in the same way as described in Sec. VII by making contact with a reference system with the same interaction and disorder.

APPENDIX B: THERMODYNAMICAL CONSISTENCY

Here, we briefly discuss the thermodynamical consistency of approximations within the SFT generalized to disordered systems. To be definite, we concentrate on the particle number as an example. The reasoning closely follows Ref. 61.

There are two ways by which the configurational average of the quantum-statistical expectation value of the particle number

$$N_{t,P,U} = \int d\boldsymbol{\eta}\, P(\boldsymbol{\eta}) N_{t,\boldsymbol{\eta},U} = \int d\boldsymbol{\eta}\, P(\boldsymbol{\eta}) \text{tr}(\rho_{t,\boldsymbol{\eta},U} N) \quad (B1)$$

can be obtained: (i) $N_{t,P,U}$ is calculated on the "zero-particle level" as the μ derivative of the averaged grand potential

$$N_{t,P,U} = -\frac{\partial \Omega_{t,P,U}}{\partial \mu}, \qquad (B2)$$

or (ii) $N_{t,P,U}$ is calculated on the "one-particle level" by frequency integration of the one-particle averaged retarded Green's function:

$$N_{t,P,U} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega\, f(\omega) \text{Im Tr}\, \Gamma_{t,P,U}(\omega + i0^+), \quad (B3)$$

where $f(\omega) = 1/(e^{\omega/T} + 1)$ is the Fermi function. Thermodynamical consistency means that both ways must yield the same result. This is not clear *a priori* as within the SFT $\Omega_{t,P,U}$ and $\Gamma_{t,P,U}$ are approximate quantities.

As in Ref. 61, however, it can be argued that there is a twofold μ dependence of $\Omega_{t,P,U}$: an *explicit* μ dependence which in Eq. (60) is due to the free Green's function $G_{t,0,0}^{-1} = \omega + \mu - t$ and an *implicit* μ dependence due to the μ dependence of the disorder self-energy at the stationary point.

Now, if and only if an overall shift ε' of the on-site energies in the reference system is treated as a variational parameter, the derivative with respect to the implicit μ dependence vanishes, and one is left with the explicit one:

$$N_{t,P,U} = -\frac{\partial \Omega_{t,P,U}}{\partial \mu} = -\frac{\partial \Omega_{t,P,U}}{\partial \mu_{\mathrm{expl.}}} =$$
$$-\frac{\partial}{\partial \mu_{\mathrm{expl.}}} \operatorname{Tr} \ln \frac{1}{\omega + \mu_{\mathrm{expl.}} - t - S_{t',P,U}} \quad \text{(B4)}$$

according to Eq. (60). Carrying out the differentiation and using $\Gamma_{t,P,U} = (G_{t,0,0}^{-1} - S_{t',P,U})^{-1}$, one immediately arrives at Eq. (B3), which proves the equivalence with Eq. (B2).

Typically, only a distinguished set of parameters are treated as variational parameters in a practical calculation. The argument shows the necessity to include ε' in the set of variational parameters if thermodynamical consistency is required for the particle number. The argument straightforwardly generalizes to all one-particle operators coupling linearly with a parameter λ' to the reference-system Hamiltonian.

APPENDIX C: CAUSALITY

The causality of all (approximate) dynamical quantities (configuration-dependent as well as averaged Green's functions and configuration-dependent and or independent self-energies) is inevitable for having well-defined self-energy functionals and expressions involving $\operatorname{Tr} \ln(\cdots)$, in particular. A frequency-dependent quantity is termed to be causal if it is analytical in the entire complex ω plane except for first-order poles on the real axis with positive residues. Equivalently, we can demand that after retardation $\omega \to \omega + i0^+$ (ω real), the imaginary part be negative definite.

Causality is easily verified, for example, for all quantities which appear in the self-energy functional Eq. (51) when

evaluated on its domain (see Sec. VIII). The last three terms on the rhs only involve exact and therewith causal quantities as arguments of $\operatorname{Tr} \ln(\cdots)$ (as these are taken from the reference system). Note that the configuration average of a configuration-dependent exact quantity is causal

Let $G(\omega)$ be the exact Green's function of a model H. We have the Lehmann representation[10] $G(\omega) = Q g(\omega) Q^\dagger$ with ω-independent matrices Q (Q not quadratic, see Ref. 93) and a diagonal matrix $g(\omega)$ with elements $g_{nn}(\omega) = 1/(\omega - \omega_n)$, where ω_n are the poles of G. Consider $\Gamma(\omega) = \langle G(\omega) \rangle$ averaged over only two configurations, for simplicity, i.e., consider $\Gamma(\omega) = p_1 Q_1 g_1(\omega) Q_1^\dagger + p_2 Q_2 g_2(\omega) Q_2^\dagger$ with $p_1, p_2 \geqslant 0, p_1 + p_2 = 1$. With $Q \equiv (\sqrt{p_1} Q_1, \sqrt{p_2} Q_2)$ and

$$\gamma(\omega) \equiv \begin{pmatrix} g_1(\omega) & 0 \\ 0 & g_2(\omega) \end{pmatrix}$$

we then immediately have the representation $\Gamma(\omega) = Q \gamma(\omega) Q^\dagger$ from which the causality of $\Gamma(\omega)$ is easily verified.

The only possible source of causality violation is left for the first term on the rhs of Eq. (51). However, it is easily shown that (i) a causal $\Gamma'(\omega)$ (the exact averaged Green's function of the reference system) implies a causal $S(\omega)$. The main point is that the retarded quantity $S(\omega + i0^+) = \omega + \mu - t' - \Gamma'(\omega + i0^+)^{-1}$ has a negative definite imaginary part since the imaginary part of $\Gamma'(\omega + i0^+)^{-1}$ is positive definite according to a lemma given in Ref. 27. Furthermore, (ii) it can be shown that the causality of $S(\omega)$ implies the causality of $\Gamma(\omega) \equiv [G_0(\omega)^{-1} - S(\omega)]^{-1}$ for *arbitrary* $G_0 = (\omega + \mu - t)^{-1}$. Namely, with $S(\omega) = G_0'(\omega)^{-1} - \Gamma'(\omega)^{-1}$ and $\Gamma'(\omega) = Q' \gamma'(\omega) Q'^\dagger$, we have the representation $\Gamma(\omega) = 1/\{[Q' \gamma'(\omega) Q'^\dagger]^{-1} - (t - t')\}$ and thus (see Ref. 93) $\Gamma(\omega) = Q'[\gamma'(\omega)^{-1} - Q'^\dagger(t - t')Q']^{-1} Q'^\dagger$ from which it is obvious that $\Gamma(\omega)$ is analytical with the exception of first-order real poles with positive residues.

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