The self-consistent Dyson equation and self-energy functionals: failure or new opportunities?

Walter Tarantino, Pina Romaniello, J. A. Berger, and Lucia Reining

1Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA/DSM and European Theoretical Spectroscopy Facility (ETSF), 91128 Palaiseau, France.
2Laboratoire de Physique Théorique, CNRS, IRSAMC, Université Toulouse III - Paul Sabatier and European Theoretical Spectroscopy Facility (ETSF), 118 Route de Narbonne, F-31062 Toulouse Cedex, France
3Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université Toulouse III - Paul Sabatier, CNRS and European Theoretical Spectroscopy Facility (ETSF), 118 Route de Narbonne, F-31062 Toulouse Cedex, France

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Perturbation theory using self-consistent Green’s functions is one of the most widely used approaches to study many-body effects in condensed matter. On the basis of general considerations and by performing analytical calculations for the specific example of the Hubbard atom, we discuss some key features of this approach. We show that when the domain of the functionals that are used to realize the map between the non-interacting and the interacting Green’s functions is properly defined, there exists a class of self-energy functionals for which the self-consistent Dyson equation has only one solution, which is the physical one. We also show that manipulation of the perturbative expansion of the interacting Green’s function may lead to a wrong self-energy as functional of the interacting Green’s function, at least for some regions of the parameter space. These findings confirm and explain numerical results of Kozik et al. for the widely used skeleton series of Luttinger and Ward [Phys. Rev. Lett. 114, 156402]. Our study shows that it is important to distinguish between the maps between sets of functions and the functionals that realize those maps. We demonstrate that the self-consistent Green’s functions approach itself is not problematic, whereas the functionals that are widely used may have a limited range of validity.

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INTRODUCTION

In quantum many-body theory observables can in principle be calculated as expectation values or weighted sums over expectation values of operators, using many-body wavefunctions. However, a many-body wavefunction for more than a few electrons is a huge object, much too large to be calculated or even stored [1]. Therefore several ways have been developed to avoid the explicit calculation of wavefunctions. One of the strategies is the use of functionals: it relies on the insight that observables can in principle be expressed as functionals of some quantities \( Q \) that are more compact than the full \( N \)-body wavefunction \( \Psi(r_1, ..., r_N) \). The problem is then split in three parts: first, to find the quantity \( Q \) that encodes sufficient information to calculate the wanted observable \( O \), then to work out the functional relation between \( Q \) and \( O, O = F[Q] \), and, finally, to determine the value \( \tilde{Q} \) that a system takes, such that \( \tilde{O} = F[\tilde{Q}] \) can be calculated. The most striking example is density functional theory (DFT), where the charge density \( n(r) \) plays the role of \( Q \). Although \( n \) has much less degrees of freedom than \( \Psi(r_1, ..., r_N) \), the Hohenberg-Kohn theorem guarantees that it encodes all information necessary for calculating any wanted observable. Moreover, the Kohn-Sham approach provides a handy tool to get a sufficiently accurate estimate of \( n(r) \) for any system. However, the explicit expression of almost all observables in terms of \( n(r) \) is unknown. An alternative to \( n(r) \) is the equilibrium one-body Green’s function \( G(r, \sigma, t, \sigma', t') \). Contrary to the density, it is non-local in space, spin and time (or frequency dependent, for its Fourier transform), but it is still much more compact than the many-body wavefunction. Moreover, it has the advantage that all expectation values of one-body operators, as well as the total energy, have a simple, known expression in terms of it.

To determine the value that the one-body Green’s function takes for the system of interest, a common approach is to solve the Dyson equation \( G = G_0 + G_0 \Sigma G \), where \( \Sigma \) is a non-local and frequency-dependent function, called self-energy. Perturbation Theory offers a way to calculate the (formal) perturbative expansion of \( \Sigma \) in the Coulomb interaction \( v \), yielding a series of functionals of \( v \) and the non-interacting Green’s function \( G_0 \): \( \Sigma = vG_0 + vG_0vG_0G_0 + \ldots \). Alternatively, one can consider the self-consistent Dyson equation (SCDE)

\[ \Sigma = vG_0 \]

1 For emphasizing the algebraic structure of the equations, spin indices, space and time coordinates, as well as integrals and summations, and exact numerical coefficients will be omitted henceforth in this section. This will also apply to equations \[16\] and \[28-31\] of later sections.
\[ G = G_0 + G_0 S[G] G, \] with \( S \) the so called ‘self-energy functional’, giving rise to the self-consistent approach \[2\]. Its formal justification can be given in terms of Legendre transformations \[3\], while the reference computable scheme is the one proposed by Luttinger and Ward \[4\], in which the self-energy functional is explicitly built as an infinite sum of Feynman diagrams (sometimes referred to as the ‘skeleton series’) obtained by formal manipulation of the perturbative expansion of the Green’s function.

Due to the unknown properties of the perturbation expansion, the Luttinger-Ward approach has not found solid mathematical foundations yet. In fact, recent numerical tests performed by Kozik and collaborators on various Hubbard models \[5\] showed clear signs of its failure in regimes of strong interactions. Their results were soon connected to earlier numerical evidence of possible pathologies in the diagrammatic approach by Schäfer and collaborators \[6, 7\]. First investigations on an entirely analytical level were carried out by Stan and collaborators \[8\], and Rossi and Werner \[9\], who independently managed to qualitatively reproduce the results of Kozik et al. using two analytically treatable toy models. Those models, however, only bear the algebraic structure of the original quantum mechanical problem and cannot be directly related to a Hamiltonian. It would be then desirable to have a less system-specific view on the general problems of the self-consistent approach on one side, and a complete, analytical treatment of at least one of the particular Hamiltonians used in the work of Kozik et al. on the other side. This is the double goal of our work.

In order to achieve this goal, we first recall and discuss the conditions under which the self-consistent approach can be set in general. This is done in Section I, where we briefly review the current understanding of the foundations of the self-consistent approach and its connection to its practical realization proposed by Luttinger and Ward. We then concentrate in Section II on the Hubbard atom, which is one of the systems studied by Kozik et al. \[5\]. In order to arrive at an analytical treatment, which makes a detailed and unambiguous analysis possible, we introduce functionals that realize the maps between the non-interacting and the interacting Green’s functions on the physical domain of this specific model. It is very important indeed to make a clear distinction between the maps and the functionals that are used to realize the maps. In particular, the numerical results of \[5\] are understood as being due to a limitation of the skeleton series and the connected problem of the definition of the physical domain, whereas it remains still possible to build a valid self-energy functional and use the self-consistent approach.

More in detail, after the discussion in Section I, the presentation of the results and analysis for the Hubbard atom in Section II is organized as follows: after an introduction (II A) we present the Hubbard atom (II B), prove the one-to-one correspondence between the \( G_0 \)’s and \( G \)’s arising in this model (II C), present explicit formulas for the functionals realizing those maps (II D), and use those to solve the SCDE (II E) and the inverse problem of finding \( G_0 \) given \( G \) (II F); then we define the ‘one-frequency–skeleton’ series (II G), which, in analogy to the standard skeleton series, when evaluated at the exact \( G \), converges to the correct self-energy only in a subregion of the entire parameter space; finally, we introduce the ‘one-frequency–SIN’ series (II H), which converges to the correct self-energy wherever the one-frequency–skeleton does not, therefore offering the possibility to maintain the self-consistent approach for any interaction strength. Conclusions will be drawn at the end.

I. THE SELF-CONSISTENT APPROACH

A. Green’s functions and self-energies

While DFT offers a computationally cheap way to get a good estimate of the charge density and several other observables, the lack of a known systematic way to connect the density to any given observable represents a serious limit of the method for those who are interested in other quantities. On the other hand, the Green’s function formalism profits from Perturbation Theory, which gives a systematic, although expensive, way to write any N-body Green’s function, and hence any observable, in terms of the non-interacting one-body Green’s function \( G_0 \) and the interaction, at least at a formal level. For instance, the one-body Green’s function (from now on, simply ‘Green’s function’) is written, in a simplified notation (see footnote 1), as

\[ G = G_0 + G_0 v G_0 G_0 + G_0 v G_0 G_0 v G_0 G_0 + \ldots \] (1)

The above expansion must be regarded as a formal expression, and several problems may occur in practice. In particular, the series may have a finite radius of convergence, and hence not be suitable for strongly interacting regimes; worse yet, it may have zero radius of convergence and be asymptotic at best (see \[10\] and references therein). Furthermore, the fact that we can write \[1\] does not guarantee that also non-perturbative effects can be written in terms of \( G_0 \) only, for more information may be required.

It has been recognized early that at least some of the terms must be summed to infinite order to avoid divergent behavior. In particular, in the homogeneous electron gas one has to sum all so-called bubble diagrams, which express the polarizability of the system \[11\]. Along this line, one widely used way to incorporate at least some of the diagrams to all orders is to recast (1) in the form of a Dyson equation \[12\]

\[ G = G_0 + G_0 \Sigma G \] (2)

in which \( \Sigma \), the ‘self-energy’, is calculated via its perturbation expansion

\[ \Sigma = v G_0 + v G_0 G_0 v G_0 + \ldots \] (3)
A further step on this route is the self-consistent approach, based on the ‘self-consistent’ Dyson equation (SCDE) in which the self-energy is substituted with a functional of the Green’s function:

\[ G = G_0 + G_0 S[G] G, \]  

(4)

This approach has been put forth by Luttinger and Ward [4], who proposed a formal expression for \( S \) by manipulation of the perturbative series (what we call the Luttinger-Ward approach). The resulting functional is itself in the form of a series, sometimes called ‘skeleton series’, which we denote by

\[ S_{LW}[G] \equiv vG + vGvGvG + ... \]  

(5)

The skeleton series has the property of naturally leading to approximations to \( S \) that fulfill conservation laws for particle number, momentum and energy [13, 14], which would not guarantee. Moreover, since it involves the fully interacting \( G \), rather than \( G_0 \), one may hope that \( [5] \) has a faster convergence than \( [3] \), leading in turn to better approximations to \( G \) than \( [3] \) when truncated at the same order. However, apart from a few further developments [3], very little is known about the consistency of the Luttinger-Ward approach. In fact, the recent results of Kozik and collaborators [5] provide numerical evidence for its failure for certain regimes.

B. On the Self-Consistent Dyson Equation

Being derived within Perturbation Theory, the Luttinger-Ward approach formally applies to all quantum field theories. However, neither the original perturbative derivation, nor further non-perturbative developments fully guarantee that the self-consistent approach always leads to the Green’s function of the original Hamiltonian problem. For this to happen, four conditions have to be fulfilled:

1. given a certain interaction, all information about the specific system of interest is encoded in \( G_0 \), the sole input of \( [4] \);
2. given \( G \) and \( G_0 \), there exists a \( \Sigma \) such that \( G = G_0 + G_0 \Sigma G \) holds;
3. there exists a functional \( S \) such that \( S[G] = \Sigma \).

Those three conditions guarantee that \( X = G \) is solution of the equation

\[ X = G_0 + G_0 S[X] X. \]  

(6)

However, the equation might have other, spurious solutions, which could be either an excited state solution, a Green’s function of another system, or a function that does not correspond to any ‘physical’ Green’s function. This would not threaten the theoretical foundations of the approach, it would, however, represent a serious obstacle for its practical use. Therefore we formulate a forth condition:

4. the functional \( S \) should be such that \( [6] \) has only one solution, namely \( X = G \).

In the following, we shall make these four conditions more precise and put them in the context of current knowledge.

First, we need to give a definition of physical Green’s function. Given an interacting Hamiltonian, the \( N \)-body Green’s functions are unambiguously defined as \( 2N \)-point correlators. We focus on the zero temperature, equilibrium one-body Green’s function,

\[ G(1, 2) \equiv -i \langle \Psi | T [\hat{\psi}(1) \hat{\psi}(2)] | \Psi \rangle, \]  

(7)

where \( | \Psi \rangle \) represents the ground-state of the Hamiltonian at fixed particle number, \( T \) the time-ordering operator, \( \hat{\psi} \) the field operator in the Heisenberg representation, and 1, 2 compact arguments representing space, spin and time degrees of freedom, \( 1 \equiv (r_1, \sigma_1, t_1) \). The definition (7) does not depend on the chosen Hamiltonian. A specific \( G \) is obtained when the Hamiltonian, in its parametric form, is decided, specific values for those parameters are chosen, and all information required to fully identify the state (in particular the number of particles) is given. When dealing with the electronic many-body Hamiltonian, we say that all ‘systems’ are characterized by the same interaction (the Coulomb interaction) and they are distinguished by the external potential. We generalize this notion in the following way. Given any (parametric) Hamiltonian, different systems are obtained by varying the value of the parameters appearing in the non-interacting part, while keeping the value of the interaction fixed. This allows us to introduce the notion of ‘physical Green’s function’ as follows. Given a certain Hamiltonian with fixed value of the interaction, the set \( \{ G \} \) of physical Green’s functions is represented by all and only the functions obtained by evaluating formula (7) on all possible systems. In the out-of-equilibrium case an analogous definition holds, while, in case of finite-temperature, one should take into account that different systems are also characterized by different values of temperature. Obviously, there is no guarantee that any arbitrary function of two (multi-dimensional) arguments \( f(1, 2) \) belongs to \( \{ G \} \), i.e. that it corresponds to the Green’s function of some system. Moreover, the set \( \{ G \} \) may change according to the interaction and the type of Green’s function (zero/finite temperature, in/out of equilibrium) considered. Finally, we note that here we consider the case of the electronic many-body problem, in which the interaction is fixed once for all to Coulomb, but our discussion would not change if a different choice were made.

In the following we shall refer to elements of \( \{ G \} \) as ‘physical Green’s functions’ or, simply, ‘Green’s func-

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2 Since the set may change with the value of the interaction, a more precise notation would be \( \{ G \}_v \). Working always at fixed \( v \), however, we shall omit the subscript \( v \), for sake of notational economy.
FIG. 1. As mentioned in [8], for zero temperature, equilibrium Green’s functions \( G \), the Hohenberg-Kohn theorem, which connects the external potential \( v_{\text{ext}} \) to the corresponding (non-degenerate) ground-state wavefunction \( \Psi \) (link 1) and to the density \( n \) (link 2), guarantees that there is a one-to-one correspondence between \( v_{\text{ext}} \) and \( G \), in the following way: if we know \( v_{\text{ext}} \), we can build \( \Psi \) (link 1) and hence \( G \) (link 3); on the other hand, if we know \( G \) we then know \( n \) (link 4) and hence \( v_{\text{ext}} \) (links 2,1). Since such a correspondence \( \{ v_{\text{ext}} \} \leftrightarrow \{ G \} \) holds also in the non-interacting case \( \{ v_{\text{ext}} \} \leftrightarrow \{ G_0 \} \), it follows that \( \{ G_0 \} \leftrightarrow \{ G \} \).

Concerning the non-relativistic electronic problem in particular, because of the the simple relation connecting the charge density to the Green’s function \( n(1) = -iG(1; 1^+1) \), one can use theorems developed in the framework of Density Functional Theory [15–18] to establish the relation between \( \{ G_0 \} \) and \( \{ G \} \), which, in DFT wording, are the set of all \( v \)–representable (non-interacting and interacting, respectively) Green’s functions. As one can see in fig. [1], a simple argument points indeed to a one-to-one map between the two sets, at least in the zero-temperature equilibrium case.

Finally, given a functional \( S \) such that \( S[G] = G^{-1} - G^{-1} \), we have to distinguish two situations. If the domain of \( S \) is \( \{ G \} \), then the above conditions ensure that the SCDE has one and only one solution. If the domain of \( S \) extends beyond \( \{ G \} \) then a problem of multiple, spurious solutions might occur. The skeleton series, for instance, takes as entry any function of two arguments, unless specified differently. Since in the case of the electronic many-body problem \( \{ G \} \) does not cover the entire space of functions with two arguments, the SCDE with the skeleton series could have spurious solutions, even when the series, evaluated at a certain \( G \), gives the correct \( \Sigma \). To better understand this situation, let us discuss a few subtleties. First, consider the map \( \{ G_0 \} \rightarrow \{ G \} \), for which there exists a functional, say \( F \), that takes elements of \( \{ G_0 \} \) to the corresponding element of \( \{ G \} \), or, in formulae, \( F[G_0] = G \). If \( \{ G_0 \} \) is only a proper subset of all possible functions of two arguments, then \( F \) is not the only functional that realizes that map, for another functional \( F’ \) such that \( F’[G_0] = G \) and yet \( F[f] \neq F’[f] \) if \( f \notin \{ G_0 \} \) can exist (fig. [2]). Since the map is supposed to be one-to-one there must also be a functional or, better, a family of functionals realizing the inverse map, namely \( L[G] = G_0 \). Given two functionals such that \( F[G_0] = G \) and \( F'[G_0] = G \) that correctly realize the map \( \{ G_0 \} \rightarrow \{ G \} \), but have different behavior outside the set \( \{ G_0 \} \). In particular, in the present example \( F \) is injective \( (F[f] \neq F[g] \text{ for all } f, g \text{ in its domain}) \) while \( F’ \) is non-injective (there is at least one \( G_0 \) and one \( f \notin \{ G_0 \} \) for which \( F'[G_0] = F'[f] \)).
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FIG. 3. While \( F \) realizes the map \( \{ G_0 \} \rightarrow \{ G \} \), \( L \) and \( L' \) realize the opposite map \( \{ G_0 \} \leftarrow \{ G \} \). \( L \) is injective on its entire domain, while \( L' \) is not. Both \( L \) and \( L' \) are equal to \( F^{-1} \) on the domain limited to \( \{ G \} \), but they are different from \( F^{-1} \) when the entire domain is allowed.

FIG. 4. Left outer set: physical Green’s functions; right outer set: physical self-energies. \( S \) and \( S' \) are two distinct functionals for which \( S[G] = S'[G] = \Sigma \). \( S_{LW} \) represents the skeleton series introduced by Luttinger and Ward. It satisfies \( S_{LW}[G] = \Sigma \) but not for all physical \( G \)’s. The equality holds only for the left inner set mapped to the right inner set.

\[ \text{and } L[G] = G_0, \text{ we cannot conclude that } L = F^{-1}, \text{ since it might be that } L[f] \neq F^{-1}[f] \text{ if } f \notin \{ G \} \text{ (see fig. 3). Different functionals } L \text{ implementing the map } \{ G \} \rightarrow \{ G_0 \} \text{ would obviously lead to different } S \text{ functionals, as shown in fig. 4. For } S[f] = L[f]^{-1} - f^{-1} \text{ the equation } X = G_0 + G_0 S[X] X \text{ is equivalent to } L[X] = G_0. \text{ Therefore, it has only one solution in the set } \{ G \} \text{ but can have other solutions outside that set, the number and nature depending on the features of the chosen } L \text{. Those spurious solutions can be avoided in two ways: either we build } S \text{ on an } L \text{ that is injective on its entire domain (i.e. there are no two } f \text{ and } g \text{ for which } L[f] = L[g] \text{) or we restrict the search for solutions to the set } \{ G \}. \text{ Unfortunately, neither option is easy to realize, the first one for a lack of methods to build } L \text{ with the desired properties and the second for a lack of a complete characterization of the set } \{ G \}.^{5} \]

\[ \text{C. On the Inverse Problem} \]

If \( \{ G_0 \} \leftrightarrow \{ G \} \) holds and we are given a functional \( F \) such that \( F[G_0] = G \), one may want to use it for solving the inverse (or ‘embedding’) problem: \( F[X] = G \), in which \( G \) is given and \( G_0 \) is to be found. In general, \( F \) can be non-injective over its entire domain, and one can run into spurious solutions (see \( F' \) in fig. 2). Unless the domain of \( F \) is properly restricted, this may happen, for instance, if one attempts to solve the Dyson equation with a self-energy evaluated in perturbation theory (eqn (2-3)). On the other hand, if the functional \( F \) relies on solving a SCDE, then the corresponding inverse problem has always only one solution, the physical \( X = G_0 \), irrespective of the properties of the \( S \) appearing in the SCDE and of possible restrictions on the search for solutions. This is because the SCDE as an equation in \( G_0 \), rather than \( G \), namely \( G = X + X S[G]G \), is a linear equation whose unique solution is \( X = (S[G] + G^{-1})^{-1} \) which readily simplifies to \( X = (L[G]^{-1} - G^{-1} + G^{-1})^{-1} = L[G] = G_0 \).

\[ \text{II. SELF-CONSISTENT APPROACH TO THE HUBBARD ATOM} \]

\[ \text{A. Introduction} \]

The previous section has set the general frame. In particular, it emerges that in order to avoid spurious, unphysical solutions to the SCDE, one must either use a self-energy functional \( S[f] = L[f]^{-1} - f^{-1} \) with \( L \) injective over its entire domain, or restrict the search of solutions to the set \( \{ G \} \) where \( L \) is injective; physical Green’s functions must lie within this set.

In order to illustrate these quite abstract considerations, and in order to use them to explain current problems in the literature and search for potential solutions, we are going to analyze the self-consistent approach on a simple, solvable model: the finite temperature, half-filled Hubbard Atom which is defined in the next subsection.

The Hubbard atom has been one of the systems studied in the recent work by Kozik and collaborators. In their Letter the outcome of several numerical tests performed on Hubbard models was reported. One set of tests is devoted to probe the number and nature of solutions of the inverse problem, defined in Section II C. They found one physical and one unphysical solution. The remaining tests concern the skeleton series, which, when evaluated at the exact \( G \), converges to the correct self-energy only for weakly interacting systems. On the basis of these numerical results, two main conclusions were proposed: (i) the map \( G_0 \rightarrow G \) is not invertible; (ii) the

\[ \text{5 For instance, although the analytic structure of the equilibrium Green’s function in frequency space is known to be a sum of poles }^{13} \text{ exact constraints on coefficients of these poles are only partially known. In fact, even for the charge density, which is a part of the Green’s function, the problem of finding all necessary constraints (in this context called } v^- \text{–representability) remains unsolved (see }^{20} \text{ and references therein).} \]
skeleton series has two branches, and one may talk about
the “non-existence of the Luttinger Ward functional”.

In the following (subsection [11C] we shall prove that,
at least in the Hubbard atom, the map \( \{G_0\} \leftrightarrow \{G\} \)
holds. This will establish the self-consistent approach as
an exact and closed rewriting of the original problem to
determine the Green’s function given the Hamiltonian.
Furthermore, we shall present an actual realization of
the approach. We will first present two explicit function-
als \( F_W \) and \( L_W \) that, limited to this model, realize the
map \( \{G_0\} \rightarrow \{G\} \) and \( \{G_0\} \leftarrow \{G\} \), respectively. The
functional \( L_W \) will then be used to build a functional
\( S_W \) that allows to write down the SCDE in an explicit
form. We shall then prove that such a SCDE has one
and only one solution in the set of physical Green’s func-
tions. On the other hand, the functional \( F_W \) will be
used to show that the inverse problem \( F[X] = G \) has
spurious solutions if \( F \) is non-injective and the search
of solutions is not restricted to the set of physical non-
interacting Green’s functions. Moreover, the formal per-
turbative expansion of \( F_W \) will allow us to build the ‘one-
frequency–skeleton’ series, in analogy to the standard
skeleton series. The one-frequency–skeleton series evalu-
ated at \( G \) will be shown to converge to the correct self-
energy only in a subregion of the parameter space. Fi-
nally, we shall construct a second series (‘one-frequency–
SIN’) that complements the one-frequency–skeleton, in
the sense that, when evaluated at \( G \), it converges to the
correct self-energy wherever in the parameter space the
one-frequency–skeleton does not, and vice versa.

B. The Hubbard Atom

The Hamiltonian of the Hubbard atom is

\[
\hat{H} = \frac{U}{2} \sum_{\sigma, \sigma' = \uparrow, \downarrow} \hat{c}^{\dagger}_\sigma \sigma' \hat{c}^{\dagger}_\sigma \sigma' c_{\sigma'} c_{\sigma},
\]

(9)

where \( \hat{c}^{(f)}_\sigma \) is a fermionic annihilation (creation)
operator and \( U > 0 \) is the interaction parameter. In order
to establish a close connection to \( [5] \), we calculate the
finite temperature one-body Green’s function in the grand
canonical ensemble, which is defined as \( [21] \)

\[
G_{\alpha \beta}(\hat{x}, \tau; \hat{x}', \tau') = \frac{\text{Tr} \left\{ e^{-\beta(\hat{H} - \mu \hat{N})} \psi^{\dagger}_\alpha(\hat{x}, \tau) \psi_\beta(\hat{x}', \tau') \right\}}{\text{Tr} \left\{ e^{-\beta(\hat{H} - \mu \hat{N})} \right\}}
\]

(10)

where \( \hat{N} \) is the number operator, \( \mu \) is the chemical
potential, and \( \mathcal{T} \) orders operators according to their value of \( \tau \),

\[
\psi_\alpha(\hat{x}, \tau) \]

is the field operator and \( \beta \equiv 1/(k_B T) \) with \( T \) the
temperature and \( k_B \) the Boltzmann constant. The fre-
quency Fourier transform to imaginary frequencies yields
the Matsubara Green’s function \( [21] \). For the Hubbard
atom \( [9] \) and for a chemical potential \( \mu = U/2 \) this yields
\( G_{\sigma \sigma'}(z) = G(z) \delta_{\sigma \sigma'} \) with

\[
G(z) = \frac{1}{2} \left( \frac{1}{z + U/2} + \frac{1}{z - U/2} \right)
\]

(11)

\[
= \frac{1}{z} \frac{1}{1 - U^2/(4z^2)}
\]

(12)

with

\[
z = i \omega_n \quad \text{and} \quad \omega_n \equiv k_B \pi T (2n + 1), \quad n \in \mathbb{Z}.
\]

(13)

The corresponding non-interacting Green’s function is obtained by setting \( U \) to 0, which yields

\[
G_0(z) \equiv \frac{1}{z}.
\]

(14)

The self-energy is then defined as

\[
\Sigma(z) \equiv G_0(z)^{-1} - G(z)^{-1} = \frac{U^2}{4z}.
\]

(15)

C. The map \( \{G_0\} \leftrightarrow \{G\} \)

In a Hubbard model with \( N > 1 \) sites at finite tem-
perature, what identifies a specific system, and hence
the corresponding Green’s function, is the value of the tem-
perature \( T \), the chemical potential \( \mu \) and the value of the
hopping expressed in units of the interaction strength \( U \)
as \( t/U \). Sometimes the hopping parameter \( t \) is fixed to 1
and \( U \) let to vary. However, in case of one site, no hop-
ning is possible, so \( U \) is simply a constant that sets the
energy scale. Moreover, in our case the chemical po-
tential is also fixed, leaving the temperature \( T \) as the only
parameter that really characterizes a system. We then
say that the set of physical Green’s functions \( \{G(z)\} \)
is defined as the set of all and only the functions in \( n \in \mathbb{Z} \)
obtained from \( [11] \) and \( [13] \) by varying \( T \in (0, \infty) \). In
other words, any function of \( n \) that cannot be written as
\( [11] \) for a certain value of \( T \) will be considered an
‘unphysical’ Green’s function. The set of physical non-
interacting Green’s functions \( \{G_0(z)\} \) can then be defined
in an analogous way.

The parametrization of the two spaces in terms of the
temperature \( T \) is quite convenient in view of the analysis
of the map between them. In fact, if we define the set of
physical temperatures \{\( T; T > 0 \}\), the one-to-one–
ness of the map \( \{G_0\} \leftrightarrow \{G\} \) can be proved as a
consequence of the one-to-one–ness of the maps \( \{T\} \leftrightarrow
\{G_0\} \) and \( \{T\} \leftrightarrow \{G\} \), as follows.

Let us first look at \( \{T\} \leftrightarrow \{G_0\} \). Since we have that
physical \( G_0 \)’s are defined starting from physical tem-
peratures (i.e. for any physical temperature there is
one physical \( G_0(z) \): \( \{T\} \rightarrow \{G_0(z)\} \)), we need to prove that
every physical \( T \) corresponds to only one \( G_0(z) \). If \( T' \) and
\( T \) gave rise to the same \( G_0(z) \) we could write

\[
\frac{1}{i(2n + 1)\pi k_B T} = \frac{1}{i(2n + 1)\pi k_B T'}.
\]

(16)
B. Conclusion

But this simply reduces to $T = T'$, so there are no two physical temperatures leading to the same non-interacting Green’s function.

Concerning the map $\{T\} \leftrightarrow \{G(\cdot)\}$, we have that $\{T\} \to \{G(\cdot)\}$ is again realized by definition, while for the inverse map we must solve the equivalent of (16) which reads:

\[
\frac{1}{2} \left( \frac{1}{i(2n+1)\pi k_B T' + \frac{U}{2}} + \frac{1}{i(2n+1)\pi k_B T' - \frac{U}{2}} \right) = \frac{1}{2} \left( \frac{1}{i(2n+1)\pi k_B T + \frac{U}{2}} + \frac{1}{i(2n+1)\pi k_B T - \frac{U}{2}} \right)
\]

which per se has two solutions:

\[
T' = T \quad \text{and} \quad T' = \frac{U^2}{4\pi^2 k_B^2 (2n+1)^2 T}
\]

However, the second one is not a valid physical temperature, since it is a function in $n$ rather than a positive number. This means that a physical interacting Green’s function corresponds to only one physical temperature.

Since $\{T\} \leftrightarrow \{G_0(\cdot)\}$ and $\{T\} \leftrightarrow \{G(\cdot)\}$ holds, one can then conclude that $\{G_0(\cdot)\} \leftrightarrow \{G(\cdot)\}$.

D. Explicit Functionals

Both sets $\{G_0(\cdot)\}$ and $\{G(\cdot)\}$ only represent portions of all possible functions in $\mathbb{R}^\mathbb{C}$ It follows that there can be different functionals realizing the maps $\{G_0(\cdot)\} \leftrightarrow \{G(\cdot)\}$, characterized by inequivalent results outside those sets. A specific functional realizing the map $\{G_0(\cdot)\} \to \{G(\cdot)\}$ is

\[
F_W(n, [f]) = \frac{f(n)}{1 - f(n)^2 U^2 T^2},
\]

This functional takes as input any function $f(n)$, not just non-interacting Green’s functions. A functional realizing the inverse map $\{G_0(\cdot)\} \leftarrow \{G(\cdot)\}$ is

\[
L_W(n, [f]) = \left( i(2n+1) \frac{U}{2} \sqrt{\frac{1}{3} + \frac{f(-1)}{f(1)}} \right)^{-1}.
\]

Note that $L_W$ carries an explicit dependence on $n$, while $F_W$ does not. For economy of notation, in the following we shall denote all functionals by $\mathcal{O}(f)$, rather than $\mathcal{O}(n, [f])$, omitting to indicate a possible dependency on $n$.

The functionals $F_W$ and $L_W$ are different from the corresponding ones built in Perturbation Theory. They have restricted capabilities, for they give the correct result only when applied to Green’s functions of the Hubbard atom, viz. (11) and (14). A difference that will play a central role in our later discussion (Sections III to IIII) is that $F_W$ is completely local in (Matsubara) frequency space (the value of $F_W[\mathcal{G}]$ at a specific $n = n_0$ depends only on $G(n')$ at that $n' = n_0$), while Perturbation Theory prescribes convolutions on frequencies. On the other hand, $L_W$ is characterized by a universal (i.e. $f$-independent) function, namely $(2n+1)$, which encodes the structure common to all $G_0(\cdot)$’s, and a prefactor that depends on $f$ in a non-local way, which, evaluated at $f = \mathcal{G}$, extracts the information about the specific system.

E. Self-Consistent Dyson Equation

Using $L_W$ we can define the functional

\[
S_W[f] \equiv L_W[f]^{-1} - f(n)^{-1} = i(2n+1) \frac{U}{2} \sqrt{\frac{1}{3} + \frac{f(-1)}{f(1)}} - \frac{1}{f(n)}.
\]

From that we can build the SCDE

\[
X = G_0(\cdot) + G_0(\cdot) S_W[X] X
\]

with $X$ an unknown function of $n$ (see fig. 6). As pointed out in Section IB, (21) with (22) are equivalent to $G_0(\cdot) = L_W[X]$. Since $L_W$ is not injective given $G_0(\cdot)$, this equation has multiple solutions. However, equation (22) has only one solution if we restrict our search to the set $\{G(\cdot)\}$. To see this explicitly, we use the expression for $G_0(\cdot)$:

\[
\frac{1}{i(2n+1) k_B \pi T} = L_W[X].
\]

We enforce the correct domain on $X$ by considering only functions belonging to $\{G(\cdot)\}$. We therefore look at

\[
\frac{1}{i(2n+1) k_B \pi T} = L_W[f_z(n)]
\]

\[\text{and}
\]

6 We intentionally leave open the definition of ‘all possible functions’ is. All following statements are valid, for instance, if one considers the set of all rational functions or the bigger set of analytic functions. What matters is only to define the domain of the functionals one considers to be the physical domain.

7 $F_W$ has the same structure as the ones studied by Rossi et al. and Schäfer et al. [8] and first introduced by Stan and collaborators [8] in the context of the so called One Point Model (OPM) [22] [23], which is a mathematically simplified framework for studying the functional formulation of the Green’s function formalism. (see also [24] [25]).

8 Consider for instance $L_W[X]$ and $L_W[X + f]$ with $f$ any function for which $f(-1) = 0$. 

9 $F_W$ has the same structure as the ones studied by Rossi et al. and Schäfer et al. [8] and first introduced by Stan and collaborators [8] in the context of the so called One Point Model (OPM) [22] [23], which is a mathematically simplified framework for studying the functional formulation of the Green’s function formalism. (see also [24] [25]).
We can then write (24) as

\[ \text{problem has two solutions: the correct } X \text{ spurious one} \]

from which we can determine \( x \) where \( x \) is an unknown temperature. The evaluation of \( L_W \) defined in (20) on \( f_x(n) \) leads to

\[ L_W[f_x(n)] = \frac{1}{i(2n+1)k_B T} + \frac{1}{i(2n+1)k_B T - \frac{U}{2}} \]  

(25)

where \( x \) is an unknown temperature. The evaluation of \( L_W \) defined in (20) on \( f_x(n) \) leads to

\[ L_W[f_x(n)] = \frac{1}{i(2n+1)k_B T} \equiv G \]  

(26)

We can then write (24) as

\[ \frac{1}{i(2n+1)k_B T} = \frac{1}{i(2n+1)k_B x} \]  

(27)

from which we can determine \( x \) without ambiguities to be

\[ x = T. \]  

(28)

Plugging this value back in \( f_x(n) \) gives the final, correct answer:

\[ X = \frac{1}{2} \left( \frac{1}{i(2n+1)\pi k_B T + \frac{U}{2}} + \frac{1}{i(2n+1)\pi k_B T - \frac{U}{2}} \right). \]

F. Inverse Problem

We now look at the problem \( F_W[X] = G(z) \), in which \( G(z) \) is known and \( G_0(z) \) to be found. The inverse problem has two solutions: the correct \( X = 1/z \) and a spurious one \( X = -\frac{4z}{z^2} \), which we will denote by \( G_a(z) \). Since there is no \( T \) such that \( G_0(z) \) can be written as \( G_a(z) \), \( G_a(z) \) is an unphysical solution, as expected. The correct solution is therefore identified without ambiguity by restricting the domain to \( \{G_0(z)\} \).

If, like in [5], the domain is not properly restricted, the spurious solution survives, leading to a problem of ‘multiple solutions’ [8, 26]. As anticipated, number and nature of the spurious, unphysical solutions depend on the specific functional one uses. Since our local functional is different from the functional of Kozik and collaborators, we expect that our \( G_a(z) \) does not correspond to the unphysical solution found by these authors. Since [5] provides no direct information on their spurious solution, but only a plot with the imaginary part of the corresponding self-energy, in fig. 6 we also plot the imaginary part of the self-energy arising from our spurious solutions, namely \( \Sigma_u(z) \equiv G_a(z)^{-1} - G(z)^{-1} \). The comparison between the two self-energies shows that indeed the two spurious solutions are different.

G. Local-Skeleton Series

We will now turn to the convergence of the skeleton series, motivated by the numerical evidence provided by Kozik et al. for the fact that the skeleton series may converge to a wrong functional. An analytic proof and analysis for the full LW skeleton series is currently out of reach. However, we can obtain and analyze a qualitatively equivalent result by studying the behavior of the ‘one-frequency–skeleton’ series, built as follows.

In standard Perturbation Theory, the skeleton series arises as a formal manipulation of the terms of the expansion of the fully interacting Green’s function in terms of the non-interacting one [4]. One way to proceed can be summarized as follows: we first start with the perturbative expansion of \( G \):

\[ G = G_0 + vG_0^3 + v^2G_0^5 + ..., \]  

(29)
We then use (29) to write \( G_0 \) in terms of \( G \):

\[
G_0 = G - (v G_0^3 + v^2 G_0^5 + ...)
\]

\[
\Rightarrow G_0 = G - \left(v (G - (v G_0^3 + v^2 G_0^5 + ...))^3 + v^2 G_0^5 + ...ight)
\]

\[
\Rightarrow G_0 = G - v G^3 - v^2 (G^5 - G G_0^5) - ...
\]

\[
\Rightarrow G_0 = G - v G^3 - v^2 G^5 - ...
\]

which is then used in the perturbative expansion of the self-energy (30) to get the formal definition of the skeleton series \( S_{LW} \):

\[
\Sigma = v G_0 + v^2 G_0^3 + ...
\]

\[
\Rightarrow \Sigma = v G - v^2 G^3 - ... \equiv S_{LW}[G].
\]

This simplified notation hides the fact that what here looks like an algebraic multiplication is in fact an integral/sum over the space/time/spin degrees of freedom of the Green’s function, and each term corresponds to many terms with different combinations of multiplications or integrals over arguments. In the case of the Hubbard Atom, for instance, each term of the perturbative expansion of the Green’s function containing a certain number of \( G_0 \)‘s would involve sums of the variables \( n, n', n'' \), on which each \( G_0 \) depends. This means that Perturbation Theory gives rise to a series of non-local functionals of \( G_0 \).

However, one can also write down a different, simpler perturbative expansion. With \( \mathcal{G}(z) = F_W[\mathcal{G}_0(z)] \), expanding \( F_W \) in powers of \( U \) yields

\[
\mathcal{G}(z) = \mathcal{G}_0(z) + \mathcal{G}_0(z)^3 \frac{U^2}{4} + \mathcal{G}_0(z)^5 \frac{U^4}{16} + ...
\]

Note that this involves now actual multiplications, not convolutions. The non-local character of the general expansion prescribed from Perturbation Theory is lost, as the above expression presents a local dependence of \( \mathcal{G}(z) \) on \( \mathcal{G}_0(z) \); in other words, at a given value of \( z \), \( \mathcal{G}(z) \) only depends on \( \mathcal{G}_0(z) \) evaluated at the same \( z \). Obviously, such an expansion is valid only for the Hubbard Atom and is not as general as Many-Body Perturbation Theory. Nevertheless, it allows us to define a local series, by following the steps analogous to equations (29–30)–(31).

This leads to

\[
S_{ofs}[\mathcal{G}(z)] = \frac{U^2 \mathcal{G}(z)}{4} - \frac{U^4 \mathcal{G}(z)^3}{16} + \frac{U^6 \mathcal{G}(z)^5}{32} + \frac{5U^8 \mathcal{G}(z)^7}{256} + \frac{7U^{10} \mathcal{G}(z)^9}{512} + ...
\]

which defines the series of functionals

\[
S_{ofs}[f] = \frac{U^2 f}{4} - \frac{U^4 f^3}{16} + \frac{U^6 f^5}{32} - \frac{5U^8 f^7}{256} + ...
\]

This formal manipulation of the local series (32) allows us to qualitatively reproduce the results of Kozik et al. for the skeleton series. In our case, the one-frequency–skeleton series \( S_{ofs} \) converges partially to a spurious \( \Sigma_u(z) \), as shown in figure 7.

FIG. 7. The physical self-energy \( \Sigma(i \omega_n) = -i U^2/(4 \omega_n) \) (in red), the unphysical \( \Sigma_u(i \omega_n) = -i \omega_n \) (in orange) and various orders of the one-frequency–skeleton series \( S_{ofs}[\mathcal{G}(i \omega_n)] \), (33) (in shades of green) are represented. \( S_{ofs}[\mathcal{G}(i \omega_n)] \) converges to the physical self-energy only in the region \( U^2 \leq 4 \omega_n^2 \) (in gray).

As in the case of Kozik et al., the unphysical self-energy corresponds to the unphysical solution of the inverse problem, \( \Sigma_u(z) = \mathcal{G}_0(z)^{-1} - \mathcal{G}(z)^{-1} \) (see also figure 6). Contrary to what reported in [8] about the standard skeleton series, the convergence of \( S_{ofs} \) to the correct result always occurs in a finite range of \( \omega_n \) at fixed \( U \):

\[
\begin{align*}
S_{ofs}[\mathcal{G}(i \omega_n)] &\equiv \Sigma(i \omega_n) & \text{for } U^2 \leq 4 \omega_n^2 \\
S_{ofs}[\mathcal{G}(i \omega_n)] &\equiv \Sigma_u(i \omega_n) & \text{for } U^2 \geq 4 \omega_n^2.
\end{align*}
\]

because of the local character of \( S_{ofs} \).

Finally, it is important to emphasize that a convergence of the series to an unphysical self-energy does not necessarily imply that the corresponding SCDE \( X = \mathcal{G}_0(z) + \mathcal{G}_0(z) S_{ofs}[X]X \) has, in the same region, a spurious solution. In fact, the Dyson equation with a wrong self-energy functional may have no solutions at all. This is indeed our case, where, similar to [7–9], the series that defines \( S_{ofs} \) in (33) converges to

\[
\tilde{S}[f] = \frac{1 + \sqrt{1 + U^2 f^2}}{2f}
\]

as long as \( |f| \leq 1/U \), which is always the case for physical Green’s functions. Therefore,

\[
\begin{align*}
\tilde{S}[\mathcal{G}(i \omega_n)] &\equiv \Sigma(i \omega_n) & \text{for } U^2 \leq 4 \omega_n^2 \\
\tilde{S}[\mathcal{G}(i \omega_n)] &\equiv \Sigma_u(i \omega_n) & \text{for } U^2 \geq 4 \omega_n^2.
\end{align*}
\]

where the functional \( \tilde{S} \) is defined over a larger domain than \( S_{ofs} \). We can therefore study the Dyson equation:

\[
X = \mathcal{G}_0(i \omega_n) + \mathcal{G}_0(i \omega_n) \tilde{S}[X]X,
\]

not enough information was provided in [9] to conclude what would happen for the standard skeleton series.
which is satisfied by \( X = G(i\omega_n) \) for \( U^2 \leq 4\omega_n^2 \), also outside that region. To do that, we look at the corresponding equation in one complex variable \( x \):

\[
x = \frac{1}{i\omega} + \frac{1}{i\omega} \left( -1 + \sqrt{1 + U^2 x^2} \right) x. \tag{39}
\]

with \( \omega \in \mathbb{R} \). If (39) has no solutions in a certain region of the parameter space, neither will (38). We recast (39) as

\[
\frac{2\omega}{U} = -\frac{i}{\xi} \left( \sqrt{\xi^2 + 1} + 1 \right),
\]

with \( \xi \equiv xU \). Since we are looking at the region defined by \( U^2 > 4\omega_n^2 \), we can write

\[
1 > \left| \frac{\sqrt{\xi^2 + 1} + 1}{\xi} \right|. \tag{41}
\]

However, the right-hand side is always greater than 1, therefore this equation, and hence the original Dyson equation (38), has no solutions, Q.E.D.\(^{10}\)

### H. Local SIN Series

In the previous section, we manipulated the perturbative expansion of a local functional realizing the map \( G_0(z) \to G(z) \), in a way one would do in Perturbation Theory to build the skeleton series. We showed that the corresponding one-frequency–skeleton series does not always converge to the correct self-energy. This supports the interpretation that the numerical findings of \cite{5} do not point to a failure of the self-consistent approach itself, but are rather due to the fact that the skeleton series does not converge to the correct functional. Moreover, it suggests that the seed of this failure lies in the way the skeleton series is constructed from the perturbative expansion of \( G \).

The problem of building a correct self-energy functional demands a solution. Following Stan and collaborators \cite{8}, we attempt therefore, for the simple Hamiltonian here considered, to build a series that complements the one-frequency–skeleton \( S_{ofs} \). As outlined in Section 18, a self-energy functional \( S \) can be built via \( S[f] \equiv L[f]^{-1} - f^{-1} \) if a functional \( L \) is given such that \( L[G] = G_0 \). Such a functional can be connected to a functional \( F[G_0] = G \) via \( L[G] = F^{-1}[G] \). However, \( F \) could be non-injective on a domain bigger than \( \{G_0\} \) and one has to find the correct inverse over \( \{G\} \). In our case, we start from \( F_W \) defined in (19). This functional is not injective: its inverse is made of two branches,

\[
F_W^{-1}[f] = \begin{cases} 
\frac{2(\sqrt{U^2 f^2 + 1} - 1)}{U^2 f} & \text{for } U^2 \leq 4\omega_n^2 \\
\frac{-2(\sqrt{U^2 f^2 + 1} + 1)}{U^2 f} & \text{for } U^2 \geq 4\omega_n^2 
\end{cases} \tag{42}
\]

Neither \( F_1 \) nor \( F_2 \) are in fact a good \( L \) functional, for which \( L[G] = G_0 \). What one would need is a mixture of the two, for \( F_1^{-1}[G] = G_0 \) and \( F_2^{-1}[G] = G_0 \) on two complementary subsets of \( \{G\} \):

\[
F_1^{-1}[G(z)] = G_0(z) \quad \text{for } U^2 \leq 4\omega_n^2 \quad F_2^{-1}[G(z)] = G_0(z) \quad \text{for } U^2 \geq 4\omega_n^2 \tag{43}
\]

The local skeleton series \( S_{ofs} \) is obtained by expanding \( (F_1^{-1}[X])^{-1} - X^{-1} \) in \( U \). Instead, an expansion of \( (F_2^{-1}[X])^{-1} - X^{-1} \) leads to what we shall call the ‘one-frequency–SIN’ series and denote by \( S_{ofSIN} \). The two series are related by

\[
S_{ofSIN}[f] = -\frac{1}{f} - S_{ofs}[f]. \tag{44}
\]

which can be used to calculate \( S_{ofSIN} \) once \( S_{ofs} \) is provided.

As shown in fig. \cite{8} the one-frequency–SIN series evaluated at \( G(z) \) converges to the physical self-energy in the region where \( S_{ofs} \) converges to the unphysical one, and vice versa. It follows that the corresponding SCDE \( X = G_0(z) + G_0(z)S_{ofSIN}[X]X \) admits \( X = G(z) \) as solution in the range \( U^2 \geq 4\omega_n^2 \). An argument similar to

\(^{11}\) This is a generalization of the complementary series introduced by Stan and collaborators, which in particular lead to their strong-interaction Hartree-Fock functional (SIN-HF).

\(^{10}\) Clearly, this result relies on the closed-form character of the functional \( \{G_0\} \) we considered. The use of a truncation of the series \( S_{ofs} \), which is always done in practice, could introduce more spurious solutions; this happens for example in the simple one-point model of \cite{8} when only the lowest order contribution is used.
the one presented in the previous section allows us also to state that outside that range the equation has no solutions. It should be remarked, however, that, even in the pertinent range \( U^2 \geq 4\omega_n^2 \), the actual solution of the self-consistent Dyson equation is not as straightforward as in the \( U^2 \leq 4\omega_n^2 \)-range. In particular, \( X = G(z) \) cannot be found by simple iterative schemes such as \( X^{(n+1)} = G_0 + G_0 S_{SISIN}[X^{(n)}]X^{(n+1)} \), and more sophisticated root-finding algorithms are required.

Finally, we notice that the two functionals \( S_{ofS} \) and \( S_{SISIN} \) can be combined to make a proper self-energy functional as

\[
\tilde{S}[f] \equiv \theta(zf(z) - 1/2)\tilde{S}[f] + (1 - \theta(zf(z) + 1/2)) \left( -\frac{1}{f(z)} - \tilde{S}[f] \right) = -\frac{1}{f(z)} + \frac{1}{2} - \frac{1}{2} + \frac{U^2 f(z)}{2}\frac{1}{\sqrt{4 + U^2 f(z)^2}}
\]

(45)

for which \( \tilde{S}[G(z)] = G_0(z)^{-1} - G(z)^{-1} \) on the entire parameter space, like in the case of \( S_W \) of [21].

**CONCLUSIONS**

The self-consistent approach, i.e. the idea of calculating the one-body Green’s function for a generic Hamiltonian problem via the self-consistent Dyson equation (SCDE) [4], has motivated in the past a notable amount of research culminating in state-of-the-art methods for nuclear and condensed matter physics. However, while the usefulness of the approach and the “in-principle-exactness” of the diagrammatic series are most often taken for granted, a critical analysis and better understanding are still needed. This is also demonstrated by a recent numerical study by Kozik and collaborators [4] that indicates a failure of the only explicit implementation of the approach at our disposal, the Luttinger-Ward approach.

In the present work we discussed some general features of the self-consistent approach, and we performed analytical calculations for a specific Hamiltonian problem, the Hubbard atom. This model is among those used by Kozik et al. to test the Luttinger-Ward approach, pointing to failures in some regions of the parameter space. Our calculations allowed us to analyze these failures, explain their origin, and give indications on how the problems might be overcome.

The first question we addressed was about the possibility to use the self-consistent approach for this model, despite the failure of the LW approach found by Kozik and collaborators. We proved that this can indeed be done. First we showed that in general the approach can be used, at least in principle, whenever there is a one-to-one correspondence between physical interacting and physical non-interacting Green’s functions; then we proved that such a correspondence holds indeed in the case under examination. Since the set of (non-)interacting physical Green’s functions does not cover all possible functions of two arguments (not for the Hubbard atom, nor for the electronic many-body problem), a distinction between the map and the functional that realizes it becomes essential. The same map \( G_0 \to G \) (or \( G \to G_0 \)) can indeed be realized by functionals that take different values when evaluated outside the set of physical Green’s functionals \( \{G_0\} \) (or \( \{G\} \)). The distinction between map and functional also clarifies the apparent contradiction with the conclusion of Kozik et al. that “[...] the map \( G_0 \to G \) [is] not invertible”, which, in light of our discussion, has to be read as “the functional used to realize the map \( G_0 \to G \) becomes non-injective when evaluated on a domain larger than that of physical \( G_0 \)’s”.

Specifically for the Hubbard atom, we have constructed explicit functionals \( F_W \) and \( L_W \) that realize the maps \( G_0 \to G \) and \( G \to G_0 \), respectively, on the physical domains of the model. These are different from the usual functionals obtained from Perturbation Theory, and they have the very important property that all calculations could be done analytically. This has, among others, the advantage that one can distinguish problems of convergence from problems of principle. In particular, these functionals were used to give an explicit realization of the self-consistent approach (calculating \( G \) as solution to \( X = G_0 + G_0 S[X X] \) and the inverse problem (calculating \( G_0 \) as solution of the equation \( G = F[X] \)).

Having established that, when provided with some functionals for the maps \( G_0 \to G \) and \( G \to G_0 \), from which one can build the self-energy functional \( S \) to use in the SCDE, the next question to be addressed was whether the corresponding SCDE \( X = G_0 + G_0 S[X X] \) has unphysical solutions alongside the physical one. For the general case, we showed that the SCDE has exactly one physical solution as long as \( \{G_0\} \to \{G\} \) holds. However, since the functional \( S \) can take as input functions outside the set \( \{G\} \), spurious solutions can be avoided if either one restricts the search over the domain of physical solutions or makes sure that the functional \( L \), linked to \( S \) via \( S[f] = L[f]^{-1} - f^{-1} \), is injective over its entire domain. It should be noted that the conditions to be imposed on the search of \( G \) in order to restrict it to the physical ones are not known in the general case, which means that one can avoid spurious solutions in principle, but the problems may persist in practice. For the Hubbard atom the conditions restricting \( G \) can be formulated in a simple way, which allowed us to illustrate the uniqueness of the solution, as well as the fact that spurious solutions appear when the restriction is dropped.

Once we proved that the self-consistent approach can indeed be used to unambiguously determine \( G \), we moved to investigate the failure of the LW approach found by Kozik and collaborators. In practical applications, one usually takes for the self-energy functional \( S[X] \) some approximation to the Luttinger Ward skeleton series which has been obtained from rearranging the terms of perturbation theory. It was commonly supposed that one could
approach the correct result by including more and more terms of this series. However, a counter-example was given by the numerical results of Kozik et al.

Having a closed functional $F_W$ realizing the map \{${G_0}$\} $\rightarrow$ \{${G}$\} for the Hubbard atom, we expanded $F_W$ in powers of $U$ and derived a perturbative expansion of the Green’s function that maintains the structure of ordinary many-body perturbation theory, but does not contain frequency integrations. This allowed us to build a self-energy functional given as a series of terms similar to the skeleton series, but local in frequency, and hence named ‘one-frequency–skeleton’ series. Like $F_W$, this functional could again be handled fully analytically. Using the one-frequency–skeleton series to calculate the self-energy leads to results that are analogous to those of Ref. [3]; in particular, the series, when evaluated at a certain $G$, converges to the correct self-energy only in a limited range of parameter space, and it converges to a wrong result outside that region. We could relate this finding to the fact that the functional $F_W$ is not injective, such that its inverse, which should realize the map $G \rightarrow G_0$, has two branches. Both of them are needed to build a proper self-energy functional, since they both cover only a part of the map between the physical domains of $G$ and $G_0$. The one-frequency–skeleton series corresponds to the perturbation expansion of one of the two branches and is therefore bound to fail on the other part of the physical domain.

The complementary branch of the self-energy functional can also be expanded in terms of the interaction. For the Hubbard atom we obtained in this way the ‘one-frequency–SIN’-series. Used in the SCDE, the two one-frequency functionals both lead to the correct result on their respective subdomain, and they both yield no result at all when one tries to solve the SCDE outside those respective subdomains. However, spurious solutions can appear when the series are truncated at some order. The one-frequency–SIN functional is a straightforward generalization of a complementary self-energy functional derived in the context of one-point model (OPM) in [8]. This gives hope that it might be possible to go even further, and find a generalized SIN functional that would complement the standard skeleton series for the general problem. Of course, the one-frequency–SIN was derived from the nonperturbative expression we used to realize the map \{${G_0}$\} $\rightarrow$ \{${G}$\}, which for the general problem is not available. On the other hand, the simple relation linking the one-frequency–SIN to the one-frequency–skeleton [14], which has survived the passage from the OPM to the Hubbard atom, may indicate the possibility of building such a hypothetical generalized SIN starting from the skeleton series only, or anyway using the tools of Perturbation Theory.

This and many more interesting questions demand further investigation, in particular: For which physical systems will the skeleton series lead to serious problems? Would the corresponding SCDE always be characterized by an unphysical solution that we can easily recognize as such? How does the picture change when, as it will be the case in practice, truncations of the series are considered? How will it be possible to restrict the domain of Green’s functions in practice? And alternatively, is it worthwhile to maintain the self-consistent approach in view of its difficulties, or should one rather build self-energy functionals of the non-interacting Green’s function?

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[1] W. Kohn, Rev. Mod. Phys. 71, 1253 (1999)
[2] R. Haussmann, *Self-consistent Quantum-Field Theory and Bosonization for Strongly Correlated Electron Systems*, Lecture Notes in Physics Monographs (Springer Berlin Heidelberg, 2003).
[3] C. De Dominicis and P. C. Martin, Journal of Mathematical Physics 5, 14 (1964)
[4] J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960)
[5] E. Kozik, M. Ferrero, and A. Georges, Phys. Rev. Lett. 114, 156402 (2015)
[6] T. Schäfer, G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni, and A. Toschi, Phys. Rev. Lett. 110, 246405 (2013)
[7] T. Schäfer, S. Ciuchi, M. Wallerberger, P. Thunström, O. Gunnarsson, G. Sangiovanni, G. Rohringer, and A. Toschi, Phys. Rev. B 94, 235108 (2016)
[8] A. Stan, P. Romaniello, S. Rigamonti, L. Reining, and J. A. Berger, New Journal of Physics 17, 093045 (2015)
[9] R. Rossi and F. Werner, Journal of Physics A: Mathematical and Theoretical 48, 485202 (2015)
[10] J. Fischer, International Journal of Modern Physics A 12, 3625 (1997)
[11] M. Gell-Mann and K. A. Brueckner, Phys. Rev. 106, 364 (1957)
[12] A. Fetter and J. Walecka, *Quantum Theory of Many-particle Systems*, Dover Books on Physics (Dover Publications, 2003).
[13] G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961)
[14] G. Baym, Phys. Rev. 127, 1391 (1962)
[15] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)
[16] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965)
[17] N. D. Mermin, Phys. Rev. 137, A1441 (1965)
[18] E. Runge and E. K. U. Gross, Phys. Rev. Lett. 52, 997 (1984).
[19] H. Lehmann, Il Nuovo Cimento (1943-1954) 11, 342 (1954).
[20] E. Engel and R. Dreizler, Density Functional Theory: An Advanced Course (Texts and Monographs in Physics, Springer Berlin Heidelberg, 2011).
[21] A. Fetter and J. Walecka, Quantum theory of many-particle systems (International series in pure and applied physics, McGraw-Hill, 1971).
[22] G. Lani, P. Romaniello, and L. Reining, New Journal of Physics 14, 013056 (2012).
[23] J. A. Berger, P. Romaniello, F. Tandetzky, B. S. Mendoza, C. Brouder, and L. Reining, New Journal of Physics 16, 113025 (2014).
[24] L. G. Molinari, Phys. Rev. B 71, 113102 (2005).
[25] Y. Pavlyukh and W. Hübner, Journal of Mathematical Physics 48, 052109 (2007), http://dx.doi.org/10.1063/1.2728512.
[26] R. Eder, ArXiv e-prints (2015), arXiv:1407.6599 [cond-mat.str-el].