Multiplicity of solutions to *GW*-type approximations

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We show that the equations underlying the *GW* approximation have a large number of solutions. This raises the question, how can we find the physical solution? We provide two theorems which explain why the methods currently in use usually find the correct solution. These theorems are general enough to cover a large class of similar methods. An efficient algorithm for including self-consistent vertex corrections well beyond *GW* is described and used in a numerical validation of the two theorems. The effect of a simple mixing scheme on solutions obtained iteratively is also investigated.

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I. INTRODUCTION

The *GW* approximation [1,2] is a state-of-the-art many-body technique for accurate determination of the spectral density function. This may be directly compared with experimental data such as that from photoemission experiments. Its success in predicting the band gaps of insulators, as well as its parameter-free nature, makes it a crucial scheme in condensed matter physics, especially for *predicting* material properties.

The self-consistent *GW* approximation is a fixed point method involving multidimensional objects like the Green's function and the self-energy. It was demonstrated recently, for an artificial one-point-model [3–6], that this fixed point is not unique and that a different way of iterating the equations can lead to a different solution [3]. It was further argued that including vertex corrections [1,7–10] could exacerbate this nonuniqueness problem. This would of course have serious consequences for condensed matter physics, which relies on *GW* method for being predictive.

However, so far as we can ascertain, extra solutions for practical *GW* calculations have never been reported in the literature. It is therefore of considerable importance to understand why these methods appear to provide unique solutions and how one can go beyond *GW* without encountering unphysical solutions. In order to do this, we first present a new algorithm for computing the self-energy. We then investigate the nature of the additional solutions numerically and provide general theorems which explain why the methods currently in use do indeed lead to a unique solution, independent of the starting point [11]. Since we cover a large class of approximations, these results not only validate *GW* calculations but also provide conditions on any future developments which would go beyond the *GW* approximation.

II. HEDIN'S EQUATIONS

The starting point are the Hedin equations, which appear as Eqs. (A22)–(A25) in the appendix of the 1965 article of Hedin [1]. We rewrite them here in modern notation:

$$\Gamma(1,2;3) = \Gamma_0(1,2;3) + \frac{\delta\Sigma(1,2)}{\delta V(3)}, \tag{1}$$

$$\Sigma(1,2) = i\lambda \int G(1,4)W(1^+,3)\Gamma(4,2;3)d(3)d(4), \tag{2}$$

$$\Pi(1,2) = -i\lambda \int G(2,3)G(4,2^+)\Gamma(3,4;1)d(3)d(4), \tag{3}$$

$$\frac{\delta G(1,2)}{\delta V(3)} = \int G(1,4)G(5,2)\Gamma(4,5;3)d(4)d(5), \tag{4}$$

$$\frac{\delta W(1,2)}{\delta V(3)} = \int W(1,4)W(5,2)\frac{\delta\Pi(4,5)}{\delta V(3)}d(4)d(5). \tag{5}$$

In these equations G is the Green's function, W is the renormalized Coulomb propagator [12], Σ is the self-energy, Π is the polarization, $\Gamma_0(1,2;3) = \lambda\delta(1,2)\delta(1,3)$ is the bare vertex, Γ is the renormalized vertex, λ is the coupling constant, and the potential differential δV is the sum of the external and Hartree contributions. The notation $(1) \equiv x_1 \equiv (\mathbf{r}_1,\sigma_1,t_1)$ is used throughout [13].

Also note that we introduced the coupling constant λ such that in the noninteracting case the vertex function vanishes [13]. One could also have defined it in such a way that the Coulomb propagator vanishes. It is more traditional to do the latter, i.e., to multiply the bare Coulomb propagator with λ. However, in order to stay consistent with the quantum field theory (QFT) roots of the problem, the correct approach is to multiply the bare vertex with λ. This is equivalent to the prefactor of the gauge coupling term in QFT. Using simple transformations [introduced later in Eq. (10): use $a = 1$, $b = \lambda^2$, $c = \lambda^{-1}$] one can show that these definitions are actually equivalent. The physical meaning of this is that it does not matter whether we define the noninteracting limit by switching off the interaction of the electrons with the photons, or by setting the photon propagator to zero.

Hedin showed how one can obtain an expansion of the vertex, and hence of Σ and Π, in terms of the renormalized quantities G and W using these equations [1]. This way one gets Σ and Π as *functionals* $\Sigma[G,W]$ and $\Pi[G,W]$. In addition to the five Hedin equations, there are two coupled Dyson equations:

$$\begin{aligned} G(1,2) &= G_0(1,2) + \int G_0(1,3)\Sigma(3,4)G(4,2)d(3)d(4), \\ W(1,2) &= v(1,2) + \int v(1,3)\Pi(3,4)W(4,2)d(3)d(4), \end{aligned} \tag{6}$$

where G_0 is the Green's function of the noninteracting system (which includes the Hartree potential) and $v(1,2) = \delta(t_1 - t_2)/|\mathbf{r_1} - \mathbf{r_2}|$ is the bare Coulomb propagator.

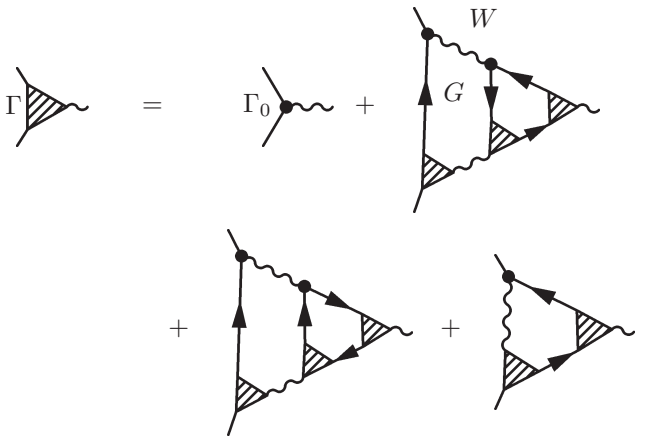
Solving the Dyson equations in conjunction with the Hedin equations yields the functionals $G[G_0,v]$ and $W[G_0,v]$.

The separation of the problem into equations for Σ and Π as functionals of G and W, as well as G and W as functionals of G_0 and v is an important conceptual step. In a later article by Hedin and Lundqvist [14], the equations are combined and the functional derivative $\delta\Sigma/\delta G$ is introduced. We should stress that this vertex equation together with Eqs. (2), (3), and the Dyson equations are not immediately useful. One also needs Eqs. (4) and (5) in order to obtain an expansion of the vertex beyond Γ_0 (alternatively one can work with a different vertex equation, that was derived in Ref. [9]).

A. Algorithms for Hedin's equations (GW approximation and beyond)

The first aim of this work is propose a useful algorithm to go well beyond the GW approximation. This algorithm has to be feasible in terms of memory and computer time. Almost all practical calculations of Hedin's equations use the GW approximation. This amounts to approximating the full vertex Γ by the bare vertex, and thus the self-energy takes on the simple form $\Sigma(1,2) = i\lambda^2 G(1,2)W(1,2)$. In the present work we describe a new algorithm for solving Hedin's equations which includes not only the GW approximation but also corrections far beyond the GW approximation.

In order that an algorithm be feasible, we need to consider the computational resources needed. The storage requirements of first order perturbation theory for the vertex scales as N^3 and the corresponding number of operations scales as N^4, where N is the number of basis functions as detailed in the next paragraph. Algorithm I presented below for calculating $\Sigma[G,W]$ and $\Pi[G,W]$ is considerably more sophisticated than the GW approximation but without worsening this scaling. Note that all the relations in the algorithm are exact apart from the two which have the derivatives of Γ removed; these would require N^4 storage. Solving Algorithm I together with the Dyson equations we refer to as the "Starfish" algorithm. It is interesting to work out which diagrams this algorithm corresponds to: finding the self-consistent solution to Starfish is equivalent to solving



(7)

self-consistently with the equations for Σ, Π, G, and W [Eqs. (2), (3), and (6)].

Algorithm 1 Hedin equations solver for $\Sigma[G,W]$ and $\Pi[G,W]$. Here the shorthand $G'(1,2;3) = \delta G(12)/\delta V(3)$, etc., is used and the function arguments are omitted.

Require: G and W
  Set $\Gamma = \Gamma_0$
  repeat
    $G' = \int G\,G\,\Gamma$
    $\Pi' = -i\lambda \int (G'\,G\,\Gamma + G\,G'\,\Gamma + G\,G\,\Gamma')$
    $W' = \int W\,W\,\Pi'$
    $\Sigma' = i\lambda \int (G'\,W\,\Gamma + G\,W'\,\Gamma + G\,W\,\Gamma')$
    $\Gamma = \Gamma_0 + \Sigma'$
  until Γ converged
  $\Sigma = i\lambda \int G\,W\,\Gamma$
  $\Pi = -i\lambda \int G\,G\,\Gamma$

III. NUMBER AND STABILITY OF SOLUTIONS

Before exploring the above algorithm numerically, we turn our attention towards the second aim of this paper, i.e., the number and nature of solutions of the Hedin equations within GW-type approximations. This question is of central importance because the predictive power of this method relies crucially on the assumption that there is a single unique solution to which the iterative process leads. If this assumption is not true then one needs to know under which conditions correct convergence can be achieved.

In order to closely examine the solutions to these equations, discretization of space-time is required. Such a discretization is done for all practical calculations; however, its impact on the equations is largely ignored; upon discretization one loses the physical meaning of these equations. As in the past, the present work assumes that there are N space-time points in total, and that limits in the time variable such as $G(4,2^+)$ are taken to mean $G(4,2)$. It will be assumed that the true physical solution can be recovered in the continuum limit when $N \to \infty$. The Dirac delta function in Eq. (1) now becomes a Kronecker delta function. One could just as well imagine using a basis other than (x,σ,t), for instance an orbital-frequency basis in order to perform such a discretization. In this discrete space, all eigenstates and eigenvalues of the Hamiltonian are *analytic* functions of λ on the whole real axis [15]. Consequently phenomena like phase transitions can be described only in the $N \to \infty$ limit.

The equations to be solved now form a closed system of *polynomial equations*. This enables us to state and prove several general theorems. To do so we define a concise notation. Let

$$F \equiv (G,W,\Pi,\Sigma,\Gamma) \in \mathbb{C}^n$$

be the vector of all dependent (or unknown) variables. Here $n = 4N^2 + N^3$ is the number of unknowns. We regard the

matrices G_0 and v (and the bare vertex) as known and fixed. Equations (2), (3), and (6), and a vertex equation like Eq. (7), can now be written in a compact form as $F = \mathfrak{g}(F)$ or $\mathfrak{h}(F) = 0$ with $\mathfrak{h}(F) \equiv \mathfrak{g}(F) - F$, where $\mathfrak{g} = (\mathfrak{g}_1, \ldots, \mathfrak{g}_n)$ is a set of polynomials in several variables.

It is important to point out that most of the following considerations do not depend on the precise form of the vertex equation. For example the trivial vertex equation $\Gamma = \Gamma_0$ corresponding to the GW approximation is also allowed here. In this case one can eliminate the vertex from the equations and redefine $F, \mathfrak{g}$ and $\mathfrak{h}$ in order to include only the smaller set of quantities and equations. Similarly, if one were to fix W in the Starfish algorithm then F would be (G, Σ, Γ) and the equations for W and Π could be eliminated.

As we are interested in the dependence of these equations and their solutions on the coupling strength λ, the equations to be solved are

$$F = \mathfrak{g}^\lambda(F) \quad \text{or} \quad \mathfrak{h}^\lambda(F) = 0. \tag{8}$$

The solution is unique for the noninteracting case and we call this F^0.

We now want to establish the number of solutions to Eq. (8) for the interacting case. An upper bound is provided by Bézout's theorem [16], which states that the maximum number of solutions to a system of polynomial equations (if finite) is equal to the product of the total degree of each equation. Thus the GW approximation with fixed W has at most 2^{N^2} solutions, and the Starfish algorithm, also for fixed W, has at most $7^{N^3} 2^{2N^2}$ solutions. A similar observation for the number of solutions of the equations underlying Hartree-Fock calculations was made in Ref. [17]. There a *lower* bound for the number of solutions was also provided, which grew exponentially with the number of electrons in the system. For the case of Hartree-Fock and density functional theory calculations it has already been shown numerically that one can obtain more than one solution [18–20].

Buchberger's algorithm is a systematic method for determining the exact number of roots by decomposing the equations into a Gröbner basis [21]. This procedure is, however, computationally very demanding and can be performed only for small (and therefore nonphysical) N. If, for example, $N = 2$ then the GW approximation with fixed W turns out to have precisely 6 solutions for generic G_0 and W. Likewise, for $N = 1$ the Starfish algorithm yields 3 solutions. From these considerations, it seems quite surprising that self-consistent GW works at all for realistic values of N. We will now provide two theorems that may explain this apparent success.

Theorem 1. For all choices of Eq. (8) (e.g., GW), the solutions have the following properties:

(i) Equation(8) has one solution F^λ_{phys} that tends to F^0 in the noninteracting limit:

$$F^\lambda_{\text{phys}} \underset{\lambda \to 0}{\longrightarrow} F^0.$$

(ii) All other solutions tend to infinity:

$$\inf \left\{ \|F\| \,:\, \mathfrak{h}^\lambda(F) = 0,\ F \neq F^\lambda_{\text{phys}} \right\} \underset{\lambda \to 0}{\longrightarrow} \infty,$$

where $\|\cdot\|$ is, say, the Euclidean vector norm.

(iii) F^λ_{phys} is an analytic function w.r.t. λ in a vicinity of $\lambda = 0$.

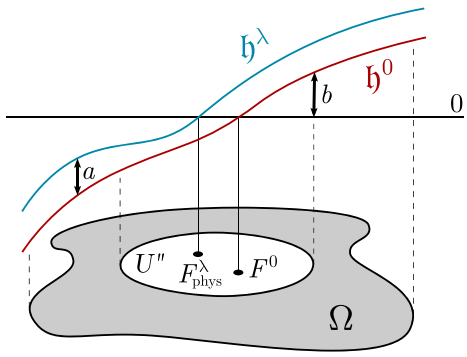


FIG. 1. (Color online) Schematic of the reasoning used in Theorem 1. Polynomial functions $\mathfrak{h}^0$ and $\mathfrak{h}^\lambda$ are drawn in red and blue on the domain $\Omega \subset \mathbb{C}^n$. The arrow at a represents the largest pointwise separation between $\mathfrak{h}^\lambda$ and $\mathfrak{h}^0$ on $\Omega \setminus U''$. The arrow at b represents $\inf_{F \in \Omega \setminus U''} \|\mathfrak{h}^0(F)\|$.

This behavior suggests that at least in some low coupling regime F_{phys} is indeed the physical solution while all others are far away from the correct result.

Proof. In the noninteracting case the Jacobian $\partial \mathfrak{h} / \partial F$ is a triangular matrix having -1's on the diagonal. Hence its determinant is not zero. In this situation the implicit function theorem [22] implies that one can solve for F as a function of λ in a neighborhood $U = U' \times U'' \subset \mathbb{C}^{n+1}$ of $(0, F^0) \in U$. It also implies that this function is analytic and that there is no other solution in U. This proves (i) and (iii).

Now for any compact set Ω where $\Omega \subset \mathbb{C}^n$ one can restrict λ such that $\mathfrak{h}^\lambda$ and $\mathfrak{h}^0$ are pointwise closer to each other in $\Omega \setminus U''$ than $\inf_{F \in \Omega \setminus U''} \|\mathfrak{h}^0(F)\| \neq 0$. This is schematically illustrated in Fig. 1. Then $\mathfrak{h}^\lambda$ has no zero in $\Omega \setminus U''$ and by the previous paragraph only F^λ_{phys} in U''. Since this can be done for any Ω this proves (ii). ■

Even though the above theorem suggests that a single well defined solution for GW (and beyond) exists in small coupling limit, it does not indicate how one can get to this solution and if converging to this solution is guaranteed. In practice, Eq. (8) is solved iteratively. That is, one starts with some initial guess F_0 which is inserted into the right hand side of $F = \mathfrak{g}(F)$, obtaining a new guess. Iterating this procedure defines a sequence

$$F_{i+1} = \mathfrak{g}(F_i). \tag{9}$$

A natural starting point for this is the non-interacting solution $F_0 = F^0$, but this is by no means necessary. For GW and similar schemes to work in any situation this sequence must converge to a fixed point, that is a solution to the equations. However, *a priori* it is unknown if the calculation will actually converge, and if a fixed point obtained this way actually corresponds to the *physical* solution. We now show that for weak coupling convergence to the unique solution is guaranteed.

Theorem 2. For small λ the physical solution F_{phys} is an attractive fixed point of Eq. (9). The size of the attracting region goes to infinity as $\lambda \to 0$.

Here *size* can be understood as the diameter of the largest ball that is contained in the attracting region.

Proof. It is sufficient to show that for any starting point we can restrict λ such that convergence to F_{phys} is guaranteed. For $a,b,c \in \mathbb{R}$ we define the following transformation:

$$\begin{aligned} G_0' &= aG_0, & v' &= bv, & \Gamma_0' &= c\Gamma_0, \\ G' &= aG, & W' &= bW, & \Gamma' &= c\Gamma, \\ \Sigma' &= a^{-1}\Sigma, & \Pi' &= b^{-1}\Pi, & \lambda' &= c\lambda, \end{aligned} \tag{10}$$

with $a^2bc^2 = 1$. (We will use these transformations in this section only to avoid confusion of the meaning of the primes with the derivatives as used earlier.) This transformation leaves Eq. (9) invariant:

$$F_{i+1}' = \mathfrak{g}'(F_i').$$

We now apply the transformation with, say, $a = \lambda^{1/4}, b = \lambda^{1/2}$, $c = \lambda^{-1/2}$. This way $\mathfrak{g}'$ depends on λ explicitly and implicitly through a, b, and c. Observe that *all* coefficients appearing in $\mathfrak{g}'$ tend to zero as $\lambda \to 0$. This is not true for the transformed starting values since the self-energy becomes larger due to the transformation. This is repaired by the first iteration: the quantities $F_1{}' = \mathfrak{g}'(F_0{}')$ tend to zero as $\lambda \to 0$. In this situation Banach's fixed point theorem can be applied, with the map $\mathfrak{g}'$ defined in an appropriate neighborhood of zero that contains $F_1{}'$. We can conclude that for small λ the transformed quantities tend to a fixed point. Since the transformation can be inverted, this remains true for the original quantities. By Theorem 1 for small λ the solution F_{phys} is the solution nearest to the noninteracting one. Hence the fixed point obtained is indeed F_{phys}. ■

Both theorems apply not only to the mentioned examples but to a large class of algorithms: it has already been demonstrated that they apply to different vertex equations. Another example would be the Dyson equations in solved form, e.g., $G = (1 - G_0\Sigma)^{-1}G_0$. This does not change the proof of Theorem 1 at all. For Theorem 2 one would need the additional assumption that in the first step the matrix inverse exists. Then it will also exist in subsequent steps provided λ is small enough and, owing to the same arguments as before, F_i would converge to the physical solution.

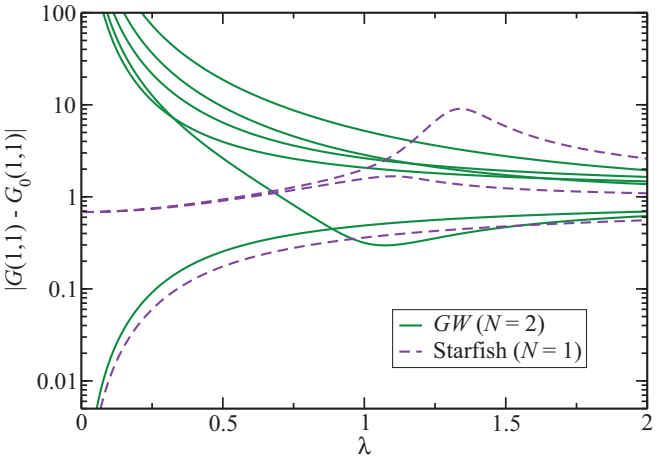


FIG. 2. (Color online) Plot of the distance of a matrix element of the Green's function to the non-interacting one versus the coupling strength λ for all possible solutions of GW with $N = 2$ and Starfish with $N = 1$, for random G_0 and W. W is kept fixed in both cases. Only one solution tends to the non-interacting one for the weak coupling limit.

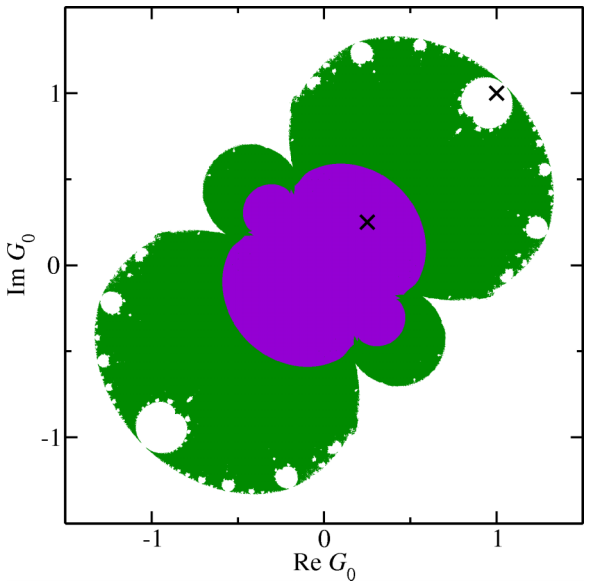


FIG. 3. (Color online) Domain of convergence of GW (green) and Starfish (purple) with $N = 1$ for input values of G_0 in the complex plane, when using the noninteracting solution as starting point. Here $v = 1$ and $\lambda = 1$. The crosses mark the chosen G_0 for investigating the starting point dependence while fixing G_0; see Fig. 4.

IV. NUMERICAL INVESTIGATION

Numerical checks of the above theorems were performed for both self-consistent GW and the Starfish algorithm. In

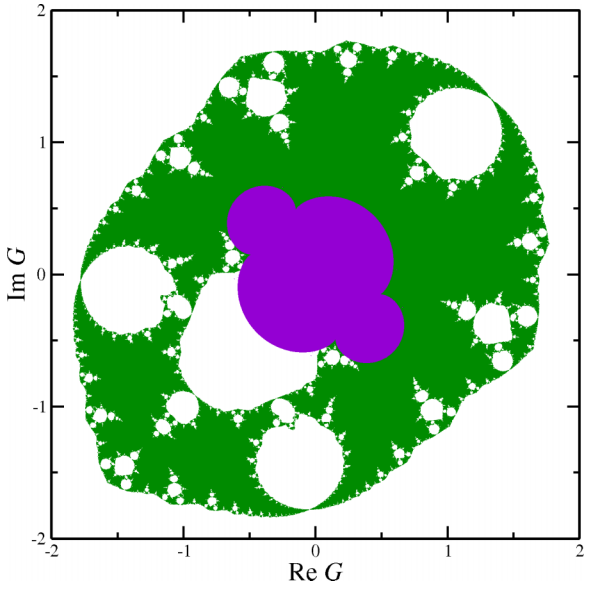


FIG. 4. (Color online) Domain of convergence of GW (green) and Starfish (purple) with $N = 1$ for different starting points of the fixed point cycle. The values of G_0 are fixed to $1 + i$ for GW and $1/4 + i/4$ for Starfish, as indicated by the crosses in Fig. 3.

order to demonstrate the multiplicity of solutions we need to obtain all of them, which is possible only for a very small N. For GW we set $N = 2$ and for Starfish we use $N = 1$. Plotted in Fig. 2 are *all* the solutions for these algorithms as a function of λ. The numerical input, in this case G_0 and W, were chosen to be random complex numbers, and W was kept fixed (which is common practice for real GW calculations). As mentioned earlier, there are 6 solutions in the GW case. Of these, 5 tend to infinity and the remaining solution tends to G_0 as $\lambda \to 0$. This is a visualization of Theorem 1. For Starfish 2 of the 3 solutions tend to a constant. This may appear to be in violation of the theorem but in this case the vertex Γ (and therefore F) diverges.

We can also examine the domains of convergence for both of these algorithms. For $N = 1$ we fix $v = 1$ and $\lambda = 1$ and plot the region of convergence of G_0 for the fully self-consistent GW and Starfish algorithm (for which W is also computed self-consistently) in Fig. 3. It can be observed that the region of stability shrinks for the higher-order method. Also noteworthy is that the region has a fractal boundary (this may be unsurprising since for case $G_0W = 1$ the domain is the Mandelbrot set). Perhaps more interesting is the region of *starting points* for which the algorithms converge. These are plotted in Fig. 4 for the same v and λ but this time with $G_0 = 1 + i$ for GW and $G_0 = 1/4 + i/4$ for Starfish, and with a variable starting point for G. These points are indicated by crosses in Fig. 3. Once again the region of convergence is smaller for Starfish, but in both cases *only one* solution is found, irrespective of the starting point. This is a numerical confirmation of Theorem 2. Note that for GW a situation was picked where the noninteracting starting point does *not* lead to convergence. Hence this can be considered a large coupling situation. But still there seems to be only one stable fixed point. The boundary of the region is also fractal (this corresponds to

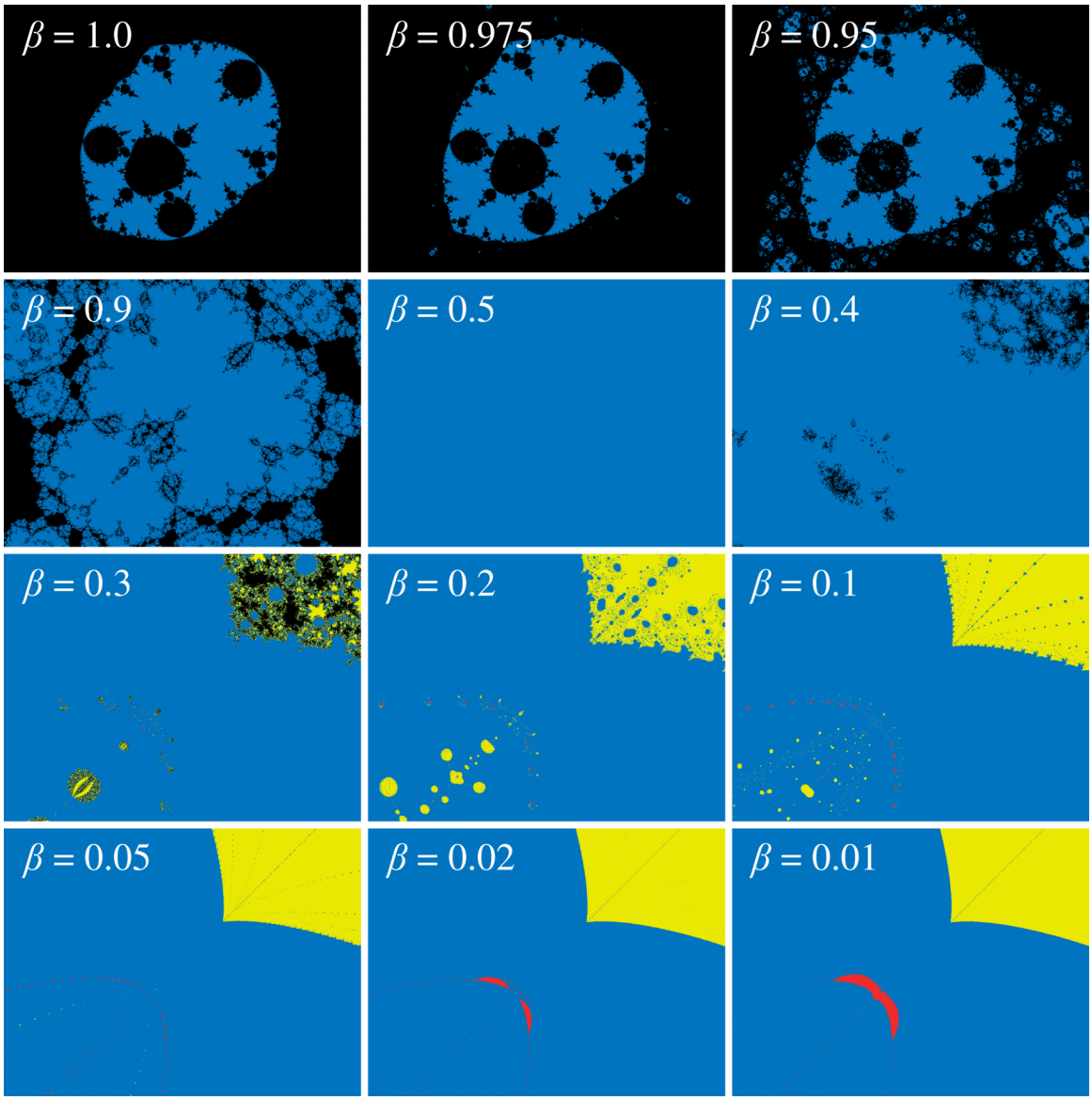


FIG. 5. (Color online) Domain of convergence of GW as a function of the mixing parameter β. Three different solutions are plotted with different colors: blue, yellow, and red. Black indicates nonconvergence.

the Julia set). Given the complexity of this boundary, even for the simple case of the GW approximation with $N = 1$, it appears impossible that in the general case one can find conditions on the starting point that will ensure convergence.

A. Mixing

In most realistic calculations of the self-consistent GW approximation, the previous and current quantities are mixed with one another using various mixing schemes [23]. This can both ensure convergence to the fixed point as well as accelerate it. In our notation, this is equivalent to modifying Eq. (9) as follows:

$$F_{i+1} = \beta \mathfrak{g}(F_i) + (1 - \beta)(F_i), \tag{11}$$

where, in general, β is a matrix. The modified map $\tilde{\mathfrak{g}} \equiv \beta \mathfrak{g} + (1 - \beta)I$ yields $\tilde{\mathfrak{h}}(F) = \beta(\mathfrak{g}(F) - F) = \beta \mathfrak{h}$. Thus if β is an invertible matrix then the fixed points of $\mathfrak{g}$ are preserved. We also note that a fixed point is asymptotically stable if all the eigenvalues of its Jacobian $\tilde{J} = \partial \tilde{\mathfrak{h}} / \partial F = \beta J$ have negative real parts. If any eigenvalue has a positive real part, then the fixed point is unstable. One may therefore choose the matrix β such that the eigenvalues of $\tilde{J}$ have arbitrary real parts. In this way particular fixed points can be made either stable or unstable as desired.

To illustrate the utility of mixing we recalculate the stability regions in Fig. 4 for the GW approximation by mixing the Green's function alone,

$$G_{i+1} = \beta G_i + (1 - \beta) G_i,$$

with β taken to be a positive real number. The effect of this is plotted in Fig. 5.

Two interesting aspects are observed: first, the domain of convergence increases dramatically with decreasing mixing parameter β; and second, *different solutions* emerge as a function of β (these are indicated by three different colors in the plot). Note that for $\beta = 1$ only one solution was found. These observations may have consequences for realistic GW calculations, namely that adjusting the mixing parameter can fundamentally change the obtained solution. In our simple example, we chose β to be a positive real number but it could also have been negative, complex, a diagonal matrix with nonzero entries, or a general invertible matrix.

V. CONCLUSION

We have argued that truncating Hedin's equations to some order yields systems of polynomial equations which have a large number of solutions. As an example of this, the Starfish algorithm was introduced which includes vertex corrections beyond GW and consequently has even more fixed point solutions. Two theorems were presented that shed some light on the general behavior of these fixed points. In particular we have shown that there is exactly one solution that tends to the noninteracting case for small coupling, while all others are divergent in this limit. Numerical tests of self-consistent GW and the Starfish algorithm for small N demonstrated that the system also converges uniquely to one fixed point even for fairly large coupling. Furthermore, the region of stability may be fractal in nature, indicating that finding simple necessary and sufficient conditions for ensuring convergence of GW calculations *a priori* may be impossible. Last, we found that mixing current and previous solutions with a certain mixing parameter not only increases the radius of convergence but also allows different solutions to be obtained. This observation may be of use in realistic GW calculations to assist in finding these other solutions and investigate their properties.

ACKNOWLEDGMENTS

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[12] We stress that W and W_0 are two-point objects in contrast to the interactions being four point objects.

[13] Introducing two more integrations and using the bare vertex one can rewrite Eqs. (2) and (3) such that they involve tensor contractions only. That way, all our equations of interest, Eqs. (1)–(7) are basis independent, though the bare vertex becomes more complicated in a different basis. Also the coupling constant λ no longer appears anywhere else than in the definition of the bare vertex Γ_0.

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