

Nonequilibrium self-energy functional theory

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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 achieved by starting from a reformulation of the original equilibrium theory in terms of double-time Green's functions on the Keldysh-Matsubara contour. With the help of a generalized Luttinger-Ward functional, we construct a functional $\widehat{\Omega}[\Sigma]$ which is stationary at the physical (nonequilibrium) self-energy Σ and which yields the grand potential of the initial thermal state Ω at the physical point. Nonperturbative approximations can be defined by specifying a reference system that serves to generate trial self-energies. These self-energies are varied by varying the reference system's one-particle parameters on the Keldysh-Matsubara contour. In the case of thermal equilibrium, this approach reduces to the conventional SFT. Contrary to the equilibrium theory, however, “unphysical” variations, i.e., variations that are different on the upper and the lower branches of the Keldysh contour, must be considered to fix the time dependence of the optimal physical parameters via the variational principle. Functional derivatives in the nonequilibrium SFT Euler equation are carried out analytically to derive conditional equations for the variational parameters that are accessible to a numerical evaluation via a time-propagation scheme. Approximations constructed by means of the nonequilibrium SFT are shown to be inherently causal, internally consistent, and to respect macroscopic conservation laws resulting from gauge symmetries of the Hamiltonian. This comprises the nonequilibrium dynamical mean-field theory but also dynamical-impurity and variational-cluster approximations that are specified by reference systems with a *finite* number of degrees of freedom. In this way, nonperturbative and consistent approximations can be set up, the numerical evaluation of which is accessible to an exact-diagonalization approach.

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I. INTRODUCTION

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, e.g., to the concept of thermalization,¹ to dynamical phase transitions,^{2,3} and other open problems in quantum statistics,⁴ 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 oxides⁵⁻⁷ or by the dynamics of ultracold atomic gases trapped in optical lattices.⁸⁻¹⁰

For correlated lattice-fermion models with local interactions, such as the Hubbard model¹¹⁻¹³ as a prototype, a conceptually appealing and pragmatic theoretical idea is the mean-field approach.¹⁴ With the invention of dynamical mean-field theory (DMFT),¹⁵⁻¹⁸ we have *the* optimal mean-field theory at hand that comprises a number of important properties, including its nonperturbative character and its internal consistency. Those features are also shared by the nonequilibrium (NE) generalization of the DMFT,^{19,20} which has already been applied successfully to a number of problems.²¹⁻²⁵

On the operational level, DMFT (both for equilibrium and for nonequilibrium) 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) techniques²⁶ nowadays represent a standard tool to treat the many-body impurity problem efficiently and accurately. Employing exact diagonalization²⁷

(ED) as a “solver” represents a competitive alternative in the case of single-band and multiband²⁸ 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 theory²⁹⁻³² (SFT) 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 (see Refs. 33 and 34 for example).

In the nonequilibrium 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.^{26,35} Simplified, e.g., perturbative approximations such as the iterative perturbation theory,²⁰ the noncrossing approximation,^{23,24} or simplified models, such as the Falicov-Kimball model,^{19,22} have been considered instead, as well as a nonequilibrium

variant of the dual-fermion approach.³⁶ For the study of steady-state properties, a nontrivial extension of ED-based DMFT has been suggested recently.³⁷ 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 nonhomogeneous function of two time variables with certain analytical properties. One indeed can find mapping strategies which are accurate and systematic at short times³⁸ but, in general, and in particular for the long-time limit, the reduction of the Hamiltonian representation of the Weiss field to a *small* number of parameters remains somehow *ad hoc*.

The goal of this 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 nonequilibrium case. Preceding attempts in this direction are not satisfactory yet. The nonequilibrium cluster-perturbation theory^{39–41} does make use of the exact diagonalization of a finite reference system out of equilibrium and provides the one-particle propagator for a nonequilibrium 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^{42,43} 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 nonequilibrium self-energy functional theory (NE-SFT): First, a functional $\hat{\Omega}[\Sigma]$ of the double-time nonequilibrium 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 nonequilibrium 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 Ω 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 nonequilibrium 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 nonequilibrium generalization of the variational cluster approach (VCA). Adding baths, one should, in the limit of a continuum of bath degrees of freedom, also recover nonequilibrium analogs of the cellular DMFT (Ref. 44) and

the dynamical cluster approximation.⁴⁵ 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 Kadanoff^{46,47} answers this question for approximations that are “ Φ -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 Φ , the question as to whether it is conserving must be addressed carefully since generic approximations within the NE-SFT can not be obtained by re-summations of diagram classes.

The paper is organized as follows: After summarizing some concepts of nonequilibrium Green’s functions that are needed to set up the theory in Sec. II, we discuss the essential properties of the Luttinger-Ward functional for the nonequilibrium case in Sec. III which is necessary to construct the dynamical variational principle of nonequilibrium SFT in Sec. IV. This is followed by a discussion of how to construct approximations within the NE-SFT in Sec. V. Section VI then shows the relation to nonequilibrium DMFT, in particular.

Some of the above steps are preparatory and will be presented in analogy to the equilibrium SFT as far as possible. The reader may compare the central Eqs. (19) and (26) with their equilibrium counterparts (cf. Ref. 32, for example). They do not, however, give sufficient consideration to the intrinsic formal structure of the full nonequilibrium SFT. The essential following part of the paper is therefore concerned with questions related to the causal structure of the theory, with the concept of variations in “unphysical” directions as well as with the need to carry out the (functional) derivatives with respect to the variational parameters *analytically* [see the discussion following Eq. (32)]. This paves the way for an efficient numerical evaluation of different impurity or cluster approximations, which will be published independently. Finally, the analytical proof of the conserving nature of *any* approach that is constructed within the framework of the NE-SFT represents an important result.

The concept of physical and transverse variations is introduced in Sec. VII. The Euler equation of the NE-SFT is worked out in Sec. VIII and used to understand the relation of the NE-SFT to the conventional equilibrium SFT in Sec. IX and for setting up a concept for the numerical evaluation of the theory in Sec. X. Its internal consistency is addressed in Sec. XI. Finally, the question of macroscopic conservation laws is discussed in detail in Sec. XII. Conclusions are given in Sec. XIII.

II. NONEQUILIBRIUM GREEN’S FUNCTION

The self-energy functional approach relies on functionals that are formally defined by means of all-order perturbation theory. Therefore, we first summarize the concept of (nonequilibrium) Green’s functions^{48–51} as far as necessary for

our purposes. Out of the various available formulations,^{52–56} we will basically follow the formal setup by Wagner.⁵³

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

$$\rho = \frac{\exp(-\beta\mathcal{H}_{\text{ini}})}{\text{tr}\exp(-\beta\mathcal{H}_{\text{ini}})}, \quad (1)$$

with $\mathcal{H}_{\text{ini}} = H_{\text{ini}} - \mu N$, where

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

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

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

For the sets of time-dependent hopping and interaction parameters, we write \mathbf{T} and \mathbf{U} for short, and, whenever necessary or convenient, we indicate the dependence of the Hamiltonian on those parameters as $H_{\mathbf{T},\mathbf{U}}$.

In the Heisenberg picture with respect to $\mathcal{H}(t) \equiv H_{\text{fin}}(t) - \mu N$, an arbitrary, possibly time-dependent observable $A(t)$ is given by

$$A_{\mathcal{H}}(t) = U(t_0, t) A(t) U(t, t_0). \quad (4)$$

Here, $U(t, t') = \mathcal{T} \exp(-i \int_{t'}^t dz \mathcal{H}(z))$ is the time-evolution operator for real times $t > t'$ and $U(t, t') = \tilde{\mathcal{T}} \exp(-i \int_{t'}^t dz \mathcal{H}(z))$ for $t < t'$, where \mathcal{T} ($\tilde{\mathcal{T}}$) is the chronological (antichronological) time-ordering operator. For a complex “time” $t_0 - i\tau$ with $0 \leq \tau \leq \beta$, we define $U(t_0 - i\tau, t_0) = \exp(-\mathcal{H}_{\text{ini}}\tau)$. Noting that $\exp(-\beta\mathcal{H}_{\text{ini}}) = U(t_0 - i\beta, t_0)$, the time-dependent expectation value of the observable $A(t)$, namely $\langle A \rangle(t) = \text{tr}[\rho A_{\mathcal{H}}(t)]$, can be written as

$$\langle A \rangle_{\mathbf{T},\mathbf{U}}(t) = \frac{\text{tr} \{ \mathcal{T}_C \exp[-i \int_C dz' \mathcal{H}_{\mathbf{T},\mathbf{U}}(z')] A(t) \}}{\text{tr} \{ \mathcal{T}_C \exp[-i \int_C dz' \mathcal{H}_{\mathbf{T},\mathbf{U}}(z')] \}}. \quad (5)$$

Here, the time integration is carried out along the contour \mathcal{C} in the complex time plane (see Fig. 1), which extends from $z' = t_0$ to ∞ 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

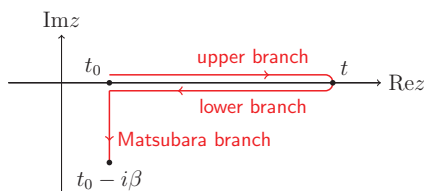


FIG. 1. (Color online) Three-branch contour \mathcal{C} in the complex time plane (see text for discussion).

the upper and the lower branches as the Keldysh contour. For a concise notation, we define $H(z)$ for contour times z as $H(z) = H_{\text{fin}}(t)$ if $z = t > t_0$ and as $H(z) = H_{\text{ini}}$ if $z = t_0 - i\tau$ with $0 \leq \tau \leq \beta$. In the same way, we define $T_{\alpha\beta}(z)$ and $U_{\alpha\beta\delta\gamma}(z)$. \mathcal{T}_C denotes the ordering operator along the contour and, after expanding the exponential, places an operator $\mathcal{H}(z_1)$ to the left of $\mathcal{H}(z_2)$ if z_1 is “later” than z_2 , where $t_0 - i\beta$ is the “latest” time. Obviously, \mathcal{T}_C replaces \mathcal{T} on the upper and $\tilde{\mathcal{T}}$ on the lower branch.

When the contour ordering operator \mathcal{T}_C acts on $A(t)$ in the numerator of Eq. (5), it places $A(t)$ at the position $z = t$ on \mathcal{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 $z' < t$ (see Fig. 1), 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 $\text{tr}\exp(-\beta\mathcal{H}_{\text{ini}})$.

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

$$iG_{\mathbf{T},\mathbf{U};\alpha\alpha'}(z, z') = \langle \mathcal{T}_C c_{\alpha, \mathcal{H}}(z) c_{\alpha', \mathcal{H}}^{\dagger}(z') \rangle. \quad (6)$$

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 $\mathcal{H}(t)$, z, z' denote arbitrary points on the contour, and \mathcal{T}_C is the time ordering of annihilation and creation operators on \mathcal{C} which yields an additional (fermionic) sign for each transposition. Note that the Green's function also depends on β and μ via the initial thermal state. These dependencies are implicit in the notations.

The “free” Green's function $\mathbf{G}_{\mathbf{T},0}$ is obtained by setting $\mathbf{U} = 0$ in Eq. (6). Using the Heisenberg equation of motion for the annihilation operator, we find

$$G_{\mathbf{T},0;\alpha\alpha'}^{-1}(z, z') = \delta_{\alpha\alpha'} \delta_{\mathcal{C}}(z, z') i \partial_{z'} - \delta_{\mathcal{C}}(z, z') [T_{\alpha\alpha'}(z') - \mu \delta_{\alpha\alpha'}], \quad (7)$$

where $\delta_{\mathcal{C}}$ 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

$$\mathbf{G}_{\mathbf{T},\mathbf{U}} = \mathbf{G}_{\mathbf{T},0} + \mathbf{G}_{\mathbf{T},0} \circ \Sigma_{\mathbf{T},\mathbf{U}} \circ \mathbf{G}_{\mathbf{T},\mathbf{U}}, \quad (8)$$

which is short for

$$G_{\mathbf{T},\mathbf{U};\alpha\alpha'}(z, z') = G_{\mathbf{T},0;\alpha\alpha'}(z, z') + \sum_{\beta\beta'} \int_{\mathcal{C}} d\bar{z} d\bar{z}' \times G_{\mathbf{T},0;\alpha\beta}(z, \bar{z}) \Sigma_{\mathbf{T},\mathbf{U};\beta\beta'}(\bar{z}, \bar{z}') G_{\mathbf{T},\mathbf{U};\beta'\alpha'}(\bar{z}', z'), \quad (9)$$

i.e., the circle \circ stands for the convolution along \mathcal{C} .

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

$$iG_{\mathbf{T},\mathbf{U};\alpha\alpha'}(z, z') = \frac{\langle \mathcal{T}_C e^{-i \int_C dz'' \mathcal{H}_{0,\mathbf{U}}(z'')} c_{\alpha}(z) c_{\alpha'}^{\dagger}(z') \rangle_{\mathbf{T},0}}{\langle \mathcal{T}_C e^{-i \int_C dz'' \mathcal{H}_{0,\mathbf{U}}(z'')} \rangle_{\mathbf{T},0}}. \quad (10)$$

Here, the time dependence of all operators is due to $\mathcal{H}_{\mathbf{T},0}$ only. Likewise, the expectation value $\langle \dots \rangle_{\mathbf{T},0}$ is defined with

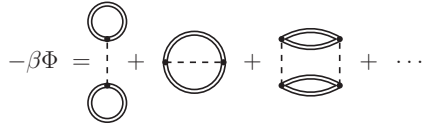


FIG. 2. Diagrammatic definition of the Luttinger-Ward functional $\widehat{\Phi}_U[\mathbf{G}]$. Double lines: fully interacting propagator \mathbf{G} . Dashed lines: interaction \mathbf{U} . See text for discussion.

the “free” density operator $\exp(-\beta\mathcal{H}_{T,0})/\text{tr}\exp(-\beta\mathcal{H}_{T,0})$. Hence, Wick’s theorem applies and therewith the standard techniques of perturbation theory.⁵³

III. LUTTINGER-WARD FUNCTIONAL

The nonequilibrium Luttinger-Ward functional $\widehat{\Phi}_U[\mathbf{G}]$ can be defined by means of all-order perturbation theory in close analogy to the equilibrium case.⁵⁷ It is obtained as the limit of the infinite series of closed renormalized skeleton diagrams (see Fig. 2), and is thus given as a functional of the contour-ordered Green’s function. Note that functionals are indicated by a hat. Usually, the skeleton-diagram expansion can not be summed up to get a closed form for $\widehat{\Phi}_U[\mathbf{G}]$, 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 nonequilibrium path-integral formalism may be used for an entirely nonperturbative construction. Again, this can be done analogously to the equilibrium case.⁵⁸ Both variants allow us to derive the following four properties that will be used extensively for constructing the nonequilibrium SFT:

(i) The Luttinger-Ward functional vanishes in the noninteracting limit

$$\widehat{\Phi}_U[\mathbf{G}] \equiv 0 \quad \text{for } \mathbf{U} = 0 \quad (11)$$

since there is no zeroth-order diagram.

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

$$\frac{\delta \widehat{\Phi}_U[\mathbf{G}]}{\delta \mathbf{G}(1,2)} = \frac{1}{\beta} \widehat{\Sigma}_U[\mathbf{G}](2,1) \quad (12)$$

with the shorthand notation $i \equiv (\alpha_i, z_i)$. Diagrammatically, the functional derivative corresponds to the removal of a propagator from each of the Φ diagrams. Taking care of topological factors,⁵⁷ one ends up with the skeleton-diagram expansion of the self-energy which, independently from the definition [Eq. (8)] gives the self-energy as a functional of the Green’s function $\widehat{\Sigma}_U[\mathbf{G}]$. Evaluating the functional $\widehat{\Sigma}$ at the exact (“physical”) Green’s function $\mathbf{G}_{T,U}$ yields the physical self-energy

$$\widehat{\Sigma}_U[\mathbf{G}_{T,U}] = \Sigma_{T,U}. \quad (13)$$

(iii) Since any diagram in the series depends on \mathbf{U} and on \mathbf{G} only, the Luttinger-Ward functional is “universal,” i.e., it is independent of \mathbf{T} . Two systems with the same interaction \mathbf{U} but different one-particle parameters \mathbf{T} are described by the same Luttinger-Ward functional. This implies that the functional $\widehat{\Sigma}_U[\mathbf{G}]$ is universal, too.

(iv) If evaluated at the physical Green’s function $\mathbf{G}_{T,U}$ of the system with Hamiltonian $H_{T,U}$, the Luttinger-Ward functional provides a quantity

$$\widehat{\Phi}_U[\mathbf{G}_{T,U}] = \Phi_{T,U}. \quad (14)$$

Note that $\Phi_{T,U}$ depends on the initial equilibrium state of the system only, as contributions from the Keldysh branch cancel each other (for details, see Sec. VIII). $\Phi_{T,U}$ is related to the grand potential of the system via the expression

$$\Omega_{T,U} = \Phi_{T,U} + \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{\varepsilon_0,0}^{-1} \circ \mathbf{G}_{T,U}) - \frac{1}{\beta} \text{Tr} (\Sigma_{T,U} \circ \mathbf{G}_{T,U}). \quad (15)$$

Here, we defined the trace as

$$\text{Tr} \mathbf{A} = \sum_{\alpha} \int_{\mathcal{C}} dz A_{\alpha\alpha}(z, z^+), \quad (16)$$

where z^+ is infinitesimally later than z on \mathcal{C} . The factor $\mathbf{G}_{\varepsilon_0,0}^{-1}$ with $\varepsilon_0 \rightarrow \infty$ has to be introduced to regularize the $\text{Tr} \ln$ term as discussed in Appendix A. It will be omitted in the following as it does not affect the results. Equation (15) can be derived using a coupling-constant integration⁵⁷ or by integrating over the chemical potential μ .⁵⁸ The proof is completely analogous to the equilibrium case.

IV. DYNAMICAL VARIATIONAL PRINCIPLE

We assume the functional $\widehat{\Sigma}_U[\mathbf{G}]$ is invertible *locally* to construct the Legendre transform of the Luttinger-Ward functional

$$\widehat{F}_U[\Sigma] = \widehat{\Phi}_U[\widehat{G}_U[\Sigma]] - \frac{1}{\beta} \text{Tr} (\Sigma \circ \widehat{G}_U[\Sigma]). \quad (17)$$

Here, $\widehat{G}_U[\widehat{\Sigma}_U[\mathbf{G}]] = \mathbf{G}$. With Eq. (12), one has

$$\frac{\delta \widehat{F}_U[\Sigma]}{\delta \Sigma(1,2)} = -\frac{1}{\beta} \widehat{G}_U[\Sigma](2,1). \quad (18)$$

We now define the self-energy functional as

$$\widehat{\Omega}_{T,U}[\Sigma] = \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{T,0}^{-1} - \Sigma)^{-1} + \widehat{F}_U[\Sigma]. \quad (19)$$

Its functional derivative is [use Eq. (A2)]

$$\frac{\delta \widehat{\Omega}_{T,U}[\Sigma]}{\delta \Sigma} = \frac{1}{\beta} (\mathbf{G}_{T,0}^{-1} - \Sigma)^{-1} - \frac{1}{\beta} \widehat{G}_U[\Sigma]. \quad (20)$$

The equation

$$\widehat{G}_U[\Sigma] = (\mathbf{G}_{T,0}^{-1} - \Sigma)^{-1} \quad (21)$$

is a (highly nonlinear) conditional equation for the self-energy of the system $H_{T,U}$. Equations (8) and (13) show that it is satisfied by the physical self-energy $\Sigma = \Sigma_{T,U}$. Note that the left-hand side of Eq. (21) is independent of \mathbf{T} but depends on \mathbf{U} (due to the universality of $\widehat{G}_U[\Sigma]$), while the right-hand side is independent of \mathbf{U} but depends on \mathbf{T} via $\mathbf{G}_{T,0}^{-1}$.

The obvious problem of finding a solution of Eq. (21) is that there is no closed form for the functional $\widehat{G}_U[\Sigma]$. Solving

Eq. (21) is equivalent, however, to a search for the stationary point of the grand potential as a functional of the self-energy:

$$\frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}]}{\delta \boldsymbol{\Sigma}} = 0. \quad (22)$$

This equation is the starting point for nonequilibrium 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 $\boldsymbol{\Sigma}$ 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 (21). As will become clear in the following, 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 $\Sigma_{\alpha\alpha'}(z, z')$.

V. CONSTRUCTING APPROXIMATIONS

Even though the Luttinger-Ward functional and its Legendre transform $\widehat{F}_U[\boldsymbol{\Sigma}]$ are generally unknown, it is possible to evaluate the self-energy functional (19) exactly on a certain subspace of self-energies: To this end, we compare the self-energy functional of the original system with the self-energy functional of a reference system, given by a Hamiltonian $H' \equiv H_{\lambda', U}$, which differs from the original Hamiltonian $H_{T,U}$ only in its one-particle parameters λ' , but shares its interaction part. In the following, primed quantities refer to the reference system. The respective self-energy functional is

$$\widehat{\Omega}_{\lambda', U}[\boldsymbol{\Sigma}] = \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{\lambda', 0}^{-1} - \boldsymbol{\Sigma})^{-1} + \widehat{F}_U[\boldsymbol{\Sigma}]. \quad (23)$$

Since $\widehat{F}_U[\boldsymbol{\Sigma}]$ is universal, we can eliminate $\widehat{F}_U[\boldsymbol{\Sigma}]$ and write

$$\begin{aligned} \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}] &= \widehat{\Omega}_{\lambda', U}[\boldsymbol{\Sigma}] + \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{T,0}^{-1} - \boldsymbol{\Sigma})^{-1} \\ &\quad - \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{\lambda', 0}^{-1} - \boldsymbol{\Sigma})^{-1}. \end{aligned} \quad (24)$$

The previous expression is still exact, but the self-energy functional for the reference system is not available in a closed form, even for very simple cases, as e.g. the atomic limit of the Hubbard model. However, we can nevertheless make use of Eq. (24) if both the exact self-energy $\boldsymbol{\Sigma}_{\lambda', U}$ and the self-energy functional of the reference system, evaluated at the exact self-energy, i.e., $\widehat{\Omega}_{\lambda', U}[\boldsymbol{\Sigma}_{\lambda', U}] = \Omega_{\lambda', U}$, are accessible. Using Dyson's equation [Eq. (8)] for the reference system, we find for the self-energy functional of the original system if evaluated at a trial self-energy taken from the reference system and parametrized by the set of variational parameters λ'

$$\begin{aligned} \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda', U}] &= \Omega_{\lambda', U} + \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{T,0}^{-1} - \boldsymbol{\Sigma}_{\lambda', U})^{-1} \\ &\quad - \frac{1}{\beta} \text{Tr} \ln (\mathbf{G}_{\lambda', U}). \end{aligned} \quad (25)$$

This shows that an exact evaluation of the general nonequilibrium self-energy functional is possible on the restricted space of trial self-energies spanned by any reference system with the same interaction part, provided that the contour-ordered

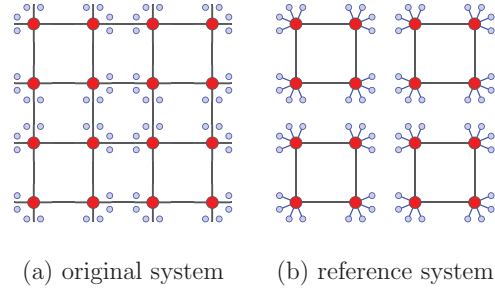


FIG. 3. (Color online) Schematic representation of the original system (a) and of a generic reference system (b). Large red circles: correlated sites with Hubbard-type local interaction U . Small blue circles: uncorrelated “bath” sites, i.e., $U = 0$. Bold black lines: intracluster hopping. Thin blue lines: hybridization, i.e., hopping between correlated and bath sites in the reference system. Note that in the original system (a) bath sites are decoupled from the correlated ones. Their presence is helpful for formal reasons to ensure equal Hilbert space dimensions in (a) and (b).

self-energy and Green's function as well as the initial-state grand potential of the reference system can be computed exactly.

The time-dependent optimal variational parameters $\lambda'_{\text{opt}}(z)$ have to be determined via the Euler equation

$$\left. \frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda', U}]}{\delta \lambda'(z)} \right|_{\lambda'(z)=\lambda'_{\text{opt}}(z)} = 0. \quad (26)$$

We thus have (approximate) access to the initial-state grand potential $\widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}}, U}]$ as well as to the final-state dynamics via the one-particle Green's function

$$\mathbf{G}^{\text{SFT}} \equiv (\mathbf{G}_{T,0}^{-1} - \boldsymbol{\Sigma}_{\lambda'_{\text{opt}}, U})^{-1} \quad (27)$$

on the Keldysh branch. The choice of the reference system specifies the type of approximation. Approximations generated in this way are nonperturbative by construction.

The Hamiltonian $H_{\lambda', U}$ of the reference system must have the same interaction part as the one of the original system and, for any practical application, must allow for an exact calculation of the trial self-energy $\boldsymbol{\Sigma}_{\lambda', U}$ and of the Green's function $\mathbf{G}_{\lambda', U}$ by analytical or numerical means. Typically, this is achieved by cutting the original lattice into disconnected clusters with a small number of sites L_c (Fig. 3). To enlarge the number of variational degrees of freedom locally without changing the interaction part, a number L_b of uncorrelated “bath sites” may be added to each of the reference system's correlated sites and coupled to the correlated sites via a finite hybridization. It is convenient to have equal Hilbert spaces and thus to formally include the bath sites in the original system as well but without a coupling to the physical sites (Fig. 3). In the case of a local (Hubbard-type) interaction and for sufficiently small L_c and L_b , the reference system can be treated by exact-diagonalization techniques.

VI. DYNAMICAL MEAN-FIELD THEORY

Nonequilibrium dynamical mean-field theory is recovered within the SFT framework when we choose the reference system as a set of completely decoupled correlated sites ($L_c = 1$) with an infinite number of bath sites ($L_b = \infty$), i.e.,

as a set of decoupled single-impurity Anderson models. For $L_c = 1$, the trial self-energies are local, i.e., diagonal with

respect to the spatial indices, and the Euler equation (26) thus explicitly reads as

$$0 = \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'(z)} = \frac{1}{\beta} \sum_{i,\sigma_1\sigma_2} \int_{\mathcal{C}} dz_1 dz_2 [(G_{T,0}^{-1} - \Sigma_{\lambda',U})^{-1} - G_{\lambda',U}]_{ii,\sigma_1\sigma_2}(z_1, z_2) \frac{\delta \Sigma_{\lambda',U;ii,\sigma_2\sigma_1}(z_2, z_1^+)}{\delta \lambda'(z)}. \quad (28)$$

Here, i is a site index and σ_i refers to the local orbital and spin degrees of freedom.

Equation (28) would be trivially satisfied if the square brackets in the integrand vanished. Because the vanishing of the square brackets is nothing but the standard self-consistency equation of DMFT,^{18–20} we see that nonequilibrium SFT yields (nonequilibrium) 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 λ' . The representability of the DMFT action by an actual impurity Hamiltonian with $L_b = \infty$ is not straightforward to see for nonequilibrium Green's functions, but can be shown under rather general conditions.³⁸

When one considers finite single-impurity models with a small number of bath orbitals, the square brackets in Eq. (28) will in general not vanish because the discrete pole structure of the impurity Green's function can not 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 us to generate nonperturbative 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 (see, e.g., Refs. 33 and 34).

VII. PHYSICAL AND TRANSVERSE VARIATIONS

The variational problem [Eq. (26)] is posed on the whole contour \mathcal{C} , i.e., the self-energy functional must be stationary with respect to variations of the parameters $\lambda'(z)$ *separately* on the Matsubara branch and on both branches of the Keldysh contour. This generates one imaginary-time and two independent real-time Euler equations which are obtained by writing $\widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}] \equiv \widehat{\Omega}_{T,U}[\Sigma_{\lambda'_+, \lambda'_-, \lambda'_M, U}]$ as a functional of the single-particle parameters $\lambda_{\pm}(t)$ on the upper/lower branch of the contour (for real t), as well as of the parameters $\lambda'_M(t_0 - i\tau)$ on the Matsubara branch. Using a simple transformation of variables,

$$\begin{aligned} \lambda'_{\text{phys}}(t) &= \frac{1}{2}[\lambda'_+(t) + \lambda'_-(t)], \\ \lambda'_{\text{trans}}(t) &= \frac{1}{2}[\lambda'_+(t) - \lambda'_-(t)], \end{aligned} \quad (29)$$

the real-time equations become equivalent to $\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda'_{\text{phys}}, \lambda'_{\text{trans}}, \lambda'_M, U}]/\delta \lambda'_{\text{phys/trans}}(t) = 0$.

The separation into variations with respect to λ'_{phys} (“physical variations”) and λ'_{trans} (“transverse variations”) has a simple motivation: In the end, we are only interested in solutions of the Euler equation by a physical parameter set $\lambda'(z)$, i.e., one that corresponds to an actual *Hamiltonian*. These parameters

must thus satisfy $\lambda'_+(t) = \lambda'_-(t)$, i.e., $\lambda'_{\text{trans}}(t) = 0$. In addition, $\lambda'_{\text{trans}}(t_0 - i\tau)$ must not depend on imaginary time (this is discussed in Sec. IX). Transverse variations $\delta \lambda'_{\text{trans}}(t) \neq 0$ shift the parameters away from the physical manifold, while physical variations remain therein.

Let us first consider variations of $\lambda'_{\text{phys}}(t)$. Interestingly, one can show that the self-energy functional is always stationary with respect to physical variations when evaluated at a physical parameter set, which satisfies $\lambda'_{\text{trans}}(t) = 0$, i.e.,

$$\left. \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda'_{\text{phys}}, \lambda'_{\text{trans}}, \lambda'_M, U}]}{\delta \lambda'_{\text{phys}}(t)} \right|_{\lambda'_{\text{trans}}(t)=0} = 0. \quad (30)$$

To prove Eq. (30), we first note that any Green's function defined by Eq. (6) is symmetric with respect to a shift of the largest time argument on the Keldysh contour from the upper to the lower branch, i.e.,

$$\begin{aligned} X(t_0 - i\tau, t^+) &= X(t_0 - i\tau, t^-), \\ X(t', t^+) &= X(t', t^-) \quad \text{for } t > t', \end{aligned} \quad (31)$$

and similar for the first time argument (t^{\pm} denotes a time argument on the upper/lower branch at t). This symmetry relation, which is often formulated as a fundamental relation between retarded, advanced, and time-ordered components of the Green's functions,⁵⁴ immediately follows from the fact that the forward and backward time evolutions cancel each other after the rightmost operator on the Keldysh contour (see also the discussion of Fig. 1). The same property holds for the convolution $A \circ B$ of any two contour functions A and B if it holds for A and B individually, and thus for any function of X [cf. Eq. (A1)]. Furthermore, it is easy to see that in the expression (16) for the trace all integrations over the Keldysh branch cancel for any function with the symmetry (31). Thus, the self-energy functional (19), when evaluated at physical parameters, depends on the Matsubara part of $\Sigma_{\lambda',U}$ only. This immediately implies the stationarity condition (30).

Stationarity with respect to physical variations locally restricts the solution to the physical manifold. Thus, a second equation is needed to fix the solution within the physical manifold. This “second” equation is given by the condition that the self-energy functional be stationary with respect to the transverse variations, if evaluated at a physical parameter set:

$$\left. \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda'_{\text{phys}}, \lambda'_{\text{trans}}, \lambda'_M, U}]}{\delta \lambda'_{\text{trans}}(t)} \right|_{\lambda'_{\text{trans}}(t)=0} = 0. \quad (32)$$

Equation (32) is the central equation of the nonequilibrium SFT.

Let us stress once more that the functional derivative with respect to $\lambda'_{\text{trans}}(t)$ is a derivative into a “nonphysical”

direction in parameter space. This has important conceptual consequences for the numerical evaluation of the theory. In the vast majority of previous *equilibrium* SFT studies, the grand potential $\widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]$ has been computed for different (static) parameter sets λ' , and algorithms to find a stationary point of a multidimensional scalar function $\lambda' \mapsto \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]$ have been employed (see Ref. 59, for example). In the nonequilibrium case, a similar strategy would require us to work explicitly with Green's functions that are defined with a different Hamiltonian for the forward and backward time evolutions. A more convenient strategy, which is worked out in the following, is to carry out the functional derivative analytically and to solve the resulting Euler equation by numerical means. The analytical expressions for the functional derivatives are then given by higher-order correlation functions evaluated at the physical parameters.

VIII. EVALUATION OF THE EULER EQUATION

We focus on Eq. (25) again and perform the functional derivative in Eq. (26) analytically. This is most conveniently done by considering the variational parameters as functions of the contour variable, i.e., $\lambda'(z)$ with $z \in \mathcal{C}$, instead of treating $\lambda_{\pm}(t)$ and $\lambda_M(t_0 - i\tau)$ separately.

Using the chain rule, we find

$$\frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'_{\alpha_1 \alpha_2}(z)} = \text{Tr} \left(\frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \Sigma_{\lambda',U}} \circ \frac{\delta \Sigma_{\lambda',U}}{\delta \lambda'_{\alpha_1 \alpha_2}(z)} \right). \quad (33)$$

The first factor is given by Eq. (20) but can be rewritten in a more convenient way. We define the difference between the one-particle parameters of the original and of the reference system as

$$V(z) = T(z) - \lambda'(z). \quad (34)$$

With this, we immediately have [see Eq. (7)]

$$G_{\lambda',0}^{-1}(1,2) = G_{T,0}^{-1}(1,2) + \delta_{\mathcal{C}}(z_1, z_2) V_{\alpha_1 \alpha_2}(z_2). \quad (35)$$

Here, we use the standard notation $1 \equiv (\alpha_1, z_1)$, etc. With the definition of the SFT Green's function [Eq. (27)] and with Dyson's equation for the reference system, we get

$$G^{\text{SFT}} = G_{\lambda',U} + G_{\lambda',U} V \circ G^{\text{SFT}}. \quad (36)$$

This equation constitutes the nonequilibrium cluster-perturbation theory.³⁹ One may formally consider perturbation theory with respect to V and define the corresponding T matrix as

$$Y_{\lambda',T,U}(z_1, z_2) = V(z_1) \delta_{\mathcal{C}}(z_1, z_2) + V(z_1) G^{\text{SFT}}(z_1, z_2) V(z_2). \quad (37)$$

The related Lippmann-Schwinger equation is

$$G^{\text{SFT}} = G_{\lambda',U} + G_{\lambda',U} \circ Y_{\lambda',T,U} \circ G_{\lambda',U}. \quad (38)$$

This eventually yields

$$\frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \Sigma_{\lambda',U}} = \frac{1}{\beta} G_{\lambda',U} \circ Y_{\lambda',T,U} \circ G_{\lambda',U} \quad (39)$$

for the first factor in Eq. (33).

To evaluate the second factor, the Dyson equation for the reference system is used once more to get $\Sigma_{\lambda',U} =$

$G_{\lambda',0}^{-1} - G_{\lambda',U}^{-1}$. The λ' dependence of the inverse free Green's function is simple: $G_{\lambda',0}^{-1}(1,2) = \delta_{\mathcal{C}}(z_1, z_2) \delta_{\alpha_1, \alpha_2} i \partial_{z_2} - \delta_{\mathcal{C}}(z_1, z_2) [\lambda'_{\alpha_1 \alpha_2}(z_2) - \delta_{\alpha_1 \alpha_2} \mu]$. We thus get

$$\begin{aligned} & \frac{\delta \Sigma_{\lambda',U}(3,4)}{\delta \lambda'_{\alpha_1 \alpha_2}(z_1)} \\ &= -\delta_{\mathcal{C}}(z_3, z_4) \delta_{\alpha_3 \alpha_1} \delta_{\mathcal{C}}(z_4, z_1) \delta_{\alpha_4 \alpha_2} \\ &+ \iint d5 d6 G_{\lambda',U}^{-1}(3,5) \frac{\delta G_{\lambda',U}(5,6)}{\delta \lambda'_{\alpha_1 \alpha_2}(z_1)} G_{\lambda',U}^{-1}(6,4). \quad (40) \end{aligned}$$

The functional derivative of the Green's function is computed in the Appendix B and given by Eq. (B2).

Combining this with Eq. (39), we finally get the derivative of the self-energy functional with respect to $\lambda'(z_1)$ in the form

$$\begin{aligned} & \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'_{\alpha_1 \alpha_2}(z_1)} \\ &= -\frac{1}{\beta} \iint d3 d4 Y_{\lambda',T,U}(4,3) L_{\lambda',U}(3,2,1^+,4)|_{z_2=z_1}, \quad (41) \end{aligned}$$

where

$$\begin{aligned} L_{\lambda',U}(1,2,3,4) &= G_{\lambda',U}(2,4) G_{\lambda',U}(1,3) \\ &- G_{\lambda',U}(1,4) G_{\lambda',U}(2,3) + G_{\lambda',U}^{(2)}(1,2,3,4) \quad (42) \end{aligned}$$

is the two-particle (four-point) vertex function with external legs and $G_{\lambda',U}^{(2)}$ is the two-particle Green's function of the reference system [see Eq. (B3)].

Therewith, we have the Euler equation of the nonequilibrium SFT:

$$\iint d3 d4 Y_{\lambda'_{\text{opt}},T,U}(4,3) L_{\lambda'_{\text{opt}},U}(3,2,1^+,4)|_{z_2=z_1} = 0. \quad (43)$$

This result will be needed both for the numerical determination of the stationary point and for working out the relation between nonequilibrium and conventional equilibrium SFT.

IX. THERMAL EQUILIBRIUM AND INITIAL STATE

Nonequilibrium SFT reduces to the conventional equilibrium formalism for a system where $T(z)$ and $U(z)$ are constant on the entire contour \mathcal{C} , i.e., for the case $H_{\text{fin}}(t) = \text{const} = H_{\text{ini}}$. To prove this fact explicitly, we have to show that a stationary point of the equilibrium SFT functional, which determines *time-independent* optimal parameters λ'_{opt} , is also a stationary point of the more general nonequilibrium Euler equation (26), i.e., of Eq. (43), when $T(z)$ and $U(z)$ are constant.

Equilibrium SFT is obtained from the more general nonequilibrium formalism by restricting the functional (25) to the Matsubara branch of the contour and, furthermore, by considering time-independent and physical variations only, i.e., the trial self-energy $\Sigma_{\lambda',U}$ is obtained as the Matsubara self-energy of a Hamiltonian with constant parameters λ' , and the parameters are varied to make $\widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]$ stationary. In the language of the more general nonequilibrium SFT formalism, those variations correspond to a variation $\delta \lambda(z)$ which is constant along the whole contour, i.e.,

$$\frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'} = \int_{\mathcal{C}} dz \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'(z)}. \quad (44)$$

Note that the integrations over the upper and lower branches of the Keldysh contour cancel, as discussed in connection with Eq. (30). We now suppose that the original Hamiltonian is time independent, and that λ'_{opt} is a solution of the equilibrium SFT formalism, i.e., the single variational equation $\partial \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]/\partial \lambda'_{\lambda'_{\text{opt}}} = 0$ is satisfied.

To see that the parameters λ'_{opt} also represent a solution of the nonequilibrium SFT, we must show that all other variations, including physical, transverse, and Matsubara ones, vanish as well. For this it is sufficient to show that the general variational equation becomes time-translationally invariant, i.e., that the expression

$$\frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'(z)} \Big|_{\lambda'(z)=\lambda'_{\text{opt}}} \quad (45)$$

does not depend on z .

Consider a z on the Matsubara branch first. Invariance under translations of imaginary time is most easily seen from the explicit expression (41) for the variational derivative: For $z_1 = t_0 - i\tau_1$, the integrals in Eq. (41) reduce to the Matsubara branch. Furthermore, the two functions L and Y in the integrand are translationally invariant in imaginary time as they are evaluated at τ -independent parameters λ' . More precisely, we can write $L(\tau_3, \tau_1, \tau_1^+, \tau_4) \equiv \tilde{L}(\tau_3 - \tau_1, \tau_4 - \tau_1)$ and $Y(\tau_3, \tau_4) \equiv \tilde{Y}(\tau_3 - \tau_4)$ with functions \tilde{L} and \tilde{Y} that are antiperiodic under $\tau \rightarrow \tau + \beta$. After a shift of variables, it is easily seen that the integral in Eq. (41) does not depend on z_1 .

For z_1 on the Keldysh branch, on the other hand, time-translational invariance of Eq. (45) can be seen from a Lehmann representation (or spectral representation) of the functions L and Y . The explicit calculation is more tedious and presented in Appendix C.

For a general nonequilibrium situation with $H_{\text{fin}}(t) \neq \text{const}$, the above argument can be used to show that the causality principle is satisfied by the nonequilibrium SFT: Satisfying the general variational equation (26) for all variations of $\lambda'(t_0 - i\tau)$ on the Matsubara branch requires that the optimal parameters on the Matsubara branch are τ independent and must be given by a solution of the equilibrium SFT. This shows that the description of the initial state is independent from the final-state dynamics.

We also note that, as in the equilibrium case, the self-energy functional evaluated at the stationary point $\widehat{\Omega}_{T,U}[\Sigma_{\lambda'_{\text{opt}},U}]$ has a clear physical meaning: It represents the (approximate) grand potential of the initial thermal state. Provided that there are several stationary points for a given set of (time-dependent) parameters of the original system, the one with the lowest grand potential in the initial state describes the thermodynamically stable initial state and the emerging final-state dynamics. Furthermore, provided that the same type of reference system is considered, the (approximate) description of the initial state is on equal footing with the one for the final state. Concluding, the nonequilibrium SFT is a true extension of the equilibrium SFT.

X. PROPAGATION SCHEME

A numerical evaluation of the Euler equation (26) seems like a formidable task because already the time dependence

of a single one-particle parameter of the reference system provides an infinite variational space. However, the variational principle of the nonequilibrium SFT has an inherent causal structure which allows it to determine the optimal parameters at successively increasing (physical) times, without modifying the result at earlier times. This causal structure is most easily visible from Eq. (43): The integrals over z_3 and z_4 extend over the entire contour \mathcal{C} but can be cut at $z_1 = t_1^\pm$ such that t_1 is the (physically) latest time (see discussion in Sec. VII). As all $\lambda'(z)$ -dependent quantities in the integrand are exact correlation functions of the reference system, Eq. (43) involves $\lambda'(z)$ at earlier times $t < t_1$ only. Hence, the conditional equation for $\lambda'_{\text{opt}}(z_1)$ and thus $\lambda'_{\text{opt}}(z_1)$ itself depends on $\lambda'_{\text{opt}}(z)$ with $t < t_1$ only.

For a numerical evaluation of the theory, one has to start from the Euler equation on the Matsubara branch only and perform a conventional equilibrium SFT calculation (cf. Sec. IX). This sets the initial conditions for determination of the time-dependent optimal variational parameters $\lambda'_{\text{opt}}(t)$. Provided that the parameters have already been determined at times earlier than a given physical time t , one has to fix $\lambda'_{\text{opt}}(t)$ by solving Eq. (43) with $z_1 = t_1^\pm$. This is somewhat inconvenient as the integrand in Eq. (43) only implicitly depends on $\lambda'_{\text{opt}}(t)$. The dependence can be made explicit, however, by means of a simple trick: Since Eq. (43) must hold for all z_1 , and since it holds at the initial time t_0 (the starting point is a stationary point of the equilibrium SFT), it suffices to require the *time derivative* of $\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]/\delta \lambda'(z)$, as given by Eq. (41), to vanish instead of the function itself. This will lead to an expression which involves $\lambda'_{\text{opt}}(t)$ explicitly.

According to Eqs. (41) and (42), the time derivative $(d/dt)\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]/\delta \lambda'(t^\pm)$ can be obtained from the corresponding equations of motion for the four-point vertex function $L_{\lambda',U}$. Commuting the respective annihilation and creation operators with the one-particle part of the Hamiltonian results in matrix products with λ' . Commuting with the interacting part, however, gives rise to higher-order products of annihilation and creation operators which we denote by $\hat{\psi}$ or $\hat{\psi}^\dagger$, respectively: $[c(1), H'_1(1)] \equiv \hat{\psi}(1)$ and $[H'_1(1), c^\dagger(1)] \equiv \hat{\psi}^\dagger(1)$. After differentiating with respect to time, the Euler equation on the Keldysh branch acquires the form

$$0 = i\beta \partial_z \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'(z)} = [\mathbf{K}_{\lambda'}^{(0)}, \lambda'](z) + \mathbf{K}_{\lambda'}^{(1)}(z), \quad (46)$$

where we have defined

$$\begin{aligned} \mathbf{K}_{\lambda';\alpha_2\alpha_1}^{(0)}(z_1) &= \iint d3 d4 Y_{\lambda',T,U}(4,3) L_{\lambda',U}(3,2,1^+,4)|_{z_2=z_1} \quad (47) \end{aligned}$$

and

$$\begin{aligned} \mathbf{K}_{\lambda';\alpha_2\alpha_1}^{(1)}(z_1) &= \iint d3 d4 Y_{\lambda',T,U}(4,3) \\ &\quad \times [L_{\lambda',U}(3,2,1_\psi^+,4) - L_{\lambda',U}(3,2_\psi,1^+,4)]|_{z_2=z_1}. \quad (48) \end{aligned}$$

Here, indexing orbital and time arguments with ψ means that the associated operators in the respective correlation functions

are replaced by $\hat{\psi}$ or $\hat{\psi}^\dagger$, respectively. For example,

$$iG_{\lambda',U}(1,\psi,2) = \langle \mathcal{T}_C \hat{\psi}(1)c^\dagger(2) \rangle \quad (49)$$

and

$$iG_{\lambda',U}(1,2,\psi) = \langle \mathcal{T}_C c(2)\hat{\psi}^\dagger(1) \rangle. \quad (50)$$

The contour integrations in $\mathbf{K}_{\lambda'}^{(0)}$ and $\mathbf{K}_{\lambda'}^{(1)}$ are confined to times (physically) earlier than z_1 . Hence, Eq. (46) provides an explicit equation for the optimal parameters $\lambda'_{\text{opt}}(t)$ at a given time t in terms of the parameters at earlier times which can be used to obtain the optimal solution by successively increasing t , starting from the equilibrium SFT solution for the initial state.

XI. INTERNAL CONSISTENCY

The SFT provides access to time-dependent expectation values of arbitrary one-particle observables as well as to the grand potential of the initial thermal state. An *exact* relation between both quantities can be derived by formally extending the grand canonical density operator to the whole Keldysh-Matsubara contour, such that the partition function reads as $Z_{T,U} = \text{tr}(\mathcal{T}_C e^{-i \int_C dz \mathcal{H}_{T,U}(z)})$ (see also discussion in Sec. II). The grand potential $\Omega_{T,U} = -\beta^{-1} \ln Z_{T,U}$ then becomes a functional of the (contour) time-dependent single-particle parameters of the model. We now consider an arbitrary one-particle observable of the form $A(z) = \sum_{\alpha\beta} a_{\alpha\beta}(z) c_\alpha^\dagger c_\beta$ which couples linearly to the Hamiltonian $H_{T,U}(z) = H_{T,U}^{(0)}(z) + \lambda_A(z)A(z)$ via a time-dependent parameter $\lambda_A(z)$. The set of one-particle parameters $\tilde{\mathbf{T}}(z)$ comprises $\lambda_A(z)$ as well as the remaining parameters $\tilde{\mathbf{T}}(z)$. Then, the expectation value of $A(z)$ can be obtained via the linear-response relation

$$\langle A(z) \rangle_{T,U} = -i\beta \left. \frac{\delta \Omega_{T,U}}{\delta \lambda_A(z)} \right|_{\lambda_A(z)=0}, \quad (51)$$

where only the variational derivative in the ‘‘transverse’’ but not in the ‘‘physical’’ contributes, as discussed in Sec. VII.

On the other hand, the expectation value may be computed from the one-particle Green’s function as

$$\langle A(z) \rangle_{T,U} = -i \text{tr}[\mathbf{a}(z) \mathbf{G}_{T,U}(z, z^+)]. \quad (52)$$

The SFT provides approximate expressions for the grand potential as well as for the expectation value. However, one can show that these approximations are consistent, i.e.,

$$\left. \frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}},U}]}{\delta \lambda_A(z)} \right|_{\lambda_A(z)=0} = \frac{1}{\beta} \text{tr}[\mathbf{a}(t) \mathbf{G}^{\text{SFT}}(z, z^+)], \quad (53)$$

where \mathbf{G}^{SFT} is the SFT Green’s function [Eq. (27)]. Here, $\widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}},U}]$ is the grand potential at the optimal parameters of the reference system which still can be considered as a functional of the time-dependent parameters of the original system and of $\lambda_A(z)$ in particular. Equation (53) represents a generalization of the ‘‘thermodynamical consistency’’ that has been shown in the context of the equilibrium formalism already.⁶⁰

To prove Eq. (53), we note that its left-hand side has a twofold dependence on $\lambda_A(z)$: (i) via the free Green’s function of the original model $\mathbf{G}_{T,0}^{-1}$, which enters the second term in

Eq. (25), and (ii) via the optimized parameters $\lambda'_{\text{opt}}(z)$, which depend on the time-dependent parameters in the final state of the original system. Consequently, there are two terms resulting from the derivative:

$$\begin{aligned} \frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}},U}]}{\delta \lambda_A(z)} &= \frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}},U}]}{\delta \lambda'_{\text{opt}}} \circ \frac{\delta \lambda'_{\text{opt}}}{\delta \lambda_A(z)} \\ &+ \frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}},U}]}{\delta \mathbf{T}} \circ \frac{\delta \mathbf{T}}{\delta \lambda_A(z)}. \end{aligned} \quad (54)$$

Internal consistency is achieved because of the stationarity of the self-energy functional at $\lambda'_{\text{opt}}(z)$, which implies that the first term must vanish. Using Eqs. (19) and (A2), the functional derivative with respect to $\mathbf{T}(z)$ in the second term is found to be

$$\frac{\delta \widehat{\Omega}_{T,U}[\boldsymbol{\Sigma}_{\lambda'_{\text{opt}},U}]}{\delta \mathbf{T}(z)} = \frac{1}{\beta} \mathbf{G}^{\text{SFT}}(z, z^+). \quad (55)$$

The second factor yields $a_{\alpha\beta}(t)$, which proves Eq. (53).

XII. CONSERVATION LAWS

Approximations can not be expected *a priori* to respect fundamental conservation laws that result from the invariance of the Hamiltonian under certain continuous groups of unitary transformations. In fact, conservation of the total particle number, the total spin, or the total energy are certainly violated within simple non-self-consistent or nonvariational schemes such as the nonequilibrium cluster-perturbation theory, apart from certain highly symmetric situations such as given by the Hubbard model on a bipartite lattice at half-filling.^{39–41} A general theory for real-time dynamics must therefore address the question under which conditions an approximation is conserving.

With respect to self-consistent perturbative approximations, this question has been answered by Baym and Kadanoff:^{46,47} a diagrammatic approximation is defined by a certain truncation of the skeleton-diagram expansion of the self-energy, which yields the self-energy as a functional of the Green’s function. Combined with Dyson’s equation, which provides an independent relation between self-energy and Green’s function, the problem can be solved using an iterative and self-consistent approach. A perturbative approximation is found to be conserving if the (truncated) skeleton-diagram expansion of the self-energy is obtained as the functional derivative of an approximate Luttinger-Ward functional that itself is constructed by truncations and resummations within diagrammatic weak-coupling perturbation theory, i.e., the self-energy must be Φ -derivable. Φ -derivable approximations are conserving.

Contrary, approximations generated within the framework of the SFT are nonperturbative and do not rely on diagrammatic resummations. While the Luttinger-Ward functional is essential for the construction of the SFT, and while the SFT self-energy is obtained as its functional derivative, approximations are generated in a very different way as compared to perturbation theory. Namely, instead of truncating the Luttinger-Ward functional diagrammatically, it is restricted to a submanifold of self-energies generated by some (simpler) reference system. The SFT self-energy is derived from this

restricted Φ functional. Hence, approximations constructed within the SFT are “ Φ -derivable” but in a different sense as compared to weak-coupling theory.

Note that the DMFT, as the most prominent approximation in this context, represents an exception. DMFT can be understood as an approximation generated within the SFT framework (see Sec. VI). At the same time, DMFT is a Φ -derivable approximation in the spirit of Baym and Kadanoff as it can be constructed diagrammatically from a truncated Luttinger-Ward functional involving local propagators only.

In the following, we will modify and adapt the essential ideas of Baym and Kadanoff to analyze under which circumstances an *arbitrary* approximation constructed within the SFT framework is conserving. The important point observed by Baym and Kadanoff is that the fundamental conservation laws, reformulated in terms of the self-energy and the Green’s function, result from invariances of the Luttinger-Ward functional under appropriate gauge transformations of the Green’s function:

$$0 = \delta \widehat{\Phi}_U[G_{T,U}] = \frac{1}{\beta} \text{Tr}(\Sigma_{T,U} \circ \delta G_{T,U}). \quad (56)$$

Within SFT, the self-energy functional is in fact constructed with the help of the Luttinger-Ward functional [see Eqs. (17) and (19)]. However, it does not inherit its gauge invariance. Nevertheless, the Euler equation provides the analog of Eq. (56) at the stationary point:

$$\begin{aligned} 0 &= \delta \widehat{\Omega}_{\lambda',U}[\Sigma_{\lambda',U}]|_{\lambda'=\lambda'_{\text{opt}}} \\ &= \frac{1}{\beta} \text{Tr}[(G^{\text{SFT}} - G_{\lambda',U}) \circ \delta \Sigma_{\lambda',U}]|_{\lambda'=\lambda'_{\text{opt}}}, \end{aligned} \quad (57)$$

i.e., by construction the variation of the grand potential $\widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]$ with respect to an *arbitrary* set of one-particle parameters of the reference system λ' vanishes, if evaluated at the optimal parameters. Thus, the goal is to identify a certain class of parameter variations which generates, via Eq. (57), the necessary conditions on the SFT Green’s function and the self-energy from which the conservation laws derive.

A. Particle number and spin

Particle number and spin conservation can be treated simultaneously. The integral quantities N_{tot} and S_{tot} can be expressed as

$$A = \sum_i A_i \quad (58)$$

in terms of local quantities A_i , the local occupation number and the local spin, n_i and $S_i^{(\eta)}$ ($\eta \in \{x, y, z\}$),

$$A_i = \sum_{\sigma\sigma'} a_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}, \quad (59)$$

using the notation

$$a_{\sigma\sigma'} = \delta_{\sigma\sigma'} \quad (60)$$

in the case $A_i = n_i$ and

$$a_{\sigma\sigma'} = \frac{1}{2} \sigma_{\sigma\sigma'}^{(\eta)} \quad (61)$$

in the case $A_i = S_i^{(\eta)}$. Here, i refers to the sites of the lattice model, $\sigma, \sigma' = \uparrow, \downarrow$ to the spin degrees of freedom, and $\sigma^{(\eta)}$ stands for the three Pauli matrices.

Consider a system with Hamiltonian $H_{T,U}$ and the time-dependent expectation value of the local quantity A_i as given by Eq. (5). With the help of the one-particle Green’s function, the expectation value can be written as

$$\langle A_i \rangle_{T,U}(t) = -i \sum_{\sigma\sigma'} a_{\sigma\sigma'} G_{T,U,ii,\sigma'\sigma}(t, t^+). \quad (62)$$

Its equation of motion is readily obtained from the equation of motion for the Green’s function [i.e., from Eqs. (7) and (8), or see Ref. 55]. We find

$$\begin{aligned} \partial_t \langle A_i \rangle_{T,U}(t) &= \sum_{\sigma\sigma'} a_{\sigma\sigma'} [G_{T,U}, \mathbf{T}]_{ii,\sigma'\sigma}(t, t^+) \\ &+ \sum_{\sigma\sigma'} a_{\sigma\sigma'} [G_{T,U} \circ \Sigma]_{ii,\sigma'\sigma}(t, t^+), \end{aligned} \quad (63)$$

where $[\dots, \dots]$ is the commutator and $[\dots \circ \dots]$ indicates that aside from the commutator a contour integration is implied.

For a Hubbard-type model with local interaction, the second commutator vanishes identically. Equation (63) thus attains the form of a continuity equation where the first commutator represents the divergence of the charge current or spin current. It vanishes if summed over all sites i due the cyclic property of the trace, and we are left with $\partial_t \langle A \rangle_{T,U}(t) = 0$, i.e., conservation of the total particle number or spin.

Within SFT, the real-time dynamics of one-particle observables is determined by the approximate Green’s function G^{SFT} , as given by Eq. (27). The SFT self-energy is the self-energy of a reference system with one-particle parameters λ' . Both are taken at optimal parameter values λ'_{opt} satisfying the SFT Euler equation (26). Thus, our goal is to show that

$$\sum_{\sigma\sigma'} a_{\sigma\sigma'} [G^{\text{SFT}} \circ \Sigma_{\lambda'_{\text{opt}},U}]_{ii,\sigma'\sigma}(t, t^+) = 0. \quad (64)$$

This would be sufficient to ensure that an approximation constructed within the SFT framework respects the conservation of particle number and spin even locally.

To this end, we consider the following gauge transformations of the one-particle parameters of the reference system $\lambda' \mapsto \tilde{\lambda}'$:

$$\begin{aligned} \boldsymbol{\varepsilon}'(z) &\mapsto \tilde{\boldsymbol{\varepsilon}}'(z) = \boldsymbol{\varepsilon}'(z) - \partial_z \chi(z), \\ \mathbf{T}'(z) &\mapsto \tilde{\mathbf{T}}'(z) = e^{i\chi(z)} \mathbf{T}'(z) e^{-i\chi(z)}, \end{aligned} \quad (65)$$

where $\boldsymbol{\varepsilon}'$ denotes the (spatially) diagonal part of λ' and \mathbf{T}' its off-diagonal part. The gauge transformation is generated by a spatially diagonal contour function χ of the form

$$\chi_{ij,\sigma\sigma'}(z) = \delta_{ij} \chi_i(z) a_{\sigma\sigma'}. \quad (66)$$

To ensure a Hermitian reference system, χ must be real but can be chosen arbitrary in other respects. Note that χ commutes with $\boldsymbol{\varepsilon}'$, which will become important later. This is trivially satisfied in the case $A_i = n_i$ [see Eq. (60)], and also holds in the case $A_i = S_i^{(\eta)}$ [see Eq. (61)] provided that $\boldsymbol{\varepsilon}'$ is independent of spin indices. The latter is a necessary condition to ensure total spin conservation *in the reference system*.

The next step is to show that the above gauge transformation of the one-particle parameters λ' implies that the exact Green’s

function $G' \equiv G_{\lambda',U}$ and the exact self-energy $\Sigma' \equiv \Sigma_{\lambda',U}$ of the reference system transform as

$$G'(z_1, z_2) \mapsto \tilde{G}'(z_1, z_2) = e^{i\chi(z_1)} G'(z_1, z_2) e^{-i\chi(z_2)} \quad (67)$$

and

$$\Sigma'(z_1, z_2) \mapsto \tilde{\Sigma}'(z_1, z_2) = e^{i\chi(z_1)} \Sigma'(z_1, z_2) e^{-i\chi(z_2)}. \quad (68)$$

We first note that Eq. (67) implies Eq. (68), which is verified by referring to the (exact) skeleton-diagram expansion $\tilde{\Sigma}' = \tilde{\Sigma}_U[\tilde{G}']$: Inserting the transformed \tilde{G}' , the phase factors of the incoming and the outgoing propagators cancel at each internal vertex. Only at the two links for the external legs the phase factors do not find a counterpart. This leaves us with the two phase factors at the transformed self-energy in Eq. (68). In order to verify Eq. (67), it is sufficient to show that the transformed Green's function and the transformed self-energy satisfy the equation of motion for the transformed parameters:

$$i\partial_{z_1} \tilde{G}'(z_1, z_2) = \delta_C(z_1, z_2) + \tilde{\lambda}'(z_1) \tilde{G}'(z_1, z_2) + (\tilde{\Sigma}' \circ \tilde{G}')(z_1, z_2). \quad (69)$$

This is a straightforward calculation which makes use of the fact that χ commutes with \mathbf{e}' . See Appendix D for details.

A first-order variation of the one-particle parameters of the reference system, given by $\delta\chi(z)$, leads to the following first-order variation of the self-energy [cf. Eq. (68)]:

$$\delta\Sigma'(z_1, z_2) = i\delta\chi(z_1)\Sigma'(z_1, z_2) - i\Sigma'(z_1, z_2)\delta\chi(z_2). \quad (70)$$

This leads to a first-order variation $\delta\hat{\Omega}_{T,U}[\Sigma_{\lambda',U}]$ which vanishes for optimal values of the variational parameters λ' , provided that the variation $\delta T' = i\delta\chi T' - iT'\delta\chi$ and $\delta\mathbf{e}' = -\partial_z\delta\chi$ of the reference parameters induced by Eq. (65) are chosen to part of our variational space. We insert Eq. (70) into the SFT Euler equation, as given by Eq. (57), and use Eq. (66) to get

$$\begin{aligned} 0 &= \beta\delta\hat{\Omega}_{T,U}[\Sigma_{\lambda',U}]|_{\lambda'=\lambda'_{\text{opt}}} \\ &= -i \sum_{i,\sigma\sigma'} \int_C dz a_{\sigma\sigma'} ([G^{\text{SFT}} \circ \Sigma_{\lambda'_{\text{opt}},U}] \\ &\quad + [G_{\lambda'_{\text{opt}},U} \circ \Sigma_{\lambda'_{\text{opt}},U}])_{ii,\sigma'\sigma}(z, z^+) \delta\chi_i(z) |_{\lambda'=\lambda'_{\text{opt}}}. \end{aligned} \quad (71)$$

Since this holds for arbitrary first-order variations $\delta\chi_i(z)$, the term $\sum_{\sigma\sigma'} a_{\sigma\sigma'}(\dots)$ must vanish. Consider the second term in the brackets: The condition $\sum_{\sigma\sigma'} a_{\sigma\sigma'} [G_{\lambda'_{\text{opt}},U} \circ \Sigma_{\lambda'_{\text{opt}},U}]_{ii,\sigma'\sigma}(z, z^+) = 0$ is just equivalent with local particle number and spin conservation *in the reference system* [see the discussion after Eq. (63)]. Therefore, *if* this is satisfied, the first term in the brackets must vanish as well, i.e., Eq. (64) is inferred. It is quite intuitive that particle number and spin conservation is respected by an approximation within the SFT only if it is exactly satisfied for the reference system that has been chosen to specify the approximation. We conclude that within the SFT, particle number and spin conservation is proliferated from the reference system, where it must hold exactly, to the original system, where it holds when formulated with the approximate SFT Green's function and self-energy.

The conservation laws are ensured by stationarity of the SFT grand potential with respect to the parameter variations defined by Eq. (65). Note that \mathbf{e}' and T' are not varied independently, i.e., particle number and spin conservation require stationarity with respect to variations along certain *directions* in the parameter space. In particular, complex hopping-parameter variations must be taken into account. Stationarity with respect to other directions can, of course, be imposed additionally.

Consider the Hubbard model and a variational cluster approximation (VCA) as an example. This results from the reference system shown in Fig. 3 for a cluster consisting of L_c correlated sites but no additional bath degrees of freedom. The conservation laws are respected if arbitrarily time-dependent and mutually independent variations for each of the onsite energies are considered as well as the resulting variations of the intracluster hopping parameters as prescribed by Eq. (65). Essentially, the same holds for approximations where additional bath degrees of freedom are considered to enlarge the parameter space.

The calculations above also show that conservation of the *total* particle number and the *total* spin are respected with site-independent variations, i.e., with a site-independent $\chi_i(z) = \chi(z)$ only. For the case of the particle number, this is equivalent with an arbitrarily time-dependent but *spatially homogeneous* variation of the onsite energies only as the phase factors in the transformation law for the off-diagonal parameters cancel each other. Analogously, the total spin is conserved within SFT if an arbitrarily time-dependent but *spatially homogeneous* magnetic field coupling to the total spin of the reference system is treated as a variational parameter.

For models with local interactions but several orbital degrees of freedom m , i.e., in the case of more complicated Coulomb parameters $U_{i,m_1m_2m_3m_4}$, the local variants of the conservation laws refer to the total particle number at a site $N_i = \sum_{m\sigma} c_{im\sigma}^\dagger c_{im\sigma}$ and the total spin at a site $S_i = \sum_m S_{im}$ with $S_{im} = (1/2) \sum_{\sigma\sigma'} c_{im\sigma}^\dagger \sigma_{\sigma\sigma'} c_{im\sigma'}$ as well as to the corresponding charge and spin currents. Here, the relevant variational parameters are the conjugated fields ε_i and \mathbf{B}_i coupling to N_i and S_i , respectively. Note that models with off-site Coulomb-interaction terms are in principle beyond the scope of the SFT (however, see Ref. 61) as the presence of intersite interactions prevents a simple decomposition of the lattice problem into independent cluster problems.

B. Energy

The case of energy conservation is more elaborate. This is related to the fact that the SFT is a variational approach which focuses on one-particle quantities, i.e., on the variational optimization of the one-particle self-energy and thus of the one-particle Green's function, while the interaction part of the total energy is a two-particle quantity. Fortunately, it can be expressed in terms of the one-particle Green's function and self-energy using the equation of motion. We can therefore proceed analogously to particle number and spin conservation and again try to make use of the ideas of Baym and Kadanoff.^{46,47} Complications are nevertheless to be expected and found in fact.

The kinetic (and potential) energy $E_{\text{kin}}(t) = \langle H_{T,0}(t) \rangle$ and the interaction energy $E_{\text{int}}(t) = \langle H_{0,U}(t) \rangle$ of the system can be written as (see Refs. 46 and 47, for example)

$$E_{\text{kin}}(t) = -i \text{tr}[\mathbf{T}(t)\mathbf{G}(t,t^+)], \quad (72)$$

$$E_{\text{int}}(t) = -\frac{i}{4} \text{tr}[(\mathbf{\Sigma} \circ \mathbf{G} + \mathbf{G} \circ \mathbf{\Sigma})(t,t^+)]. \quad (73)$$

The former directly follows from the definition of the Green's function. For the latter, we made use of the equation of motion for the Green's function and Dyson's equation. Note that we have written $\mathbf{G} \equiv \mathbf{G}_{T,U}$ and $\mathbf{\Sigma} \equiv \mathbf{\Sigma}_{T,U}$ for short. The total energy of the system is $E_{\text{tot}}(t) \equiv \langle H(t) \rangle = E_{\text{kin}}(t) + E_{\text{int}}(t)$. In the following, we assume that the interaction parameters \mathbf{U} are time independent (see also discussion in Sec. XII C). Using $\partial_t E_{\text{tot}}(t) = \langle \partial_t H(t) \rangle$, this immediately implies the following energy-balance relation:

$$\frac{\partial E_{\text{tot}}(t)}{\partial t} = \sum_{\alpha\beta} \frac{\partial T_{\alpha\beta}(t)}{\partial t} \langle c_{\alpha}^{\dagger}(t)c_{\beta}(t) \rangle. \quad (74)$$

Next, we express both the left-hand side and the right-hand side of Eq. (74) in terms of $\mathbf{\Sigma}$ and \mathbf{G} . Using the equation of motion again, the time derivatives of $E_{\text{kin}}(t)$ and $E_{\text{int}}(t)$ can be computed. From Eq. (72), we get

$$\begin{aligned} \frac{\partial E_{\text{kin}}(t)}{\partial t} &= \sum_{\alpha\beta} T_{\alpha\beta}([\mathbf{G}, \mathbf{T}]_{\beta\alpha}(t,t^+) + [\mathbf{G} \circ \mathbf{\Sigma}]_{\beta\alpha}(t,t^+)) \\ &\quad - i \text{tr} \left(\frac{\partial \mathbf{T}(t)}{\partial t} \mathbf{G}(t,t^+) \right) \\ &= \sum_{\alpha\beta} T_{\alpha\beta}[\mathbf{G} \circ \mathbf{\Sigma}]_{\beta\alpha}(t,t^+) - i \text{tr} \left(\frac{\partial \mathbf{T}(t)}{\partial t} \mathbf{G}(t,t^+) \right). \end{aligned} \quad (75)$$

Here, the first term in the first line vanishes due the cyclic property of the trace. Exploiting once more the equation of motion and the complex-conjugated equation, we find

$$\begin{aligned} \frac{\partial E_{\text{kin}}(t_1)}{\partial t_1} &= i \sum_{\alpha_1} \int d2 \left[\left(\frac{\partial}{\partial t_1} G(1,2) \right) \Sigma(2,1^+) \right. \\ &\quad \left. + \Sigma(1,2) \frac{\partial}{\partial t_1} G(2,1^+) \right] \\ &\quad - i \text{tr} \left(\frac{\partial \mathbf{T}(t_1)}{\partial t_1} \mathbf{G}(t_1,t_1^+) \right). \end{aligned} \quad (76)$$

Note that the last summand just equals the right-hand side of Eq. (74). This equation can easily be combined with the time derivative of the interaction energy [Eq. (73)]. After applying the product rule, the energy-balance relation [Eq. (74)] is

$$\begin{aligned} \delta \Sigma'(2,1) &= \int_C dz \left[\frac{3}{4} \Sigma'(2,1) \left(\frac{\partial}{\partial z_2} \delta(z_2 - z) \right) + \frac{3}{4} \Sigma'(2,1) \left(\frac{\partial}{\partial z_1} \delta(z_1 - z) \right) \right. \\ &\quad \left. + \left(\frac{\partial}{\partial z_2} \Sigma'(2,1) \right) \delta(z_2 - z) + \left(\frac{\partial}{\partial z_1} \Sigma'(2,1) \right) \delta(z_1 - z) \right] \delta\theta(t). \end{aligned} \quad (81)$$

expressed as⁴⁷

$$\begin{aligned} &-\frac{3}{4} \sum_{\alpha_1} \int d2 \frac{\partial}{\partial t_1} [\Sigma(1,2)G(2,1^+) + G(1,2)\Sigma(2,1^+)] \\ &\quad + \sum_{\alpha_1} \int d2 \left(\frac{\partial \Sigma(1,2)}{\partial t_1} G(2,1^+) + G(1,2) \frac{\partial \Sigma(2,1^+)}{\partial t_1} \right) \\ &= 0. \end{aligned} \quad (77)$$

An approximation constructed within the SFT will respect energy balance if Eq. (77) holds but with $\mathbf{\Sigma}$ replaced by $\mathbf{\Sigma}_{\lambda'_{\text{opt}},U}$ and with \mathbf{G} replaced by \mathbf{G}^{SFT} . Thus, the goal is to find a class of transformations of the one-particle parameters such that their corresponding first-order variations around the stationary point generate the above equation as the SFT Euler equation. In principle, this can be achieved with

$$\lambda'(z) \mapsto \tilde{\lambda}'(z) = i(1 - \dot{\theta}^{-1/2})\partial_z + \frac{i}{4}\dot{\theta}^{-3/2}\ddot{\theta} + \dot{\theta}^{1/2}\lambda'(\theta), \quad (78)$$

where $\theta(z)$ is an arbitrary real function on the contour with $\partial_z \theta(z) \neq 0$ which describes a transformation of the time scale. Note that due to the term $\propto \partial_z$ the action of $\tilde{\lambda}'(z)$ is nonlocal in time. This is a severe complication if $\tilde{\lambda}'(z)$ should represent parameters of an actual impurity Hamiltonian, as discussed in Sec. XII C. It is nevertheless illustrative to see how energy conservation can be derived if the self-energy functional is stationary under the variations defined by Eq. (78).

The time-dependent transformation of the one-particle parameters induces a corresponding transformation of the exact Green's function $\mathbf{G}' \equiv \mathbf{G}_{\lambda',U}$ and of the exact self-energy $\mathbf{\Sigma}' \equiv \mathbf{\Sigma}_{\lambda',U}$ of the reference system. For \mathbf{G}' , we have

$$\mathbf{G}'(z_1, z_2) \mapsto \tilde{\mathbf{G}}'(z_1, z_2) = \dot{\theta}_1^{1/4} \mathbf{G}'(\theta_1, \theta_2) \dot{\theta}_2^{1/4}, \quad (79)$$

where the shorthand notation $\theta_1 = \theta(z_1)$ and $\dot{\theta}_1 = \partial_{z_1} \theta(z_1)$, etc., is used. Via the skeleton-diagram expansion $\mathbf{\Sigma}' = \tilde{\mathbf{\Sigma}}_U[\mathbf{G}']$, this induces the following transformation of the self-energy:

$$\mathbf{\Sigma}'(z_1, z_2) \mapsto \tilde{\mathbf{\Sigma}}'(z_1, z_2) = \dot{\theta}_1^{3/4} \mathbf{\Sigma}'(\theta_1, \theta_2) \dot{\theta}_2^{3/4}. \quad (80)$$

Namely, any internal vertex at time z_i connects to four propagators and thereby collects a factor $\dot{\theta}_i$ by which the implicit z_i integration can be transformed into a θ_i integration. The factors $\dot{\theta}_1^{3/4}$ and $\dot{\theta}_2^{3/4}$ in Eq. (80) result from the three incoming and outgoing propagators at the two ‘‘external’’ vertices. Now, Eq. (79) is verified by showing that the asserted expression for the transformed Green's function $\tilde{\mathbf{G}}'(z_1, z_2)$ together with Eq. (80) satisfies the equation of motion for transformed one-particle parameters [Eq. (78)]. A proof for this can be found in Appendix E.

The first-order variations of $\mathbf{\Sigma}'$ induced by this transformation, $\delta \mathbf{\Sigma}' = \delta \mathbf{\Sigma}'(\theta_1, \theta_2) / \delta \theta|_{\theta=t} \circ \delta \theta$, are given by

Inserting this into the Euler equation (26), integrating by parts, and exploiting the δ functions, we are left with

$$\begin{aligned}
0 = \beta\delta\widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]|_{\lambda'=\lambda'_{\text{opt}}} &= \int_{\mathcal{C}} dz_1 \left\{ -\frac{3}{4} \sum_{\alpha_1} \int d2 \frac{\partial}{\partial z_1} (\Sigma_{\lambda',U}(1,2)G^{\text{SFT}}(2,1^+) + G^{\text{SFT}}(1,2)\Sigma_{\lambda',U}(2,1^+)) \right. \\
&+ \sum_{\alpha_1} \int d2 \left[\left(\frac{\partial}{\partial z_1} \Sigma_{\lambda',U}(1,2) \right) G^{\text{SFT}}(2,1^+) + G^{\text{SFT}}(1,2) \frac{\partial}{\partial z_1} \Sigma_{\lambda',U}(2,1^+) \right] \\
&+ \frac{3}{4} \sum_{\alpha_1} \int d2 \frac{\partial}{\partial z_1} (\Sigma_{\lambda',U}(1,2)G_{\lambda',U}(2,1^+) + G_{\lambda',U}(1,2)\Sigma_{\lambda',U}(2,1^+)) \\
&\left. - \sum_{\alpha_1} \int d2 \left[\left(\frac{\partial}{\partial z_1} \Sigma_{\lambda',U}(1,2) \right) G_{\lambda',U}(2,1^+) + G_{\lambda',U}(1,2) \frac{\partial}{\partial z_1} \Sigma_{\lambda',U}(2,1^+) \right] \right\}_{\lambda'=\lambda'_{\text{opt}}} \delta\theta(z_1). \quad (82)
\end{aligned}$$

At the stationary point, this holds for all variations $\delta\theta(z_1)$. Hence, the term in the curly brackets must vanish. We assume that the energy-balance relation is satisfied *in the reference system* as expressed by Eq. (77), with $\Sigma \equiv \Sigma_{T,U}$ replaced by $\Sigma_{\lambda',U}$ and with $G \equiv G_{T,U}$ replaced by $G_{\lambda',U}$. This implies that the last two terms in Eq. (82) vanish and therewith the first two terms in the curly brackets must vanish which is just equivalent with total-energy balance within the SFT. We conclude that within the SFT, the energy-conservation law is proliferated from the reference system to the original system, if stationarity of the self-energy functional under the variations defined by Eq. (78) can be enforced.

C. Discussion

However, there are two important points that need further discussion. First, we recall that the interaction parameters must be assumed as time independent $U = \text{const}$ to show that the nonequilibrium SFT respects conservation of energy. In the case of a time-dependent interaction $U(t)$ (and assuming the one-particle parameters as constant for a moment), the energy-balance relation will involve a two-particle correlation function

$$\frac{\partial E_{\text{tot}}(t)}{\partial t} = \sum_{\alpha\beta\gamma\delta} \frac{\partial U_{\alpha\beta\delta\gamma}(t)}{\partial t} \langle c_{\alpha}^{\dagger}(t)c_{\beta}^{\dagger}(t)c_{\gamma}(t)c_{\delta}(t) \rangle, \quad (83)$$

which can not (easily) be expressed in terms Σ and G . Therefore, without further approximations, it is impossible to set up (and prove) an energy-balance equation within SFT in this case.

An exception worth mentioning is a time dependence of the simple form $U_{\alpha\beta\delta\gamma}(t) = \kappa(t)U_{\alpha\beta\delta\gamma}$ where we furthermore assume $\kappa(t) = \dot{\varphi}^{-1}(t)$ with $\dot{\varphi}(t) \equiv \partial_t \varphi(t) \neq 0$. In this case, the time dependence can be shifted to the one-particle parameters by a transformation of the time scale: $H(t) \mapsto \tilde{H}(t) = \dot{\varphi}(t)H[\varphi(t)]$ and $|\tilde{\psi}(t)\rangle = |\psi[\varphi(t)]\rangle$ which leaves the Schrödinger equation form invariant:

$$[i\partial_t - \tilde{H}(t)]|\tilde{\psi}(t)\rangle = \dot{\varphi}(t)[i\partial_{\varphi} - H(\varphi)]|\psi(\varphi)\rangle = 0. \quad (84)$$

The second point to be discussed is that according to the presence of the contour derivative ∂_z in the transformation law Eq. (78), time-nonlocal one-particle parameters of the reference system are generated by a generic transformation

of the time scale $\theta(z)$. Within the present (Hamiltonian) formalism, time-nonlocal parameters $\lambda'(z_1, z_2)$ must be generated effectively by considering additional bath degrees of freedom in the reference system, i.e., $\lambda'(z_1, z_2)$ must be understood as a corresponding hybridization function

$$\lambda'(z_1, z_2) = V'(z_1)G'_0(z_1, z_2)V'(z_2), \quad (85)$$

where G'_0 is the noninteracting bath Green's function and V' the hybridization matrix element. However, a time-nonlocal term of the form ∂_z can presumably not be represented with the help of a *finite* number of bath degrees of freedom (see also Ref. 38 for a discussion). On the other hand, with the consideration of a *continuum* of bath sites, one is essentially restricted to DMFT or to cellular DMFT as approximations that can be constructed within the SFT framework. This conflicts with the original intention to construct variational and consistent approximations using reference systems with a few degrees of freedom only which are accessible to an exact-diagonalization technique.

However, the argument can also be turned by stating that the degree to which energy conservation is violated within an SFT-based approximation can be controlled systematically by increasing the number of variational degrees of freedom in the reference system. Adding bath degrees of freedom, for example, is expected to substantially improve the degree to which energy conservation is respected. Furthermore, the analysis in Sec. XII B shows that a substantial violation of energy conservation should not be expected *for short times*. Here, the system's dynamics is dominated by high-energy excitations and is thus only weakly affected by a discrete level structure.

Another option is to enforce energy conservation. As the SFT is a variational approach, energy conservation can easily be imposed as an additional constraint that is used to fix the time dependence of one of the variational parameters. This represents an *ad hoc* but physically motivated modification of the original theory by which the search for optimal values of the remaining variational parameters is confined to a subspace where $E_{\text{tot}} = \text{const}$. Here, $E_{\text{tot}} = E_{\text{tot}}[\lambda'](z)$ is given by Eqs. (72) and (73) with G and Σ replaced by G^{SFT} and $\Sigma_{\lambda',U}$. The SFT variational principle, Eq. (26), is replaced by

$$E_{\text{tot}}[\lambda'](z) - \text{const} = 0 \quad (86)$$

and

$$\frac{\delta}{\delta \lambda'(z)} \left(\widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}] - \int_{\mathcal{K}} dz' \xi(z') E_{\text{tot}}[\lambda'](z') \right) = 0, \quad (87)$$

where $\xi(z)$ is a Lagrange multiplier on the Keldysh branch \mathcal{K} . Alternatively, for driven systems with an explicitly time-dependent Hamiltonian, one may impose Eq. (77), again formulated in terms of \mathbf{G}^{SFT} and $\Sigma_{\lambda',U}$, as a constraint. Again, variations in the transverse direction must be considered [i.e., $\lambda_+(t) = -\lambda_-(t)$], followed by an evaluation on the physical manifold [i.e., $\lambda_+(t) = \lambda_-(t)$, $\xi_+ = \xi_-$], as discussed in Sec. VII. Furthermore, Eqs. (86) and (87) have an inherent causal structure analogous to the full SFT equations and may thus be solved by a similar propagation algorithm as discussed in Sec. X. An overall time-dependent scaling of the hopping parameters may be considered as a variational parameter taken to satisfy the constraint, but there is no obvious optimal choice.

XIII. 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 also extends different approximations within a single theoretical framework. This comprises “two-site” approximations^{29,62} and the linearized DMFT,⁶³ dynamical impurity approximations (DIA),^{29,33,34} but also dynamical mean-field theory (DMFT) and its cluster extensions, i.e., the cellular DMFT (C-DMFT),^{30,44,64} as well as the dynamical cluster approximation⁴⁵ (DCA) (see also Ref. 31 for deriving the DCA within SFT), and finally the cluster-perturbation theory^{65,66} (CPT) and its variational extension, the variational cluster approach (VCA).⁶⁷ The SFT has been extended into several directions, e.g., to systems with nonlocal interactions,⁶⁸ to disordered³¹ and to bosonic systems.^{69,70}

This study has shown how to generalize the SFT and the different approximations that can be constructed within the SFT to the general nonequilibrium case. This nonequilibrium SFT addresses problems of transient real-time dynamics in lattice-fermion systems far from equilibrium. It provides approximations to describe the dynamics of single-particle observables in a state that evolves from an initial thermal state after a sudden quench or after an arbitrarily time-dependent and strong perturbation. As for the equilibrium theory, the approximations generated are nonperturbative, consistent in itself, and can be improved systematically. In fact, the nonequilibrium SFT reduces to the equilibrium approach in the case of an equilibrium setup, and it comprises the equilibrium SFT which describes the initial equilibrium state from which the subsequent final-state dynamics evolves. The same holds for each of the different approximations.

Essentially, the main starting point for the nonequilibrium generalization 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 which exhibits several important aspects that have no counterpart in the equilibrium formalism.

The first essential and important difference as compared to equilibrium SFT consists in the fact that the Euler equation that fixes the variational parameters results from “transverse” variations that involve trial self-energies away from the “physical” manifold, while stationarity with respect to “physical” variations turns out to be trivial. Another point concerns the functional $\widehat{\Omega}[\Sigma]$ itself. Evaluating the self-energy functional at the (physical) stationary point yields the grand potential of the initial thermal state. The value of the functional thereby has a clear physical meaning which may be used to decide between several solutions of the Euler equation.

It is remarkable that even the most simple approximations, such as the nonequilibrium variant of the two-site DIA, can be shown to respect the conservation laws resulting from the U(1) and SU(2) symmetries of the original Hamiltonian. This demonstrates that there is a class of approximations that are “conserving” in the sense of Baym and Kadanoff but nonperturbative at the same time, apart from the nonequilibrium DMFT, which can be understood as a Φ -derivable diagrammatic technique *and* as an approximation within the nonequilibrium SFT framework.

As the nonequilibrium SFT represents a variational approach that is based on one-particle quantities, it is not surprising that complications show up in the context of total-energy conservation. Energy conservation can be ensured with the help of time-nonlocal variational parameters or can be enforced by means of a constrained variation: as an *ad hoc* but physically motivated alternative. We expect, however, that there is no substantial violation of total-energy conservation in the short-time domain anyway.

Finally, the nonequilibrium SFT has an inherently causal structure, i.e., approximations do respect the physical causality principle. This not only is satisfying fundamentally but also important for the numerical implementation of the theory. A time-propagation algorithm has been proposed here which requires the exact computation of one- and more-particle time-dependent correlation functions for the reference system that specifies the approximation.

While the practical usefulness and the reliability of such approximations has to be awaited, we do not see severe obstacles for an implementation using reference systems with a small number of degrees of freedom. A very simple nonvariational variant of the nonequilibrium VCA has been implemented already.^{39–41} This essentially consists in the numerical solution of the CPT equation (36). From the computational point of view, we expect that the CPT equation also represents the bottleneck in case of a fully variational NE-VCA.

Clearly, the implementation of cluster and of impurity approximations is more involved compared to the direct mapping of the DMFT hybridization function to a single-impurity Anderson model,³⁸ but the many favorable properties of the NE-SFT make it a very promising way to employ an exact-diagonalization solver in the context of nonequilibrium dynamical mean-field or cluster-mean-field approaches. Work along these lines is in progress.

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APPENDIX A: ANALYTICAL FUNCTIONS OF CONTOUR FUNCTIONS

Analytical functions of contour functions $X(z, z')$ are formally defined as

$$f(X) = \sum_n \frac{f^{(n)}(0)}{n!} X^{on}, \quad (\text{A1})$$

where the notations $X^{on} = \underbrace{X \circ \dots \circ X}_{n \text{ times}}$ and $X^{o0} = \mathbf{1}$ are used.

We immediately have

$$\frac{\delta \text{Tr}[f(X)]}{\delta X(1,2)} = f'(X)(2,1^+). \quad (\text{A2})$$

By setting \hbar to one, time is measured in units 1/energy, and hence the contour integration carries the unit 1/energy, too. Therefore, for a meaningful definition of f via Eq. (A1), its argument X must have energy units. This ensures that each \circ -power of X has the same unit.

With the trivial inverse Green's function

$$G_{\varepsilon_0,0;\alpha\alpha'}^{-1}(z, z') = \delta_{\alpha\alpha'} \delta_C(z, z') (i\partial_{z'} + \mu - \varepsilon_0), \quad (\text{A3})$$

the term $G_{\varepsilon_0,0}^{-1} \circ G_{T,U}$ carries energy units, and the principal branch of the logarithm $\ln(G_{\varepsilon_0,0}^{-1} \circ G_{T,U})$ is well defined for any ε_0 . For $\varepsilon_0 \rightarrow \infty$, it represents a regularization of the ill-defined expression $\ln G_{T,U}$. In particular, we find that this is related to the grand potential

$$\Omega_{T,0} = \frac{1}{\beta} \text{Tr} \ln (G_{\varepsilon_0,0}^{-1} \circ G_{T,0}) \quad (\text{A4})$$

in the noninteracting case [see also Eq. (15)].

APPENDIX B: DEPENDENCE OF THE GREEN'S FUNCTION ON THE ONE-PARTICLE PARAMETERS

To exhibit the full λ' dependence of the Green's function of the reference system $G_{\lambda',U}(z_1, z_2)$, one may switch to an “inverted” interaction picture where the roles of the “free” and the “interacting” parts are interchanged. With this choice, all expectation values and time dependencies are due to $H_{0,U}$, whereas all one-particle terms of the Hamiltonian enter via the S matrix only. Therewith, analogously to Eq. (10), the Green's function can be written as

$$iG_{\lambda',U;\alpha_1\alpha_2}(z_1, z_2) = \frac{\langle \mathcal{T}_C e^{-i \int_C dz \mathcal{H}_{\lambda',0}(z)} c_{\alpha_1}(z_1) c_{\alpha_2}^\dagger(z_2) \rangle_{0,U}}{\langle \mathcal{T}_C e^{-i \int_C dz \mathcal{H}_{\lambda',0}(z)} \rangle_{0,U}}. \quad (\text{B1})$$

Here, one can directly read off the functional derivative with respect to λ' :

$$\frac{\delta G_{\lambda',U}(1,2)}{\delta \lambda'_{\alpha_3\alpha_4}(z_3)} = G_{\lambda',U}(1,2) G_{\lambda',U}(4,3^+) |_{z_4=z_3} - G_{\lambda',U}^{(2)}(1,4,3^+,2) |_{z_4=z_3}, \quad (\text{B2})$$

where

$$G_{\lambda',U}^{(2)}(1,2,3,4) = (-i)^2 \langle \mathcal{T}_C c(1) c(2) c^\dagger(3) c^\dagger(4) \rangle \quad (\text{B3})$$

is the two-particle Green's function of the reference system.

APPENDIX C: TIME INDEPENDENCE OF THE EULER EQUATION IN THE EQUILIBRIUM CASE

In the following, we show the time independence of the Euler equation on the Keldysh contour in the equilibrium case, i.e.,

$$\left. \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'_{\alpha_1\alpha_2}(z_1)} \right|_{\lambda'_{\text{opt}}=\text{const}} = \left. \frac{\partial \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\partial \lambda'_{\alpha_1\alpha_2}} \right|_{\lambda'_{\text{opt}}=\text{const}}, \quad (\text{C1})$$

where $z_1 = t_1$ is the physically largest time on the Keldysh contour. To this end, we start with Eq. (41) and make all contour integrations explicit:

$$-\beta \frac{\delta \widehat{\Omega}_{T,U}[\Sigma_{\lambda',U}]}{\delta \lambda'_{\alpha_1\alpha_2}(t_1)} = \int d3 \int d4 Y_{\lambda',T,U}(4,3) L_{\lambda',U}(3,2,1^+,4) |_{z_2=z_1} = \sum_{\alpha_3\alpha_4} \int d z_3 Y_{43}^\delta(z_3) L_{3214}(z_3, t_1, t_1^+, z_3^+) \quad (\text{C2})$$

$$+ \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_3} dt_4 Y_{43}^<(t_4, t_3) L_{3214}^{3>}(t_3, t_1, t_1^+, t_4) \quad (\text{C3})$$

$$+ \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_{t_3}^{t_1} dt_4 Y_{43}^>(t_4, t_3) L_{3214}^{3<}(t_3, t_1, t_1^+, t_4) \quad (\text{C4})$$

$$- \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_1} dt_4 Y_{43}^<(t_4, t_3) L_{3214}^{2>}(t_3, t_1, t_1^+, t_4) \quad (\text{C5})$$

$$- \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_1} dt_4 Y_{43}^>(t_4, t_3) L_{3214}^{2<}(t_3, t_1, t_1^+, t_4) \quad (\text{C6})$$

$$+ \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_{t_3}^{t_1} dt_4 Y_{43}^<(t_4, t_3) L_{3214}^{1>}(t_3, t_1, t_1^+, t_4) \quad (\text{C7})$$

$$+ \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_3} dt_4 Y_{43}^>(t_4, t_3) L_{3214}^{1<}(t_3, t_1, t_1^+, t_4) \quad (\text{C8})$$

$$- i \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_0^\beta d\tau_4 Y_{43}^>(t_0 - i\tau_4, t_3) L_{3214}^{2<}(t_3, t_1, t_1^+, t_0 - i\tau_4) \quad (\text{C9})$$

$$+ i \sum_{\alpha_3\alpha_4} \int_{t_0}^{t_1} dt_3 \int_0^\beta d\tau_4 Y_{43}^>(t_0 - i\tau_4, t_3) L_{3214}^{1<}(t_3, t_1, t_1^+, t_0 - i\tau_4) \quad (\text{C10})$$

$$- i \sum_{\alpha_3\alpha_4} \int_0^\beta d\tau_3 \int_{t_0}^{t_1} dt_4 Y_{43}^{<}(t_4, t_0 - i\tau_3) L_{3214}^{2>}(t_0 - i\tau_3, t_1, t_1^+, t_4) \quad (\text{C11})$$

$$+ i \sum_{\alpha_3\alpha_4} \int_0^\beta d\tau_3 \int_{t_0}^{t_1} dt_4 Y_{43}^{<}(t_4, t_0 - i\tau_3) L_{3214}^{1>}(t_0 - i\tau_3, t_1, t_1^+, t_4) \quad (\text{C12})$$

$$+ (-i)^2 \sum_{\alpha_3\alpha_4} \int_0^\beta d\tau_3 \int_0^{\tau_3} d\tau_4 Y_{43}^{<}(t_0 - i\tau_4, t_0 - i\tau_3) L_{3214}^{1>}(t_0 - i\tau_3, t_1, t_1^+, t_0 - i\tau_4) \quad (\text{C13})$$

$$+ (-i)^2 \sum_{\alpha_3\alpha_4} \int_0^\beta d\tau_3 \int_{\tau_3}^\beta d\tau_4 Y_{43}^>(t_0 - i\tau_4, t_0 - i\tau_3) L_{3214}^{1<}(t_0 - i\tau_3, t_1, t_1^+, t_0 - i\tau_4). \quad (\text{C14})$$

Here, we have split up the T matrix \mathbf{Y} into a singular, lesser, and greater part:

$$\mathbf{Y}_{\lambda', T, U}(z_1, z_2) = \mathbf{V}(z_1) \delta_C(z_1, z_2) + \mathbf{V}(z_1) \mathbf{G}^{\text{SFT}}(z_1, z_2) \mathbf{V}(z_2) \quad (\text{C15})$$

$$=: \mathbf{Y}_{\lambda', T, U}^\delta(z_1) \delta_C(z_1, z_2) + \Theta_C(z_1, z_2) \mathbf{Y}_{\lambda', T, U}^>(z_1, z_2) + \Theta_C(z_2, z_1) \mathbf{Y}_{\lambda', T, U}^{<}(z_1, z_2), \quad (\text{C16})$$

where $\Theta_C(z, z')$ denotes the Heaviside step function on the contour. For the two-particle vertex function $\mathbf{L}_{\lambda', U}$ [Eq. (42)], the notation $L^{i\gtrless}(z_3, z_1, z_1^+, z_4)$ indicates that z_1 is the i th time on the contour and that z_3 is a later/earlier contour time than z_4 . Note that we write $L_{3214}^{i\gtrless}$ which is short for $L_{\alpha_3\alpha_2\alpha_1\alpha_4}^{i\gtrless}$ and that the indexing with the parameters λ' and U has been suppressed for brevity.

To evaluate the above integrations in equilibrium, we express the T matrix via its spectral representation⁷¹ with the respective spectral function \mathbf{A}^Y :

$$\mathbf{Y}^{\gtrless}(z_1, z_2) = i \int d\omega e^{-i\omega(z_1 - z_2)} f^{\gtrless}(\omega) \mathbf{A}^Y(\omega), \quad (\text{C17})$$

with $f^<(\omega) = f(\omega)$ and $f^>(\omega) = f(\omega) - 1$ and where $f(\omega)$ is the Fermi function. This also implies

$$f^>(\omega) = -e^{\omega\beta} f^<(\omega). \quad (\text{C18})$$

For the two-particle vertex function, we choose the Lehmann representation by inserting the completeness relation $\mathbf{1} = \sum_m |m\rangle \langle m|$ between all operators. We find

$$L^{3>}(3, 2, 1^+, 4)_{z_2=z_1} = \sum_{mnlk} \left[-M_{3214}^{mnlk} e^{-\beta E_m} e^{-\beta E_k} e^{i(E_m + E_k - E_n - E_l)z_1} e^{i(E_n - E_m)z_3} e^{i(E_l - E_k)z_4} \right. \\ \left. + \tilde{M}_{3214}^{mnlk} e^{-\beta E_m} e^{-\beta E_k} e^{i(E_m - E_n)z_3} e^{i(E_n - E_m)z_4} - N_{3214}^{mnlk} e^{-\beta E_m} e^{i(E_m - E_k)z_1} e^{i(E_k - E_l)z_3} e^{i(E_l - E_m)z_4} \right], \quad (\text{C19})$$

$$L^{3<}(3, 2, 1^+, 4)_{z_2=z_1} = \sum_{mnlk} \left[-M_{3214}^{mnlk} e^{-\beta E_m} e^{-\beta E_k} e^{i(E_m + E_k - E_n - E_l)z_1} e^{i(E_n - E_m)z_3} e^{i(E_l - E_k)z_4} \right. \\ \left. - \tilde{M}_{3214}^{mnlk} e^{-\beta E_n} e^{-\beta E_k} e^{i(E_m - E_n)z_3} e^{i(E_n - E_m)z_4} + \tilde{N}_{3214}^{mnlk} e^{-\beta E_m} e^{i(E_m - E_k)z_1} e^{i(E_l - E_m)z_3} e^{i(E_k - E_l)z_4} \right], \quad (\text{C20})$$

and similar expressions for $L^{1\gtrless}$ and $L^{2\gtrless}$. For the amplitudes, we used the shorthand notations

$$M_{3214}^{mnlk} = \frac{(-i)^2}{Z^2} \langle m | c_1^\dagger | n \rangle \langle n | c_3 | m \rangle \langle k | c_2 | l \rangle \langle l | c_4^\dagger | k \rangle, \quad (\text{C21})$$

$$\tilde{M}_{3214}^{mnlk} = \frac{(-i)^2}{Z^2} \langle m | c_3 | n \rangle \langle n | c_4^\dagger | m \rangle \langle k | c_1^\dagger | l \rangle \langle l | c_2 | k \rangle, \quad (\text{C22})$$

$$N_{3214}^{mnlk} = \frac{(-i)^2}{Z^2} \langle m | c_1^\dagger | n \rangle \langle l | c_4^\dagger | m \rangle \langle n | c_2 | k \rangle \langle k | c_3 | l \rangle, \quad (\text{C23})$$

$$\tilde{N}_{3214}^{mnlk} = \frac{(-i)^2}{Z^2} \langle m | c_1^\dagger | n \rangle \langle k | c_4^\dagger | l \rangle \langle n | c_2 | k \rangle \langle l | c_3 | m \rangle. \quad (\text{C24})$$

Let us first focus on those terms involving only greater and lesser parts of $Y_{\lambda', T, U}$ [Eqs. (C3)–(C14)] and evaluate them for each amplitude [Eqs. (C21)–(C24)] separately. For this purpose, we write all summands (C3)–(C14) in the compact form

$$i \sum_{\alpha_3 \alpha_4} \sum_{m n k l} \sum_X \int d\omega f(\omega) A_{43}^Y(\omega) X_{3214}^{m n k l} \mathcal{R}_{m n k l}^X(\omega, t_1). \quad (\text{C25})$$

To this end, we have made use of Eq. (C18) and factored out all common terms for each combination of amplitudes $X_{3214}^{m n k l}$, where X stands for M, \tilde{M}, N , or \tilde{N} . The remaining exponential factors, resulting from the time-evolution operator and the density matrix when introducing the Lehmann representation, and the two time integrations along the different branches are collected in the term $\mathcal{R}_{m n k l}^X(\omega, t_1)$ for each X . As an example, we give an expression for $\mathcal{R}_{m n k l}^N(\omega, t_1)$ in the following and tag each summand according to its origin in the above expression for $-\beta \delta \widehat{\Omega}_{T, U}[\Sigma_{\lambda', U}]/\delta \lambda'_{\alpha_1 \alpha_2}(t_1)$:

$$\begin{aligned} \mathcal{R}_{m n k l}^N(\omega, t_1) &= -e^{-\beta E_m} (-\mathcal{I}_c^N + \mathcal{I}_{a'}^N + \mathcal{I}_{b_1}^N - \mathcal{I}_a^N) \quad (\text{from C3}) \\ &+ e^{-\beta(E_l - \omega)} (-\mathcal{I}_c^N + \mathcal{I}_{b_1}^N + \mathcal{I}_{b_2}^N - \mathcal{I}_a^N) \quad (\text{from C6}) \\ &- e^{-\beta E_k} (-\mathcal{I}_c^N + \mathcal{I}_{b_2}^N + \mathcal{I}_{c'}^N - \mathcal{I}_{a'}^N) \quad (\text{from C7}) \\ &+ (e^{-\beta E_m} - e^{-\beta(E_l - \omega)}) (\mathcal{I}_{b_1}^N - \mathcal{I}_a^N) \quad (\text{from C9}) \\ &+ (e^{-\beta E_k} - e^{-\beta(E_l - \omega)}) (\mathcal{I}_{b_2}^N - \mathcal{I}_a^N) \quad (\text{from C12}) \\ &+ [(e^{-\beta E_m} - e^{-\beta E_k}) \mathcal{I}_{a'}^N + (e^{-\beta E_k} + e^{-\beta(E_l - \omega)}) \mathcal{I}_a^N]. \quad (\text{from C13}) \end{aligned}$$

Here, the results of the different integrals are given by

$$\mathcal{I}_a^N := \mathcal{I}_{a, m n k l}^N(\omega, t_1) = \frac{1}{E_l - E_m - \omega} \frac{1}{E_k - E_l + \omega} e^{i(E_m - E_k)(t_1 - t_0)}, \quad (\text{C26})$$

$$\mathcal{I}_{a'}^N := \mathcal{I}_{a', m n k l}^N(\omega, t_1) = \frac{1}{E_l - E_m - \omega} \frac{1}{E_k - E_m} e^{i(E_m - E_k)(t_1 - t_0)}, \quad (\text{C27})$$

$$\mathcal{I}_{b_1}^N := \mathcal{I}_{b_1, m n k l}^N(\omega, t_1) = \frac{1}{E_l - E_m - \omega} \frac{1}{E_k - E_l + \omega} e^{i(E_m - E_l + \omega)(t_1 - t_0)}, \quad (\text{C28})$$

$$\mathcal{I}_{b_2}^N := \mathcal{I}_{b_2, m n k l}^N(\omega, t_1) = \frac{1}{E_l - E_m - \omega} \frac{1}{E_k - E_l + \omega} e^{i(E_l - E_k - \omega)(t_1 - t_0)}, \quad (\text{C29})$$

$$\mathcal{I}_c^N := \mathcal{I}_{c, m n k l}^N(\omega) = \frac{1}{E_l - E_m - \omega} \frac{1}{E_k - E_l + \omega}, \quad (\text{C30})$$

$$\mathcal{I}_{c'}^N := \mathcal{I}_{c', m n k l}^N(\omega) = \frac{1}{E_l - E_m - \omega} \frac{1}{E_k - E_m}. \quad (\text{C31})$$

By collecting prefactors, we find that all explicitly t_1 -dependent parts drop out and that only those containing \mathcal{I}_c^N and $\mathcal{I}_{c'}^N$ contribute. Analogous calculations lead to the same result for M, \tilde{M} , and \tilde{N} , and we thus conclude

$$\mathcal{R}_{m n k l}^X(\omega, t_1) = \mathcal{R}_{m n k l}^X(\omega) \quad \forall X. \quad (\text{C32})$$

The singular part $\sum_{\alpha_3 \alpha_4} \int d z_3 Y_{43}^{\delta}(z_3) L_{3214}(z_3, t_1, t_1^+, z_3^+)$ [Eq. (C2)] is evaluated straightforwardly and also turns out to be independent of the time t_1 . This completes the proof of Eq. (C1).

APPENDIX D: FORM INVARIANCE OF THE EQUATION OF MOTION UNDER GAUGE TRANSFORMATIONS

Here, we show the form invariance of the equation of motion for the Green's function under the gauge transformations (65). To verify the transformed equation of motion [Eq. (69)], we first compute the left-hand side:

$$i \partial_{z_1} \tilde{\mathbf{G}}'(z_1, z_2) = e^{i\chi(z_1)} i \partial_{z_1} \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)} - [\partial_{z_1} \chi(z_1)] e^{i\chi(z_1)} \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)}. \quad (\text{D1})$$

To treat the second term on the right-hand side of Eq. (69), we distinguish between (spatially) diagonal and off-diagonal parts of the one-particle parameters and apply the respective transformation laws [Eq. (65)]. This yields

$$\begin{aligned} \tilde{\boldsymbol{\lambda}}'(z_1) \tilde{\mathbf{G}}'(z_1, z_2) &= \tilde{\boldsymbol{\varepsilon}}'(z_1) \tilde{\mathbf{G}}'(z_1, z_2) + \tilde{\mathbf{T}}'(z_1) \tilde{\mathbf{G}}'(z_1, z_2) = \boldsymbol{\varepsilon}'(z_1) e^{i\chi(z_1)} \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)} \\ &+ e^{i\chi(z_1)} \mathbf{T}'(z_1) e^{-i\chi(z_1)} e^{i\chi(z_1)} \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)} - [\partial_{z_1} \chi(z_1)] e^{i\chi(z_1)} \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)} \\ &= e^{i\chi(z_1)} \boldsymbol{\lambda}'(z_1) \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)} - [\partial_{z_1} \chi(z_1)] e^{i\chi(z_1)} \mathbf{G}'(z_1, z_2) e^{-i\chi(z_2)}. \quad (\text{D2}) \end{aligned}$$

In the last step, we made use of the commutativity of $\boldsymbol{\varepsilon}'$ and χ . The second terms in Eqs. (D1) and (D2) cancel each other. Finally, we have $(\tilde{\boldsymbol{\Sigma}}' \circ \tilde{\mathbf{G}}')(z_1, z_2) = e^{i\chi(z_1)} (\boldsymbol{\Sigma}' \circ \mathbf{G}')(z_1, z_2) e^{-i\chi(z_2)}$ and $\delta_C(z_1, z_2) = e^{i\chi(z_1)} \delta_C(z_1, z_2) e^{-i\chi(z_2)}$. Thus, we conclude that the transformed equation of motion is solved by the transformed Green's function and self-energy if the original one was solved by the original quantities.

APPENDIX E: FORM INVARIANCE OF THE EQUATION OF MOTION UNDER TRANSFORMATIONS OF THE TIME SCALE

Here, we show the form invariance of the equation of motion for the Green's function under the transformations of the time scale [Eq. (78)]. To verify the transformed equation of motion,

$$i\partial_{z_1}\tilde{\mathbf{G}}'(z_1, z_2) = \delta_C(z_1, z_2) + \tilde{\lambda}'(z_1)\tilde{\mathbf{G}}'(z_1, z_2) + (\tilde{\Sigma}' \circ \tilde{\mathbf{G}}')(z_1, z_2), \quad (\text{E1})$$

we first compute the left-hand side:

$$\begin{aligned} i\partial_{z_1}\tilde{\mathbf{G}}'(z_1, z_2) &= i\partial_{z_1}(\dot{\theta}_1^{1/4}\mathbf{G}'(\theta_1, \theta_2)\dot{\theta}_2^{1/4}) = \frac{i}{4}\dot{\theta}_1^{-3/4}\ddot{\theta}_1\mathbf{G}'(\theta_1, \theta_2)\dot{\theta}_2^{1/4} + i\dot{\theta}_1^{5/4}\partial_{\theta_1}\mathbf{G}'(\theta_1, \theta_2)\dot{\theta}_2^{1/4} \\ &= \dot{\theta}_1^{3/4}\left(\frac{i}{4}\dot{\theta}_1^{-3/2}\ddot{\theta}_1\mathbf{G}'(\theta_1, \theta_2) + i\dot{\theta}_1^{1/2}\partial_{\theta_1}\mathbf{G}'(\theta_1, \theta_2)\right)\dot{\theta}_2^{1/4}. \end{aligned} \quad (\text{E2})$$

With Eq. (78), we find

$$\begin{aligned} \tilde{\lambda}'(z_1)\tilde{\mathbf{G}}'(z_1, z_2) &= \left(i(1 - \dot{\theta}_1^{-1/2})\partial_z + \frac{i}{4}\dot{\theta}_1^{-3/2}\ddot{\theta}_1 + \dot{\theta}_1^{1/2}\lambda'(\theta_1)\right)\dot{\theta}_1^{1/4}\mathbf{G}'(\theta_1, \theta_2)\dot{\theta}_2^{1/4} \\ &= \left(\frac{i}{4}(1 - \dot{\theta}_1^{-1/2})\dot{\theta}_1^{-3/4}\ddot{\theta}_1 + \frac{i}{4}\dot{\theta}_1^{-5/4}\ddot{\theta}_1 + \dot{\theta}_1^{3/4}\lambda'(\theta_1) + i(1 - \dot{\theta}_1^{-1/2})\dot{\theta}_1^{5/4}\partial_{\theta_1}\right)\mathbf{G}'(\theta_1, \theta_2)\dot{\theta}_2^{1/4} \\ &= \dot{\theta}_1^{3/4}\left(\frac{i}{4}\dot{\theta}_1^{-3/2}\ddot{\theta}_1\mathbf{G}'(\theta_1, \theta_2) + i\dot{\theta}_1^{1/2}\partial_{\theta_1}\mathbf{G}'(\theta_1, \theta_2)\right)\dot{\theta}_2^{1/4} - \dot{\theta}_1^{3/4}(i\partial_{\theta_1}\mathbf{G}'(\theta_1, \theta_2) - \lambda'(\theta_1)\mathbf{G}'(\theta_1, \theta_2))\dot{\theta}_2^{1/4}. \end{aligned} \quad (\text{E3})$$

Combining both equations leaves us with the following expression:

$$i\partial_{z_1}\tilde{\mathbf{G}}'(z_1, z_2) - \tilde{\lambda}'(z_1)\tilde{\mathbf{G}}'(z_1, z_2) = \dot{\theta}_1^{3/4}(i\partial_{\theta_1}\mathbf{G}'(\theta_1, \theta_2) - \lambda'(\theta_1)\mathbf{G}'(\theta_1, \theta_2))\dot{\theta}_2^{1/4}. \quad (\text{E4})$$

Furthermore, using the substitution rule, we find both $(\tilde{\Sigma}' \circ \tilde{\mathbf{G}}')(z_1, z_2) = \dot{\theta}_1^{3/4}(\Sigma' \circ \mathbf{G}')(\theta_1, \theta_2)\dot{\theta}_2^{1/4}$ and $\delta(z_1, z_2) = \dot{\theta}_1\delta(\theta_1, \theta_2) = \dot{\theta}_1^{3/4}\delta(\theta_1, \theta_2)\dot{\theta}_2^{1/4}$. Thus, assembling all parts completes the proof.

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¹T. Kinoshita, T. Wenger, and D. S. Weiss, *Nature (London)* **440**, 900 (2006).

²A. Mitra, S. Takei, Y. B. Kim, and A. J. Millis, *Phys. Rev. Lett.* **97**, 236808 (2006).

³S. Diehl, A. Tomadin, A. Micheli, R. Fazio, and P. Zoller, *Phys. Rev. Lett.* **105**, 015702 (2010).

⁴A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys.* **59**, 1 (1987).

⁵S. Iwai, M. Ono, A. Maeda, H. Matsuzaki, H. Kishida, H. Okamoto, and Y. Tokura, *Phys. Rev. Lett.* **91**, 057401 (2003).

⁶L. Perfetti, P. A. Loukakos, M. Lisowski, U. Bovensiepen, H. Berger, S. Biermann, P. S. Cornaglia, A. Georges, and M. Wolf, *Phys. Rev. Lett.* **97**, 067402 (2006).

⁷S. Wall, D. Prabhakaran, A. T. Boothroyd, and A. Cavalleri, *Phys. Rev. Lett.* **103**, 097402 (2009).

⁸D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, *Phys. Rev. Lett.* **81**, 3108 (1998).

⁹I. Bloch, J. Dalibard, and W. Zwerger, *Rev. Mod. Phys.* **80**, 885 (2008).

¹⁰N. Strohmaier, D. Greif, R. Jördens, L. Tarruell, H. Moritz, T. Esslinger, R. Sensarma, D. Pekker, E. Altman, and E. Demler, *Phys. Rev. Lett.* **104**, 080401 (2010).

¹¹M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963).

¹²J. Hubbard, *Proc. R. Soc. London, Ser. A* **276**, 238 (1963).

¹³J. Kanamori, *Prog. Theor. Phys.* **30**, 275 (1963).

¹⁴P. Weiss, *J. Phys. Theor. Appl.* **6**, 661 (1907).

¹⁵W. Metzner and D. Vollhardt, *Phys. Rev. Lett.* **62**, 324 (1989).

¹⁶A. Georges and G. Kotliar, *Phys. Rev. B* **45**, 6479 (1992).

¹⁷M. Jarrell, *Phys. Rev. Lett.* **69**, 168 (1992).

¹⁸A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).

¹⁹J. K. Freericks, V. M. Turkowski, and V. Zlatić, *Phys. Rev. Lett.* **97**, 266408 (2006).

²⁰P. Schmidt and H. Monien, arXiv:cond-mat/0202046.

²¹M. Eckstein, M. Kollar, and P. Werner, *Phys. Rev. Lett.* **103**, 056403 (2009).

²²N. Tsuji, T. Oka, and H. Aoki, *Phys. Rev. Lett.* **103**, 047403 (2009).

²³M. Eckstein and P. Werner, *Phys. Rev. B* **82**, 115115 (2010).

²⁴P. Werner and M. Eckstein, *Phys. Rev. B* **86**, 045119 (2012).

²⁵A. Amaricci, C. Weber, M. Capone, and G. Kotliar, *Phys. Rev. B* **86**, 085110 (2012).

²⁶E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, *Rev. Mod. Phys.* **83**, 349 (2011).

²⁷M. Caffarel and W. Krauth, *Phys. Rev. Lett.* **72**, 1545 (1994).

²⁸A. Liesch and H. Ishida, *J. Phys.: Condens. Matter* **24**, 053201 (2012).

²⁹M. Potthoff, *Eur. Phys. J. B* **32**, 429 (2003).

³⁰M. Potthoff, M. Aichhorn, and C. Dahnen, *Phys. Rev. Lett.* **91**, 206402 (2003).

³¹M. Potthoff and M. Balzer, *Phys. Rev. B* **75**, 125112 (2007).

³²M. Potthoff, in *Strongly Correlated Systems: Theoretical Methods*, Springer Series in Solid-State Sciences, Vol. 171, edited by A. Avella and F. Mancini (Springer, Berlin, 2012), pp. 303–339.

³³K. Pozgajcic, arXiv:cond-mat/0407172.

³⁴M. Eckstein, M. Kollar, M. Potthoff, and D. Vollhardt, *Phys. Rev. B* **75**, 125103 (2007).

- ³⁵P. Werner, T. Oka, and A. J. Millis, *Phys. Rev. B* **79**, 035320 (2009).
- ³⁶C. Jung, A. Lieder, S. Brener, H. Hafermann, B. Baxevanis, A. Chudnovskiy, A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, *Ann. Phys. (NY)* **524**, 49 (2012).
- ³⁷E. Arrigoni, M. Knap, and W. von der Linden, *Phys. Rev. Lett.* **110**, 086403 (2013).
- ³⁸C. Gramsch, K. Balzer, M. Eckstein, and M. Kollar, arXiv:1306.6315.
- ³⁹M. Balzer and M. Potthoff, *Phys. Rev. B* **83**, 195132 (2011).
- ⁴⁰M. Balzer, N. Gdaniec, and M. Potthoff, *J. Phys.: Condens. Matter* **24**, 035603 (2012).
- ⁴¹P. Jurgenowski and M. Potthoff, *Phys. Rev. B* **87**, 205118 (2013).
- ⁴²M. Knap, W. von der Linden, and E. Arrigoni, *Phys. Rev. B* **84**, 115145 (2011).
- ⁴³M. Nuss, C. Heil, M. Ganahl, M. Knap, H. G. Evertz, E. Arrigoni, and W. von der Linden, *Phys. Rev. B* **86**, 245119 (2012).
- ⁴⁴G. Kotliar, S. Y. Savrasov, G. Pálsson, and G. Biroli, *Phys. Rev. Lett.* **87**, 186401 (2001).
- ⁴⁵M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy, *Phys. Rev. B* **58**, R7475 (1998).
- ⁴⁶G. Baym and L. P. Kadanoff, *Phys. Rev.* **124**, 287 (1961).
- ⁴⁷G. Baym, *Phys. Rev.* **127**, 1391 (1962).
- ⁴⁸R. Kubo, *J. Phys. Soc. Jpn.* **12**, 570 (1957).
- ⁴⁹T. Matsubara, *Prog. Theor. Phys.* **14**, 351 (1955).
- ⁵⁰J. Schwinger, *J. Math. Phys.* **2**, 407 (1961).
- ⁵¹L. Keldysh, *Zh. Eksp. Teor. Fiz.* **47**, 1515 (1964) [*Sov. Phys.–JETP* **20**, 1018 (1965)].
- ⁵²P. Danielewicz, *Ann. Phys. (NY)* **152**, 239 (1984).
- ⁵³M. Wagner, *Phys. Rev. B* **44**, 6104 (1991).
- ⁵⁴R. van Leeuwen, N. E. Dahlen, G. Stefanucci, C. O. Almbladh, and U. von Barth, in *Time-Dependent Density Functional Theory*, edited by M. A. L. Marques, C. A. Ullrich, F. Nogueira, A. Rubio, K. Burke, and E. K. U. Gross, Vol. 706 (Springer, Berlin, 2006), pp. 33–59.
- ⁵⁵J. Rammer, *Quantum Field Theory of Nonequilibrium States* (Cambridge University Press, Cambridge, UK, 2007).
- ⁵⁶A. Kamenev, *Field theory of Nonequilibrium Systems* (Cambridge University Press, Cambridge, New York, 2011).
- ⁵⁷J. M. Luttinger and J. C. Ward, *Phys. Rev.* **118**, 1417 (1960).
- ⁵⁸M. Potthoff, *Condens. Matter Phys.* **9**, 557 (2006).
- ⁵⁹M. Balzer and M. Potthoff, *Phys. Rev. B* **82**, 174441 (2010).
- ⁶⁰M. Aichhorn, E. Arrigoni, M. Potthoff, and W. Hanke, *Phys. Rev. B* **74**, 024508 (2006).
- ⁶¹M. Aichhorn, H. G. Evertz, W. von der Linden, and M. Potthoff, *Phys. Rev. B* **70**, 235107 (2004).
- ⁶²M. Potthoff, *Phys. Rev. B* **64**, 165114 (2001).
- ⁶³R. Bulla and M. Potthoff, *Eur. Phys. J. B* **13**, 257 (2000).
- ⁶⁴A. I. Lichtenstein and M. I. Katsnelson, *Phys. Rev. B* **62**, R9283 (2000).
- ⁶⁵C. Gros and R. Valentí, *Phys. Rev. B* **48**, 418 (1993).
- ⁶⁶D. Sénéchal, D. Perez, and M. Pioro-Ladrière, *Phys. Rev. Lett.* **84**, 522 (2000).
- ⁶⁷C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff, *Phys. Rev. B* **70**, 245110 (2004).
- ⁶⁸N.-H. Tong, *Phys. Rev. B* **72**, 115104 (2005).
- ⁶⁹W. Koller and N. Dupuis, *J. Phys.: Condens. Matter* **18**, 9525 (2006).
- ⁷⁰E. Arrigoni, M. Knap, and W. von der Linden, *Phys. Rev. B* **84**, 014535 (2011).
- ⁷¹A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Mechanics* (Dover, New York, 1975).