

Self-consistent Dyson equation and self-energy functionals: An analysis and illustration on the example of the Hubbard atom

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(Received 17 March 2017; revised manuscript received 27 June 2017; published 18 July 2017)

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 noninteracting 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 a 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 (2015)]. 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.

DOI: [10.1103/PhysRevB.96.045124](https://doi.org/10.1103/PhysRevB.96.045124)

I. 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 wave functions. However, a many-body wave function 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 wave functions. 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 wave function $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$. 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 $n(\mathbf{r})$ plays the role of Q . Although $n(\mathbf{r})$ has much less degrees of freedom than $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$, the Hohenberg-Kohn theorem guarantees that the knowledge of $n(\mathbf{r})$ is sufficient to completely identify the local external potential of the specific system from which it arises. Moreover, the Kohn-Sham approach provides a handy tool to get a highly accurate estimate of $n(\mathbf{r})$ for any system. However, the explicit expression of almost all observables in terms of $n(\mathbf{r})$ is unknown. An alternative to $n(\mathbf{r})$ is the equilibrium one-body Green's function $G(\mathbf{r}, \sigma, t, \mathbf{r}', \sigma', t')$. Contrary to the density, it is nonlocal in space, spin, and time (or frequency dependent, for

its Fourier transform), but it is still much more compact than the many-body wave function. 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 [2]. 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 Eqs. (1)–(6) and (31)–(33) of later sections. $G = G_0 + G_0 \Sigma G$, where Σ is a nonlocal and frequency-dependent function, called self-energy. Perturbation theory offers a way to calculate the (formal) perturbative expansion of Σ in the Coulomb interaction v , yielding a series of functionals of v and the noninteracting Green's function G_0 , $\Sigma = vG_0 + vG_0vG_0G_0 + \dots$. Alternatively, one can consider the self-consistent Dyson equation (SCDE) $G = G_0 + G_0 S[G]G$, with S the so-called 'self-energy functional,' giving rise to the self-consistent approach [3]. Its formal justification can be given in terms of Legendre transformations [4], while the reference computable scheme is the one proposed by Luttinger and Ward [5], 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 [6] 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

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by Schäfer and collaborators [7–9]. First investigations on an entirely analytical level were carried out by Stan and collaborators [10], and Rossi and Werner [11], 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 Sec. II, 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 Sec. III on the Hubbard atom, which is one of the systems studied by Kozik *et al.* [6]. 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 noninteracting 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 Ref. [6] 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 Sec. II, the presentation of the results and analysis for the Hubbard atom in Sec. III is organized as follows: After an introduction Sec. III A we present the Hubbard atom Sec. III B, prove the one-to-one correspondence between the G_0 's and G 's arising in this model Sec. III C, present explicit formulas for the functionals realizing those maps Sec. III D, and use those to solve the SCDE Sec. III E and the inverse problem of finding G_0 given G Sec. III F; then we define the 'one-frequency–skeleton' series Sec. III 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 Sec. III 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.

II. 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 noninteracting 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 Ref. [2]), as

$$G = G_0 + G_0 v G_0 G_0 + G_0 v G_0 G_0 v G_0 G_0 + \dots \quad (1)$$

One difficulty of this expression is the need to properly define G_0 , which is far from obvious in the presence of degeneracies; the latter point is tightly linked to the problems of perturbation theory based on the Gell-Mann-Low theorem at zero temperature for systems with a degenerate noninteracting ground state (see Ref. [12] and references therein). Even when this can be sorted out, the above expression 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 Ref. [13] and references therein). Furthermore, the fact that we can write (1) does not guarantee that also nonperturbative 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 [14]. 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 [15]

$$G = G_0 + G_0 \Sigma G \quad (2)$$

in which Σ , the 'self-energy,' is calculated via its perturbation expansion

$$\Sigma = v G_0 + v G_0 G_0 v G_0 + \dots \quad (3)$$

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:

$$G = G_0 + G_0 S[G] G. \quad (4)$$

This approach has been put forth by Luttinger and Ward [5], 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

$$S_{LW}[G] \equiv v G + v G G v G + \dots \quad (5)$$

The skeleton series has the property of naturally leading to approximations to S that fulfill conservation laws for particle number, momentum, and energy [16,17], which (3) 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 [4], very little is known about the consistency of the Luttinger-Ward approach. In fact, the recent results of Kozik and collaborators [6] 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 nonperturbative 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 Σ 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 a solution of the equation

$$X = G_0 + G_0 S[X] X. \tag{6}$$

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 fourth 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. For example, for the zero temperature, equilibrium one-body Green’s function, we have

$$G(1,2) \equiv -i \langle \Psi | \mathcal{T} [\hat{\psi}^\dagger(1) \hat{\psi}(2)] | \Psi \rangle, \tag{7}$$

where $|\Psi\rangle$ represents the ground state of the Hamiltonian at fixed particle number, \mathcal{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, $1 \equiv (\mathbf{r}_1, \sigma_1, t_1)$. 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 noninteracting 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*. 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. 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 functions,’ all other functions of two arguments being ‘unphysical Green’s functions’. In an equivalent fashion, the set of ‘physical noninteracting Green’s functions’ $\{G_0\}$ can be established. It should be emphasized that this is an important difference with other works, like Ref. [6], in which this distinction is not made, and the term ‘Green’s function’ seems to include any function of two arguments, covering both ‘physical’ and ‘unphysical’ ones.

This definition allows us to reformulate the first point of our list of conditions in the following way: Given a certain Hamiltonian (with fixed value of the interaction, but all possible values of its parameters), the corresponding set $\{G_0\}$ must identify all elements of the set $\{G\}$ completely and without ambiguities. In other words, the map $\{G_0\} \rightarrow \{G\}$ must be surjective.

The second point concerns the existence of the self-energy Σ . Formally, one can write $\Sigma = G_0^{-1} - G^{-1}$, where the inverse functions G^{-1} and G_0^{-1} , from now on collectively shorthanded with $G_{(0)}^{-1}$, are defined by

$$\begin{aligned} & \int d3 G_{(0)}(1,3) G_{(0)}(3,2)^{-1} \\ & = \int d3 G_{(0)}(1,3)^{-1} G_{(0)}(3,2) = \delta(1,2). \end{aligned} \tag{8}$$

For a self-energy to exist it is therefore enough that $G_{(0)}^{-1}$ exists.

The third issue is the existence of a functional S with $S[G] = \Sigma$. For this we need that $\{G_0\} \rightarrow \{G\}$ is also injective, which makes $\{G_0\} \leftrightarrow \{G\}$ a one-to-one map. This indeed would allow us to build a functional L such that $L[G] = G_0$ and S as $S[f] \equiv L[f]^{-1} - f^{-1}$, where the inverse [in the sense of (8)] $L[f]^{-1}$ is guaranteed to exist for at least $f = G$ by the existence of the inverse of G_0 .

Concerning the nonrelativistic electronic problem in particular, because of the simple relation connecting the charge density to the Green’s function $n(1) = -iG(1; 1^+)$, one can use theorems developed in the framework of density functional theory [18–21] to establish the relation between $\{G_0\}$ and $\{G\}$, which, in DFT wording, are the set of all v -representable (noninteracting 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. For the finite temperature,

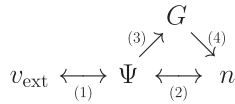


FIG. 1. As mentioned in Ref. [10], for zero temperature, equilibrium Green’s functions G , defined by (7), the Hohenberg-Kohn theorem, which connects the external potential v_{ext} to the corresponding (nondegenerate) ground-state wave function Ψ (link 1) and to the density n (link 2), guarantees that there is a one-to-one correspondence between v_{ext} and G in the following way: If we know v_{ext} , we can build Ψ (link 1) and hence G (link 3); on the other hand, if we know G we then know n via $-iG(1,1^+) = n(1)$ (link 4) and hence v_{ext} (links 2,1). Since such a correspondence $\{v_{\text{ext}}\} \leftrightarrow \{G\}$ holds also in the noninteracting case $\{v_{\text{ext}}\} \leftrightarrow \{G_0\}$, it follows that $\{G_0\} \leftrightarrow \{G\}$.

a proof of one-to-one-ness, for a more general Hamiltonian, was given by Potthoff (see Appendix A of Ref. [22]).

Finally, given a functional S such that $S[G] = G_0^{-1} - G^{-1}$, 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 [for instance, $-iG(1,1^+)$ corresponds to the charge density, which cannot be negative] the SCDE with the skeleton series could have spurious solutions, even when the series, evaluated at a certain G , gives the correct Σ . 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 formulas, $F[G_0] = G$. 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 $L[G] = G_0$, we cannot conclude that $L = F^{-1}$, since it might be that $L[f] \neq F^{-1}[f]$ if $f \notin \{G\}$ (see Fig. 3). Different functionals L implementing the map $\{G\} \rightarrow \{G_0\}$ would obviously lead to different S functionals,

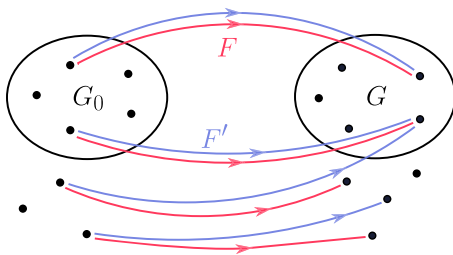


FIG. 2. Pictorial representation of two functionals F and F' that correctly realize the map $\{G_0\} \rightarrow \{G\}$, but have different behavior outside the set $\{G_0\}$. In particular, in the present example F is injective ($F[f] \neq F[g]$ for all f, g in its domain) while F' is noninjective (there is at least one G_0 and one $f \notin \{G_0\}$ for which $F'[G_0] = F'[f]$).

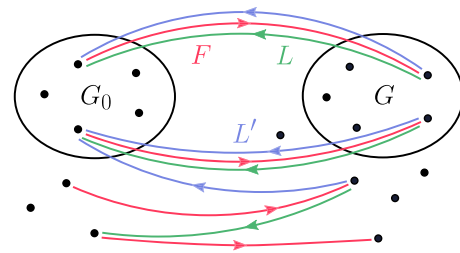


FIG. 3. While F realizes the map $\{G_0\} \rightarrow \{G\}$, L and L' realize the opposite map $\{G_0\} \leftarrow \{G\}$. L is injective on its entire domain, while L' is not. Both L and L' are equal to F^{-1} on the domain limited to $\{G\}$, but they are different from F^{-1} when the entire domain is allowed.

as shown in Fig. 4. For $S[f] = L[f]^{-1} - f^{-1}$ the equation $X = G_0 + G_0S[X]X$ is equivalent to $L[X] = G_0$. Therefore, it has only one solution in the set $\{G\}$ but can have other solutions outside that set, the number and nature depending on the features of the chosen L . Those spurious solutions can be avoided in two ways: Either we build S on an L that is injective on its entire domain (i.e., there are no two f and g for which $L[f] = L[g]$) or we restrict the search for solutions to the set $\{G\}$. Unfortunately, neither option is easy to realize, the first one for a lack of methods to build L with the desired properties and the second for a lack of a complete characterization of the set $\{G\}$.

For instance, it was suggested [23] that the spurious solutions found by Kozik *et al.* could have been identified as unphysical by looking at their analytic structure in frequency space, which for physical Green’s function is expected to be a sum of poles [24]. Although this might be true in this specific case, more generally, for what is known, the pole structure is only a *necessary* feature of physical Green’s functions, therefore we cannot exclude situations in which spurious solutions arising in other contexts come in the form of a sum of poles. In the case of nonrelativistic electrons, for instance, the problem of a complete characterization of the set $\{G\}$ covers the more specific problem of finding all necessary constraints to the charge density (in DFT context called v representability), which to date remains unsolved (see Ref. [25] and references therein).

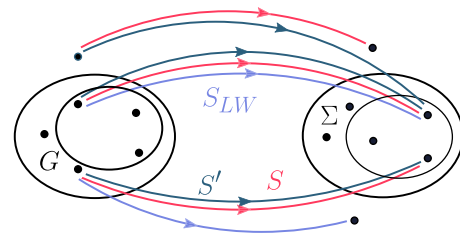


FIG. 4. Left outer set: physical Green’s functions; right outer set: physical self-energies. S and S' are two distinct functionals for which $S[G] = S'[G] = \Sigma$. S_{LW} represents the skeleton series introduced by Luttinger and Ward. It satisfies $S_{LW}[G] = \Sigma$ but not for all physical G ’s.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

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 noninjective 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 [Eqs. (2) and (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 $G = X + XS[G]G$, is a *linear* equation whose unique solution is $X = (S[G] + G^{-1})^{-1}$ which readily simplifies to $X = (L[G]^{-1} - G^{-1} + G^{-1})^{-1} = L[G] = G_0$.

III. SELF-CONSISTENT APPROACH TO THE HUBBARD ATOM

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 $S[f] \equiv L[f]^{-1} - f^{-1}$ 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 [6]. 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 Sec. 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 skeleton series has two branches, and one may talk about the ‘nonexistence of the Luttinger Ward functional.’

In the following (Sec. III C) 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 functionals 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 us 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 functions. 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 noninjective and the search of solutions is not restricted to the set of physical noninteracting Green’s functions. Moreover, the formal perturbative 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 evaluated at G will be shown to converge to the correct self-energy only in a subregion of the parameter space. Finally, 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

$$\hat{H} = \frac{U}{2} \sum_{\sigma, \sigma' = \uparrow, \downarrow} \hat{c}_{\sigma}^{\dagger} \hat{c}_{\sigma'}^{\dagger} \hat{c}_{\sigma'} \hat{c}_{\sigma}, \quad (9)$$

where $\hat{c}_{\sigma}^{(\dagger)}$ is a fermionic annihilation (creation) operator and $U > 0$ is the interaction parameter. In order to establish a close connection to [6], we calculate the finite temperature one-body Green’s function in the grand canonical ensemble, which is defined as [15]

$$G_{\sigma\sigma'}(\mathbf{r}, \tau; \mathbf{r}', \tau') = \frac{\text{Tr}\{e^{-\beta(\hat{H} - \mu\hat{N})} \mathcal{T}[\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}, \tau) \hat{\psi}_{\sigma'}(\mathbf{r}', \tau')]\}}{\text{Tr}\{e^{-\beta(\hat{H} - \mu\hat{N})}\}}, \quad (10)$$

where \hat{N} is the number operator, μ is the chemical potential, \mathcal{T} orders operators according to their value of τ , $\hat{\psi}_{\alpha}(\vec{x}, \tau)$ is the field operator and $\beta = 1/(k_B T)$ with T the temperature, and k_B is the Boltzmann constant. The frequency Fourier transform to imaginary frequencies yields the Matsubara Green’s function [15]. For the Hubbard atom (9) we have

$$G_{\sigma\sigma'}(z) = \frac{\delta_{\sigma\sigma'}}{e^{2\beta\mu} + 2e^{\beta(\mu+U)} + e^{\beta U}} \times \left(\frac{e^{\beta(\mu+U)} + e^{\beta U}}{\mu + z} + \frac{e^{2\beta\mu} + e^{\beta(\mu+U)}}{\mu - U + z} \right). \quad (11)$$

Choosing the chemical potential to be $\mu = U/2$ yields $G_{\sigma\sigma'}(z) = \mathcal{G}(z)\delta_{\sigma\sigma'}$ with

$$\mathcal{G}(z) \equiv \frac{1}{2} \left(\frac{1}{z + U/2} + \frac{1}{z - U/2} \right) \quad (12)$$

$$= \frac{1}{z} \frac{1}{1 - U^2/(4z^2)} \quad (13)$$

and

$$z \equiv i\omega_n \quad \text{and} \quad \omega_n \equiv k_B\pi T(2n + 1), \quad n \in \mathbb{Z}. \quad (14)$$

Following Kozik *et al.*, we define the corresponding noninteracting Green’s function by setting U to 0, which yields

$$\mathcal{G}_0(z) \equiv \frac{1}{z}. \quad (15)$$

The self-energy is then defined as

$$\Sigma(z) \equiv \mathcal{G}_0(z)^{-1} - \mathcal{G}(z)^{-1} = \frac{U^2}{4z}. \quad (16)$$

Strictly speaking, the noninteracting Green's function should be calculated at the same chemical potential as the interacting one [namely by setting $U \rightarrow 0$ in (11) and then choosing the chemical potential $\mu = U/2$] and should therefore read

$$\mathcal{G}_0(z) = \frac{1}{z + U/2}. \quad (17)$$

With this choice, the self-energy would contain an additional term $-U/2$ with respect to (16), stemming from the difference of the inverse of the two noninteracting Green's functions. This is simply a constant shift, which has no influence on our discussion. Here we adopt the definition of Kozik *et al.*, namely (15), in order to facilitate the comparison with that work.

C. The map $\{\mathcal{G}_0\} \leftrightarrow \{\mathcal{G}\}$

In a Hubbard model with $N > 1$ sites at finite temperature, what identifies a specific system, and hence the corresponding Green's function, is the value of the temperature T , the chemical potential μ 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 hopping is possible, so U is simply a *constant* that sets the energy scale. Moreover, in our case the chemical potential 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 $\{\mathcal{G}(z)\}$ is defined as the set of all and only the functions in $n \in \mathbb{Z}$ obtained from (12) and (14) by varying $T \in (0, \infty)$. In other words, any function of n that cannot be written as (12) for a certain value of T will be considered an 'unphysical' Green's function. The set of physical noninteracting Green's functions $\{\mathcal{G}_0(z)\}$ 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 space of physical temperatures $\{T; T > 0\}$, the one-to-one-ness of the map $\{\mathcal{G}_0(z)\} \leftrightarrow \{\mathcal{G}(z)\}$ can be proved as a consequence of the one-to-one-ness of the maps $\{T\} \leftrightarrow \{\mathcal{G}_0(z)\}$ and $\{T\} \leftrightarrow \{\mathcal{G}(z)\}$, as follows.

Let us first look at $\{T\} \leftrightarrow \{\mathcal{G}_0(z)\}$. Since we have that physical \mathcal{G}_0 's are defined starting from physical temperatures (i.e., for any physical temperature there is one physical $\mathcal{G}_0(z)$: $\{T\} \rightarrow \{\mathcal{G}_0(z)\}$), we need to prove that every physical T corresponds to only one $\mathcal{G}_0(z)$. If T' and T gave rise to the same $\mathcal{G}_0(z)$ we could write

$$\frac{1}{i(2n+1)\pi k_B T} = \frac{1}{i(2n+1)\pi k_B T'}. \quad (18)$$

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

Concerning the map $\{T\} \leftrightarrow \{\mathcal{G}(z)\}$, we have that $\{T\} \rightarrow \{\mathcal{G}(z)\}$ is again realized by definition, while for the inverse

map we must solve the equivalent of (18) which reads:

$$\begin{aligned} & \frac{1}{2} \left(\frac{1}{i(2n+1)\pi k_B T' + \frac{U}{2}} + \frac{1}{i(2n+1)\pi k_B T' - \frac{U}{2}} \right) \\ &= \frac{1}{2} \left(\frac{1}{i(2n+1)\pi k_B T + \frac{U}{2}} + \frac{1}{i(2n+1)\pi k_B T - \frac{U}{2}} \right) \end{aligned} \quad (19)$$

which *per se* has two solutions:

$$T' = T \quad \text{and} \quad T' = \frac{U^2}{4\pi^2 k_B^2 (2n+1)^2 T}. \quad (20)$$

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 $\{T\} \leftrightarrow \{\mathcal{G}_0(z)\}$ and $\{T\} \leftrightarrow \{\mathcal{G}(z)\}$ holds, one can then conclude that $\{\mathcal{G}_0(z)\} \leftrightarrow \{\mathcal{G}(z)\}$.

D. Explicit functionals

Both sets $\{\mathcal{G}_0(z)\}$ and $\{\mathcal{G}(z)\}$ are only a subset of the set of all rational functions or the even bigger set of analytic functions. It follows that there can be different functionals realizing the maps $\{\mathcal{G}_0(z)\} \leftrightarrow \{\mathcal{G}(z)\}$, characterized by inequivalent results outside those sets. A specific functional realizing the map $\{\mathcal{G}_0(z)\} \rightarrow \{\mathcal{G}(z)\}$ is

$$F_W(n, [f]) \equiv \frac{f(n)}{1 - f(n)^2 \frac{U^2}{4}}. \quad (21)$$

F_W is in fact a simple *function* which has the same structure of the ones studied by Rossi *et al.* and Schäfer *et al.* [8,11] and first introduced by Stan and collaborators [10] in the context of the so called one point model (OPM) [26,27]. The functional takes as input any function $f(n)$, not just noninteracting Green's functions. It cannot accommodate, however, all possible variations, for example, with respect to a spin-dependent external potential; so it cannot give rise to the Hubbard atom Green's function of, for instance [28], and cannot be used to explore the vertex of the Bethe-Salpeter equation, like in Ref. [8]. However, it is perfectly sufficient for the purpose of our work here. A functional realizing the inverse map $\{\mathcal{G}_0(z)\} \leftarrow \{\mathcal{G}(z)\}$ is

$$L_W(n, [f]) \equiv \left(i(2n+1) \frac{U}{2} \sqrt{-\frac{\frac{1}{3} + \frac{f(-1)}{f(1)}}{3 + \frac{f(-1)}{f(1)}}} \right)^{-1}. \quad (22)$$

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. (12) and (15). A difference that will play a central role in our later discussion (Secs. III F to III H) is that F_W is completely *local* in (Matsubara) frequency space (the value of $F_W[G]$ at a

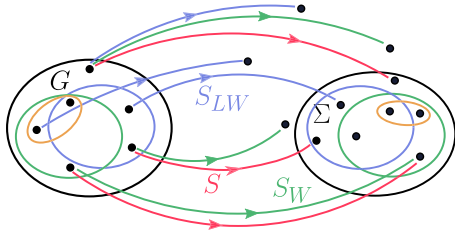


FIG. 5. A self-energy functional S realizes the map $\{G\} \rightarrow \{\Sigma\}$ for all physical G 's (black sets). Just like the skeleton series S_{LW} satisfies $S_{LW}[G] = \Sigma$ only for certain G 's (blue subsets), so does S_W for which $S_W[G] = \Sigma$ (green subsets). Contrary to S_{LW} , the subset for which $S_W[G] = \Sigma$ (orange subsets) includes all G 's of the Hubbard atom.

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 $\mathcal{G}_0(z)$'s, and a prefactor that depends on f in a nonlocal 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

$$S_W[f] \equiv L_W[f]^{-1} - f(n)^{-1} \\ = i(2n + 1) \frac{U}{2} \sqrt{-\frac{\frac{1}{3} + \frac{f(-1)}{f(1)}}{3 + \frac{f(-1)}{f(1)}} - \frac{1}{f(n)}}. \quad (23)$$

From that we can build the SCDE

$$X = \mathcal{G}_0(z) + \mathcal{G}_0(z)S_W[X]X \quad (24)$$

with X an unknown function of n (see Fig. 5). As pointed out in Sec. II B, (23) with (24) are equivalent to $\mathcal{G}_0(z) = L_W[X]$.

L_W is not injective: For instance, $L_W[X] = L_W[X + f]$ with f any function for which $f(-1) = 0$. It follows that, given $\mathcal{G}_0(z)$, this equation has multiple solutions. However, Eq. (24) has only one solution if we restrict our search to the set $\{\mathcal{G}(z)\}$. To see this explicitly, we use the expression for $\mathcal{G}_0(z)$:

$$\frac{1}{i(2n + 1)k_B\pi T} = L_W[X]. \quad (25)$$

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

$$\frac{1}{i(2n + 1)k_B\pi T} = L_W[f_x(n)] \quad (26)$$

with

$$f_x(n) \equiv \frac{1}{2} \left(\frac{1}{i(2n + 1)\pi k_B x + \frac{U}{2}} + \frac{1}{i(2n + 1)\pi k_B x - \frac{U}{2}} \right), \quad (27)$$

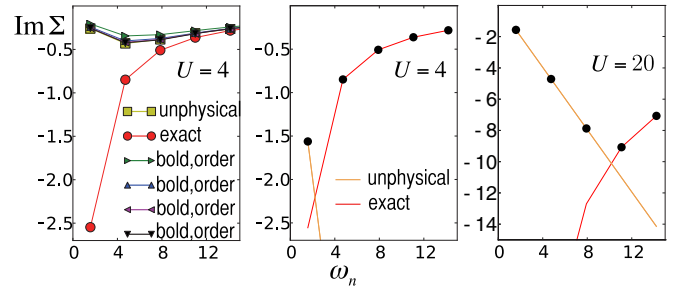


FIG. 6. Left panel: third panel of Fig. 3 from Ref. [6], representing the physical (red) and the unphysical (black) self-energies corresponding to the physical and the unphysical solutions to the inverse problem $F_{\text{QMC}}[X] = G$, with F_{QMC} the functional defined by the Quantum Monte Carlo code used in Ref. [6] to calculate G from a given G_0 . Second and third panel: physical (red) and unphysical (orange) self-energies corresponding to the physical and unphysical solutions to $F_W[X] = G$, for two different values of U .

where x is an unknown temperature. The evaluation of L_W defined in (22) on $f_x(n)$ leads to

$$L_W[f_x(n)] = \frac{1}{i(2n + 1)k_B\pi x}. \quad (28)$$

We can then write (26) as

$$\frac{1}{i(2n + 1)k_B\pi T} = \frac{1}{i(2n + 1)k_B\pi x} \quad (29)$$

from which we can determine x without ambiguities to be

$$x = T. \quad (30)$$

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 $F_W[X] = \mathcal{G}(z)$, in which $\mathcal{G}(z)$ is known and $\mathcal{G}_0(z)$ is to be found. The inverse problem has two solutions: the correct $X = 1/z$ and a spurious one $X = -\frac{4z}{U^2}$, which we will denote by $\mathcal{G}_u(z)$. Since there is no T such that $\mathcal{G}_0(z)$ can be written as $\mathcal{G}_u(z)$, $\mathcal{G}_u(z) \notin \{\mathcal{G}_0(z)\}$, $\mathcal{G}_u(z)$ is an unphysical solution, as expected. The correct solution is therefore identified without ambiguity by restricting the domain to $\{\mathcal{G}_0(z)\}$. If, like in Ref. [6], the domain is not properly restricted, the spurious solution survives, leading to a problem of ‘multiple solutions’ [10,23]. 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 $\mathcal{G}_u(z)$ does not correspond to the unphysical solution found by these authors. Since Ref. [6] 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 $\Sigma_u(z) \equiv \mathcal{G}_u(z)^{-1} - \mathcal{G}(z)^{-1}$. 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 noninteracting one [5]. One way to proceed can be summarized as follows: we first start with the perturbative expansion of G :

$$G = G_0 + vG_0^3 + v^2G_0^5 + \dots, \quad (31)$$

We then use (31) to write G_0 in terms of G :

$$\begin{aligned} G_0 &= G - (vG_0^3 + v^2G_0^5 + \dots) \\ \Rightarrow G_0 &= G - (v(G - (vG_0^3 + v^2G_0^5 + \dots))^3 + v^2G_0^5 + \dots) \\ \Rightarrow G_0 &= G - vG^3 - v^2(G^5 + GG^4) - \dots \\ &\dots \\ \Rightarrow G_0 &= G - vG^3 - v^2G^5 - \dots \end{aligned} \quad (32)$$

which is then used in the perturbative expansion of the self-energy (3) to get the formal definition of the skeleton series S_{LW} :

$$\begin{aligned} \Sigma &= vG_0 + v^2G_0^3 + \dots \\ \Rightarrow \Sigma &= vG - v^2G^3 - \dots \equiv S_{\text{LW}}[G]. \end{aligned} \quad (33)$$

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'', \dots on which each G_0 depends. This means that Perturbation Theory gives rise to a series of *nonlocal* 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

$$\mathcal{G}(z) = \mathcal{G}_0(z) + \mathcal{G}_0(z)^3 \frac{U^2}{4} + \mathcal{G}_0(z)^5 \frac{U^4}{16} + \dots \quad (34)$$

Note that this involves now *actual* multiplications, not convolutions. The *nonlocal* 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

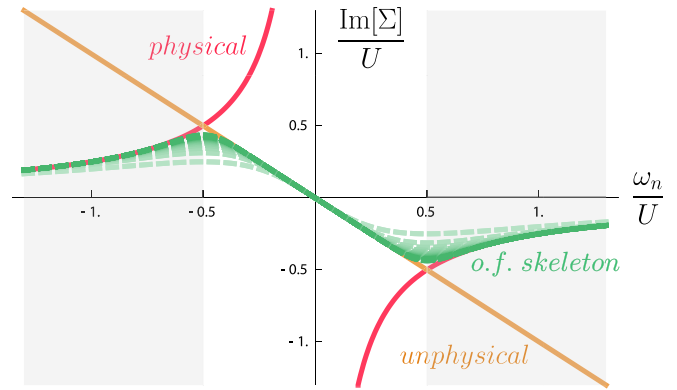


FIG. 7. The physical self-energy $\Sigma(i\omega_n) = -iU^2/(4\omega_n)$ (in red), the unphysical $\Sigma_u(i\omega_n) = -i\omega_n$ (in orange) and various orders of the one-frequency–skeleton series $S_{\text{ofs}}[\mathcal{G}(i\omega_n)]$ (35) (in shades of green) are represented. $S_{\text{ofs}}[\mathcal{G}(i\omega_n)]$ converges to the physical self-energy only in the region $U^2 \leq 4\omega_n^2$ (in gray).

perturbation theory. Nevertheless, it allows us to define a *local* series, by following the steps analogous to Eqs. (31)–(33). This leads to

$$\begin{aligned} S_{\text{ofs}}[\mathcal{G}(z)] &= \frac{U^2\mathcal{G}(z)}{4} - \frac{U^4\mathcal{G}(z)^3}{16} + \frac{U^6\mathcal{G}(z)^5}{32} \\ &\quad - \frac{5U^8\mathcal{G}(z)^7}{256} + \frac{7U^{10}\mathcal{G}(z)^9}{512} + \dots \end{aligned} \quad (35)$$

which defines the series of functionals

$$S_{\text{ofs}}[f] \equiv \frac{U^2 f}{4} - \frac{U^4 f^3}{16} + \frac{U^6 f^5}{32} - \frac{5U^8 f^7}{256} + \dots \quad (36)$$

This formal manipulation of the local series (34) 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 the correct self-energy, partially to a spurious $\Sigma_u(z)$, as shown in Fig. 7. As in the case of Kozik *et al.*, the unphysical self-energy corresponds to the unphysical solution of the inverse problem, $\Sigma_u(z) = \mathcal{G}_u(z)^{-1} - \mathcal{G}(z)^{-1}$ (see also Fig. 6).

Contrary to what was reported in Ref. [6] about the standard skeleton series, the convergence of S_{ofs} to the correct result always occurs in a finite range of ω_n at fixed U :

$$\begin{aligned} S_{\text{ofs}}[\mathcal{G}(i\omega_n)] &= \Sigma(i\omega_n) \quad \text{for } U^2 \leq 4\omega_n^2 \\ S_{\text{ofs}}[\mathcal{G}(i\omega_n)] &= \Sigma_u(i\omega_n) \quad \text{for } U^2 \geq 4\omega_n^2. \end{aligned} \quad (37)$$

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 $X = \mathcal{G}_0(z) + \mathcal{G}_0(z)S_{\text{ofs}}[X]X$ 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 [8,10,11], the series that defines S_{ofs} in (35) converges to

$$\check{\Sigma}[f] \equiv \frac{-1 + \sqrt{1 + U^2 f^2}}{2f} \quad (38)$$

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

$$\begin{aligned} \check{S}[\mathcal{G}(i\omega_n)] &= \Sigma(i\omega_n) \quad \text{for } U^2 \leq 4\omega_n^2 \\ \check{S}[\mathcal{G}(i\omega_n)] &= \Sigma_u(i\omega_n) \quad \text{for } U^2 \geq 4\omega_n^2, \end{aligned} \quad (39)$$

where the functional \check{S} is defined over a larger domain than S_{of_s} . We can therefore study the Dyson equation:

$$X = \mathcal{G}_0(i\omega_n) + \mathcal{G}_0(i\omega_n)\check{S}[X]X, \quad (40)$$

which is satisfied by $X = \mathcal{G}(i\omega_n)$ 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 :

$$x = \frac{1}{i\omega} + \frac{1}{i\omega} \left(\frac{-1 + \sqrt{1 + U^2 x^2}}{2x} \right) x \quad (41)$$

with $\omega \in \mathbb{R}$. If (41) has no solutions in a certain region of the parameter space, neither will (40). We recast (41) as

$$\frac{2\omega}{U} = -\frac{i(\sqrt{\xi^2 + 1} + 1)}{\xi}, \quad (42)$$

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

$$1 > \left| \frac{\sqrt{\xi^2 + 1} + 1}{\xi} \right|. \quad (43)$$

However, the right-hand side is always greater than 1, therefore this equation, and hence the original Dyson Eq. (40), has no solutions, *Q.E.D.* Clearly, this result relies on the closed-form character of the functional (38) we considered. The use of a truncation of the series S_{of_s} , which is always done in practice, could introduce more spurious solutions; this happens for example in the simple one-point model of [10] when only the lowest order contribution is used. However, a complete analysis of the equation with truncations of a self-energy functional is beyond the purposes of this work.

H. Local SIN series

In the previous section, we manipulated the perturbative expansion of a local functional realizing the map $\mathcal{G}_0(z) \rightarrow \mathcal{G}(z)$, 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 [6] 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 [10], we attempt therefore, for the simple Hamiltonian here considered, to build a series that *complements* the one-frequency-skeleton S_{of_s} . As outlined in Sec. II B, 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

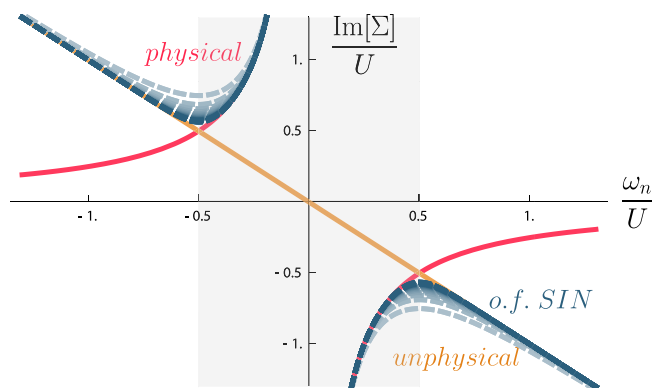


FIG. 8. The physical self-energy $\Sigma(i\omega_n) = -iU^2/(4\omega_n)$ (in red), the unphysical $\Sigma_u(i\omega_n) = -i\omega_n$ (in orange), and various orders of the one-frequency-SIN series $S_{ofSIN}[\mathcal{G}(i\omega_n)]$ (46) (in shades of blue) are represented. $S_{ofSIN}[\mathcal{G}(i\omega_n)]$ converges to the physical self-energy only in the region $U^2 \geq 4\omega_n^2$ (in gray).

could be noninjective 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 (21). This functional is not injective: its inverse is made of two branches,

$$\begin{aligned} F_1^{-1}[f] &\equiv \frac{2(\sqrt{U^2 f^2 + 1} - 1)}{U^2 f} \\ F_2^{-1}[f] &\equiv -\frac{2(\sqrt{U^2 f^2 + 1} + 1)}{U^2 f}. \end{aligned} \quad (44)$$

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 $\{G\}$:

$$\begin{aligned} F_1^{-1}[\mathcal{G}(z)] &= \mathcal{G}_0(z) \quad \text{for } U^2 \leq 4\omega_n^2 \\ F_2^{-1}[\mathcal{G}(z)] &= \mathcal{G}_0(z) \quad \text{for } U^2 \geq 4\omega_n^2. \end{aligned} \quad (45)$$

The local skeleton series S_{of_s} 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

$$S_{ofSIN}[f] = -\frac{1}{f} - S_{of_s}[f]. \quad (46)$$

which can be used to calculate S_{ofSIN} once S_{of_s} is provided.

As shown in fig. 8, the one-frequency-SIN series evaluated at $\mathcal{G}(z)$ converges to the physical self-energy in the region where S_{of_s} converges to the unphysical one, and vice versa. It follows that the corresponding SCDE $X = \mathcal{G}_0(z) + \mathcal{G}_0(z)S_{ofSIN}[X]X$ admits $X = \mathcal{G}(z)$ as solution in the range $U^2 \geq 4\omega_n^2$. An argument similar to 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, $X = \mathcal{G}(z)$ can not be found by simple iterative schemes such as

$X^{(n+1)} = G_0 + G_0 S_{\text{ofSIN}}[X^{(n)}]X^{(n+1)}$, and more sophisticated root-finding algorithms are required.

Finally, we notice that the two functionals S_{ofs} and S_{ofSIN} can be combined to make a proper self-energy functional as

$$\begin{aligned} \tilde{S}[f] &\equiv \theta(zf(z) - 1/2)\check{S}[f] \\ &\quad + (1 - \theta(zf(z) - 1/2))\left(-\frac{1}{f(z)} - \check{S}[f]\right) \\ &= -\frac{1}{f(z)} + \frac{1}{2} \frac{U^2 f(z)}{-1 + \text{sgn}(zf(z) - \frac{1}{2})\sqrt{1 + U^2 f(z)^2}} \end{aligned} \quad (47)$$

for which $\tilde{S}[\mathcal{G}(z)] = \mathcal{G}_0(z)^{-1} - \mathcal{G}(z)^{-1}$ on the entire parameter space, like in the case of S_W of (23).

IV. 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 [6] 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 noninteracting 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 $G_0 \rightarrow G$ (or $G \rightarrow G_0$) can indeed be realized by functionals that take different values when evaluated *outside* the set of physical Green's functions $\{G_0\}$ (or $\{G\}$). The distinction between map and functional also clarifies the apparent contradiction with the conclusion of Kozik *et al.* that “[...] the map $G_0 \rightarrow G$ [is] not invertible,” which, in light of our discussion, has to be read as “the functional used to realize the map $G_0 \rightarrow G$ becomes noninjective 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 $G_0 \rightarrow G$ and $G \rightarrow G_0$, 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 $G_0 \rightarrow G$ and $G \rightarrow G_0$, 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 spurious, unphysical solutions alongside the physical one. For the general case, we showed that the SCDE has exactly one physical solution as long as $\{G_0\} \leftrightarrow \{G\}$ 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 counterexample 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. [6]; 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 a one-point model in Ref. [10]. 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 (46), 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 noninteracting Green’s function?

ACKNOWLEDGMENTS

The authors would like to thank all attendees to the Workshop “Multiple Solutions in Many-Body Theories” held in Paris the 13th and 14th of June 2016 for interesting discussions. The research leading to these results has received funding from the European Research Council under the European Union’s Seventh Framework Programme (FP/2007–2013)/ERC Grant Agreement No. 320971.

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