Effective action approach to strongly correlated fermion systems

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We construct a new functional for the single particle Green’s function, which is a variant of the standard Baym Kadanoff functional. The stability of the stationary solutions to the new functional is directly related to aspects of the irreducible particle hole interaction through the Bethe Salpeter equation. A startling aspect of this functional is that it allows a simple and rigorous derivation of both the standard and extended dynamical mean field (DMFT) equations as stationary conditions. Though the DMFT equations were formerly obtained only in the limit of infinite lattice coordination, the new functional described in the work, presents a way of directly extending DMFT to finite dimensional systems, both on a lattice and in a continuum. Instabilities of the stationary solution at the bifurcation point of the functional, signal the appearance of a zero mode at the Mott transition which then couples to physical quantities resulting in divergences at the transition.

I. INTRODUCTION

Functional methods have long been used as a tool to study interacting systems. These involve techniques ranging from simple weak coupling perturbative methods to strong coupling expansions. Often, since it is not possible to sum the entire series of diagrams one takes recourse to various approximation schemes in the hope that they will capture some of the essential physics. In addition, functional methods, have a long history of systematizing these approximations. A direct way of testing the validity of any approximation is through the effective action approach to interacting systems. Typically, the effective action is obtained in terms of some relevant variable, for e.g. the density, magnetization, the order parameter, the single particle Greens function etc., as a perturbative series in the interaction. A well known and frequently used functional is the Baym Kadanoff functional \( \Gamma_{bk} \), which is the effective action for the single particle Green’s function \( G \). \( \Gamma_{bk} \) gives the free energy of the system at its stationary point which are known to be saddle points and not extrema. In order to use variational approximations on these functionals, the functional should be convex. This is the case when one performs Legendre transformations with respect to time or frequency independent quantities as in density functional theory. Very recently, a functional of the Green’s function whose minimum gives the local Green’s function of the Hubbard model on the Bethe lattice was investigated by one of us. This functional has several desirable properties, in particular it is a true extremum at the physical local Greens function. This motivates us to search for generalizations of the functional of Ref. to finite dimensions.

In this paper, we present a new functional \( \Gamma_{new} \) for the single particle Green’s function, for which we can show that its saddle point is in fact an extremum, in the case that the irreducible vertex function in the particle hole channel has a definite sign (see below for a precise definition). This functional has many other useful properties primarily in the context of dynamical mean field methods which can now be naturally viewed as an approximation to this functional. The paper is organized as follows: first we introduce the Baym Kadanoff functional and our proposed functional and obtain the conditions under which the saddle points of this functional are extrema. We then proceed to show that the dynamical mean field theory (DMFT) equations are a simple outcome of certain simple approximations on our functional, hence providing some justification for direct extensions of dynamical mean field theory to finite dimensions. We also discuss some potential applications pertaining to the Mott transition and the problem of adapting tight binding basis for dynamical mean field calculations.

II. THE BAYM KADANOFF FUNCTIONAL

Consider the partition function \( Z \) (or equivalently the free energy \( W \)) of a system of electrons moving in a crystal potential \( V_c(x) \) with Coulomb interactions \( V \)

\[
Z = \exp[-\beta W] = \int D[\psi^\dagger] \exp[-\int dx \psi^\dagger(x) [\partial_x - \frac{\nabla^2}{2m} + V_c(x)] \psi(x) - \frac{1}{2} \int dx dx' \psi^\dagger(x) \psi^\dagger(x') V(x-x') \psi(x) \psi(x)]
\]  (1)
Here \( x = (x, \tau) \) denotes the space-imaginary time coordinates. Our formulation is fairly general, it applies to both lattice models or continuum models. In the lattice case, the space coordinate \( x \) labels lattice sites and the integral symbol should be interpreted as a summation symbol over the lattice sites. We have omitted additional quantum numbers that can be carried by the field \( \psi \), such as spin and also orbital quantum numbers, in order not to clutter the notation.

The effective action for the single Green’s function \( G \) i.e., Baym Kadanoff functional, is defined as the Legendre transform of \( W \) with respect to the interacting single particle electron Green’s function \( G(x, y) \) i.e.,

\[
\Gamma_{bk}[G] = W[J] + JG
\]

where, \( W[J] \) denotes the free energy in the presence of an external source field \( J \) coupled to the electron Green’s function. Using the condition \( J = \delta \Gamma_{bk}/\delta G \) to eliminate \( J \) in (2), we obtain the Baym Kadanoff functional

\[
\Gamma_{bk} = [\text{Tr} \log G - \text{Tr}[G_0^{-1} - G^{-1}]]G + \Phi[G]
\]

where, \( G_0 \) is the non-interacting Green’s function and \( \Phi[G] \) is the sum of all two particle irreducible diagrams constructed using the interaction and \( G \). Stationarity yields the Dyson equation

\[
G^{-1} = G_0^{-1} - \Sigma[G]
\]

where \( \Sigma(x, y) = \delta \Phi/\delta G(y, x) \). At the saddle point (3), \( \Gamma_{bk} \) is just the free energy of the system. An effective action approach is most useful when the saddle points are extrema. This is related to the stability of stationary solutions, which demands that leading order fluctuations around the stationary solution (3), increase the energy. To obtain a formal criterion for stability, we first consider the fluctuations around the stationary solution

\[
\delta \Gamma = \Gamma[G + \delta G] - \Gamma[G] = \int \int \delta G(y, x) \frac{\delta^2 \Gamma}{\delta G(y, x) \delta G(u, v)} \delta G(v, u)
\]

where \( \Gamma \) is any functional. In the functional treatment, it is essential to note that any quantity \( O(x, y) \) is defined as \( O(x, y) = \langle x | O | y \rangle \) and hence should be viewed as a matrix in \( x \) and \( y \).

To examine the stability of a saddle point of the functional it is convenient to introduce a matrix \( \hat{C} \) which acts on the Matsubara frequencies without affecting the spatial coordinates i.e., \( \hat{C} \chi(i\omega_n, x, y) = \chi(-i\omega_n, x, y) \). Using the following property of Green’s functions \( G(i\omega_n, x, y)^* = G(-i\omega_n, x, y) \), which we assume to hold for the trial Green’s functions as well, we can rewrite (3) as

\[
\delta \Gamma = \sum_{n, m} \delta G(i\omega_n)^* \chi(i\omega_n, i\omega_m) \delta G(i\omega_m)
\]

The matrix \( \chi = \hat{C} \chi \) is defined by \( \chi = \delta^2 \Gamma/\delta G^2 \). While the frequency indices have been made explicit, matrix multiplication in the real or momentum space indices is implied. For the saddle point to be an extremum (maximum or minimum) the form defined by (3) has to be negative (positive). For \( \Gamma_{bk} \)

\[
\frac{\delta^2 \Gamma_{bk}}{\delta G(x, y) \delta G(u, v)} = -G^{-1}(y, u)G^{-1}(v, x) + \Gamma^{ph}(xy; uv)
\]

Here \( \Gamma^{ph}(xy; uv) = \langle xy | \Gamma^{ph} | vu \rangle = \delta^2 \Phi/\delta G(x, y) \delta G(u, v) \), is the irreducible vertex which describes the irreducible particle hole interaction in the two particle channel and should be viewed as a tensor in the indices \( x, y, u, v \). The analog of (3) in momentum space is

\[
\chi_{bk}(p_1, p_2, p_3, p_4) = -G^{-1}(p_2, p_3)G^{-1}(p_4, p_1) + \Gamma^{ph}(p_1, p_2, p_3, p_4)
\]

where, \( p = (p, i\omega_p) \) with \( \omega_p \) being the Matsubara frequencies. For \( \Gamma = \Gamma_{bk} \), using (8) in (3), we see that even in the non-interacting case, where \( \Phi \) is zero, the first term in (8) makes \( \Gamma_{bk} \) unbounded from below. To further illustrate this lack of stability in \( \Gamma_{bk} \), we consider the simple example of an electron gas with Coulomb interactions \( V(x) = V(x)\delta(t) \). Let \( V(q) \) be the Fourier transform of \( V(x) \). In the Hartree approximation, \( \Phi \) is frequency independent and and rewriting the spin and momentum indices explicitly,

\[
\Gamma^{ph}(p_1, p_2, p_3, p_4) = \delta(p_1 + p_3 - p_2 - p_4)V(p_3 - p_4)
\]

Substituting this in (9)
where, $G^{-1}(p) = i\omega_p - \epsilon_p$ and $\epsilon_p$ is the dispersion of the particles shifted by the Hartree self energy term $NV(0)$, with $N$ being the total number of particles.

We see from (10) that $\hat{\chi}_{bk}$, in the sector of zero total energy and momentum, $\hat{\chi}_{bk}$ decouples into $2 \times 2$ blocks in the non-interacting limit, with zero diagonal matrix elements and equal off diagonal matrix elements $\omega_n^2 + \epsilon^2$. Consequently, (6) has positive and negative eigenvalues even in the non-interacting case. The Hartree term adds the constant $NV(0)$ to all entries of $\hat{\chi}_{bk}$ . This results in the stationary solution remaining a saddle point rather than an extremum for small values of the interaction. Moreover, (10) shows that attractive interactions tend to further destabilize $\Gamma_{bk}$.

### III. A NEW FUNCTIONAL

To construct a functional with a different stability matrix, we modify $\Gamma_{bk}$ as follows:

\[
\Gamma_{\text{new}} = \Gamma_{bk} - \text{Tr} \log(1 - JG) - \text{Tr} JG
\]

In simple terms, we have changed the value of the functional away from the saddle point, by adding certain source dependent terms which vanish quadratically as the source is turned off. Note that though $\Gamma_{\text{new}}$ is closely related to $\Gamma_{bk}$, it is not a simple Legendre transform of the free energy in the presence of a source coupled to a simple composite operator. Using the relation $J = \delta \Gamma_{bk} / \delta G = G^{-1} - G_0^{-1} + \delta \Phi / \delta G$ in (11) we get

\[
\Gamma_{\text{new}} = -\text{Tr} \log[G_0^{-1} - \frac{\delta \Phi}{\delta G}] - \text{Tr} G \frac{\delta \Phi}{\delta G} + \Phi
\]

It is straightforward to check that though $\Gamma_{\text{new}}$ and $\Gamma_{bk}$ yield (3) and the same free energy at stationarity, their higher order derivatives evaluated at stationarity are different. This has profound implications for the stability.

The stability of a stationary solution is again described by (5, 6), with $\Gamma$ replaced by $\Gamma_{\text{new}}$. In the non-interacting case, $\Gamma_{\text{new}}$ is trivially a constant. The second derivative of $\Gamma_{\text{new}}$ at stationarity is

\[
\frac{\delta^2 \Gamma_{\text{new}}}{\delta G(x, y) \delta G(u, v)} = -\Gamma^{ph}(xy; uv) + \int_{abmn} G(a, m)\Gamma^{ph}(mn; xy)G(n, b)\Gamma^{ph}(ba; uv)
\]

A diagrammatic representation of the above equation is shown in Fig. 1. The integration over a variable $x$ denotes

![Diagram](image)

**FIG. 1.** Diagrammatic representation of the (13)

In momentum space, (13) reads

\[
\chi_{\text{new}}(l, m, p, q) = -\Gamma^{ph}(l, m, p, q) + \int_{k_1, k_2, k_3, k_4} G(k_1, k_2)\Gamma^{ph}(k_2, k_3, l, m)G(k_3, k_4)\Gamma^{ph}(k_4, k_1, p, q)
\]

where $\chi_{\text{new}}$ is the Fourier transform of the second derivative of $\Gamma_{\text{new}}$. In the translationally invariant case, defining the momentum transfer $Q = l - m = q - p$ (14) simplifies to (Fig. 2)

\[
\chi_{\text{new}}(l, p; Q) = [-\Gamma^{ph}(l, p; Q) + \int_k G(k - \frac{Q}{2})\Gamma^{ph}(k, l; Q)G(k + \frac{Q}{2})\Gamma^{ph}(k, p; Q)]
\]

For the stability analysis we limit ourselves to consider the case of zero transfer frequency $\omega_Q = 0$ since it is natural to expect that the leading instability sets in first at zero frequency. This is known to be the case of the two dimensional Hubbard model within the full parquet approximation as investigated by Bickers. To derive the conditions under which the stationary point is an extremum, we analyze the form of $\chi_{\text{new}}$, and then derive general stability conditions for it. The matrix $\Gamma^{ph}$ obeys the property $\Gamma^{ph\dagger} = \hat{C}\Gamma^{ph}\hat{C}$ and so do (GG) and $\chi_{\text{new}}$, implying that $\hat{\chi}_{\text{new}}$ and $\hat{C}\Gamma^{ph}$ are hermitian matrices. The particle hole kernel which enters in the Bethe Salpeter equation can be rewritten as
\[ (1 - G G_{ph}) = \sum \lambda_i |\phi_i\rangle \langle \phi_i | \] with all the eigenvalues \( \lambda_i \) positive as required by the stability requirements of the particle hole kernel. Moreover, \( \chi_{new} = -\sum \lambda_i C T^{ph} |\phi_i\rangle \langle \phi_i | \). If \( C T^{ph} \) is positive definite (negative definite), \( \chi_{new} \) is negative (positive) definite and hence the stationary solution denotes a maximum (minimum). Applying the same argument to \( \Gamma_{bk} \), we note that the functional is an extremum only if the Hermitian matrix \( C G G \) is positive or negative definite. Referring back to the previous section, we see that this is not the case even in the non-interacting limit where this operator has eigenvalues of both sign. To summarize, the instability of the stationary solutions of \( \Gamma_{new} \) is linked to physical instabilities in the particle hole sector. Since the eigenvalues of the Bethe Salpeter equation are always positive when the solution is stable, instabilities are signaled by the vanishing of an eigenvalue for the first time.

We now illustrate the stability analysis of \( \Gamma_{new} \) in the Hartree approximation. Using \( \chi_{new} \) in \( \Gamma_{new} \), we see that

\[ \chi_{new}(l, m, p, q) = \delta(l - m + p - q) \int_{k} G(k)G(k + l - m)V(1 - m)V(m - 1) - V(1 - m) \] (16)

As before we will consider the case of zero frequency and momentum transfer. Summing over the internal frequencies \( i \omega_k \) in \( \chi_{new} \) we obtain

\[ \chi_{new}(l, p; Q) = V(Q)[-1 + V(Q)] \int_{k} \left\{ n(k - Q) - n(k + Q) \right\} \right\} \right\} \] (17)

where, \( n(k) \) is the Fermi occupation function with the Hartree shifted chemical potential. Taking the \( Q \to 0 \) limit,

\[ \chi_{new}(l, p; 0) = -V(0)[1 - V(0) \int_{k} \frac{\partial n(k)}{\partial \epsilon_k}] \] (18)

Note that \( \chi_{new} \) viewed as a matrix in Matsubara frequencies has constant entries, and so does \( \chi_{new} \). All the eigenvalues of this matrix are zero with the exception of one single eigenvalue proportional to

\[ -V(0)[1 + V(0)N(\mu)] \] (19)

where \( N(\mu) \) is the density of states corresponding to the Hartree shifted chemical potential. From \( \chi_{new} \), we see that the Hartree approximation is again unstable for repulsive interactions. However, it is stable for attractive interactions \( V \to -V \), and becomes unstable when \( V(0)N(\mu) \to 1 \) triggering an instability in the particle-hole sector. This is the well known phase separation instability of fermions with attractive interactions. To investigate superconducting instabilities one would have to introduce anomalous Green’s functions, and extend the recent work of Janis, who considered the Baym Kadanoff functional, to our functional. A more comprehensive discussion of the stability of \( \Gamma_{new} \) and the relative stability of \( \Gamma_{new} \) and \( \Gamma_{bk} \) is left for future work.

![FIG. 2. Diagrammatic representation of \( \Gamma_{new} \) in momentum space](image)

**IV. DYNAMICAL MEAN FIELD THEORY AS AN APPROXIMATION**

We now focus on the various applications of the new functional introduced in this paper. Despite the simple structure of both \( \Gamma_{bk} \) and \( \Gamma_{new} \), it is often impractical and intractable to sum over the infinite series of diagrams that contribute to \( \Phi[G] \). Rather, various approximation schemes are used to obtain \( \Gamma_{bk} \) (\( \Gamma_{new} \)) and hence \( G \). The validity of these approximations depend on whether \( \Phi[G_{new}] \) (or \( \Phi[G_{new}] \)) for \( \Gamma_{new} \) are positive or not. Typical approximations range from Hartree Fock and RPA methods at weak coupling to atomic limits for strong coupling. Recent years have seen the development of Dynamical mean field theory (DMFT) which is one of the very few methods available to study correlated electron systems in the weak, strong and intermediate coupling regimes. Though this method is exact only in the limit of infinite dimensions, it has been very successful in describing the physics of realistic three dimensional systems, like the transition metal oxides. DMFT is formulated on a lattice and is characterized by self-consistency conditions (henceforth referred to as the DMFT equations) on the full local Green’s functions. The form of these depend on the non-interacting density of states of the lattice considered. These equations were derived using the cavity
method or local perturbation theory in infinite dimensions. Consequently, issues regarding the fluctuations around the DMFT, extension to finite dimensional lattices and systems in the continuum, have been difficult to analyze.

Some of the above issues can be resolved if DMFT is viewed as an approximation to $\Gamma_{\text{new}}$. Here, for the first time, we show that the DMFT equations can be derived directly from $\Gamma_{\text{new}}$, by making the ansatz that $G$ is completely local i.e., $G(r, r', i\omega_n) = G(r, r, i\omega_n)\delta(r - r')$. Notice that our approach is fairly general. If we have in mind a lattice model the delta function $\delta(r - r')$ should be understood as a Kronecker delta function, while if we have a multiband model in mind $G_0$ and $G$ should be viewed as matrices in the band and spin indices. Using the above ansatz, the stationarity condition for $\Gamma_{\text{new}}$ yields

$$G(r, r, i\omega_n) = (G_0^{-1} - \frac{\delta \Phi}{\delta G})^{-1}(r, r)$$

where the second term within the square brackets is a diagonal matrix with entries $\delta \Phi/\delta G = \delta \Phi/\delta G(r, r, i\omega_n)$. The above equation should be viewed as a matrix in the spatial coordinates. Interestingly, (20) are exactly the DMFT equations postulated in Ref. 7 for non-translationally invariant systems.

The local ansatz applied to $\Gamma_{bh}$ yields the following equation

$$G^{-1}(r, r, i\omega_n) = G_0^{-1}(r, r, i\omega_n) - \frac{\delta \Phi}{\delta G(r, r)}$$

The crucial point is that (20) and (21) become inequivalent in the local $G$ approximation. This becomes transparent in momentum space. Consider a translationally invariant system with $G_0^{-1} = i\omega_n - \epsilon_k$ where $\epsilon_k$ is the energy dispersion of the non-interacting system. Rewriting (20) in momentum space,

$$G(i\omega_n) = \int \frac{\rho(\epsilon)d\epsilon}{(i\omega_n - \epsilon - \frac{\delta \Phi}{\delta G(i\omega_n)} )}$$

where, $G(r, r, i\omega_n) \equiv G(i\omega_n)$ and $\rho(\epsilon)$ is the non-interacting density of states. On the other hand, using the above form of $G_0^{-1}$ in (21) clearly leads to unphysical conditions. Replacing $\rho$ in (22) by a lattice density of states in the limit of large dimensions yields the standard DMFT equations. The potential applications need to be explored further.

V. BASIS OPTIMIZATION CRITERIA IN DMFT CALCULATIONS

Model Hamiltonians presuppose a choice of tight binding basis and hence model parameters. In a previous paper, we argued that starting from the full Hamiltonian we can construct a functional of the local Green’s function which yields the true local Green’s function of the problem at stationarity. There, DMFT viewed as a theory for the local Green’s function, is an exact theory but the functional which needs to be constructed is not known explicitly (beyond a general diagrammatic series discussed in ref. 8). Here we adopt a different approach and would like to view dynamical mean field theory as an approximation to a simple functional. When the saddle point fluctuations are positive, we can gauge the quality of different approximations.

We first notice as in Ref. 8 that different choices of tight binding orbitals $\phi_\alpha$ where $\alpha$ denotes the band index, can be used to represent the exact one particle Green’s function

$$G(r, r', i\omega_n) = \sum_{R_1, R_2} \phi_\alpha(r - R_1)G_{\alpha\beta}(R_1, R_2, i\omega_n)\phi_\beta(r' - R_2)$$

We can then insert the following approximate trial Green’s function into our functional

$$G(r, r', i\omega_n) = \sum_{R_1, R_2} \phi_\alpha(r - R_1)G_{\alpha\beta}(R_1, R_2, i\omega_n)\phi_\beta(r' - R_2)\delta(R_1, R_2)$$

compute the trial value of $\Gamma_{\text{new}}$ and optimize with respect to the $G_{\alpha\beta}$ first by solving the DMFT equations which expresses the local lattice self energy

$$\Sigma_{\alpha\beta}(R_1, R_1, i\omega_n) = \frac{\delta \Phi}{\delta G_{\alpha\beta}(R_1, R_1, i\omega_n)}$$

in terms of $G_{\alpha\beta}(R_1, R_1, i\omega_n)$. Another choice of orbitals would lead to a different trial function, so a functional perspective offers the possibility of optimizing the basis of orbitals specifically for DMFT calculations.
VI. DERIVATION OF EXTENDED DYNAMICAL MEAN FIELD EQUATIONS

Ordinary dynamical mean field theory treats longer range interactions at the level of the Hartree approximation. An extended dynamical mean field approach has been suggested to partially remove this shortcoming. Recent work on the effects of long range Coulomb interactions within DMFT have shown that they can substantially modify the behavior near a Mott transition, changing the nature of the transition from a continuous one for short range interactions, to a discontinuous one. In the light of these works and given the relevance of long range interactions, we present a functional derivation of extended DMFT equations along the lines of Sec. IV.

We consider the system of electrons with some non-local interaction. Decoupling the repulsive quartic interaction term in (1) using a Hubbard Stratanovich field \( \phi \), we get

\[
Z = \int D[\psi \psi^\dagger] \exp[-\frac{1}{2} \int dx \psi^\dagger(x)[\partial_t - \nabla^2 + V(x)]\psi(x) - \int dx dy \phi(x) \Pi^{'-1}_0(x-y) (x-y) \phi(y) - i \int dx \phi(x) \psi^\dagger(x) \psi(x) \]
\[
\tag{26}
\]

If we chose \( \Pi_0(x,y) = V(x-y) \) to be instantaneous in time, then upon integrating out the field \( \phi \) we recover the interacting electron system of (1). This decoupling can be extended to attractive interactions between the electrons by retaining the same repulsive interaction between the phonons (so as to obtain a positive dispersion) and replacing the factor \( i \) in (26) by unity.

Physically, \( \phi \) can be interpreted as a phonon field with a particular dispersion determined by \( \Pi_0 \). In fact, we can start with (26) as a general action describing interacting electrons and phonons, the limit of static Coulomb interactions being obtained as a limiting case. In momentum space, the term quadratic in the phononic field is \( \phi(q) \Pi^{-1}_0(q) \phi(-q) \) with \( \Pi_0 \) being the Fourier transform of the interaction. We now have a system of interacting fermionic and bosonic fields. Similar to Sec. II, we calculate the free energy \( W[J,K] \) of the electron-phonon system, where \( J \) and \( K \) are the source fields for the electron Green’s function \( G \) and the phonon Green’s function \( \Pi \) respectively. Note that in the present case, the phonon Green’s function is nothing but the full density density correlator or two particle Green’s function of the electrons. The effective action functional i.e., the equivalent of the Baym Kadanoff functional for such a coupled system is now given by the double Legendre transform of \( W[J,K] \)

\[
\Gamma[G, \Pi] = \text{Tr} \log G - \text{Tr}[G_0^{-1} G^{-1}] - \frac{1}{2} \text{Tr} \log \Pi + \frac{1}{2} \text{Tr} \Pi_0^{-1} \Pi + \Phi[G, \Pi] \]
\[
\tag{27}
\]

\( \Phi \) is the sum of all two particle irreducible diagrams constructed using the electron-phonon vertex. The source fields are fixed by the following conditions:

\[
J = G^{-1} - G_0^{-1} + \frac{\delta \Phi}{\delta G}, \quad K = \Pi^{-1} - \Pi_0^{-1} - 2 \frac{\delta \Phi}{\delta \Pi}
\]
\[
\tag{28}
\]

The saddle point conditions on the above functional are given by (28) with \( J \) and \( K \) set equal to zero. The stability condition for this functional is given by

\[
\int \int \sum_{i,j} \delta X_i(v,x) \frac{\delta^2 \Gamma}{\delta X_i(x,y) \delta X_j(y,u)} \delta X_j(u,v) \geq 0
\]
\[
\tag{29}
\]

where \( X_i \) refer to \( G \) and \( \Pi \). Following (11) we introduce a slightly modified functional

\[
\Gamma_{\text{new}}[G, \Pi] = \Gamma - \text{Tr} \log(1 - JG) - \text{Tr} JG + \frac{1}{2} [\text{Tr} \log(1 - K\Pi) + \text{Tr} K\Pi]
\]
\[
\tag{30}
\]

Substituting (28) in (30), we get

\[
\Gamma_{\text{new}}[G, \Pi] = - \text{Tr} \log \left( G_0^{-1} - \frac{\delta \Phi}{\delta G} \right) - \text{Tr} G \frac{\delta \Phi}{\delta G} + \frac{1}{2} \text{Tr} \log \left( \Pi_0^{-1} + 2 \frac{\delta \Phi}{\delta \Pi} \right) - \text{Tr} \Pi \frac{\delta \Phi}{\delta \Pi} + \Phi[G, \Pi]
\]
\[
\tag{31}
\]

These extra terms tend to stabilize the functional by adding positive terms to \( \Gamma \). The saddle point equations of (31) are
The saddle point solutions are obtained by equating the above equations to zero. The relevant solution is $G^{-1} = G_0^{-1} - \delta \Phi / \delta G$ and $\Pi^{-1} = \Pi_0^{-1} + 2\delta \Phi / \delta D$ since (31) demands that when $J = K = 0$, $\delta \Gamma_{new} / \delta X = \delta \Gamma / \delta X$. The second order derivatives are given by

$$
\frac{\delta^2 \Gamma_{new}}{\delta G \delta G} = \left[ G \frac{\delta^2 \Phi}{\delta G \delta G} G - \frac{\delta^2 \Phi}{\delta G \delta G} \right] - 2\Pi \frac{\delta^2 \Phi}{\delta G \delta \Pi} \Pi \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} - 2\Pi \frac{\delta^2 \Phi}{\delta G \delta \Pi} \Pi \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} \tag{34}
$$

$$
\frac{\delta^2 \Gamma_{new}}{\delta \Pi \delta \Pi} = -\left[ 2\Pi \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} \Pi + \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} \right] + G \frac{\delta^2 \Phi}{\delta G \delta \Pi} G \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} \tag{35}
$$

$$
\frac{\delta^2 \Gamma_{new}}{\delta G \delta \Pi} = G \frac{\delta^2 \Phi}{\delta G \delta \Pi} G \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} - 2\Pi \frac{\delta^2 \Phi}{\delta G \delta \Pi} \Pi \frac{\delta^2 \Phi}{\delta \Pi \delta \Pi} \tag{36}
$$

To obtain the extended mean field equations, we make the ansatz: $G(r, r', i\omega_n) = G(r, r, i\omega_n) \delta(r - r')$ and $\Pi(r, r', i\omega_n) = \Pi(r, r, i\omega_n) \delta(r - r')$. Minimizing with respect to $G$ and $\Pi$ we get

$$
G(r, r, i\omega_n) = [G_0^{-1} - \frac{\delta \Phi}{\delta G}]^{-1}(r, r) \tag{37}
$$

$$
\Pi(r, r, i\omega_n) = [\Pi_0^{-1} + 2\frac{\delta \Phi}{\delta \Pi}]^{-1}(r, r) \tag{38}
$$

As before, $\delta \Phi / \delta G$ and $\delta \Phi / \delta \Pi$ are local self energies and should be viewed as diagonal matrices in the space coordinates. In the translationally invariant case, the above reduce to the following equations

$$
G(i\omega_n) = \int_q \frac{dq}{G_0^{-1}(q, \omega_n) - \delta \Phi / \delta G} \tag{39}
$$

$$
\Pi(i\omega_n) = \int_q \frac{dq}{\Pi_0^{-1}(q) + 2\delta \Phi / \delta \Pi} \tag{40}
$$

These are precisely the extended dynamical mean field equations obtained in Ref. [3]. We therefore, see that all the dynamical mean field theories can be seen as consequences of local approximations made on the new functionals. An analysis of stability similar to the one leading to the conditions on (31) is left for future work.

### A. Mott transition

Recently, the Mott (metal-insulator) transition in the infinite dimensional Hubbard model was revisited from a Landau Ginzburg perspective. The central idea consisted of the introduction of a Landau functional whose saddle point gives the (local) Green’s function of the problem. The Mott transition is then viewed as bifurcations of the stationary points of this functional as the parameters of the theory are varied. This approach was used to clarify various issues related to the zero temperature Mott transition in infinite dimensions, and to study the finite temperature Mott transition at half filling in the infinite dimensional Hubbard model.

Here we suggest that the functional $\Gamma_{new}$ discussed in this paper, be viewed as a generalization of the Landau functional discussed in Ref. [3] to finite dimensions, and use it to extend some of the lessons learnt in infinite dimensions to finite dimensions. In particular, we elaborate on a connection between the existence of a Mott transition and the divergence of the charge compressibility, conjectured on the basis of pioneering numerical work by Furukawa and Imada. They discovered that the approach to the Mott transition in two dimensions as a function of doping is characterized by a divergent compressibility. By varying the hopping integrals, they demonstrated that this is a general phenomena characteristic of the approach to the Mott transition. Here we use the following argument. The Mott transition is but a bifurcation of the stationary solutions of $\Gamma_{new}$ i.e. solutions of $\delta \Gamma_{new}[G] / \delta G = 0$, as a control parameter $\alpha$ (which could stand for chemical potential, temperature or $U$) is varied. For a bifurcation to take place the matrix $\chi_{new} = \frac{\delta^2 \Gamma_{new}}{\delta G(x,y) \delta G(u,v)}$ has to be non invertible since otherwise the equation:
\[ \delta G = - \left( \frac{\delta^2 \Gamma_{\text{new}}}{\delta G \delta G} \right)_c^{-1} \left( \frac{\delta^2 \Gamma_{\text{new}}}{\delta G \delta \alpha} \right)_c \delta \alpha \] (40)

could be uniquely solved for \( \delta G \). In [10], the subscript \( c \) denotes the quantities evaluated at criticality. We have seen in Sec. [11] that when \( \chi_{\text{new}} \) ceases to be invertible, an instability sets in the particle hole channel at zero momentum. This implies a divergent compressibility unless there exist matrix elements which cancel the contribution of the vanishing eigenvalue of the Bethe Salpeter kernel, which signals the instability. This argument directly relates the existence of a Mott transition to the divergence of the compressibility supporting the observation of Ref. [12]. We stress however that while our argument is fairly general and very appealing in the light of the numerical results of Ref. [12], it is based on assumptions which need to be verified on a case by case basis. In fact, even in infinite dimensions, the Landau functional at zero temperature has some very singular bifurcations in its phase diagram at which the compressibility does not diverge. This issue as well as the computation of matrix elements in specific bifurcations requires a problem specific analysis which at this stage can be performed rigorously only in the limit of infinite dimensions [13].

Finally it would be useful to extend the analysis to spin dependent Green’s functions. This would allow us to understand the effects of magnetism in many cases, examples being the doping driven Mott transition in two dimensions, where one approaches a magnetically ordered state and the problem of the antiferromagnetic metal to antiferromagnetic insulator transition in infinite dimensions that we have studied recently [14].

VII. CONCLUSION

To summarize, we have constructed a new functional for the single particle Green’s function and investigated its use as a variational free energy. We found that stability of the saddle point solutions was linked to the Bethe-Salpeter equation in the particle hole sector. From the perspective of applications, the use of \( \Gamma_{\text{new}} \) allows us to derive DMFT and extended DMFT, directly in finite dimensions, for non translationally invariant geometries. Functional methods provide simple connections between one particle Green’s functions and particle hole instabilities, and we use these ideas to discuss the compressibility near the Mott transition. Finally, we have shown that under some circumstances it is possible to understand whether the stationary points of \( \Gamma_{\text{new}} \) are extrema or saddle points. We feel that this is a significant advantage, over the Baym-Kadanoff functional \( \Gamma_{bk} \), when used to generate non perturbative approximations using trial Green functions. There is a great deal of freedom, in adding sources to \( \Gamma_{bk} \) so as to convert its stationary points into extrema, and constructions along the lines of our paper, but with different additions of sources, so as to obtain more general stability conditions than the ones we were able to obtain are well worth pursuing.

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