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Two-particle irreducible effective action approach to nonlinear current-conserving approximations in driven systems

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Abstract

Using closed-time-path two-particle irreducible coarse-grained effective action (CTP 2PI CGEA) techniques, we study the response of an open interacting electronic system to time-dependent external electromagnetic fields. We show that the CTP 2PI CGEA is invariant under a simultaneous gauge transformation of the external field and the full Schwinger–Keldysh propagator, and that this property holds even when the loop expansion of the CTP 2PI CGEA is truncated at arbitrary order. The effective action approach provides a systematic way of calculating the propagator and response functions of the system, via the Schwinger–Dyson equation and the Bethe–Salpeter equations, respectively. We show that, due to the invariance of the CTP 2PI CGEA under external gauge transformations, the response functions calculated from it satisfy the Ward–Takahashi hierarchy, thus warranting the conservation of the electronic current beyond the expectation value level. We also clarify the connection between nonlinear response theory and the WT hierarchy, and discuss an example of an ad hoc approximation that violates it. These findings may be useful in the study of current fluctuations in correlated electronic pumping devices.

1. Introduction

In this paper, we are interested in the response of an open electronic system to time-dependent external electromagnetic fields. Although our analysis is quite general and can be applied to a variety of condensed matter systems, we have in mind a system of *strongly* interacting electrons subjected to external driving fields and in contact with two ideal reservoirs of non-interacting electrons. This could be a picture of the so-called interacting electron pumping devices, which are currently attracting much interest both experimentally and theoretically [1]. In these devices, a direct current can be generated by applying slowly oscillating external fields to the central electrons, even in the absence of a bias voltage difference between reservoirs. These are very interesting systems to study from the theoretical point of view, since they represent a unique and challenging combination of strongly correlated particles and quantum transport, and for which the study of current conservation beyond the expectation value level is nontrivial. A typical situation where one needs to go beyond the expectation value of the current is when dealing

with current fluctuations. It is with these applications in mind that the following considerations were developed.

The main purpose of this work is to determine the basic requirements that a field-theoretical approach to *open driven* systems must satisfy in order to produce current-conserving results (in the sense of the WT hierarchy developed in section 2) in transport calculations *going beyond linear response*. Another aim we have in mind is to clarify the close relation that exists between current conservation and response theory, especially in the nonlinear regime. In order to analyse these issues, we combine the so-called external gauge invariance method with the closed-time-path 2PI coarse-grained effective action (CTP 2PI CGEA), suitable for the description of strongly interacting quantum open systems both in and out of equilibrium [2–6].

The area of non-equilibrium physics in interacting systems is gaining increasing interest nowadays, particularly time-dependent quantum transport in correlated systems [7–11]. The so-called *time propagation method* [7] constitutes a significant advance in this area. It consists in first determining the (interacting) equilibrium Green function and

then propagating it by using the Kadanoff–Baym equations. This is equivalent [7, 8] to solving the Bethe–Salpeter equation for the particle–hole propagator (which is related to the first-order response function of the system), but numerically much less expensive. This is a powerful method in which external fields are treated exactly to all orders while many-body interactions are treated perturbatively. In this paper, we adopt another method to study non-equilibrium transport through correlated systems, in which both the external fields and the many-body interactions are treated perturbatively. Since it is based on an expansion of the Green function in powers of the external fields, it is only valid for weak external fields. On the other hand, it allows us to focus on current conservation beyond the expectation value level (i.e. conservation of current fluctuations). In this aspect the present work goes beyond previous analyses such as those described in [7–11].

This paper is organized as follows. In section 2 we present the Ward–Takahashi (WT) hierarchy, which is the most general form of current conservation beyond the expectation value level for a system driven by external fields. We discuss two possible ways (based on effective action techniques) of generating approximations to the non-equilibrium many-body problem that satisfy the WT hierarchy. One of such methods, relying on the external gauge invariance of the effective action, is used throughout the paper. In section 3 we introduce the 2PI CGEA of the system, closely following [2]. In section 4 we prove that the exact and truncated effective actions are external gauge-invariant. Using these theoretical tools, we show in section 5 that for any approximation to the Schwinger–Dyson equation (obtained from a truncation of the loop expansion of the 2PI CGEA) there exists a corresponding approximation to the Bethe–Salpeter equations (which give the vertex functions), such that the WT hierarchy holds. The WT identities are systematically obtained from the external gauge symmetry of the 2PI CGEA. In this section we also clarify the relation between the WT hierarchy and current-conserving nonlinear response theory. In section 6 we show, using a simple example, how ad hoc approximations to the 2PI CGEA (not resulting from a truncation of its loop expansion) violate the WT hierarchy. A brief summary is given in section 7.

2. Ward–Takahashi hierarchy and current conservation

In many-particle systems, and particularly in quantum transport theories, n -point vertex functions play a fundamental role, since they represent generalized currents which satisfy the hierarchy of Ward–Takahashi identities [12]. This hierarchy is satisfied to all orders in the exact theory, thus guaranteeing local gauge invariance and the conservation of the associated charges.

There are two equivalent ways of obtaining the WT identities. The first one, due to Rivier and Pelka [12] (see also [13]), relies on the equation of motion of the n -particle Green’s function (GF). In the second one, due to Kadanoff and Baym [14, 15], the two-point GF is expanded in powers of a fictitious non-local external field (for a recent development see [10]). To zeroth order in the expansion, the classical

continuity equation is recovered (i.e. the mean current is divergenceless); to first order in the external field, the usual WT identity relating the three-point vertex to the two-point propagator is obtained. Higher-order terms in the expansion reproduce the hierarchy of WT identities obtained by the first method. We note that the second approach is not directly related to Baym’s Φ -derivable approximation [2, 14, 16], because in principle no approximation is involved. It is just an equivalent way of deriving the WT hierarchy which is based on a functional approach and not on the equations of motion for the propagators.

In its most general form, the generalized continuity equation (WT hierarchy) can be written as (we use the simplified notation $1 = (t_1, \mathbf{r}_1)$ and employ Schwinger–Keldysh non-equilibrium formalism [2–5, 17–20]):

$$\begin{aligned} \partial_\mu^z \Lambda_{(n)}^\mu(1 \cdots n, 1' \cdots n'; z) &= i^n e \{ -\delta(z - n') G_n(1 \cdots n, 1' \cdots (n-1')z) + \cdots \\ &+ (-1)^n \delta(z - 1') G_n(1 \cdots n, 2' \cdots z) + \cdots \\ &+ \delta(z - n) G_n(1 \cdots (n-1)z, 1' \cdots n') - \cdots \\ &- (-1)^n \delta(z - 1) G_n(2 \cdots z, 1' \cdots n') \} \end{aligned} \quad (1)$$

where

$$\begin{aligned} \Lambda_{(n)}^\mu(12 \cdots n, 1'2' \cdots n'; z) &= \langle T_c j^\mu(z) \psi(1) \psi(2) \cdots \psi(n) \psi^\dagger(n') \cdots \psi^\dagger(2') \psi^\dagger(1') \rangle \end{aligned} \quad (2)$$

is the $(n+1)$ -point vertex function with current insertion at $z = (t_z, \mathbf{r}_z)$:

$$\begin{aligned} j^\mu(z) &= -e \lim_{z' \rightarrow z} D^\mu(z, z') \psi^\dagger(z') \psi(z); \\ D^i(z, z') &= (2i)^{-1} (\nabla_z^i - \nabla_{z'}^i) \quad \mu = i = 1, 2, 3, \\ D^0(z, z') &= 1 \quad \mu = 0 \end{aligned} \quad (3)$$

and G_n are real-time propagators defined as usual:

$$\begin{aligned} G_n(1 \cdots n, 1' \cdots n') &= i^{-(n)} \langle T_c \psi(1) \cdots \psi(n) \psi^\dagger(n') \cdots \psi^\dagger(1') \rangle. \end{aligned} \quad (4)$$

Note that $\Lambda_{(n=0)}^\mu(z) = \langle j^\mu(z) \rangle$ and that

$$D^i(z, z')[A] = -i \{ \nabla_z^i - \nabla_{z'}^i - ie[A^i(z) + A^i(z')] \} / 2 \quad (5)$$

in the presence of external fields.

In equations (2) and (4), T_c is the closed-time-path time ordering operator, ψ and ψ^\dagger are field operators in the Heisenberg representation, and $\langle \cdots \rangle$ stands for an average taken with respect to the density matrix of the system in the remote past. The classical continuity equation and the usual WT identity [21] correspond to the cases $n = 0$ and $n = 1$ of equation (1), respectively:

$$\partial_\mu^z \langle j^\mu(z) \rangle = 0 \quad (6)$$

and

$$\partial_\mu^z \Lambda_{(1)}^\mu(1, 1'; z) = ie[-\delta(z, 1') G(1, z) + \delta(z, 1) G(z, 1')], \quad (7)$$

$G(1, 1')$ being the single-particle propagator.

As already mentioned, in the exact theory equation (1) holds for arbitrary n . The hierarchy of n -particle propagators

take into account that field excitations can be created and annihilated in the second-quantization formalism, thus acting as source terms for the generalized currents represented by the vertex functions. In other words, in the exact theory, particle number is *strongly* conserved, not only in the mean. This fact has an important consequence in quantum transport theories based on response theory to an external field, which is the main subject of this work. For a many-particle system in the presence of an external field, the hierarchy for the exact propagators implies that the current, as defined by equation (3), is conserved to all orders in the external perturbation, with linear response theory corresponding to the special case $n = 1$.

It is impossible, in general, to obtain the propagators of an interacting field theory exactly and some approximations must be made. In the weak-coupling regime, no conflict arises between conservation laws and perturbative expansions based on Feynman diagrams, because conserved quantities are conserved order by order in the expansion¹. On the other hand, for a strong coupled theory re-summation concepts are usually needed [2, 16], and warranting conservation laws then becomes a nontrivial issue. Symmetries satisfied at the exact level may not be satisfied by approximate propagators, thereby violating (generalized) current conservation dictated by the hierarchy in equation (1).

A systematic way of generating conserving approximations (at the classical level, i.e. $n = 0$) was given by Baym [14] and corresponds to his well-known Φ -derivable scheme. The self-energy is obtained from a functional Φ consisting of an infinite series of two-particle irreducible (2PI) closed diagrams, constructed from full propagators and bare vertices [16]. The solutions obtained from truncating the Φ functional are such that, if Φ is invariant under a simultaneous symmetry transformation of the classical field and propagator, the expectation values of the respective Noether currents are conserved [2, 14, 23]. We emphasize that this situation corresponds to the case $n = 0$ of the WT hierarchy, given by equation (6). Therefore, the conservation of generalized currents encoded in the WT hierarchy is not automatically warranted in this approach. Moreover, in certain situations (e.g. in theories exhibiting spontaneous symmetry breaking) the hierarchy is already violated at the level of the self-energy (corresponding to $n = 1$) which does not satisfy the Nambu–Goldstone theorem [2, 24, 25]. The reason is simple: the n -point functions obtained by functional differentiation in a Φ -derivable approximation may not be equal to the one-particle irreducible [2] (1PI) functions that satisfy the WT hierarchy.

To our knowledge, there are two possible approaches to overcome this problem present in Φ -derivable approaches².

¹ Of course, no conflict arises for non-interacting particles, since in that case the lifetime of field excitations is infinite. See [22] for a discussion of second-order response theory in non-interacting systems.

² We refer to approaches to solve the problem that still belong to the two-particle irreducible class. Of course, one could in principle solve the problem of local symmetries (WT identities) by treating the dynamics of higher-order correlations. This would require n -particle irreducible effective actions, with $n > 2$ (see [4] and [26]). However, we think that the relation between nonlinear response and current conservation is clearly appreciated in the 2PI formalism, which is also technically feasible as compared to $n > 2$ effective actions. It remains to investigate the possibility of relating higher-order response functions (and the response of higher-order correlations) to higher-order effective actions in the n -particle hierarchy.

In the one put forward by van Hees and Knoll [24], a non-perturbative approximation for the 1PI quantum effective action is obtained on top of a self-consistent solution to Schwinger–Dyson equations (SDE) derived from the truncated 2PI effective action. The vertex functions obtained in the usual way from this 1PI effective action fulfil the WT identities. The extra terms not accounted for in the Φ -derivable approximation and required to satisfy the identities are encoded in a Bethe–Salpeter equation (BSE) and higher vertex equations (see [27] for a calculation of conductivity in QED). The second approach [28, 29] is based on the concept of *external gauge invariance* and provides a systematic way of generating consistent SDE and BSEs that automatically satisfy WT identities. Most importantly in the context of transport theories of strongly interacting systems, the derivation of the SDE and the BSEs can be done, in principle, to any order in the external field coupled to the system. Therefore, the latter is especially suited for the study of response theory beyond first order and its relation to current conservation beyond the expectation value level, and will be employed here.

3. CTP 2PI coarse-grained effective action

In this section, we introduce the closed-time-path 2PI effective action [2–6, 19] for a specific fermionic system open to an environment. A detailed presentation of effective action techniques and the CTP formalism can be found in [2].

The system we are interested in consists of a central region with interacting electrons described by fields (ψ^\dagger, ψ) and coupled to an external field. This central region is connected to two ideal reservoirs of non-interacting electrons described by fields $(\phi_\alpha^\dagger, \phi_\alpha)$, with $\alpha = (L, R)$ denoting the left or right reservoir. The reservoirs are assumed to remain in equilibrium at all times.

The CTP classical action of the system is $S[\bar{\psi}, \psi, \bar{\phi}, \phi] = S_\psi + S_\phi + S_c$, with

$$\begin{aligned} S_\psi &= c_{AB} \bar{\psi}^A C_{AB}^{-1} \psi^B + S_{\text{int}}[\bar{\psi}, \psi] \\ S_\phi &= c_{AB} \bar{\phi}^A B_{AB}^{-1} \phi^B \quad S_c = c_{AB} \bar{\psi}^A T_{AB} \phi^B + \text{h.c.} \end{aligned} \quad (8)$$

where

$$S_{\text{int}}[\bar{\psi}, \psi] = \frac{1}{24} U_{ABCD} \bar{\psi}^A \psi^B \bar{\psi}^C \psi^D \quad (9)$$

U_{ABCD} being the completely antisymmetrized bare interaction local vertex. For the moment, we shall not specify the structure of the four-fermion vertex U_{ABCD} since its precise form will not be needed until section 6. T_{AB} is a local coupling parameter between the central region and the reservoirs.

We are using a DeWitt notation [2, 30] with $A = (x, a)$, $x = (t_x, r_x, \sigma)$ and $a = (1, 2)$ [or $(+, -)$] being CTP indices indicating the branch within the closed-time contour. For the fields describing electrons inside the reservoirs, an additional index α must be included in the CTP indices (A, B) , but for simplicity we leave it implicit. Repeated indices are assumed to be integrated or summed. $(\bar{\psi}, \psi)$ and $(\bar{\phi}, \phi)$ are Grassmann variables and c_{ab} is a CTP metric $c_{ab} = \text{diag}(1, -1)$, while $c_{AB} = c_{ab} \delta(x_A, x_B)$. C_{AB} and B_{AB} are the free CTP

propagators corresponding to S_ψ and S_ϕ . They satisfy (we set $\hbar, m, c = 1$ in what follows)

$$\begin{aligned} c_{AB}\square B_{BC} &= i\delta_A^C \\ c_{AB}\tilde{\square} C_{BC} &= i\delta_A^C \end{aligned} \quad (10)$$

where $\square(1) = i\partial_{t_1} - h_0(1)$ while $\tilde{\square}(1) = i\partial_{t_1} - \tilde{h}_0(1)$, h_0 and \tilde{h}_0 being single-particle Hamiltonians corresponding to the reservoirs and the central region, respectively. Explicitly, they are

$$\begin{aligned} h_0(1) &= -\frac{1}{2}\nabla_1^2 \quad \text{and} \\ \tilde{h}_0(1) &= \frac{1}{2}[-i\nabla_1 + eA_i(1)]^2 + eA_0(1) \end{aligned} \quad (11)$$

where $A_\mu(z)$ is the external classical field and $i = (1, 2, 3)$. Note that it is not necessary to add CTP indices to the external field, since this is a physical source, and in any case we would obtain $A_{\mu,1} = A_{\mu,2}$. It is important to remark that, since A_μ is external, it is not treated as a dynamical field.

From the classical action of equation (8), we form the CTP generating functional Z_{CTP} with local and bi-local external sources J_A and K_{AB} , respectively. Since we are interested in the dynamics inside the central region coupled to reservoirs, only the fields $(\bar{\psi}, \psi)$ describing the ‘system’ will be coupled to the external sources. Z_{CTP} contains all the information about the non-equilibrium many-body system since all closed-time path correlators can be calculated from it [2]. When written as a path integral over field configurations it is

$$\begin{aligned} Z_{\text{CTP}}[J, K] &= \int [D\bar{\phi}][D\phi][D\bar{\psi}][D\psi] \exp i(S[\bar{\psi}, \psi, \bar{\phi}, \phi] \\ &\quad + \bar{J}_A \psi^A + \bar{\psi}^A J_A + \frac{1}{2} K_{AB} \bar{\psi}^A \psi^B) \end{aligned} \quad (12)$$

where (\bar{J}_A, J_A) and K_{AB} are fermionic and bosonic sources, respectively. The measure corresponding to each field, for example ψ , actually stands for $[D\psi_a]$ with $a = (1, 2)$ the branch index. The CTP boundary condition of the path integral giving Z_{CTP} , namely the continuity of field histories in the remote future, is implicit. We assume that the initial state is prepared in the remote past, corresponding to the *in-vacuum* [2, 3]. Note that (\bar{J}_A, J_A) act as Lagrange multipliers constraining the deviations of $(\bar{\psi}, \psi)$ from their mean values, while K_{AB} constrains their fluctuations [5]. This is the main idea behind n PI effective action techniques, namely to treat $1 \cdots n$ -point correlators on the same footing [2, 5, 26]. By using the 2PI CGEA, only the one- and two-point correlators are treated as dynamical variables and therefore obtained variationally; higher correlations (with $n > 2$) are calculated from them. Note that the use of the 2PI CGEA to obtain equations of motion for mean fields and propagators represents an enormous simplification of the usual perturbation expansion. Moreover, non-perturbative approximation schemes based on expansions of the 2PI EA provide powerful calculational tools where standard expansion schemes break down [2, 6].

Any correlation function of the many-body system can be obtained from Z_{CTP} by functional differentiation with respect to (\bar{J}_A, J_A) and then setting all sources to zero. For example,

the CTP two-point propagator of the central region is

$$\begin{aligned} \langle T_c \psi^A (\psi^B)^\dagger \rangle &= \frac{\delta^2 Z_{\text{CTP}}[J, K]}{i\delta_R \bar{J}_A i\delta_L J_B} \Big|_{[\bar{J}, J, K]=0} \\ &= \int [D\bar{\phi}][D\phi][D\bar{\psi}][D\psi] \psi^A \bar{\psi}^B \exp i(S[\bar{\psi}, \psi, \bar{\phi}, \phi]), \end{aligned} \quad (13)$$

with $\delta_{R,L}$ denoting right and left differentiation, respectively. Note that there is no need to use contour-ordering operators in the second line of equation (13), since the path integral automatically arranges operators in the correct order.

Since the reservoirs’ fields enter the action quadratically, we can integrate them out exactly in Z_{CTP} , thus defining a new generating functional for CTP propagators belonging to the system. This *coarse-grained* generating functional is

$$\tilde{Z}_{\text{CTP}}[J, K] = \int [D\bar{\psi}][D\psi] \exp i(\tilde{S}[\bar{\psi}, \psi] + \text{sources}) \quad (14)$$

where the effective classical action is given by

$$\tilde{S}[\bar{\psi}, \psi] = \tilde{S}_\psi = c_{AB} \bar{\psi}^A D_{AB}^{-1} \psi^B + S_{\text{int}}[\bar{\psi}, \psi] \quad (15)$$

with

$$D_{AB}^{-1} = C_{AB}^{-1} + i\Sigma_{\phi, AB}. \quad (16)$$

The self-energy Σ_ϕ describes the influence of the reservoirs on the particles’ dynamics inside the system and it is given explicitly by

$$\Sigma_{\phi, AD} = T_{AB}^* B_{BC} T_{CD} \quad (17)$$

where B is given by equations (10). It is a complex quantity whose imaginary part represents the tunnelling rate of particles from the central region to the reservoirs. Note that Σ_ϕ can be easily calculated since it depends on the equilibrium CTP propagators of the reservoir composed of non-interacting electrons. The CTP propagators corresponding to the system are calculated from \tilde{Z}_{CTP} using the analogue of equation (13) with the replacement $S \rightarrow \tilde{S}$.

From \tilde{Z}_{CTP} we define the CTP generating functional of connected propagators W_{CTP} in the usual way, i.e. $\tilde{Z}_{\text{CTP}} = \exp iW$, and then apply a double Legendre transform to obtain the 2PI-CTP effective action of the system. The sources (J, K) are connected to the mean field and full propagators (denoted by G) through

$$\begin{aligned} \frac{\delta W}{\delta \bar{J}_A} = \hat{\psi}^A = 0 \quad \frac{\delta W}{\delta J_A} = \hat{\psi}^A = 0 \\ \frac{\delta W}{\delta K_{AB}} = \frac{1}{2} G_{AB} \end{aligned} \quad (18)$$

where we have used that the fermionic mean fields $(\hat{\psi}, \hat{\bar{\psi}}) = 0$ since no symmetry breaking occurs. By performing the double Legendre transform on W and then using the background field method we can write the CTP 2PI CGEA of the system as [2] (Tr and ln operations are understood in a functional sense)

$$\Gamma[G, A] = i\text{Tr} \ln G - iD_{AB}^{-1} G^{AB} + \Gamma_2[G] \quad (19)$$

where A is the external classical field introduced before. We note that the CTP 2PI CGEA depends explicitly on the external

field only through $D^{-1}[A]$; this will be important in what follows.

In equation (19), $\Gamma_2[G]$ encodes all quantum corrections and consists of vacuum 2PI closed diagrams with full propagators in internal lines and vertices corresponding to a theory with shifted classical action $S[\hat{\bar{\psi}} + \bar{\psi}, \hat{\psi} + \psi]$ (neglecting constant and linear terms), where $(\bar{\psi}, \psi)$ denote fluctuations. The diagrams are vacuum because the mean value of the fluctuation fields is zero by construction. Note that, because of the vanishing of the mean fields, the shifted classical action vanishes when evaluated at $(\hat{\bar{\psi}}, \hat{\psi})$. Therefore, the vertices contributing to Γ_2 are identical to those of the original classical action, namely the quartic one with U as the coupling parameter. The case of non-interacting electrons corresponds in this scheme to $\Gamma_2 = 0$.

The Schwinger–Dyson equations for the CTP propagators follow directly from $\Gamma[G, A]$:

$$\frac{\delta\Gamma}{\delta G_{AB}} = -\frac{1}{2}K_{AB} \quad (20)$$

where the physical case corresponds to vanishing external sources $K = 0$. Defining the self-energy

$$\Sigma_{AB} = -2\delta\Gamma_2/\delta G^{AB} \quad (21)$$

we can rewrite the SDE in the usual way:

$$G_{AB}^{-1} = D_{AB}^{-1} + i\Sigma_{AB}, \quad (22)$$

Σ_{AB} being one-particle irreducible by construction.

In this paper, we shall not go beyond second order in the interaction parameter U , corresponding in this theory to a three-loop expansion. To this order, Γ_2 is in our compact notation

$$\Gamma_2 = -\frac{1}{8}U_{ABCD}G_{AB}G_{CD} + i\frac{1}{48}U_{ABCD}U_{EFGH}G_{AE}G_{BF}G_{CG}G_{DH}. \quad (23)$$

The first term corresponds to the so-called *double-bubble* diagram and the second term to the *basketball* diagram. In the SDE, the first term yields the time-dependent Hartree–Fock approximation, while the second is non-local and complex (therefore including fluctuation damping) [2, 3, 5]. We will return to these approximations when proving the external gauge invariance of the CTP 2PI CGEA, in section 4, and also in section 6.

4. External gauge invariance of the CTP 2PI EA

The crucial observation that allows us to relate the CTP 2PI CGEA of the open system to nonlinear transport through it is that $\Gamma[G, A]$ is invariant under a gauge transformation of the external field A_μ . Following Bando *et al* ([28]), we will call this *external gauge invariance* (EGI) of the 2PI EA. We will first give a brief proof of the EGI of the *exact* 2PI CGEA, where exact means that Γ_2 is expanded to all loop orders in equation (19). Then, we will prove that, even when the loop expansion of Γ_2 is truncated at certain order, the truncated 2PI EA still remains EGI.

Under a local transformation $U(1) = \exp i e\varphi(1)$, the external field and the full propagator transform as [25, 29] (we omit the CTP indices for the moment)

$$A_\mu \rightarrow A'_\mu = U A_\mu U^{-1} - i(\partial_\mu U)U^{-1} \quad (24)$$

$$G(1, 2) \rightarrow G'(1, 2) = U(1)G(1, 2)U^{-1}(2).$$

It is rather straightforward to prove that, if we retain all terms in the loop expansion of Γ_2 , then the 2PI CGEA is EGI [2, 6, 25]. This can be simply understood by recalling that the exact 2PI CGEA is precisely the generating functional of 1PI propagators. The proof of the EGI of the exact 2PI CGEA is based on the fact that, under a gauge transformation of the fields $(A_\mu, \bar{\psi}, \psi)$, the CTP generating functional $\tilde{Z}_{\text{CTP}}[J, K]$ as given in equation (14) is invariant. This is because the transformation is equivalent to a change of integration variables in the path integral, whose Jacobian is trivial due to the unitarity of the transformation ($\det U = 1$). Since the classical (effective) action $\tilde{S}[\bar{\psi}, \psi]$ is external gauge-invariant, only the source terms are transformed. For a local infinitesimal variation of the fields $\zeta = (A_\mu, \bar{\psi}, \psi)$, given in compact notation by

$$\delta\zeta = e(0, -i\varphi\bar{\psi}, i\varphi\psi) + (\partial_\mu\varphi, 0, 0) \quad (25)$$

we obtain from equation (14)

$$\delta\tilde{Z}_{\text{CTP}} = 0 = \langle \bar{J}_A \delta\psi^A + \delta\bar{\psi}^A J_A + \frac{1}{2}K_{AB}\delta\bar{\psi}^A\psi^B + \frac{1}{2}K_{AB}\bar{\psi}^A\delta\psi^B \rangle, \quad (26)$$

with

$$\langle \dots \rangle = \int [D\bar{\psi}][D\psi](\dots) \exp i(\tilde{S}[\bar{\psi}, \psi] + \text{sources}). \quad (27)$$

Using that

$$\frac{\delta\Gamma}{\delta\bar{\psi}^A} = -J_A + \frac{1}{2}K_{AB}\psi^B$$

$$\frac{\delta\Gamma}{\delta\psi^A} = \bar{J}_A - \frac{1}{2}K_{AB}\bar{\psi}^B \quad \frac{\delta\Gamma}{\delta G_{AB}} = -\frac{1}{2}K_{AB}, \quad (28)$$

which follows since W and Γ are Legendre transforms of each other, we can turn equation (26) into an equation for Γ :

$$\sum_{\alpha=2,3} \delta\zeta_\alpha \frac{\delta\Gamma}{\delta\zeta^\alpha} + \frac{\delta\Gamma}{\delta G_{AB}} \delta G^{AB} = 0 \quad (29)$$

where the variation of the full propagator is given by

$$\delta G^{AB} = \delta\langle\psi^A\bar{\psi}^B\rangle = \langle\delta\psi^A\bar{\psi}^B + \psi^A\delta\bar{\psi}^B\rangle. \quad (30)$$

According to equation (25), equation (30) is the infinitesimal version of the transformation rule for G given in equations (24). Therefore, equation (29) shows that the exact 2PI CGEA is gauge-invariant under equations (24).

We turn now to the invariance of the 2PI effective action which results from a truncation in the loop expansion of the quantum correction Γ_2 . For completeness, we will also show explicitly that the first two terms in equation (19), the one-loop

terms, are EGI. We start with the first term of $\Gamma[G, A]$, which is clearly EGI:

$$\text{Tr} \ln G \rightarrow \text{Tr} \ln(UGU^{-1}) = \text{Tr}[U(\ln G)U^{-1}] = \text{Tr} \ln G. \quad (31)$$

The EGI of the second term of equation (19) is proved by noting that D^{-1} transforms as G under equations (24). This follows directly from the equation of motion for the system's free propagator C , given in equations (10), and the fact that Σ_ϕ is invariant under the external gauge transformation. The latter is a consequence of the equation of motion satisfied by B , the reservoir's free propagator, and the dependence of Σ_ϕ on this propagator, given in equation (17).

The third term contributing to $\Gamma[G, A]$ is $\Gamma_2[G]$, the sum of 2PI vacuum diagrams with G in internal lines. The proof of external gauge invariance proceeds as before and relies on the transformation law for propagators and the structure of the 2PI EA. To be explicit, we rewrite the first term of equation (23) taking into account that the interaction vertex U_{ABCD} is local. Using the locality of the bare vertex we obtain for the double-bubble diagram

$$\Gamma_2^{(1)} = -\frac{\tilde{U}}{8} G_{AB} G_{BA} \quad (32)$$

which shows that, as already mentioned, the self-energy derived from it is local. It is clear from the above expression that, under the external gauge transformation given in equations (24), $\Gamma_2^{(1)}$ is invariant. The structure of higher terms in the loop expansion of Γ_2 is such that the EGI holds to arbitrary order.

The main conclusion of this discussion is that, even though the system is open to reservoirs, its 2PI coarse-grained effective action is, order by order in the loop expansion, invariant under the gauge transformation given in equations (24). As we shall see, this makes the combination of the CTP 2PI-CG effective action approach and the external gauge invariance a powerful technique to study strongly interacting driven systems beyond linear response. We should remark that, in the presence of non-vanishing mean fields, the 2PI CGEA may not be EGI order by order in a loop expansion [2, 6, 25].

5. WT hierarchy from external gauge invariance

We have seen that the CTP 2PI CGEA describing the system is left invariant under an external gauge transformation, and that this property holds to all orders in the (loop) expansion of the quantum corrections given by Γ_2 . This implies that the SDE derived functionally from the 2PI effective action is automatically external gauge-covariant. Most importantly, this is true for an *arbitrary* external classical field. This will be the key property to relate this symmetry to nonlinear response, thus generating approximations which satisfy the WT hierarchy to arbitrary order. We will show that the external gauge covariance is also inherited by the BSE for vertex functions, which as a consequence of EGI will satisfy the Ward–Takahashi hierarchy.

Gauge invariance of the effective action $\Gamma[G, A]$ implies

$$\Gamma[G, A] = \Gamma[G', A'] \quad (33)$$

where a prime denotes external gauge-transformed quantities according to equations (24). The SDE for the CTP propagators is given by $\delta\Gamma/\delta G_{AB} = 0$ and, due to the EGI of the 2PI CGEA, it is (external) gauge-covariant:

$$\frac{\delta\Gamma[G, A]}{\delta G_{AB}} = U^{-1} \frac{\delta\Gamma[G', A']}{\delta G'_{AB}} U. \quad (34)$$

This property of the 2PI CGEA has an important consequence. It implies that the variational procedure by which one obtains the SDE from the 2PI CGEA is independent of the external gauge. That is to say, if $G_{AB}[A]$ is a solution of the SDE in the background classical field A , i.e.

$$\left. \frac{\delta\Gamma[G, A]}{\delta G_{AB}} \right|_{G_{AB}=G_{AB}[A]} = 0, \quad (35)$$

then the solution corresponding to a transformed external field $A' = UAU^{-1} - i(\partial U)U^{-1}$ is precisely $G' = UGU^{-1}$:

$$\left. \frac{\delta\Gamma[G', A']}{\delta G'_{AB}} \right|_{G'_{AB}=UG_{AB}[A]U^{-1}} = 0. \quad (36)$$

More explicitly, EGI of the 2PI CGEA implies

$$G[A'] = UG[A]U^{-1}. \quad (37)$$

We will now make a connection between EGI and nonlinear response. For notational simplicity, CTP indices are omitted in the following. The solution $G[A]$ to the SDE can be expanded in powers of the external field A_μ (see [18, 20, 31]):

$$\begin{aligned} G[A](X, Y) &= G[0](X, Y) + iA_\mu \Pi_3^\mu + \frac{i^2}{2} A_\mu A_\nu \Pi_4^{\mu\nu} \\ &+ \frac{i^3}{3} A_\mu A_\nu A_\rho \Pi_5^{\mu\nu\rho} \dots \\ &= \sum_{n=0} \frac{i^n}{n!} \int d1 \dots dn A_{\mu_1}(1) \dots A_{\mu_n}(n) \Pi_{(n+2)}^{\mu_1 \dots \mu_n} \\ &\times (1, \dots, n; X, Y), \end{aligned} \quad (38)$$

where in the third line we have made explicit the internal (integration) $(1, \dots, n)$ and the external (X, Y) variables. The dummy indices μ, ν, ρ , etc, of the first two lines are denoted by μ_1, \dots, μ_n in the third.

The 'response' functions $\Pi_{(n+2)}$ encode the variation of the full propagator with the external field. We note that it is possible [18, 31], in principle, to expand higher-order correlation functions similarly to the two-point function as given in equations (38), but in this paper we shall only deal with $G[A](X, Y)$. Equations (38) are given in the so-called [18, 31] single-time representation of CTP correlators, which is simpler for calculations than the 'physical' or r/a representation. Both representations are related by a similarity transformation characterized by an orthogonal matrix [17, 18] $Q = (\hat{1} - i\sigma_2)/\sqrt{2}$ with

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (39)$$

and are completely equivalent to each other:

$$\begin{aligned} E_{i_1 \dots i_n}(1 \dots n) &= 2^{n/2-1} Q_{i_1 \alpha_1} \dots Q_{i_n \alpha_n} E_{\alpha_1 \dots \alpha_n}(1 \dots n) \\ E_{\alpha_1 \dots \alpha_n}(1 \dots n) &= 2^{1-n/2} Q_{\alpha_1 i_1}^T \dots Q_{\alpha_n i_n}^T E_{i_1 \dots i_n}(1 \dots n) \end{aligned} \quad (40)$$

where $E(1 \dots n)$ denotes a n -point CTP function, α_j (i_j) corresponds to the single-time (physical) representation and repeated indices are assumed to be summed. To give an example of equations (40), for the propagators in the physical

$$\tilde{G} = \begin{pmatrix} 0 & G_a \\ G_r & G_c \end{pmatrix} \quad (41)$$

and in the single-time

$$\tilde{G} = \begin{pmatrix} G_{++} & G_{+-} \\ G_{-+} & G_{--} \end{pmatrix} \quad (42)$$

representations we have [2]

$$\begin{aligned} \tilde{G}_{11} &= \frac{1}{2}(G_{++} + G_{--} - G_{+-} - G_{-+}) = 0 \\ \tilde{G}_{12} &= G_a = \frac{1}{2}(G_{++} - G_{-+} + G_{+-} - G_{--}) \\ \tilde{G}_{21} &= G_r = \frac{1}{2}(G_{++} - G_{+-} + G_{-+} - G_{--}) \\ \tilde{G}_{22} &= G_c = \frac{1}{2}(G_{++} + G_{--} + G_{+-} + G_{-+}) \\ &= G_{+-} + G_{-+} = G_{++} + G_{--}. \end{aligned} \quad (43)$$

The first equality in equations (43) is valid in general: any CTP function in the physical representation with all its indices set to ‘1’ satisfies $\tilde{G}_{11 \dots 1} = 0$. The last line results from the identity $G_{+-} + G_{-+} = G_{++} + G_{--}$, which follows from the normalization of the step function $\theta(1, 2) + \theta(2, 1) = 1$. In these expressions, G_r , G_a and G_c are retarded, advanced and correlation functions, respectively:

$$\begin{aligned} G_r(1, 2) &= -i\theta(1, 2)\{\psi(1), \psi^\dagger(2)\} \\ G_a(1, 2) &= -i\theta(2, 1)\{\psi(1), \psi^\dagger(2)\} \\ G_c(1, 2) &= -i\{\psi(1), \psi^\dagger(2)\} \end{aligned} \quad (44)$$

where $\{, \}$ is the anticommutator and θ the step function, while $G_{++}, G_{--}, G_{+-}, G_{-+}$ are the chronological (Feynman), antichronological (Dyson), lesser and greater correlations:

$$\begin{aligned} G_{++}(1, 2) &= -i\langle T\psi(1)\psi^\dagger(2) \rangle \\ G_{+-}(1, 2) &= i\langle \psi^\dagger(2)\psi(1) \rangle \\ G_{-+}(1, 2) &= -i\langle \psi(1)\psi^\dagger(2) \rangle \\ G_{--}(1, 2) &= -i\langle \tilde{T}\psi(1)\psi^\dagger(2) \rangle, \end{aligned} \quad (45)$$

with (T, \tilde{T}) denoting the chronological and antichronological time ordering operator. Using this transformation rule, it is a simple matter to re-express equations (38) (and what follows from them) in the physical representation (see [18] and [20]), but for clarity we will continue employing the single-time representation.

We note that, as discussed in [18], in the physical representation the observables are given by retaining only

the ‘2’ component of the n -point function $\tilde{G}(1 \dots n)$, i.e. by the correlation functions $\tilde{G}_{2 \dots 2}$. For example, the two-point observable ($n = 2$) is the fully symmetrized correlation function $\tilde{G}_{22}(X, Y) = G_c(X, Y)$, given in equations (43). Using the relation between the physical and single-time representations, the response of the correlation two-point function \tilde{G}_{22} is immediately obtained:

$$\tilde{G}_{22}[A](X, Y) = \tilde{G}_{22}[0](X, Y) + i\tilde{\Pi}_{221}^\mu(X, Y; 1)A_\mu(1) + \dots \quad (46)$$

It is worth remarking that the use of the closed-time path method automatically ensures that the response functions are causal (see, for instance, [2] and [18])³.

Returning now to equations (38), the response functions are given by

$$\begin{aligned} \Pi_{(n+2)}^{\mu_1 \dots \mu_n}(1, \dots, n; X, Y) \\ = i^{-n} \frac{\delta G(X, Y; A)}{\delta A_{\mu_1}(1) \dots \delta A_{\mu_n}(n)} \Big|_{[A_{\mu_1} \dots A_{\mu_n}] = 0} \end{aligned} \quad (47)$$

and correspond to $(n + 2)$ -point functions with n current vertices inserted at locations $(1, \dots, n)$ where interactions between the current and the external classical field take place. In more detail, the response functions for $n = 1, 2$ are

$$\begin{aligned} \Pi_3^\mu(X, Y; z) &= -i\langle T_c j^\mu(z)\psi(X)\psi^\dagger(Y) \rangle \quad \text{and} \\ \Pi_4^{\mu\nu}(X, Y; z, w) &= -\langle T_c j^\mu(z)j^\nu(w)\psi(X)\psi^\dagger(Y) \rangle. \end{aligned} \quad (48)$$

Note that $-i\Pi_2(X, Y)$ corresponds to the propagator in the absence of the external field, which can be written as $G[0](X_i, Y_i; X_0 - Y_0)$ due to time-translation invariance of the system in equilibrium.

The structure of $\Pi_{(n+2)}$ as given in equations (48) follows because functional differentiation with respect to A_μ yields a current insertion to which the external field couples. In functional language we have that

$$\begin{aligned} \frac{\delta G(X, Y; A)}{\delta A_{\mu_1}(1) \dots \delta A_{\mu_n}(n)} \Big|_{[A_{\mu_1} \dots A_{\mu_n}] = 0} &= \int [D\psi][d\bar{\psi}] \psi(X)\bar{\psi}(Y) \\ &\times \frac{\delta}{\delta A_{\mu_1}(1) \dots \delta A_{\mu_n}(n)} \Big|_{[A_{\mu_1} \dots A_{\mu_n}] = 0} \\ &\times \exp i(\tilde{S}[\bar{\psi}, \psi] + \text{sources}). \end{aligned} \quad (49)$$

Equation (49) automatically leads to equations (48) since

$$\begin{aligned} \frac{\delta}{\delta A_{\mu_1}(1) \dots \delta A_{\mu_n}(n)} \Big|_{[A_{\mu_1} \dots A_{\mu_n}] = 0} \exp i(\tilde{S}[\bar{\psi}, \psi] + \text{sources}) \\ = (-i)^n j_{\mu_1}(1) \dots j_{\mu_n}(n) \exp i(\tilde{S}[\bar{\psi}, \psi, A = 0] + \text{sources}). \end{aligned} \quad (50)$$

The functions $\Pi_{(n+2)}$ are obtained from the SDE by functional differentiation with respect to A_μ (and then setting $A = 0$). This results in the BSEs for the response functions. For example, the BSE that determines Π_3 is

$$\frac{\delta G^{-1}}{\delta A_\mu} = \frac{\delta D^{-1}}{\delta A_\mu} + i \frac{\delta \Sigma}{\delta A_\mu} \quad (51)$$

³ The causality of the response functions is easily proved in the physical representation, and follows directly from the structure of the generating functional of CTP correlation functions.

where both sides of the equation are evaluated at $A_\mu = 0$. Using that $G(1, 2)G^{-1}(2, 1') = \delta(1, 1')$ (where the coordinate 2 is integrated), which implies

$$\frac{\delta G^{-1}(1, 2)}{\delta A_\mu(3)} = - \int d4 d5 G^{-1}(1, 4) \frac{\delta G(4, 5)}{\delta A_\mu(3)} G^{-1}(5, 2) \quad (52)$$

and defining

$$\tilde{\Pi}_{(n+2)}^{\mu_1 \dots \mu_n} = G^{-1} \Pi_{(n+2)}^{\mu_1 \dots \mu_n} G^{-1}, \quad (53)$$

the BSE for Π_3 can be written as

$$\tilde{\Pi}_3^\mu = - \frac{\delta D^{-1}}{\delta A_\mu} - i \frac{\delta \Sigma}{\delta A_\mu}. \quad (54)$$

Since the self-energy Σ is defined through Γ_2 , it is a functional of the full propagator G and therefore the last term in equation (54) involves Π_3 . Namely

$$\begin{aligned} \tilde{\Pi}_3^\mu(X, Y; z) &= - \frac{\delta D^{-1}}{\delta A_\mu} - i \frac{\delta \Sigma}{\delta G} \frac{\delta G}{\delta A_\mu} \\ &= - \frac{\delta D^{-1}(X, Y)}{\delta A_\mu(z)} - i \frac{\delta \Sigma(X, Y)}{\delta G(V, W)} \frac{\delta G(V, W)}{\delta A_\mu(z)} \\ &= - \frac{\delta D^{-1}(X, Y)}{\delta A_\mu(z)} - i \frac{\delta \Sigma(X, Y)}{\delta G(V, W)} \Pi_3^\mu(V, W; z), \end{aligned} \quad (55)$$

where in the last two lines the coordinates are shown explicitly (V and W are integrated). This is an integral equation that determines Π_3 once the quantity $\delta \Sigma / \delta G$ is known. Taking further functional derivatives of the SDE with respect to A_μ (and setting $A = 0$) results in a set of integral equations for $n > 1$ response functions. Note that Σ is directly obtained from $\Gamma[G, A]$, so the SD and BS equations are fully consistent with each other.

As we have seen, the combination of the SDE and the BSEs completely determines the full propagator and the response functions $\Pi_{(n+2)}$. The SDE is obtained from the 2PI CGEA, while the BSEs are obtained from the SDE by differentiation with respect to the external field. The important point is that, because the 2PI CGEA is invariant under external gauge transformations, both the full propagator and response functions obtained this way are external gauge-covariant. As we will show below, the EGI property of the 2PI CGEA implies that G and $\Pi_{(n+2)}$, as obtained from $\Gamma[G, A]$, satisfy the WT hierarchy. This provides the required link between current conservation in nonlinear response and the external gauge invariance of the 2PI CGEA, and also a powerful and systematic way of studying nonlinear response in strongly interacting systems coupled to ideal reservoirs.

To see the connection between EGI and the WT hierarchy, recall that external gauge invariance of the effective action means $G[A'] = UG[A]U^{-1}$. Inserting the expansion in powers of the external field given in equations (38) into both sides of this identity we get

$$\begin{aligned} G[0] + iA'_\mu \Pi_3^\mu + \frac{i^2}{2} A'_\mu A'_\nu \Pi_4^{\mu\nu} + \dots \\ = \sum_{n=0} \frac{i^n}{n!} \int d1 \dots dn A'_{\mu_1}(1) \dots A'_{\mu_n}(n) \end{aligned}$$

$$\begin{aligned} &\times \Pi_{(n+2)}^{\mu_1 \dots \mu_n}(1, \dots, n; X, Y) \\ &= UG[0]U^{-1} + iA'_\mu U \Pi_3^\mu U^{-1} + \frac{i^2}{2} A'_\mu A'_\nu U \Pi_4^{\mu\nu} U^{-1} + \dots \\ &= \sum_{n=0} \frac{i^n}{n!} \int d1 \dots dn A_{\mu_1}(1) \dots A_{\mu_n}(n) \\ &\times [U(X) \Pi_{(n+2)}^{\mu_1 \dots \mu_n}(1, \dots, n; X, Y) U^{-1}(Y)]. \end{aligned} \quad (56)$$

Note that equation (56) explicitly shows that the response functions $\Pi_{(n+2)}$ are external gauge-covariant. In particular, for an infinitesimal external gauge transformation $U(X) \approx 1 + ie\varphi(X)$ the transformed external field is

$$A'_\mu(X) = A_\mu(X) + \partial_\mu \varphi(X), \quad (57)$$

so equation (56) becomes

$$\begin{aligned} &\sum_{n=0} \frac{i^n}{n!} \int [dn] \prod_{i=1}^n \{A_{\mu_i}(i) + \partial_{\mu_i} \varphi(i)\} \Pi_{(n+2)}^{\mu_1 \dots \mu_n} \\ &= \sum_{n=0} \frac{i^n}{n!} \int [dn] \prod_{i=1}^n A_{\mu_i}(i) \{ \Pi_{(n+2)}^{\mu_1 \dots \mu_n} \\ &\quad + ie[\varphi(X) \Pi_{(n+2)}^{\mu_1 \dots \mu_n} - \Pi_{(n+2)}^{\mu_1 \dots \mu_n} \varphi(Y)] \} \end{aligned} \quad (58)$$

where we have suppressed the arguments of $\Pi_{(n+2)}^{\mu_1 \dots \mu_n}(1 \dots n; X, Y)$ and defined $[dn] = d1 \dots dn$ for brevity. Comparing terms of the same order in A_μ on both sides of this expression we get

$$\begin{aligned} \Pi_2(X, Y) + i \int d1 [\partial_\mu^1 \varphi(1)] \Pi_3^\mu(X, Y; 1) \\ = \Pi_2(X, Y) + ie[\varphi(X) \Pi_2(X, Y) - \Pi_2(X, Y) \varphi(Y)] \end{aligned} \quad (59)$$

for the zeroth-order term and

$$\begin{aligned} &\int d1 d2 [\partial_\nu^2 \varphi(2)] \Pi_4^{\mu\nu}(X, Y; 1, 2) A_\mu(1) \\ &= \int d1 e[\varphi(X) \Pi_3^\mu(X, Y; 1) - \Pi_3^\mu(X, Y; 1) \varphi(Y)] A_\mu(1) \end{aligned} \quad (60)$$

for the linear term. Higher-order terms have a similar structure but can become quite involved. The main point to emphasize is that the EGI of the 2PI CGEA implies relationships among the response functions, shown explicitly in equation (58).

Assuming that φ vanishes at infinity, we can integrate by parts the second term in equation (59) (zeroth order in A_μ) to obtain

$$\begin{aligned} &i \int d1 \varphi(1) \partial_\mu^1 \Pi_3^\mu(X, Y; 1) \\ &= -ie[\varphi(X) \Pi_2(X, Y) - \Pi_2(X, Y) \varphi(Y)] \end{aligned} \quad (61)$$

which implies

$$\partial_\mu^z \Pi_3^\mu(X, Y; z) = -e \Pi_2(X, Y) [\delta(X - z) - \delta(Y - z)] \quad (62)$$

or, in more detail,

$$\begin{aligned} \partial_\mu^z \langle T_c j^\mu(z) \psi(X) \bar{\psi}(Y) \rangle &= e \langle T_c \psi(X) \bar{\psi}(Y) \rangle \\ &\times [\delta(Y - z) - \delta(X - z)]. \end{aligned} \quad (63)$$

This is precisely the identity corresponding to $n = 1$ in the WT hierarchy given by equation (1), that is, equation (7). We see that, even at zeroth order in the external field, the relation

between the three-point vertex and the two-point function, equation (63), is satisfied due to the EGI of the 2PI EA.

Similarly, for the linear term, equation (60) implies the following identity:

$$-\int d2\partial_v^2 \Pi_4^{\mu\nu}(X, Y; 1, 2)\varphi(2) = e[\varphi(X)\Pi_3^\mu(X, Y; 1) - \Pi_3^\mu(X, Y; 1)\varphi(Y)] \quad (64)$$

which leads by the same calculation as in the zeroth-order case to a WT identity between the three- and four-point response functions (equivalent to equation (1) for $n = 2$):

$$\partial_v^z \Pi_4^{\mu\nu}(X, Y; 1, z) = e[\delta(Y - z) - \delta(X - z)]\Pi_3^\mu(X, Y; 1). \quad (65)$$

It is clear that this procedure could be continued to higher-order terms in A_μ , thus generating higher-order WT identities. We note that the hierarchy obtained for the response functions $\Pi_{(n+2)}$ is completely equivalent to that involving $\Lambda_{(n)}$, given in equation (1), as expected since, ultimately, they both enforce current conservation. As can be seen from their definitions, equations (2) and (47), the relation between vertex and response functions can be compactly written as

$$\Pi_{(n+2)}^{\mu_1 \dots \mu_n}(X, Y; z_1 \dots z_n) = (-e)^{(n-1)} \prod_{\alpha=2}^n \lim_{z'_\alpha \rightarrow z_\alpha} D^{\mu_\alpha}(z'_\alpha, z_\alpha) \times \Lambda_{(n)}^{\mu_1}(X z_2 \dots z_n, Y z'_2 \dots z'_n; z_1) \quad (66)$$

for $n \geq 2$ and

$$\begin{aligned} \Pi_{(3)}^\mu(X, Y; z) &= \Lambda_{(1)}^\mu(X, Y; z) & \text{for } n = 1, \\ \Pi_{(2)}(X, Y) &= iG[0](X, Y) & \text{for } n = 0, \end{aligned} \quad (67)$$

where the operator $D^{\mu_\alpha}(z'_\alpha, z_\alpha)$ is defined in equation (3). Defining the operator (with $n \geq 2$ and $2 \leq \alpha \leq n$)

$$F_n^{\mu_2 \dots \mu_n}(\{z'_\alpha, z_\alpha\}) = (-e)^{(n-1)} \prod_{\alpha=2}^n \lim_{z'_\alpha \rightarrow z_\alpha} D^{\mu_\alpha}(z'_\alpha, z_\alpha) \quad (68)$$

that appears in equation (66) acting on $\Lambda_{(n)}^{\mu_1}$, noting that this operator does not depend on z_1 (the ‘external’ coordinate in $\Lambda_{(n)}$), and using the property of the Green’s function G_n :

$$\begin{aligned} F_n^{\mu_2 \dots \mu_n}(\{z'_\alpha, z_\alpha\})G_n(1 \dots z_\alpha \dots n, 1' \dots z'_\alpha \dots n') \\ = F_n \langle T_c \psi(1) \dots \psi(z_\alpha) \dots \psi(n) \bar{\psi}(n') \dots \bar{\psi}(z'_\alpha) \dots \bar{\psi}(1') \rangle \\ = \langle T_c j^{\mu_2}(z_2) \dots j^{\mu_n}(z_n) \psi(1) \bar{\psi}(1') \rangle \\ = \Pi_{(n+2)}^{\mu_2 \dots \mu_n}(1, 1'; z_2 \dots z_n) \end{aligned} \quad (69)$$

the equivalence between WT hierarchies can be proven using equation (66) (the calculation is tedious but rather straightforward).

Therefore, the external gauge invariance of the 2PI CGEA enforces the WT hierarchy necessary for current conservation beyond the expectation value level. By expanding the full propagator (solution to the SDE) in powers of the external field, we can calculate current-conserving response functions as solutions to the BSEs obtained from the SDE. The key point is that the EGI of the 2PI CGEA implies the covariance of the full propagator and the response vertex functions, and this results in the WT relationships among them. We emphasize

that such a procedure relies on an expansion of $G[A]$ in powers of the external field A , so it is valid only for weak external fields.

We end this section by indicating how to calculate the current induced by the external classical field. The average current which evolves by the action of the external field is given by equation (3), which can be re-expressed in terms of the lesser Green function G_{+-} :

$$\begin{aligned} \langle j^\mu(z) \rangle &= -e \lim_{z' \rightarrow z} D^\mu(z, z')[A] \langle \psi^\dagger(z') \psi(z) \rangle \\ &= ie \lim_{z' \rightarrow z} D^\mu(z, z')[A] G_{+-}(z, z') \end{aligned} \quad (70)$$

where $D^\mu[A]$ is given in equation (5) and one should recall that G_{+-} must be calculated in the presence of the external field [22]. The lesser Green function appearing in the expression for the current can be calculated directly from the expansion given in equations (38). In this way, the induced average current can be systematically calculated to arbitrary order in the external classical field. The approach based on the 2PI EA and its loop truncation, adopted here, guarantees that the WT hierarchy is fulfilled.

6. Approximate 2PI effective actions and current conservation

As shown in section 3, the virtue of the 2PI CGEA method is that it provides a systematic way of encompassing interacting fields and current-conserving nonlinear response theory in a unified way. In particular, truncations to the loop expansion of the 2PI CGEA are, to arbitrary order, external gauge-invariant. Therefore, any such approximation will preserve the WT hierarchy. In this section, we give a concrete example of an ad hoc approximation to the 2PI CGEA, i.e. not obtained from a truncation in the loop expansion, and analyse the consequences for current conservation.

To be specific, we consider the following bare interaction vertex in S_{int} as appearing in equation (9):

$$U_{ABCD} = c_{abcd} \bar{\delta}_{t,r} \bar{\delta}_\sigma \tilde{U} \quad (71)$$

where

$$c_{abcd} = \begin{cases} 1 & \text{if } a, b, c, d = + \\ -1 & \text{if } a, b, c, d = - \\ 0 & \text{otherwise} \end{cases} \quad (72)$$

is a CTP tensor. In equation (71) we have grouped delta functions as follows:

$$\begin{aligned} \bar{\delta}_{t,r} &= \delta(t_A - t_B) \delta(t_A - t_C) \delta(t_A - t_D) \\ &\quad \times \delta(r_A - r_B) \delta(r_A - r_C) \delta(r_A - r_D) \\ &= \delta(X_A - X_B) \delta(X_A - X_C) \delta(X_A - X_D) \end{aligned} \quad (73)$$

and (σ stands for spin projection)

$$\bar{\delta}_\sigma = \delta_{\sigma_A, \sigma_B} \delta_{\sigma_C, \sigma_D}. \quad (74)$$

This vertex describes a ‘Hubbard-like’ local interaction $n_\uparrow(r)n_\downarrow(r)$, where $n_\sigma(r)$ is the electron number operator at position r .

It will be convenient for what follows to write the quantum correction to the 2PI EA as

$$\Gamma_2[G] = \sum_{i=1}^{\infty} \Gamma_2^{(i)} \quad (75)$$

where $\Gamma_2^{(i)}$ is of order \tilde{U}^i . We note that, due to the fact that fermion mean fields vanish, an expansion of Γ_2 in powers of U is equivalent to a loop expansion (this is no longer true when symmetry breaking occurs, see, e.g., [2]). The $O(U)$ diagram corresponds to the double-bubble, which is two-loop, while the $O(U^2)$ one corresponds to the basketball, which is three-loop. Both diagrams are given in equation (23). Since the CTP self-energy is obtained by functionally differentiating Γ_2 with respect to the full propagator, the contributions to the self-energy can also be classified according to equation (75). According to equation (71), for $i = 1$ we have

$$\begin{aligned} \Sigma_{AB}^{(1)} &= \Sigma_{ab}^{(1)}(X_A, X_B) = \frac{1}{4} U_{ABCD} G_{CD} \\ &= \frac{1}{4} \tilde{U} c_{abcd} \sum_{\sigma_C, \sigma_D} \int dX_C dX_D \delta(X_A - X_B) \\ &\quad \times \delta(X_A - X_C) \delta(X_A - X_D) \delta_{\sigma_A \sigma_B} \delta_{\sigma_C \sigma_D} G_{cd}(X_C, X_D) \\ &= \frac{1}{2} \tilde{U} c_{abcd} \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} G_{cd}(X_A, X_B). \end{aligned} \quad (76)$$

We note that the exchange part of Σ_{AB} is absent because the interaction occurs between particles with opposite spin projection.

From this equation, the $(+, -)$ components of the CTP self-energy are immediately obtained:

$$\begin{aligned} \Sigma_{++}^{(1)}(X_A, X_B) &= \tilde{U} \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} G_{++}(X_A, X_B) \\ \Sigma_{--}^{(1)}(X_A, X_B) &= -\tilde{U} \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} G_{--}(X_A, X_B) \quad (77) \\ \Sigma_{+-}^{(1)} &= \Sigma_{-+}^{(1)} = 0 \end{aligned}$$

where the last line follows from the definition of the CTP tensor c_{abcd} and shows the well-known fact that the quasiparticle lifetime is infinite in the Hartree approximation.

One can proceed similarly for $i = 2$ to obtain (we omit the calculation since it is completely analogous to the $i = 1$ case)

$$\begin{aligned} \Sigma_{++}^{(2)}(X_A, X_B) &= -i\tilde{U}^2 \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} [G_{++}(X_A, X_B)]^3 \\ \Sigma_{--}^{(2)}(X_A, X_B) &= -i\tilde{U}^2 \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} [G_{--}(X_A, X_B)]^3 \\ \Sigma_{+-}^{(2)}(X_A, X_B) &= i\tilde{U}^2 \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} [G_{+-}(X_A, X_B)]^3 \\ \Sigma_{-+}^{(2)}(X_A, X_B) &= i\tilde{U}^2 \delta(X_A - X_B) \delta_{\sigma_A \sigma_B} [G_{-+}(X_A, X_B)]^3 \end{aligned} \quad (78)$$

showing that this approximation includes fluctuation damping since the lesser and greater components of the self-energy are nonzero. The full CTP self-energy to order U^2 is then given by $\Sigma^{(1)} + \Sigma^{(2)}$.

As we have shown in previous sections, the truncation of the loop (U) expansion of $\Gamma_2[G]$ does not violate the external gauge invariance of the full 2PI EA, therefore providing approximate propagator and vertex functions that satisfy the WT hierarchy. We will now discuss, in the context of the 2PI EA description presented in this work, an ad hoc approximation known in non-equilibrium perturbation theory

applied to transport through quantum dots (see [1, 32] and references therein) and show why it does not preserve current conservation.

In the language of the 2PI EA formalism, the approximation involves two separate steps. In the first one, the quantum correction Γ_2 is approximated by the two-loop ($O(U)$) contribution, $\Gamma_2^{(1)}$. The $O(U^2)$ self-energy is calculated self-consistently either from [32] the Hartree G_{+-} (lesser correlation) or by requiring [1, 33] that the occupation of the central region evaluated with a renormalized $\Sigma^{(1)}$ (but not the Hartree one) equals the one calculated (in the next step) from the propagator dressed with $\Sigma^{(2)}$. In the second step, $\Sigma^{(2)}$ is calculated from equations (78) but with the full propagator G_{AB} replaced by that calculated from $\Sigma^{(1)}$ in the first step. In simpler terms, in this approximation the internal lines in $\Sigma^{(2)}$ are not the full propagator, as they are in the 2PI EA approach, but are either the Hartree or a similarly calculated propagator. It is easy to recognize that such an approach cannot, as it is, produce current-conserving results in general, since it breaks the variational procedure by which the full propagator is obtained from a single (truncated) functional.

The difference between the approximations to the 2PI EA based on a loop truncation and the ad hoc one can be best appreciated by comparing their SD equations. For the truncation to three loops we have

$$G_{AB}^{-1} = D_{AB}^{-1} + i\Sigma_{AB}^{(1)}[G] + i\Sigma_{AB}^{(2)}[G] \quad (79)$$

where we have made explicit that $\Sigma^{(1,2)}$ are functionals of the full CTP propagator G_{AB} , given by equations (77) and (78), respectively. For the ad hoc approximation we have instead the following system of self-consistent equations:

$$\begin{aligned} g_{AB}^{-1} &= D_{AB}^{-1} + i\Sigma_{AB}^{(1)}[g] + K \\ \tilde{g}_{AB}^{-1} &= D_{AB}^{-1} + i\Sigma_{AB}^{(1)}[g] + i\Sigma_{AB}^{(2)}[g] \quad (80) \\ \tilde{g}_{+-}(r, t; r, t) &= g_{+-}(r, t; r, t) \end{aligned}$$

where \tilde{g} is the $O(U^2)$ propagator in this approximation scheme and K is a source added in the calculation of g to enforce the condition expressed in the third line. This condition corresponds to requiring that the level occupation of the central region calculated from g and from \tilde{g} be equal. Note that if $K = 0$ then the $O(U)$ propagator, g , becomes the usual Hartree propagator. The equation of motion for \tilde{g} can be cast in a more familiar form [1, 17] using the properties of CTP propagators described in section 5. The result is $(1 = (r_1, t_1))$

$$\begin{aligned} \tilde{g}_{+-}(1, 2) &= \int d3 d4 \tilde{g}_r(1, 3) \{ \Sigma_{\phi, +-}(3, 4) \\ &\quad + \Sigma_{+-}^{(2)}[g](3, 4) \} \tilde{g}_a(4, 2) \\ \tilde{g}_{-+}(1, 2) &= \int d3 d4 \tilde{g}_r(1, 3) \{ \Sigma_{\phi, -+}(3, 4) \\ &\quad + \Sigma_{-+}^{(2)}[g](3, 4) \} \tilde{g}_a(4, 2) \quad (81) \\ \tilde{g}_r(1, 2) &= g_r(1, 2) + \int d3 d4 g_r(1, 3) \\ &\quad \times \Sigma_r^{(2)}[g](3, 4) \tilde{g}_r(4, 2), \end{aligned}$$

where the retarded $O(U^2)$ self-energy is

$$\Sigma_r^{(2)}(1, 2) = \theta(1, 2)[\Sigma_{+-}^{(2)}(1, 2) - \Sigma_{-+}^{(2)}(1, 2)] \quad (82)$$

and Σ_ϕ is given in equation (17). Using that the reservoirs are in equilibrium and non-interacting, and that the coupling matrix does not mix CTP branches, i.e. $T_{AB} = \text{diag}(T, T)$, the components of Σ_ϕ in energy–momentum space can be written as

$$\begin{aligned} \Sigma_{\phi,+}(p) &= |T|^2 B_{+-}(p) \\ &= \sum_j 2\pi i |T|^2 n(p) \delta(p_0 - p_j^2/2) \end{aligned} \quad (83)$$

$$\begin{aligned} \Sigma_{\phi,-}(p) &= |T|^2 B_{-+}(p) \\ &= - \sum_j 2\pi i |T|^2 [1 - n(p)] \delta(p_0 - p_j^2/2) \end{aligned}$$

where $n(p)$ is the Fermi–Dirac function, the momentum index j denotes single-particle energy levels and we have assumed that $T(p) = T$, independent of p . We note that the term describing the evolution of initial correlations is absent from equation (81), since we are assuming that the system is in a non-equilibrium stationary (or periodic) state maintained by the external classical field.

The equation of motion for the full propagator G has the same structure as the one for \tilde{g} , with the following replacements:

$$\begin{aligned} \tilde{g}_{+-}, \tilde{g}_{-+}, \tilde{g}_r &\rightarrow G_{+-}, G_{-+}, G_r \\ \Sigma_{+-}^{(2)}[g], \Sigma_{-+}^{(2)}[g], \Sigma_r^{(2)}[g] &\rightarrow \Sigma_{+-}[G], \Sigma_{-+}[G], \Sigma_r[G] \\ g_r &\rightarrow D_r. \end{aligned} \quad (84)$$

We will now consider the expectation value of the electronic current in the ad hoc approximation discussed so far. As emphasized in section 2, the WT hierarchy given in equation (1) is a direct consequence of the equations of motion satisfied by the *exact* propagators. This can be shown quite simply by noting that the $(n + 1)$ -point vertex function $\Lambda_{(n)}^\mu$, defined in equation (2), can be rewritten in terms of the operator $D^\mu(z, z')$, defined in equation (5):

$$\begin{aligned} \Lambda_{(n)}^\mu(1 \cdots n, 1' \cdots n'; z) &= -e i^{(n+1)} \lim_{z' \rightarrow z} D^\mu(z, z') \\ &\times G_{(n+1)}(1 \cdots n, z, 1' \cdots n', z'). \end{aligned} \quad (85)$$

The divergence of $\Lambda_{(n)}^\mu$ will therefore be given by the divergence of the operator $D^\mu(z, z')$, which follows immediately from its definition. The result is

$$\begin{aligned} \partial_\mu \Lambda_{(n)}^\mu(1 \cdots n, 1' \cdots n'; z) &= i^n e \lim_{z' \rightarrow z} \{ [i(\partial_{t_z} + \partial_{t_{z'}}) \\ &+ \frac{1}{2}(\nabla_z^2 - \nabla_{z'}^2) - A_i(z) + A_i(z')] G_{(n+1)} \\ &\times (1 \cdots z; 1' \cdots z') \} = i^n e \lim_{z' \rightarrow z} \zeta(z, z') \\ &\times G_{(n+1)}(1 \cdots z; 1' \cdots z'). \end{aligned} \quad (86)$$

This equation shows that the divergence of the expectation value of the 4-current $j^\mu(z)$, that corresponds to $n = 0$, is directly given by the action of the differential operator $\zeta(z, z')$ acting on $G_{(1)}(z, z') = G(z, z')$. Using Heisenberg's

equation of motion for the field operators ψ, ψ^\dagger it is easy to show [12, 15] that the exact propagator satisfy two differential equations:

$$\begin{aligned} [i\partial_{t_z} + \nabla_z^2 - A_i(z)]G(z, z') &= \delta(z, z') \\ &- i \int d1 U(z, 1) G_2(z1, z'1^+) \\ [-i\partial_{t_{z'}} + \nabla_{z'}^2 - A_i(z')]G(z, z') &= \delta(z, z') \\ &- i \int d1 U(1, z') G_2(z1^-, z'1) \end{aligned} \quad (87)$$

that, when subtracted, result in

$$\lim_{z' \rightarrow z} \zeta(z, z') G(1 \cdots z; 1' \cdots z') = 0, \quad (88)$$

whereby $\partial_\mu \langle j^\mu(z) \rangle = 0$ in the exact theory.

In an approximate theory, the quantity $-iUG_2$ appearing in equations (87) is replaced by the product ΣG , and so the conservation of current at the expectation value is not immediately guaranteed. It is well known [2, 14, 16, 23] that Φ -derivable approximations are such that $\partial_\mu \langle j^\mu(z) \rangle = 0$. As we have shown in previous sections, the approximations to the 2PI EA based on truncations of the loop expansion guarantee not only this condition but the entire WT hierarchy (order by order in the expansion of G with respect to the external driving field).

The approximation defined by equation (80) cannot be derived from a loop-truncated effective action, and hence equation (88) is not expected to hold. To end this section, we will briefly show how large is the divergence of the current expectation value in the ad hoc approximation. From equations (87) we have that, for an approximation based on a truncation of the loop expansion of the 2PI EA, the following identity holds:

$$\begin{aligned} \lim_{z' \rightarrow z} \zeta(z, z') G(z, z') &= \int d1 \{ G(z, 1) \Sigma^{(2)}[G](1, z) \\ &- \Sigma^{(2)}[G](z, 1) G(1, z) \} = 0 \end{aligned} \quad (89)$$

where we note that the Hartree part of the self-energy, $\Sigma^{(1)}[G]$, can be included in the left-hand side of equations (87) as an extra single-particle term, and, being local, its difference vanishes when $z' \rightarrow z$. Therefore, in equation (89) we only need to consider $\Sigma^{(2)}$. Putting $G = \tilde{g} + \tilde{G}$ and $\Sigma^{(2)}[G] = \Sigma^{(2)}[g] + \Xi$ in equation (89), and neglecting terms proportional to \tilde{G} and Ξ , we immediately obtain

$$\begin{aligned} \partial_\mu \langle \tilde{j}^\mu(z) \rangle &= e \int d1 \{ \tilde{g}(z, 1) \Sigma^{(2)}[g](1, z) \\ &- \Sigma^{(2)}[g](z, 1) \tilde{g}(1, z) \} \end{aligned} \quad (90)$$

where \tilde{j} denotes the current calculated in the ad hoc approximation. Since $\tilde{g}, \Sigma^{(2)}[g] \sim O(U^2)$, we conclude that the violation of current conservation in the mean is $O(U^4)$ or higher.

To conclude, we note that the combination of equations (86) and (89) constitutes a useful way of checking that a given approximation is conserving in the mean, and may provide some insight in the search of conserving approximations not based on loop truncations. As we have shown, it also provides a way of calculating an upper bound to the violation of mean current conservation.

7. Conclusions

In this work, we have determined the basic requirements that an approximation to a non-equilibrium many-body problem in an open and driven fermionic system must satisfy in order to achieve current conservation beyond the expectation value level. One of the most important results of this work is the close relation found between nonlinear response theory and the Ward–Takahashi hierarchy, necessary for current conservation. This connection, although already known [7–11, 14, 15], was clearly displayed by using the closed-time-path two-particle irreducible coarse-grained effective action to describe the central electrons coupled to ideal reservoirs.

We have shown that the gauge invariance of the 2PI effective action with respect to transformations of the external classical field driving the system automatically implies the WT hierarchy among the propagator and vertex functions calculated from the effective action. More importantly for practical calculations, for every approximation to the 2PI effective action that results from truncating its loop expansion, the closed-time path propagator (obtained from the Schwinger–Dyson equation) and the vertex functions (obtained from the Bethe–Salpeter equations) are such that the WT hierarchy holds.

Using a simple example, we have also discussed, in the context of the 2PI effective action formalism, the relation between ad hoc approximations (not obtained from a truncation of the loop expansion) and current conservation. Using a general expression for the divergence of the mean current, we have shown that in the ad hoc approximation considered current conservation at the expectation value level is violated at $O(U^4)$ or even at higher order.

In summary, we hope to have shown that closed-time-path 2PI effective action techniques are a powerful and systematic method to study the nonlinear response in strongly correlated open systems in weak external fields, in a current conserving way. We also hope to have shown the necessity, within the EA approach, of using loop-truncated approximations to the 2PI EA when going beyond the linear response regime. Our results may be of use in the theoretical study of quantum transport through interacting electronic pumping devices, which are nowadays receiving much attention.

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