I. INTRODUCTION

Effective functionals, such as the Landau-Ginzburg free energy functional in the vicinity of phase transitions, have long been used to study classical and quantum systems. Typically, the effective functional $F[h]$ is obtained in terms of a relevant variable $h$, such as the order parameter in the Landau-Ginzburg theory, or the electron density in the density functional theory. The optimal value of $h$ is then obtained from the requirement that the functional be stationary at the solution, $\delta F/\delta h = 0$.

In the formalism of Luttinger Ward and Baym-Kadanoff, one of the best known functional approaches for correlated electrons, a functional $\Omega[G]$ is stationary and equal to the grand potential at the exact physical value of $G$. In such a scheme, the functional dependence $\Omega[G]$ is not known exactly. It can be approximated perturbatively by summing a subset of the infinite series of skeleton diagrams that define the Luttinger-Ward functional. To obtain non-perturbative results on the other hand, one of the most effective methods is the Dynamical Mean-Field Theory (DMFT). Chitra and Kotliar have shown how this theory can be obtained by modifying the Kadanoff-Baym functional and making the local approximation on the stationarity condition. More recently, a general scheme for generating a wide class of non-perturbative approximations for the Hubbard model from a functional has been proposed by Potthoff. In this method, known as the self-energy-functional approach (SFA), a new functional $\Omega[\Sigma]$ of the self-energy $\Sigma$ is constructed, which is stationary at the physical solution. The functional itself is unknown explicitly, but Potthoff suggested a particular way of calculating a variational solution $\delta \Omega/\delta \Sigma = 0$ with the help of a reference system, typically a cluster of finite size, which can be solved exactly. This particular implementation of the self-energy functional with no bath (contrary to DMFT) goes under the name of the variational cluster approximation (VCA). DMFT and generalizations thereof, (such as Cellular Dynamical Mean-Field Theory (CDMFT)) can be obtained as various special cases of SFA corresponding to different choices of reference systems and/or approximations of the stationarity condition. (The functionals of Chitra and Kotliar and of Potthoff are in fact identical, as shown in Appendix C).

One desirable feature of functional approaches is the variational principle that guarantees that an approximate grand potential is an upper bound to the true grand potential. Such a variational principle is missing for the stationary solutions of both the Baym-Kadanoff functional and Potthoff’s self-energy functional since stationary solutions are known to be saddle points rather than extrema.

A question thus remains open up to present, whether or not it is possible to construct a functional, be it a functional of the Green function $G$ or of the self-energy $\Sigma$, such that its stationary solutions would always be extrema (say, minima) of the functional. If so, this would mean that the functional is convex at the physical solution, which is a first necessary step on the way to prove the variational principle. For an infinite-coordination Bethe lattice, this question was answered positively by Kotliar, who proved that a functional could be constructed, such that its extrema occurred at the physical local Green function of the Hubbard model. However an attempt by Chitra to find its analogue for a finite-dimensional lattice was only partially successful.

Another motivation to find convex functionals is a practical one. In VCA, the functional is definitely not convex for example when the intra-cluster chemical potential is varied. The physical solutions are then sad-
dle points. However, most efficient numerical algorithms such as e.g. the conjugate gradient method, have been designed to find extrema of a functional rather than saddle points. Although one may attempt to use such algorithms to also find saddle points (by minimizing the magnitude square of the gradients of the functional), the unphysical solutions may occur.

In this paper we reexamine the above problem and show that a convex functional can be found. In particular, we construct a new functional of the self-energy $\Omega[\Sigma]$, such that its stationary solutions are minima when the irreducible particle-hole vertex depends only on center of mass coordinates and the system is away from phase transitions in the corresponding channel. Going beyond this approximation involves complicated integrals that cannot be treated analytically, however numerical tests on a tractable version of the functional suggest that it is indeed always convex at the physical solution. Moreover, we show that such a construction is not unique and that several functionals can be constructed that differ in the higher-order terms of the expansion with respect to the self-energy.

Despite the convexity of the proposed functional, its implementation requires additional approximations and it turns out to be inadequate to detect a second-order phase transition for both Cooper pairing and antiferromagnetic instabilities. There, the new functional appears to always be convex at the paramagnetic solution, whereas in the case of second-order phase transitions, the paramagnetic solution is rightly expected to be a saddle point, with minima developing instead at a finite value of the symmetry-breaking order parameter. In other words, the sought convexity of the functional ‘overdoes’ its job, imposing too stringent conditions on the resulting physical solution.

Given that the VCA method has originally been developed to study broken symmetry phases, the aforementioned feature of the proposed new functional is especially undesirable. To cure this drawback, we propose a different, this time phenomenological, approach that ensures convexity at the physical solution and, moreover, respects the tendency of the system to develop an instability towards a broken symmetry phase. This finding opens up new perspectives in the use of the convexity property of the functional, in particular permitting to apply powerful numerical techniques, such as the conjugate gradient method, which are only guaranteed to work if the solution is known to be an extremum (and not a saddle point) of the functional.

The paper is organized as follows. First, in Section II we review the variational cluster approximation (VCA) as proposed by Potthoff, followed by a general discussion of the stability of the stationary solution and criteria for convexity in Section III. We then proceed to derive a new functional of self-energy in Section IV with the proof of its convexity given in Appendix A and the recipe for incorporating it into the VCA framework in Appendix B. The second part of Section IV is devoted to numerical tests of the proposed functional on a two-dimensional Hubbard model, which show that the functional is convex but that it fails to correctly describe second-order phase transitions into a broken symmetry phase. Triggered by this negative result, we propose in Section V an answer to the convexity problem while correcting the aforementioned failure to describe second-order phase transitions. The adequacy of this new construction is corroborated by numerical tests. More technical aspects of the work are detailed in appendices.

II. REVIEW OF THE CONVENTIONAL VCA SCHEME

Consider, following Potthoff, a general Hamiltonian $H = H_0(t) + H_I(U)$ with one-particle hopping parameters $t$ and two-particle interaction parameters $U$:

$$H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{ijkl} U_{ijkl} c_{i\sigma}^\dagger c_{k\sigma}^\dagger c_{j\sigma} c_{l\sigma}. \quad (1)$$

Here $i, j, k, l$ refer to an orthonormal and complete set of one-particle basis states. The equilibrium thermodynamics and elementary one-particle excitations of the system for temperature $T$ and chemical potential $\mu$ are fully described by the one-particle Matsubara Green function defined by the imaginary-time ordered product

$$G_\sigma(r_1, \tau_1; r_2, \tau_2) = -\langle T[G_\sigma(r_1, \tau_1)c_{\sigma}^\dagger(r_2, \tau_2)] \rangle, \quad (2)$$

where the symbol $\langle \ldots \rangle$ denotes thermal average and $G_\sigma(1, 2) \equiv G_\sigma(r_1, \tau_1; r_2, \tau_2)$ can be seen as $\langle r_1, \tau_1 | G_\sigma | r_2, \tau_2 \rangle$ or $G_{12}$, a matrix of two indices, each of which stands for both space and imaginary time.

We start by defining the Luttinger-Ward functional $\Phi[G]$, constructed formally as a sum of all closed, irreducible skeleton diagrams involving fully renormalized (“dressed”) Green functions, as illustrated in Fig. 1. We note that this functional is universal, that is, it does not depend on the kinetic part of the Hamiltonian $H_0(t)$, but only on the vertices $U$ and the Green function itself.

The important property of the Luttinger-Ward functional is that its functional derivative gives the self-energy of the system:

$$\frac{\delta \Phi[G]}{\delta G_\sigma(1, 2)} = \Sigma_\sigma(2, 1) = \Sigma_\sigma[G]. \quad (3)$$

![FIG. 1: (Color online) Luttinger-Ward functional $\Phi[G]$ constructed as a sum of renormalised skeleton diagrams with appropriate combinatorial coefficients (not shown). The Hartree approximation consists in considering the first two diagrams only of the series.](image-url)
This equation serves as a definition of the self-energy as a functional of \( G \). We can now introduce the grand potential of the system as the Baym-Kadanoff functional, defined in terms of the fully dressed Green function as follows:

\[
\Omega_{BK}[G] = \Phi[G] - \text{Tr} \left( \left(G_0^{-1} - G^{-1}\right) G \right) + \text{Tr} \ln(G).
\]

Inverting Eq. (3) (locally) to obtain the Green function as a functional of \( \Sigma \), we can now express the Luttinger-Ward functional as a functional of self-energy \( \Phi[G(\Sigma)] \). Substituting this into the expression for the Baym–Kadanoff functional and using Dyson’s equation \( G^{-1} = G_0^{-1} - \Sigma \), Potthoff proposed the following functional of the self-energy

\[
\Omega[\Sigma] = \Phi[G(\Sigma)] - \text{Tr} (\Sigma G) - \text{Tr} \ln(G_0^{-1} - \Sigma).
\]

Recognizing that the first two terms on the right hand side of the Potthoff functional represent the Legendre transform of the Luttinger-Ward functional

\[
F[\Sigma] = \Phi[G(\Sigma)] - \text{Tr} (\Sigma G),
\]

one can now rewrite the expression for the grand potential as follows:

\[
\Omega[\Sigma] = F[\Sigma] - \text{Tr} \ln(G_0^{-1} - \Sigma).
\]

Using Eqs. (3) and (4), it is easy to show that the following equation holds:

\[
\frac{\delta F[\Sigma]}{\delta \Sigma_x(1,2)} = -G_{\sigma}(2,1) = -G_{21}[\Sigma].
\]

It can be viewed as the definition of the Green function in terms of the self-energy \( \Sigma \). Using this, we immediately arrive at the conclusion that the variational derivative of the grand potential in Eq. (4) vanishes at the true physical solution:

\[
\frac{\delta \Omega[\Sigma]}{\delta \Sigma} \bigg|_{sol} = -G + (G_0^{-1} - \Sigma)^{-1} \bigg|_{sol} = 0 \tag{9}
\]

by virtue of the Dyson equation. At the physical solution, \( \Omega[\Sigma] = \Omega[G] \) is equal to the true grand potential. Therefore solving the problem amounts to finding such a function \( \Sigma \) that satisfies the above stationarity condition.

Since the Luttinger-Ward functional \( \Phi[G] \) is a universal functional of the interaction \( U \) and of the stationary value of \( G \), its Legendre transform \( F[\Sigma] \) is a universal functional of \( U \) and \( \Sigma \). In other words the value of this functional should not depend on one-body operators such as the hopping matrix \( t \). This fact is the crucial point that allows one to define VCA.

One proceeds as follows. In the case of the Hubbard model where the interaction is local, one can modify the hopping matrix elements to subdivide the infinite cluster into disjoint identical clusters. One can then compute the grand potential \( \Omega' \) and the self-energy \( \Sigma' \) of that problem exactly (for example by means of exact diagonalization). The one-body part of the cluster Hamiltonian can contain a different hopping matrix, along with site energies, chemical potential and Weiss fields, all of which are used as variational parameters. Since one can write the grand potential for the cluster problem as

\[
\Omega'[\Sigma'] = F'[\Sigma'] - \text{Tr} \ln \left( G_0'^{-1} - \Sigma' \right),
\]

the universality of the functional \( F[\Sigma] \) allows one to find its exact value for the solution of the cluster problem:

\[
F[\Sigma'] \equiv F'[\Sigma'] = \Omega' + \text{Tr} \ln \left( G_0'^{-1} - \Sigma' \right).
\]

Using this last result, the functional \( \Omega[\Sigma] \) in Eq. (7) can be evaluated exactly when \( \Sigma \to \Sigma' \):

\[
\Omega[\Sigma'] = (F'[\Sigma'] + \text{Tr} \ln(G_0^{-1} - \Sigma')) - \text{Tr} \ln(G_0^{-1} - \Sigma').
\]

Since they are the solutions of the cluster problems, the self-energies \( \Sigma' \) can be varied through the one-body terms of the clusters (which we define to also contain Weiss fields for various order parameters). These are collectively represented by the matrix \( t_{ij} \). Clearly, the self-energies obtained in this way will span only a small subspace of an infinite-dimensional space of all possible variations, namely only those that can be represented as the physical self-energies of a cluster \( \Sigma'(t') \) parametrized by the matrix \( t_{ij}' \). The corresponding stationary solution is obtained by searching for values of \( t_{ij}' \) such that

\[
\frac{d\Omega}{dt_{ij}'} = \frac{\delta \Omega}{\delta \Sigma} \cdot \frac{d\Sigma}{dt_{ij}'} = 0. \tag{13}
\]

The set of equations (12)–(13) forms the essence of the VCA quantum cluster method.

### III. STABILITY OF THE STATIONARY SOLUTION

Let us consider fluctuations around the stationary solution of an arbitrary self-energy functional:

\[
\delta \Omega = \Omega[\Sigma + \delta \Sigma] - \Omega[\Sigma] = \iint \frac{\delta^2 \Omega}{\delta \Sigma_\sigma(1',1) \delta \Sigma_\sigma'(2',2)} \delta \Sigma_\sigma(1') \delta \Sigma_\sigma'(2'). \tag{14}
\]

The spin indices have been written explicitly and must be summed over. From now on, we will not write them explicitly to have a lighter notation.

For a stationary point to be numerically stable, it must be a minimum. A maximum will also do since it suffices to change the sign. Correspondingly, the functional derivative in Eq. (14) must be negative or positive-definite, respectively. It is easy to verify that for Potthoff’s self-energy functional, Eq. (4), the second functional derivative is given by

\[
\frac{\delta^2 \Omega}{\delta \Sigma_{11} \delta \Sigma_{22'}} = \Gamma_{11';22'} + G_{12'} G_{21}, \tag{15}
\]
where $\Gamma_{11':22'}$ stands for the second functional derivative of the universal functional $F[\Sigma]$:
\[
\Gamma_{11':22'} \equiv \frac{\delta^2 F}{\delta \Sigma_{11'} \delta \Sigma_{22'}}
\]  
and is thus a tensor of the fourth rank.

It follows directly from the expression for the second functional derivative Eq. (16) that the stationary solution is a saddle point. Following the arguments of Ref. 5, this is simplest to illustrate in the absence of two-body interactions in the Hamiltonian, when $\Sigma = 0$ and $F[\Sigma] = 0$. Then the first term in Eq. (17) vanishes while in Matsubara-Fourier space the last term leads to
\[
\frac{\delta^2 \Omega}{\delta \Sigma^2} = G \left( k'_1 \right) G \left( k'_2 \right) \delta \left( k'_1 - k_2 \right) \delta \left( k'_2 - k_1 \right).
\]  
In the sector of zero total momentum and total energy ($k'_1 = -k'_2$), this quantity decouples in $2 \times 2$ blocks with zero diagonal elements and equal off-diagonal components equal to $(\omega_n^2 + \epsilon_{k_1}^2)^{-1}$. The eigenvalues are thus both positive and negative, which corresponds to a saddle point. The effect of interactions, $\Gamma_{11':22'}$, cannot cure this problem for all wave vectors and frequencies.

In the case of VCA, the relevant question concerns stability with respect to variations in the cluster parameters. It has been pointed out empirically in the original VCA proposal, that variations with respect to site energies or chemical potentials lead to saddle points. This is illustrated in Fig. 2 where the grand potential obtained from a $2 \times 2$ cluster solution is plotted as a function of the intra-cluster nearest-neighbor hopping $t'$ (Fig. 2a) and of the cluster chemical potential $\mu'$ (Fig. 2b). Clearly, the stationary solution is a minimum in the former case and a maximum in the latter. Yet, varying the cluster chemical potential $\mu'$ has been shown essential in the VCA scheme for obtaining thermodynamic consistency, which requires that the number $\langle n \rangle$ of electrons in the system has the same value when calculated from the two independent relations:
\[
\langle n \rangle = -\frac{\partial \Omega}{\partial \mu} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \ f(\omega) \ \text{Im} \ \left[ \text{Tr} G(\omega + i0^+) \right],
\]  
where $f(\omega) = [\exp(\omega/T) + 1]^{-1}$ is the Fermi function. Therefore, it is preferable to let $\mu'$ vary and somehow deal with the fact that the grand potential is known to be non-convex in this case.

The fact that the solution is a saddle point rather than an extremum has consequences for practical implementations, since there seem to exist no robust numerical search algorithms for a saddle point, whereas many such algorithms have been developed for extremal searches. It would therefore be desirable from this point of view, as well as for the reasons outlined in Section I, to find such a functional $\Omega[\Sigma]$ whose stationary solutions would be guaranteed to be extrema. In the next Section, we shall demonstrate that such a functional can indeed be formally constructed, and its convexity can be proved rigorously given certain approximations.

IV. CONVEX FUNCTIONALS $\Omega[\Sigma]$

In this section, we first derive a general expression for a convex functional. The drawback of this approach is that in practical implementations, convexity is preserved for order parameters as well. This makes it an undesirable feature in the presence of phase transitions. In the next section, we will restrict ourselves to preserving convexity as a function of the cluster chemical potential, which in practice is the main problem to be solved.

A. Analytical results for convex functionals

The main idea of the current approach is to add a term $\Delta \Omega[\Sigma]$ to the grand potential that is quadratic in $\Sigma$ and that does not alter the stationary solution of the original potential $\Omega[\Sigma]$, but renders it a positive-definite functional of the self-energy. We first introduce an auxiliary functional $f[\Sigma]$ that is defined by
\[
f[\Sigma] = f(1,2) = \frac{\delta \Omega[\Sigma]}{\delta \Sigma(2,1)} = \frac{\delta^2 \Omega[\Sigma]}{\delta \Sigma^2(2,1)} + \left( G_0^{-1} - \Sigma \right)^{-1} (1,2)
\]  
and that, by virtue of the stationarity condition Eq. (9), vanishes identically at the stationary solution of $\Omega[\Sigma]$.

It turns out that the simplest term $\Delta \Omega[\Sigma]$ that can be added to the grand potential is of the form
\[
\Delta \Omega_1 = -\frac{1}{2} \text{Tr} \left( \left[ (G_0^{-1} - \Sigma) f \right]^2 \right) = -\frac{1}{2} \text{Tr} \left( 1 + (G_0^{-1} - \Sigma) \frac{\delta F}{\delta \Sigma} \right)^2.
\]  

FIG. 2: Functional $\Omega$ for the 2D Hubbard model ($U/t = 8$) calculated from the exact-diagonalization solution of a 2x2 cluster using Eq. (12), plotted as a function of (a) cluster nearest-neighbour hopping parameter $t'$ and (b) cluster chemical potential $\mu'$. The variational solution of the problem in the space of cluster parameters $(t' = 1, \mu' = 4)$ is a saddle point instead of an extremum.
Indeed, $\Delta \Omega_1$ and its functional derivative both vanish at the stationary solutions of the grand potential, as follows from the definition of the functional $f[\Sigma]$ and, therefore, the new functional

$$\Omega_1[\Sigma] = \Omega[\Sigma] + \Delta \Omega_1[\Sigma]$$  \hspace{1cm} (21)

yields the same stationary solution as the original one. The proof of the convexity of this new functional in the special case where the irreducible particle-hole vertex is local is given in the Appendix A.

We note in passing that our choice of $\Delta \Omega[\Sigma]$ is not unique. To second order in the quantity $f[\Sigma]$, the correction $\Delta \Omega_1$ given by Eq. (21) is the same as, for example, the following one

$$\Delta \Omega_2 = \text{Tr} \ln (1 - (G_0^{-1} - \Sigma)f) + \text{Tr} \left((G_0^{-1} - \Sigma)f\right)$$ \hspace{1cm} (22)

$$= \text{Tr} \ln \left((G_0^{-1} - \Sigma) \frac{\delta F}{\delta \Sigma}\right) + \text{Tr} \left(1 + (G_0^{-1} - \Sigma) \frac{\delta F}{\delta \Sigma}\right),$$

meaning that it leaves the stationary point of the original functional unchanged and leads to exactly the same expression for the second functional derivative as Eq. (21). Note also that despite being similar in spirit to the work of Chitra and Kotliar, the above derivation is significantly different, as demonstrated in Appendix B where the connection between the Chitra–Kotliar result and the Potthoff functional is exposed.

While implementing Eqs. (21) (22) in practice, a problem arises since Eq. (19) for the auxiliary functional $f[\Sigma]$ contains a functional derivative $\delta F[\Sigma]/\delta \Sigma$ whose value is not readily available in practical calculations. Therefore, an approximation must be made in order to implement the new functional into the VCA scheme. One such elegant approximation is given in Appendix B and the conclusions of the numerical verification of its convexity is the subject of the following subsection.

### B. Drawback of this type of functionals

While numerical tests show convincingly (see Appendix B for details) that the functionals proposed in Eqs. (19) (21) are indeed convex with respect to all cluster variational parameters, including the cluster chemical potential $\mu'$, there is a major drawback. The numerical tests show one undesirable property, namely its failure to correctly predict second-order phase transitions, at least for the approximation to $f[\Sigma]$ proposed in Appendix B.

Consider Fig. 3a that shows the dependence of $\Omega_1$ and of the new functionals given by Eqs. (19) (22) on the magnitude of the antiferromagnetic Weiss field $M$. Unlike the original functional, which has a minimum at a finite value of $M$, both new functionals have a single minimum at $M = 0$, thereby favouring the paramagnetic (PM) solution. The behavior as a function of the superconducting $d$-wave Weiss field, $D$, follows the same pattern, as shown in Fig. 3b. Only the original functional $\Omega$ exhibits a minimum at non-zero value of $D$, whereas both functionals proposed in this work have no other minima except at $D = 0$. Clearly, such behavior of the new functionals is unphysical since the existence of antiferromagnetism in the Hubbard model, for example around $U = 4$ at half-filling, is solidly established.

As discussed in Appendix A we would have expected that at least in the particle-hole channel, instabilities (such as antiferromagnetism) could have been detected by the present functional. However, we had to approximate $\delta F[\Sigma]/\delta \Sigma$ to do the calculation. In some sense, the requirement of convexity here ‘overdoes’ its job by rendering the paramagnetic solution always a minimum and hence ignoring a possible instability towards a broken-symmetry phase!

### V. CURING THE PROBLEM OF CONVEXITY ARISING FROM A RESTRICTED SET OF VARIABLES

In practical implementations of VCA, the cluster chemical potential leads to a first-order saddle point even in paramagnetic states. There exist several numerical techniques that can deal with this type of problems. In the context of VCA we show a practical way to transform the saddle point coming from variation of the cluster chemical potential $\mu'$ into a minimum while preserving the ‘right’ of the system to develop a second-order phase transition. It seems to work well even in cases where the analytically-obtained approximations given in Eqs. (19) (21) fail.

Let us recall that the general form of the convex correction developed in Section IV was

$$\Delta \Omega \sim \text{Tr} \left(\frac{\delta \Omega}{\delta \Sigma}\right)^2$$ \hspace{1cm} (23)

Typically, we know from experience about the existence of a certain variational parameter $\hbar$ (here, the cluster chemical potential $\mu'$) such that the $\Omega$ lacks convexity

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**FIG. 3:** (Color online) Dependence of the original Potthoff’s functional $\Omega$ (open circles), functional $\Omega_1$ (solid red line) and $\Omega_2$ (broken blue line) on the symmetry-breaking Weiss fields conjugate to (a) antiferromagnetic staggered magnetization, (b) $d$-wave superconductivity. Results are for the Hubbard model ($U/t = 4$). Arrows denote positions of minima of $\Omega$ and maxima of $\Omega_1$. 
at the stationary solution \( h = h_0 \). Let us modify the correction in Eq. (24) as follows:

\[
\Delta \Omega \sim \text{Tr} \left( \frac{\delta \Omega}{\delta \Sigma} \cdot \frac{\partial \Sigma}{\partial h} \right)^2 = \text{Tr} \left( \frac{\partial \Omega}{\partial h} \right)^2,
\]

where we have effectively substituted the unknown functional derivative \( \delta \Omega/\delta \Sigma \) by a much simpler derivative with respect to the variational parameter \( h \), which can be easily calculated numerically.

We thus postulate the following functional

\[
\Omega_{\lambda} = \Omega + \frac{\lambda}{2} \left( \frac{\partial \Omega}{\partial h} \right)^2,
\]

where \( \lambda \) is some empirical coefficient that should be chosen such that the resulting potential \( \Omega_{\lambda} \) is a convex function of \( h \). By construction, the additional term vanishes at the stationary solution \( h = h_0 \) where \( \partial \Omega/\partial h = 0 \), and the value of the new potential coincides with the old one \( \Omega(h_0) \). For the second derivative at \( h_0 \) we have:

\[
\frac{\partial^2 \Omega_{\lambda}}{\partial h^2} \bigg|_{h=h_0} = \frac{\partial^2 \Omega}{\partial h^2} \left( 1 + \lambda \frac{\partial^2 \Omega}{\partial h^2} \right).
\]

If the original functional is already convex, \( \partial^2 \Omega/\partial h^2 > 0 \), the new functional will be convex too. If however \( \Omega \) has a maximum and not a minimum at \( h_0 \), the coefficient \( \lambda \) has to satisfy the following inequality to ensure that the new functional is convex:

\[
\lambda > \lambda_0(h) \equiv \left| \frac{\partial^2 \Omega}{\partial h^2} \right|^{-1}.
\]

In particular, note that choosing \( \lambda = 2 \lambda_0(h) \) will result in the new functional being convex everywhere and having the same absolute value of curvature as the original one: \( \partial^2 \Omega_{\lambda}/\partial h^2 = -\partial^2 \Omega/\partial h^2 \). Chosen in such a way, the behavior of the newly constructed functional \( \Omega_{\lambda} \) as a function of the cluster chemical potential \( h \equiv \mu' \) is plotted in Fig. 4.

As we see, \( \Omega_{\lambda} \) can clearly be made convex with a suitable choice of the coefficient \( \lambda \). The lowest allowed value \( \lambda_0 \) that yields a convex functional is itself a function of parameters of the model, such as Hubbard \( U \), as is clear from comparison of Fig. 4(a) and b). In particular, we find \( \lambda_0 = 5.8 \) for \( U = 4t \) and \( \lambda_0 = 9.9 \) for \( U = 8t \).

Note that by taking derivatives with respect to cluster parameters in Eq. (24) instead of the more general Eq. (26), we have substituted a strong requirement of convexity with respect to all variations in \( \Sigma \) with a much weaker one, which only requires that the functional be convex with respect to a particular parameter (or set of parameters) \( h \). Let us then see what effect this has on the dependence of \( \Omega_{\lambda} \) on a symmetry-breaking parameter, such as the superconducting Weiss field \( D \). The first derivative with respect to \( D \) reads:

\[
\frac{\partial \Omega_{\lambda}}{\partial D} = \frac{\partial \Omega}{\partial D} + \lambda \frac{\partial^2 \Omega}{\partial h \partial D} \frac{\partial \Omega}{\partial h}.
\]

All the stationary points of \( \Omega \) (where derivatives with respect to both \( \mu' \) and \( D \) vanish) are also stationary points of the new functional \( \Omega_{\lambda} \). That functional can also have additional stationary points that are not stationary points of \( \Omega \), but with the procedure suggested below to choose \( \lambda \), we found this not to be an issue.

In numerical calculations, we searched for minima of \( \Omega_{\lambda} \) and found that, indeed, one recovers as minima the same solutions (\( \mu'_0, D_0 \)) that were saddle points of \( \Omega \). To illustrate how one can choose \( \lambda \) in practice, we consider several cases. First, in Fig. 5a, \( \mu' \) is fixed at the known superconducting solution \( \mu'_0 \) and \( \lambda \) is taken either as constant or defined by the procedure in Eq. (27) that guarantees convexity. All curves have their minimum at the same value \( D = D_0 \) as expected. To gain more insight into the convergence process, we can also check whether the solution for \( D \) is stable in cases where the value of the cluster chemical potential \( \mu' \) is slightly off the true solution \( \mu'_0 \). Such a situation is illustrated in Fig. 5b, where the chemical potential \( \mu' \) is fixed at the PM value \( \mu'_\text{PM} = 2.45 \) instead of the true SC solution \( \mu'_0 = 2.28 \).

As expected from Eq. (26), both the old and the new functionals coincide at the paramagnetic solution \( D = 0 \) since by construction, \( \partial \Omega/\partial \mu' = 0 \) there. The situation is different however away from \( D = 0 \). Fixing \( \lambda = \text{const} \) (solid line in Fig. 5a) yields a minimum at an incorrect value of \( D = 0.84 \) instead of \( D_0 = 0.56 \). By contrast, a variable coefficient \( \lambda = 2 \lambda_0(\mu') \), where \( \lambda_0 \) is determined at each point from Eq. (27), gives a minimum of \( \Omega_{\lambda}(D) \) (dashed line in Fig. 5b) that is already very close to the true solution. Varying \( \mu' \) as well eventually leads to the correct solution in all cases, as mentioned above. An empirical case-by-case analysis has shown that the choice \( \lambda = 2 \lambda_0(\mu') \) gives consistently reliable results and is preferred over fixing \( \lambda \) to a constant value. Besides, such a choice avoids the ambiguity in the value of \( \lambda \) and ensures that the functional \( \Omega_{\lambda}(\mu') \) is always a convex one, according to the inequality in Eq. (27).

The knowledge of the derivatives \( \partial \Omega/\partial h \) and \( \partial^2 \Omega/\partial h^2 \) is required in order to implement the convex correction (26) with \( \lambda = 2 \lambda_0(h) \). Numerically, this requires
FIG. 5: (Color online) Dependence on the symmetry-breaking superconducting Weiss field $D$ of Potthoff’s grand potential (black dots), and of the functional in Eq. (25) constructed for two choices of the coefficient $\lambda$: the constant $\lambda = 15$ (solid red curve) and the variable $\lambda = 2\lambda_0(\mu')$ (dashed blue curve). The calculations are for the electron-doped Hubbard model (2.2% doping) with $U = 4t$ and the next-nearest neighbour hopping $t' = 0.3t$. The cluster chemical potential $\mu'$ was fixed at the value corresponding to (a) the true SC solution, $D = 0.56$, and (b) the PM solution, $D = 0$.

VI. CONCLUSIONS

It is known that physical solutions obtained with VCA are in general saddle points rather than extrema of the functional $\Omega[\Sigma]$. This is so in particular in the important practical case where the cluster chemical potential is varied. Saddle points are notoriously more difficult to find numerically than extrema. We have thus constructed a new functional that we proved to be a convex functional of the self-energy at the stationary solution, at least in the case where the irreducible particle-hole vertex depends only on the centre of mass coordinates (Appendix A). It turns out, however, that implementing the proposed functional in practice is far from simple, since it involves, as can be seen in Eq. (25), an unknown functional derivative $\delta F/\delta \Sigma$ of the Legendre transform $F[\Sigma]$ of the Luttinger-Ward functional. An approximation therefore had to be made to express this functional derivative in terms of cluster-defined quantities, as detailed in Appendix B. The corresponding numerical results in Sec. IV B show that the new functional is indeed convex even in the general non-perturbative case. However attractive this may be, the proposed functional changes qualitatively the behavior of $\Omega$ with respect to symmetry-breaking order parameters, such as magnetism or superconductivity, rendering instead the paramagnetic solution stable.

To cure this problem we proposed a functional Eq. (25) and a (non-unique) recipe to find the coefficient $\lambda$ that guaranties convexity with respect to cluster chemical potential $\mu'$ only. This approach removes the saddle point normally associated with $\mu'$, has the same physical solutions as the original problem and leaves unchanged the minimum or maximum character of the functional with respect to variations of symmetry-breaking order parameters, such as magnetism or superconductivity. Despite the non-uniqueness of the proposed convex functional and the admittedly phenomenological basis of its derivation, we argue that this is an important result. In particular, our findings open a way to the use of powerful numerical algorithms for solving for minima, such as e.g. conjugate gradients, that only work provided the functional is convex at the physical solution. We consider the use of such efficient algorithms as highly desirable for the VCA approach. The question of the existence of a functional that would give a bound for the true grand potential and thereby implement the variational principle, is left open.

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APPENDIX A: CONVEXITY OF THE ANALYTICAL FUNCTIONAL

We aim to prove the convexity of the new proposed functional $\Omega_i[\Sigma]$ given by either of Eqs. (25) ($i = 1$) or $\Omega_i[\Sigma]$ ($i = 2$). At the true solution where $\delta \Omega_i/\delta \Sigma = f[\Sigma] = 0$, the knowledge of the functional $\Omega$ at three points. For this reason, the computational cost of evaluating $\Omega$ at a given point in parameter space is three times that of the original functional $\Omega$. However, the minima of the proposed functional may now be searched more efficiently using powerful numerical methods designed for extrema search, such as the conjugate gradient method. 

It is known that physical solutions obtained with VCA are in general saddle points rather than extrema of the functional $\Omega[\Sigma]$. This is so in particular in the important practical case where the cluster chemical potential
for the indices not explicitly written. We then use the definition
\[
\frac{\delta^2 \Omega_i}{\delta \Sigma_{11} \delta \Sigma_{22'}} \bigg|_{t=0} = \frac{\delta^2 \Omega}{\delta \Sigma_{11'} \delta \Sigma_{22'}} - \text{Tr} \left[ G^{-1} \frac{\delta f}{\delta \Sigma_{11'}} G^{-1} \frac{\delta f}{\delta \Sigma_{22'}} \right] \tag{A1}
\]
with \(G^{-1} = (G_0^{-1} - \Sigma)\) and matrix multiplication implied for the indices not explicitly written. We then use the

\[
\left( G_0^{-1} - \Sigma \right)_{33'} \cdot \Gamma_{43';11'} \cdot \left( G_0^{-1} - \Sigma \right)_{44'} \cdot \Gamma_{34';22'} = \text{Tr} \left[ G^{-1} \Gamma_{11'}^{T} G^{-1} \Gamma_{22'}^{T} \right]. \tag{A4}
\]

where the transpose applies only to the indices involved in the matrix multiplication.

Irreducible vertices are usually easier to approximate. So it is useful to work with the second functional derivative of the Luttinger-Ward functional \(\Phi[G]\) with respect to the single-particle Green function:

\[
\Gamma_{11';22'}^{\text{ph}} = \frac{\delta^2 \Phi[G]}{\delta G_{11} \delta G_{22'}} = \frac{\delta \Sigma_{11'}}{\delta G_{22'}} \tag{A5}
\]

where we have used the property Eq. [3] of the Luttinger-Ward functional. The superscript in the notation \(\Gamma^{\text{ph}}\) indicates that this symmetric matrix \((\Gamma^{\text{ph}}_{12;34} = \Gamma^{\text{ph}}_{34;12})\)

is the irreducible particle-hole vertex, i.e.:

\[
\Pi^{-1}_{12;34} = \delta_{13} \delta_{24} - G_{22'} \Gamma^{\text{ph}}_{23';34} G_{3'1}, \tag{A6}
\]

where \(\Pi\) is the full (reducible) particle-hole vertex. In the language of Feynman diagrams, the latter can be cast as shown in Fig. 6.

It is required on physical grounds that the reducible particle-hole vertex \(\Pi\) should be positive-definite at zero frequency for stability in the particle-hole channel and hence it follows that its inverse obeys the same property. If there is an instability that affects the particle-hole channel directly or indirectly, it should still be visible in \(\Pi^{-1}\).

Using the identity \(\delta F/\delta \Sigma = -G\) and the definition of \(\Gamma\) given by Eq. (10), we obtain (with summation over repeated indices implied) that

\[
\Gamma_{12;1'2'}^{\text{ph}} = \frac{\delta (G)}{\delta G_{11'}} \frac{\delta \Sigma_{1'2'}}{\delta G_{33}} \tag{A7}
\]

which again has the structure of matrix multiplication if the pairs of indices on either side of the semi-colon are flattened (combined as one). Using this result we obtain

\[
\text{Tr} (G^{-1} \Gamma_{11'}^{T} G^{-1} \Gamma_{22'}^{T}) \text{Tr} (G^{\text{ph}}_{22'} G^{\text{ph}}_{33'}) = \delta_{13} \delta_{1'3'} = I. \tag{A9}
\]

Using this last identity and Eq. (A3) for \(\delta^2 \Omega_i/\delta \Sigma^2\), we find:

\[
- \frac{\delta^2 \Omega_i}{\delta \Sigma_{11'} \delta \Sigma_{22'}} \text{Tr} (G^{\text{ph}}_{22'} G^{\text{ph}}_{33'}) = \delta_{13} \delta_{1'3'} - G_{14} \Gamma^{\text{ph}}_{44';33'} G_{4'1'}. \tag{A10}
\]

As has been pointed out above, the right-hand side of this equation is positive-definite at zero frequency, following from the requirement that the kernel of the particle-hole

![FIG. 6: Bethe-Salpeter equation for the particle-hole vertex \(\Pi\) in the language of Feynman diagrams.](image-url)
Let us now concentrate on $L_{22;33} [G] = \text{Tr}(G_{22}^\text{ph} G_{33}^\text{ph})$ appearing on the left hand side of the last equation (A10). We assume that the irreducible particle-hole vertex is local (like in the Random Phase Approximation), i.e.

$$
- \frac{\delta^2 \Omega}{\delta \Sigma_{11} \delta \Sigma_{22}} G_{6;5} \Gamma_{22;5;5}^\text{ph} G_{5;6} \Gamma_{6;6;33}^\text{ph} = - \frac{\delta^2 \Omega}{\delta \Sigma_{11} \delta \Sigma_{22}} \tilde{\Gamma}_{25}^\text{ph} G_{6;5} G_{5;6} \tilde{\Gamma}_{6;3}^\text{ph}
$$

with this approximation, we can write for the left-hand side of the stability equation (A10):

$$
\Gamma_{11;22}^\text{ph} = \delta_{11} \delta_{22} \Gamma_{12}^\text{ph}
$$

Taking the Fourier-Matsubara transform, we find

$$
\tilde{L}(Q,i\omega_n) = \tilde{\Gamma}^\text{ph}(Q,i\omega_n) \left[ \int \sum_{i\omega_n} G(k,i\omega_n) G(k+Q,i\omega_n+i\omega_n) \right] \tilde{\Gamma}^\text{ph}(Q,i\omega_n)
$$

where the dressed Lindhard function $\chi(Q,i\omega_n)$ (no vertex correction) denotes the value of the integral (defined with the minus sign) in the last equation. Using the spectral representation one can show that $\chi(Q,i\omega_n)$ for a system at equilibrium is always positive for all Matsubara frequencies. Also, $\tilde{\Gamma}^\text{ph}(Q,i\omega_n)$ is real, as follows from its spectral properties, so $\left( \tilde{\Gamma}^\text{ph}(Q,i\omega_n) \right)^2$ is positive. It is thus clear that the quantity $\tilde{L}(Q,i\omega_n)$ must be negative-definite, with possible exception of phase transitions that, in this simple approximation, could appear in the particle-hole channel. Comparing this with the identity given by Eq. (A10):

$$
- \frac{\delta^2 \Omega}{\delta \Sigma \delta \Sigma} \cdot L[G] = 1 - G \tilde{\Gamma}^\text{ph} G,
$$

and remembering that its right hand side is positive-definite, we arrive at the conclusion that, at least in the above approximation for the particle-hole vertex, the object $\delta^2 \Omega/\delta \Sigma^2$ must also be positive-definite at zero frequency. This in turn means that our proposed grand potential $\Omega[\Sigma]$, defined by Eq. (21) and either expressions (20) or (22), is a convex functional of the self-energy within this approximation.

It should be noted that being a convex functional of the self-energy is not necessarily the same as being a convex functional of a given cluster parameter $h'$. Indeed, differentiating again the first derivative $d\Omega/dh'$ given by

$$
- \frac{\delta^2 \Omega}{\delta \Sigma \delta \Sigma} (Q,i\omega_n) \cdot \tilde{L}(Q,i\omega_n) = 1 + \chi(Q,i\omega_n) \tilde{\Gamma}^\text{ph}(Q,i\omega_n)
$$

Eq. (13), one obtains

$$
d^2 \Omega_i \int \frac{d\Sigma(1)}{d\Sigma(2)} \int \frac{d\Sigma(2)}{d\Sigma(1)} \int \frac{d\Sigma(1)}{dh'} \int \frac{d\Sigma(1)}{dh} dh' dh dh' = \int \frac{d\Sigma(1)}{d\Sigma(2)} \int \frac{d\Sigma(2)}{d\Sigma(1)} \int \frac{d\Sigma(1)}{dh'} \int \frac{d\Sigma(1)}{dh} dh' dh dh'.
$$

Note that in the above, we have assumed translational invariance, and hence self-energy can be written as a function of one momentum and frequency variable only. Since the functional derivative in the first term of Eq. (A18) is almost certainly positive-definite at the stationary solution, as suggested above, the first term is guaranteed to be positive too. The situation with the second term is more complicated. Naively, it may seem that this term vanishes since, at the stationary solution, $d\Omega/\delta \Sigma$ is zero by definition. This would be true if the variational space of the cluster parameter $h'$ was sufficient to describe the
complete variational space of the functional \( \Omega[\Sigma(h')] \).
Unfortunately, and this is the main approximation entering the VCA method, this may not always be true. In fact, one may only vary \( \delta\Sigma(h') \) in a subspace that can be parametrized by the cluster parameter \( h' \), which is a small part of the whole infinite-dimensional space of variation \( \delta\Sigma \). Therefore, the solution obtained by requiring that the derivative \( \partial\Omega/\partial h' \) vanishes, is not necessarily the same as the true solution where \( \delta\Omega/\delta\Sigma = 0 \). Although we expect this contribution to be very small, it is difficult to judge the convexity of the given grand potential with respect to some cluster parameter, even if the potential is known to be a convex functional of \( \Sigma \). Since varying \( h' \) is the best one can achieve within the VCA approach we stress that numerical tests are always desirable to verify the convexity of a given functional \( \Omega[\Sigma(h')] \).

**APPENDIX B: IMPLEMENTATION OF THE CONVEX FUNCTIONAL IN VCA**

In Section 11 we proposed a correction \( \Delta\Omega_{1,2} \) to the original grand potential \( \Omega[\Sigma] \), such that it is rendered a convex functional of the self-energy. The issue that we address here is how to implement this correction in the framework of the VCA quantum cluster method.

The key element entering the expressions \(^{20,22}\) for \( \Delta\Omega \) is the auxiliary functional \( f[\Sigma] \) defined by Eq. \(^{19}\) as a functional derivative \( f[\Sigma] \equiv \delta\Omega/\delta\Sigma \). Unfortunately it is not possible to evaluate this functional derivative even numerically since we have no direct way of varying the self-energy \( \Sigma \) (however we develop a variant of this idea further in Section 11). The unknown element in \( f[\Sigma] \) Eq. \(^{19}\) is the functional derivative \( \delta F[\Sigma]/\delta\Sigma \), where \( F[\Sigma] \) is a universal functional of the self-energy, as explained in section \(^{11}\). This functional derivative can be evaluated at the ground state solution of the cluster by virtue of Eq. \(^{1}\):

\[
\frac{\delta F[\Sigma]}{\delta\Sigma} \approx \left. \frac{\delta F[\Sigma']}{\delta\Sigma'} \right|_{\text{sol}} = -G',
\]  

where, as before, we denote the quantities belonging to the cluster by prime. Now, that both terms on the right hand side of Eq. \(^{19}\) are known, we can write:

\[
f[\Sigma] \approx -G' + \frac{1}{G_0^{-1} - \Sigma} \equiv -G' + G.
\]  

We stress that this last equation is approximate. This is because the self-energy \( \Sigma' \) of the cluster solution, at which the derivative in \(^{1}\) is evaluated, is not, generally speaking, equal to the true lattice self-energy. Another way to see this is to note that, by construction, \( f[\Sigma] \) must vanish identically at the true stationary solution of the lattice, whereas it is clear that the right hand side of Eq. \(^{22}\) can only vanish if the two Green functions are equal to each other at the ground state of the cluster tiling. Rigorously speaking, this can only be the case in the limit of infinitely large cluster, where \( G' \to G \).

**FIG. 7:** (Color online) Comparisons of three different functionals for the 2D Hubbard model \((U/t_{lat} = 8)\): the original functional from Eq. \(^{12}\) (black dots), and the two functionals proposed in this work, given respectively by Eq. \(^{13}\) (solid red curve) and Eq. \(^{15}\) (dashed blue curve). The panels show (a) dependence of all three functionals on the nearest-neighbour hopping parameter \( t' \) of the cluster, (b) same for the dependence on the chemical potential \( \mu' \) of the cluster. Comparison between the two functionals proposed in this work as functions of the cluster chemical potential \( \mu' \) for (c) half-filled case, \( \mu_{lat} = 4t \), and (d) away from half-filling, \( \mu_{lat} = 3t \) (corresponds to 0.4% electron doping).

Using this approximation Eq. \(^{22}\), we can now rewrite Eq. \(^{20}\) for \( \Delta\Omega_1 \) as

\[
\Delta\Omega_1[\Sigma] = -\frac{1}{2} \text{Tr} \left[ 1 - (G_0^{-1} - \Sigma)G' \right]^2,
\]  

so that, by virtue of Eq. \(^{12}\), the new convex functional \( \Omega_1 = \Omega + \Delta\Omega_1 \) finally becomes:

\[
\Omega_1[\Sigma] \approx \Omega' - \text{Tr} \ln \left[ (G_0^{-1} - \Sigma)G' \right] - \frac{1}{2} \text{Tr} \left[ 1 - (G_0^{-1} - \Sigma)G' \right]^2.
\]  

Similarly, for the correction \( \Delta\Omega_2 \) expressed by Eq. \(^{22}\), we obtain an alternative expression for the new functional

\[
\Omega_2[\Sigma] \approx \Omega' + \text{Tr} \left[ 1 - (G_0^{-1} - \Sigma)G' \right].
\]  

The proposed functionals Eqs.\(^{13,15}\) have been implemented into the VCA scheme using the Lanczos algorithm of exact diagonalization (ED) to solve the cluster problem. The Hubbard model on a square lattice with nearest neighbor hopping \( t \) has been studied, and a cluster of \( 2 \times 2 \) sites was used in the ED scheme. While the hopping parameter \( t \) and the chemical potential \( \mu \) of the lattice model remain fixed, we have the freedom of varying the corresponding parameters of the cluster \( t' \) and \( \mu' \), whose optimal values should be found by solving the stationarity equation \(^{13}\).
Figure 7 shows the comparison between the original grand potential $\Omega$ (dotted line) and the two potentials derived in Section B, as functions of the variational hopping parameter $t'$. All three functionals appear to have minimum at the same value of $t' = t = 1$ and the proposed new functionals are convex functions of $t'$ near the solution, as is the original grand potential $\Omega$.

The dependence of the grand potential on the cluster chemical potential $\mu'$ is plotted in Fig. 7 for the half-filled case. Functional $\Omega_1$ shown by the solid line, clearly is a convex function near the stationary solution $\mu'_0 = 4t$, unlike the original grand potential $\Omega$ (dotted line) that develops a maximum at this point. The details of the behavior of the new functionals near $\mu'_0$ appear more clearly in the blow up shown in Fig. 7. The functional $\Omega_2$ (dashed line) has vanishing second derivative within machine precision around the stationary solution. The same conclusion equally holds away from half-filling, as illustrated in Fig. 7.

The above illustrations as well as many tests performed for different values of the parameters $U$, $t$ and $\mu$ all show that the proposed functional $\Omega_1$ given by Eq. (11) develops a minimum at the stationary solution with respect to both variational parameters $\mu'$ and $t'$. The functional $\Omega_2$, is less useful for practical calculations since it exhibits a vanishing second derivative with respect to $\mu'$ sufficiently close to half-filling.

Despite these encouraging results, note that the actual values of $\Omega_1$ and $\Omega_2$ at the solution, while being nearly equal, deviate appreciably from the original grand potential $\Omega$. There would be no such deviation if we could have evaluated $f[\\Sigma]$ exactly instead of approximately as we were forced to do.

**APPENDIX C: CONNECTION TO THE CHITRA–KOTLIAR FUNCTIONAL**

The purpose of this Appendix is to identify the connection that exists between Potthoff’s original functional, the new convex functional $\Omega[\\Sigma]$ proposed in this work (Sec. IV), and an earlier attempt to construct a convex functional undertaken by Chitra and Kotliar in Ref. 5. According to the latter study, one can construct an improved version of the Baym-Kadanoff functional $\Omega_{BK}[G]$ given by Eq. (4) as follows:

$$\Omega_{CK}[G] = \Phi[G] - \text{Tr}(G \frac{\delta \Phi}{\delta G}) - \text{Tr}(G_0^{-1} - \frac{\delta \Phi}{\delta G}).$$  \hspace{1cm} (C3)

Using the relation $\frac{\delta \Phi}{\delta G} = \Sigma[G]$, and the Legendre transform of the Luttinger-Ward functional as in Eq. (6)

$$F[\\Sigma] = \Phi[G[\\Sigma]] - \text{Tr} (\\Sigma G),$$  \hspace{1cm} (C4)

$\Omega_{CK}$ in Eq. (C3) becomes

$$\Omega_{CK}[G(\\Sigma)] = F[\\Sigma] - \text{Tr} (G_0^{-1} - \Sigma).$$  \hspace{1cm} (C5)

This last expression is nothing else but Potthoff’s functional $\Omega[\\Sigma]$ as given in Eq. (7). In other words, we see that the Chitra–Kotliar functional $G$, if expressed in terms of the self-energy $\\Sigma$, is equivalent to Potthoff’s $\Omega[\\Sigma]$. Although both groups begin with the Baym-Kadanoff functional to propose their own functional, they use the Dyson equation in apparently different but in fact equivalent ways.

As regards the new functionals of the self-energy introduced in this work (see Section IV), their derivation, despite being similar in spirit to that of Chitra and Kotliar, have required additional ingredients that are contained neither in the Potthoff’s grand potential $\Omega[\\Sigma]$, nor in the Chitra–Kotliar functional.

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