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## **ON NON-EQUILIBRIUM STRONG CORRELATION SYSTEMS**

The self-energy-functional theory (SFT) is generalized to describe the real-time dynamics of correlated lattice-fermion models far from thermal equilibrium. This is based on a reformulation of the original equilibrium theory in terms of double-time Green's functions on the Keldysh-Matsubara contour. It is considered equations for non-equilibrium Green's functions and corresponding solutions describing elemental excitations in considered systems.

### **1. On description of the dynamics of non-equilibrium systems**

The development of new theoretical methods to study the real-time dynamics of systems of strongly correlated fermions far from thermal equilibrium has

become more and more important recently. Apart from fundamental questions related to dynamical phase transitions (see [1] and other open problems in quantum statistics [2] this interest is to a large extent triggered by the experimental progress which made it possible to control microscopic degrees of freedom with high temporal resolution. Examples are given by femtosecond pump-probe spectroscopy from transition-metal oxides (see [3] or by the dynamics of ultracold atomic gases trapped in optical lattices [4].

For correlated lattice-fermion models with local interactions, such as the Hubbard model [5] as a prototype, a conceptually appealing and pragmatic theoretical idea is the mean-field approach [6]. With the invention of dynamical mean-field theory (DMFT) [7] we have the optimal mean-field theory at hand that comprises a number of important properties, including its non-perturbative character and its internal consistency. Those features are also shared by the non-equilibrium (NE) generalization of the DMFT [8], which has already been applied successfully to a number of problems [9].

DMFT (both for equilibrium and for non-equilibrium) requires the computation of the fermion self-energy of an effective impurity model with self-consistently determined parameters. For the equilibrium case, quantum Monte-Carlo (QMC) techniques [10] nowadays represent a standard tool to treat the many-body impurity problem efficiently and accurately. Employing exact diagonalization (ED) as a “solver” represents a competitive alternative in case of single-band models. It is easily implemented, computationally efficient and highly accurate. A disadvantage of the ED solver consists in the essentially ad hoc character of the self-consistency condition that fixes the Weiss field. This originates from the impossibility to fit a continuous Weiss field with any finite number of bath degrees of freedom, and it becomes a serious problem, if, for reasons of limited computational resources, only a small number of bath sites can be used in the effective impurity model.

The ad-hoc character of the bath representation can lead to a violation of thermodynamic consistency and conservation laws. This problem could be solved within the framework of the self-energy-functional theory (SFT) [11], where the DMFT self-consistency condition is replaced by the condition for stationarity of the system's grand potential with respect to the bath parameters of the impurity or “reference” system. Thereby the bath parameters are efficiently determined by a physically meaningful and unique procedure, which provides consistent results for impurity models with a few parameters only and recovers the full DMFT in the continuum limit. Very precise studies of phase diagrams have been done in this way.

In the non-equilibrium case, the situation is more complicated: QMC-based solvers have been employed successfully but suffer from a severe sign (or phase) problem contrary to the equilibrium case where the sign problem is absent or mild. Simplified, e.g., perturbative approximations, such as the iterative perturbation theory [9] the non-crossing approximation or simplified models, such as the Falicov-Kimball model [8] have been considered instead, as well as a non-

equilibrium variant of the dual-fermion approach. For the study of steady-state properties, a non-trivial extension of ED-based DMFT has been suggested recently [12]. The development of ED-based impurity solvers to compute the real-time evolution within DMFT is more challenging, as it is by no means obvious how to fix the time-dependent parameters to fit a given Weiss field, i.e., a given non-homogeneous function of two time variables with certain analytical properties. One indeed can find mapping strategies which are accurate and systematic at short times, but in general, and in particular for the longtime limit, the reduction of the Hamiltonian representation of the Weiss field to a small number of parameters remains somehow ad-hoc.

The goal of the present study is therefore to explore whether non-perturbative and internally consistent approximations based on the exact-diagonalization of a reference system with a finite (small) number of bath sites can be formulated by means of a proper generalization of the self-energy-functional theory to the non-equilibrium case. Preceding attempts in this direction are not satisfactory yet. The non-equilibrium cluster-perturbation theory [13] does make use of the exact diagonalization of a finite reference system out of equilibrium and provides the one-particle propagator for a non-equilibrium state of the correlated lattice model. However, the approach does not rely on a variational principle at all and does not involve any self-consistent or variational optimization of the parameters of the reference system. On the other hand, a self-consistent parameter optimization is part of a similar ED-based cluster approach, which has been formulated and applied to study the steady state of an out-of-equilibrium correlated lattice model. Here a physically motivated self-consistency condition is used which, however, is not yet shown to derive from a general variational principle that also applies to the transient dynamics.

There are several problems that must be solved in order to construct a non-equilibrium self-energy-functional theory (NE-SFT): First, a functional  $\widehat{\Omega}[\Sigma]$  of the double-time non-equilibrium self-energy must be constructed formally and shown to be stationary at the physical self-energy of the lattice model. Ideally, the functional, if evaluated at the physical self-energy, has a precise physical meaning. In the spirit of the equilibrium SFT, the functional should be accessible to an exact numerical evaluation for trial non-equilibrium self-energies generated by a reference system, which typically consists of a small number of sites such that it is tractable by exact diagonalization techniques. Next one must find conditional equations for the parameters of the reference system, by demanding stationarity of when varying the self-energy through variation of the parameters.

The NE-SFT should furthermore recover the nonequilibrium DMFT if a single-impurity Anderson model, with a continuum of bath degrees of freedom, was chosen as a reference. Apart from non-equilibrium dynamical impurity approximations (DIA) resulting from Anderson models with a finite number of bath sites, the NE-SFT should also allow for the construction of cluster approximations, such as a non-equilibrium generalization of the variational cluster

approach (VCA). Adding baths one should, in the limit of a continuum of bath degrees of freedom, also recover non-equilibrium analogues of the cellular DMFT and the dynamical cluster approximation. Finally, it will be interesting to see how the standard SFT is recovered within the general NE-SFT setup in case of an equilibrium situation.

The most important question in the context of any method addressing real-time dynamics, however, concerns macroscopic conservation laws. Do approximations derived within the NE-SFT framework respect the conservation of the total particle number, the total spin and the total energy for a U(1) and SU(2) symmetric and time-independent Hamiltonian? This "conserving" nature of approximations is not easily obtained. The seminal work of Baym and Kadanov [14] answers this question for approximations that are "derivable", including DMFT and self-consistent perturbation theory, such as the second-order Born approximation. While the construction of the NE-SFT makes use of the Luttinger-Ward functional  $\Phi$ , the question whether it is conserving must be addressed carefully since generic approximations within the NE-SFT cannot be obtained by resummations of diagram classes.

## 2. Non-equilibrium Green's functions

The self-energy-functional approach relies on functionals that are formally defined by means of all-order perturbation theory. Therefore, we summarize the concept of (non-equilibrium) Green's functions as far as necessary for our purposes. Out of the various available formulations we will basically follow the formal setup by Wagner [15].

We assume that the system at initial time  $t_0$  is prepared in a thermal state with inverse temperature  $\beta$  and chemical potential  $\mu$ , as given by a density operator

$$\rho = \frac{\exp(-\beta H_{ini})}{\text{Tr} \exp(-\beta H_{ini})} \quad (1)$$

with  $H_{ini} = H_{ini} - \mu N$ , where

$$H_{ini} = \sum_{\alpha\beta} T_{\alpha\beta}^{(ini)} c_{\alpha}^{+} c_{\beta} + \frac{1}{2} \sum_{\alpha\beta\delta\gamma} U_{\alpha\beta\delta\gamma}^{(ini)} c_{\alpha}^{+} c_{\beta}^{+} c_{\gamma} c_{\delta} \quad (2)$$

is the initial Hamiltonian and  $N$  the total particle number operator. Greek indices refer to one-particle basis states, which typically are characterized by a lattice site, an orbital index and a spin-projection quantum number. For times  $t > t_0$  the system's time evolution shall be governed by the possibly time-dependent Hamiltonian

$$H_{fin} = \sum_{\alpha\beta} T_{\alpha\beta}^{(fin)} c_{\alpha}^{+} c_{\beta} + \frac{1}{2} \sum_{\alpha\beta\delta\gamma} U_{\alpha\beta\delta\gamma}^{(fin)} c_{\alpha}^{+} c_{\beta}^{+} c_{\gamma} c_{\delta}. \quad (3)$$

For the sets of time-dependent hopping and interaction parameters we write  $T$  and  $U$  for short, and, whenever necessary or convenient, we indicate the

dependence of the Hamiltonian on those parameters as  $H_{T,U}$ . In the Heisenberg picture with respect to  $H(t) = H_{fm}(t) - \mu N$ , an arbitrary, possibly time-dependent observable  $A(t)$  is given by

$$A_H(t) = U(t_0, t)A(t)U(t, t_0)$$

Here  $U(t, t') = T \exp\left(-i \int_{t'}^t dz H(z)\right)$  is the time evolution operator for times

$t < t'$ , where  $T(\tilde{T})$  is chronological (anti-chronological) time-ordering operator. Noting that  $\exp(-\beta H_{ini}) = U(t_0 - i\beta, t_0)$ , the time-dependent expectation value of the observable  $A(t)$ , namely  $\langle A \rangle(t) = \text{Tr}(\rho A_H(t))$ , can be written as

$$\langle A \rangle(t) = \frac{\text{Tr}\left(T_C \exp\left(\int_C dz' H_{T,U}(z')\right) A(t)\right)}{\text{Tr}\left(T_C \exp\left(\int_C dz' H_{T,U}(z')\right)\right)} \quad (4)$$

Here, the time integration is carried out along the contour  $C$  in the complex time plane, which extends from  $z' = t_0$  to  $z' = \infty$  along the real axis (upper branch) and back to  $z' = t_0$  (lower branch) and finally from  $z' = t_0$  to  $z' = t_0 - i\beta$  along the imaginary axis (Matsubara branch). We also refer to the upper and the lower branch as the Keldysh contour. For a concise notation, we define  $H(z)$  for contour times  $z$  as  $H(z) = H_{fm}(t)$  if  $z = t > t_0$  and as  $H(z) = H_{ini}(t)$  if  $z = t_0 - i\tau$  with  $0 \leq \tau \leq \beta$ . In the same way, we define  $T_{\alpha\beta}(z)$  and  $U_{\alpha\beta\delta\gamma}(z)$ .  $T_C$  denotes the ordering operator along the contour and, after expanding the exponential, places an operator  $H(z_1)$  to the left of  $H(z_2)$  if  $z_1$  is "later" than  $z_2$ , where  $t_0 - i\beta$  is the "latest" time. Obviously,  $T_C$  replaces  $T$  on the upper and  $\tilde{T}$  on the lower branch.

When the contour ordering operator  $T_C$  acts on  $A(t)$  in the numerator of Eq. (5), it places  $z_2$  at the position  $z = t_0$  on  $C$ , where the expectation value is evaluated. Because the integrations along the upper and the lower branches cancel each other in the interval  $t < z' < \infty$ , the integration along the Keldysh branch is limited to  $z' < t$ , and it does not matter whether  $A(t)$  is placed at  $z = t$  on the upper or the lower branch of the contour. For the denominator, only the Matsubara branch contributes and results in  $\text{Tr}(-\beta H_{ini})$ .

For a system specified by the parameters  $\dots$  and  $U$  we define the elements of the contour-ordered Green's function  $G_{T,U}$  as

$$iG_{T,U;\alpha\alpha'}(z, z') = \langle T_C c_{\alpha,H} c_{\alpha',H}^+ \rangle. \quad (5)$$

Here  $\langle \dots \rangle = \text{Tr}(\rho \dots)$  denotes the expectation value in the initial state. Furthermore, the annihilation and creation operators are given in their Heisenberg

picture with respect to  $H(t)$ ,  $z$ ,  $z'$  denote arbitrary points on the contour, and  $T_C$  is the time ordering of annihilation and creation operators on  $C$  which yields an additional (fermionic) sign for each transposition. Note that the Green's function also depends on  $\beta$  and  $\mu$  via the initial thermal state. These dependencies are implicit in the notations.

The "free" Green's function  $G_{T,0}$  is obtained by setting  $U=0$  in Eq. (5). Using the Heisenberg equation of motion for the annihilation operator, we find

$$G_{T,T,0;\alpha\alpha'}^{-1}(z,z') = \delta_{\alpha,\alpha'} \delta_C(z,z') - i\partial_z (T_{\alpha\alpha'}(z') - \mu\delta_{\alpha\alpha'}) \quad (6)$$

where  $\delta_C$  is the contour delta-function, and the matrix inverse refers to both one-particle basis indices and time variables. With the help of the free and the interacting Green's functions we can also introduce the self-energy via the Dyson equation

$$G_{T,U} = G_{T,0} + G_{T,0} \circ \Sigma_{T,U} \circ G_{T,U}. \quad (7)$$

By switching to the interaction picture, the interacting Green's function can be cast into the form:

$$iG_{T,U;\alpha\alpha'}(z,z') = \frac{\left\langle T_C e^{-i\int_C dz'' H_{0,U}(z'')} c_\alpha(z) c_{\alpha'}^\dagger(z') \right\rangle_{T,0}}{\left\langle T_C e^{-i\int_C dz'' H_{0,U}(z'')} \right\rangle_{T,0}}. \quad (8)$$

Here the time dependence of all operators is due to  $H_{T,0}$  only. Likewise, the expectation value  $\langle \dots \rangle_{T,0}$  is defined with the "free" density operator  $\exp(\exp(-\beta H_{T,0}) / \text{Tr}(-\beta H_{T,0}))$ . Hence, Wick's theorem applies and therewith the standard techniques of perturbation theory.

### 3. Luttinger-Ward functional

The non-equilibrium Luttinger-Ward functional  $\Phi_U[G]$  can be defined by means of all-order perturbation theory in close analogy to the equilibrium case. It is obtained as the limit of the infinite series of closed renormalized skeleton diagrams, and is thus given as a functional of the contour-ordered Green's function. Usually the skeleton-diagram expansion cannot be summed up to get a closed form for  $\Phi_U[G]$ , and the explicit functional dependence is unknown even for the most simple types of interactions like the Hubbard interaction. As an alternative to the diagrammatic definition of the Luttinger-Ward functional, a non-equilibrium path-integral formalism may be used for an entirely non-perturbative construction. Again, this can be done analogously to the equilibrium case. Both variants allow deriving the following four properties that will be used extensively for constructing the non-equilibrium SFT.

The Luttinger-Ward functional vanishes in the non-interacting limit

$$\Phi_U[G]=0 \text{ for } U=0, \quad (9)$$

since there is no zero-order diagram.

The functional derivative of the Luttinger-Ward functional with respect to its argument is

$$\frac{\delta\Phi_U[G]}{\delta G(1,2)} = \frac{1}{2}\Sigma_U G(1,2), \quad (10)$$

with the short-hand notation  $i=(\alpha_i, z_i)$ . Diagrammatically, the functional derivative corresponds to the removal of a propagator from each of the  $\Phi$  diagrams. Taking care of topological factors, one ends up with the skeleton-diagram expansion of the self-energy which, independently from the definition, Eq. (7), gives the self-energy as a functional of the Green's function  $\Sigma_U[G]$ . Evaluating the functional  $\Sigma$  at the exact ("physical") Green's function  $G_{T,U}$  yields the physical self-energy

$$\Sigma_U[G_{T,U}] = \Sigma_{T,U} \quad (11)$$

Since any diagram in the series depends on  $U$  and on  $G$  only, the Luttinger-Ward functional is "universal", i.e., it is independent of  $T$ . Two systems with the same interaction  $U$  but different one-particle parameters  $T$  are described by the same Luttinger-Ward functional. This implies that the functional  $\Sigma_U[G]$  is universal, too.

If evaluated at the physical Green's function  $G_{T,U}$  of the system with Hamiltonian  $H_{T,U}$ , the Luttinger-Ward functional provides a quantity  $\Phi_U[G_{T,U}] = \Phi_{T,U}$ .  $\Phi_{T,U}$  depends on the initial equilibrium state of the system only, as contributions from the Keldysh branch cancel each other. It is related to the grand potential of the system via the expression

$$\Omega_{T,U} = \Phi_{T,U} + \frac{1}{\beta} \text{Tr} \left[ \ln(G_{\varepsilon_0,0}^{-1} \circ G_{T,U}) - (\Sigma_{T,U} \circ G_{T,U}) \right]. \quad (12)$$

Here, we defined the trace as  $\text{Tr} A = \sum_{\alpha} \int_C dz A_{\alpha\alpha}(z, z^+)$ , where  $z^+$  is infinitesimally later than  $z$  on  $C$ . The factor  $G_{\varepsilon_0,0}^{-1}$  with  $\varepsilon_0 \rightarrow \infty$  has to be introduced to regularize the  $\text{Tr} \ln$  term. It will be omitted in the following, as it does not affect the results. Equation (12) can be derived using a coupling-constant integration or by integrating over the chemical potential  $\mu$ . The proof is completely analogous to the equilibrium case.

We assume the functional  $\Sigma_U[G]$  is invertible locally to construct the Legendre transform of the Luttinger-Ward functional

$$F_U[\Sigma] = \Phi_U[\Sigma] - \frac{1}{2} \text{Tr}(\Sigma \circ G_U[\Sigma]). \quad (13)$$

Here  $G_U[\Sigma_U[G]] = G$  and

$$\frac{\delta F_U[\Sigma]}{\delta \Sigma(1,2)} = -\frac{1}{2} G_U[\Sigma](2,1) \quad (14)$$

We now define the self-energy functional as

$$\Omega_{T,U}[\Sigma] = -\frac{1}{2} \text{Tr} \ln \left( G_{T,0}^{-1} - \Sigma \right)^{-1} + F_U[\Sigma]. \quad (15)$$

It's functional derivative is

$$\frac{\delta \Omega_{T,U}[\Sigma]}{\delta \Sigma(1,2)} = \frac{1}{\beta} \left[ \left( G_{T,0}^{-1} - \Sigma \right)^{-1} - G_U[\Sigma] \right]. \quad (16)$$

The equation

$$G_U[\Sigma] = \left( G_{T,0}^{-1} - \Sigma \right)^{-1} \quad (17)$$

is a (highly non-linear) conditional equation for the self-energy of the system  $H_{T,U}$ . Equations (7) and (11) show that it is satisfied by the physical self-energy  $\Sigma = \Sigma_{T,U}$ . Note that the left-hand side of Eq. (17) is independent of  $T$  but depends on  $U$  (due to the universality of  $G_U[\Sigma]$ ), while the right-hand side is independent of  $U$  but depends on  $T$  via  $G_{T,0}^{-1}$ .

The obvious problem of finding a solution of Eq. (17) is that there is no closed form for the functional  $G_U[\Sigma]$ . Solving Eq. (21) is equivalent, however, to a search for the stationary point of the grand potential as a functional of the self-energy  $\delta G_{T,U} / \delta \Sigma = 0$ . This equation is the starting point for non-equilibrium self-energy-functional theory.

Note that, while there are various symmetry relations between the elements  $\Sigma_{\alpha\alpha'}(z, z')$  of the self-energy at different times  $z$  and  $z'$ , the elements of  $\Sigma_{-}$  have to be treated as independent of each other for the functional differentiation to ensure the equivalence of the variational principle Eq. (22) with the fundamental Dyson equation Eq. (17). As will become clear below, the stationarity with respect to some of the variational directions just ensures the correct symmetry relations between the elements of  $\Sigma_{\alpha\alpha'}(z, z')$ , while the other variational directions fix the actual value of  $\Sigma_{\alpha\alpha'}(z, z')$ .

#### 4. Dynamical mean-field theory

Non-equilibrium dynamical mean-field theory is recovered within the SFT framework when we choose the reference system as a set of completely decoupled correlated sites with an infinite number of bath sites, i.e., as a set of decoupled single-impurity Anderson models. For completely decoupled correlated sites the trial self-energies are local, i.e., diagonal with respect to the spatial indices, and the Euler equation (26) thus explicitly reads as



$$\frac{1}{\beta} \sum_{i, \sigma_1 \sigma_2} \int_C dz_1 dz_2 \left[ \left( G_{T,0}^{-1} - \Sigma_{\lambda'} \right)^{-1} - G_{\lambda', U} - G_{\lambda', U} \right]_{ii', \sigma_1 \sigma_2} (z_1, z_2) \frac{\delta \Sigma_{\lambda', U; ii', \sigma_1 \sigma_2} (z_2, z_1')}{\delta \lambda' (z)} = 0. \quad (18)$$

Here,  $i$  is a site index and  $\sigma_i$  refers to the local orbital and spin degrees of freedom. Equation (18) would be trivially satisfied if the bracket in the integrand vanished. Because the vanishing of the bracket is nothing but the standard self-consistency equation of DMFT, we see that non-equilibrium SFT yields (non-equilibrium) DMFT as a stationary point provided that the DMFT self-energy can be represented as the self-energy  $\Sigma_{\lambda', U}$  of a single-impurity Anderson Hamiltonian with single-particle (bath) parameters  $\lambda'$ .

The representability of the DMFT action by an actual impurity Hamiltonian with the number uncorrelated sites 1 is not straightforward to see for non-equilibrium Green's functions but can be shown under rather general conditions.<sup>37</sup> When one considers finite single-impurity models with a small number of bath orbitals, the bracket in Eq. (18) will in general not vanish because the discrete pole structure of the impurity Green's function cannot be reconciled with the branch cuts of the Green's function for the original model. Due to the presence of the projector  $\delta \Sigma_{\lambda'} / \delta \lambda'$ , however, stationarity of the self-energy functional is nevertheless possible. This allows to generate non-perturbative and consistent approximations to DMFT by solving reference systems with a few degrees of freedom only. In the equilibrium case, this has been shown to be a highly efficient strategy.

## 5. Conclusions

Self-energy-functional theory (SFT) addresses the problem of strongly correlated fermions with local Hubbard-type interactions on a low-dimensional lattice. One of the main advantages of the standard equilibrium SFT is that it unifies and extends different approximations within a single theoretical framework. This comprises "two-site" approximations and the linearized DMFT, dynamical impurity approximations (DIA), but also dynamical mean-field theory (DMFT) and its cluster extensions, i.e., the cellular DMFT (C-DMFT) as well as the dynamical cluster approximation (DCA) and finally the cluster perturbation theory (CPT) and its variational extension, the variational cluster approach (VCA). The SFT has been extended into several directions, e.g., to systems with non-local interactions, to disordered and to bosonic systems.

The present study has shown how to generalize the SFT and the different approximations that can be constructed within the SFT to the general non-equilibrium case. Essentially, the main idea is to reformulate the entire theory in terms of the one-particle Green's functions and the self-energy on the Keldysh-Matsubara contour in the complex time plane. While the basic structure of the theory remains unchanged in this way, a much more general approach is gained.

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## **ЭКСПАНДЕРИ, СИЛЬНИ ЭКСПАНДЕРИ ТА КВАЗИВИПАДКОВІ ГРАФИ**

This paper investigates the connectivity properties of quasi-random graphs based on expanders and strong expanders.

В данній роботі досліджена зв'язність квазіслучайних графів на базі експандерів і сильних експандерів.

**Квазівипадкові графи** (частково-випадкові графи) описують системи, структура яких може змінюватись внаслідок випадкового розриву частини зв'язків [1-3]. Нехай  $G$  - звичайний граф з множиною  $G^0$  вершин і множиною  $G^1$  ребер,  $|G^0| = n$ ,  $|G^1| = m$ , квазівипадковим графом на основі графа  $G$  називається граф  $G(p)$  з множиною  $(G(p))^0 = G^0$  вершин і з випадковою множиною  $U = (G(p))^1$ , ребер для якого виконуються умови:  $Prob(u \in U) = p$  при  $u \in (G)^1$  і  $Prob(u \in U) = 0$  при  $u \notin (G)^1$ .

Величину  $\lambda = mq$ ,  $q = 1 - p$  будемо називати **декрементом** квазівипадкового графа. Очевидно, що декремент це є математичне