

Ward identity for nonequilibrium Fermi systems

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A nonequilibrium Ward identity (NE WI) connecting the scalar transport vertex correction with one-particle self-energy is derived using the global U(1) symmetry of the fermion nonequilibrium Green's functions (NGF). The nonperturbative derivation does not depend on the details of the many-body system. A renormalized multiplicative composition rule for the NGF, reflecting time coherence, is obtained and related to the NE WI. Applications involve (i) testing the consistency of approximations shown in the example of a self-consistent Born approximation for disorder scattering, and (ii) in the general quantum transport theory, the formalism permits one to assess routes to generalized master equations, in particular those based on the generalized Kadanoff-Baym ansatz.

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The Ward identity (WI), discovered by Ward¹ for QED, and its many generalizations have played a crucial role in quantum field theory and in the theory of condensed matter.¹⁻¹³ In all quantum field theories, WIs are essential for the renormalization program: they lower the number of independent renormalization constants, serve in proofs of renormalizability, and provide control over the divergent terms in perturbation schemes. Takahashi showed² that WIs are at the root of any field theory, since they are related to symmetries and conservation laws, corresponding to the gauge invariance. WIs, especially for finite energy and momentum transfers, are often called Ward-Takahashi identities.

Ward identities have also been extremely useful in condensed matter physics, first as a tool in the field-theoretic approach to developing phenomenological description of condensed matter systems based on an effective single-particle picture. In particular, they have played an important role in the Fermi liquid theory^{4,11} since they have ensured consistency of the single-particle description with many-particle correlations. WIs have been employed in connection with conserving approximations for real-time and Matsubara Green's functions^{7,6,9} for a broad variety of condensed matter systems such as metals,^{4,11} superconductors,¹³ and disordered systems^{5,13} or systems with electron-phonon interactions.³

The virtue of WIs, employed in all of the above applications, is to express, under special conditions, a higher-order quantity, like an interaction vertex, in terms of a lower-order quantity, in this case of the single-particle self-energy.

This property has made WIs a constitutive part of the consistent quantum transport theory ever since the pilot work of Langer.¹⁴ In the description of linear transport, the emphasis naturally shifts from the single-particle spectral properties to the two-particle Green's functions, yielding the linear response functions. This calls for a consistent perturbation scheme for both, and a check of this consistency is provided by equilibrium Ward identities for the so-called transport vertex corrections.⁸ These quantities are equivalent with the true linear response functions.^{5,11,13} Ward identities in this case

serve to express the response to special disturbances in terms of the single-particle characteristics.

While the use of WIs for equilibrium spectral properties and for the linear transport has been extensive, a generalization suitable for nonequilibrium systems has not been proposed so far. It is our aim to make a step in this direction and to show its usefulness.

In this paper we consider consequences of the global U(1) symmetry for the properties of the electronic nonequilibrium Green's function¹⁵⁻¹⁹ (NGF) admitting an arbitrarily large deviation from equilibrium. In a near-equilibrium case, this symmetry is known^{2,6,9,10} to lead to a Ward identity connected with particle number conservation and expressing the transport vertex for linear response to a shift in the energy zero (or, equivalently, of the chemical potential) in terms of the equilibrium self-energy. We derive an extension of this WI to all nonequilibrium processes of the broad switch-on class specified by the Keldysh initial condition: they start at a switch-on instant from equilibrium, which has been formed at an infinitely remote initial time.¹⁵⁻¹⁹

We further derive from the nonequilibrium Ward identity the renormalized semigroup composition rule for nonequilibrium Green's functions (NE RSGR) accounting for memory and coherence past and future in the system. It is shown that this necessary condition for the WI can also be deduced from the Dyson equation alone, without invoking the gauge invariance explicitly.

Finally, the use of the NE WI is examined in two important cases. (i) The self-consistent Born approximation (SCBA) for disorder scattering^{5,12,20} is used as an example how a standard application of the WI for testing consistency of physical approximations can be extended to nonequilibrium processes. (ii) The NE WI promises to be instrumental in the modern approach to quantum transport equations beyond the Boltzmann limit.¹⁷⁻¹⁹ In particular, we establish its close relationship with the well-known generalized Kadanoff-Baym ansatz (GKBA). Exact companions of the GKBA, the reconstruction equations for the NGF, are identified as a limiting case of the NE RSGR. We then use the

full NE RSGR to assess the GKBA from a still unexplored angle.

The *global* gauge symmetry is universal and does not depend on the specific many-body Hamiltonian $\mathcal{H}(t)$ (admitting any geometry, dimensionality and external fields, interactions with other quantized fields and/or direct interactions between the Fermions, any spin structure, and a continuous and discrete configuration space). The only natural requirement is that the Hamiltonian conserve the total Fermion number \mathcal{N} :

$$[\mathcal{H}(t), \mathcal{N}]_- = 0. \quad (1)$$

The formal means to make full use of this generality are simple. The fermions are described by their nonequilibrium Green's function possessing an exact or approximate self-energy. Equations for these quantities are kept in an invariant representationless form.

We work with the real-time matrix NGF and self-energy,¹⁸ rather than with the equivalent causal quantities on the Schwinger-Keldysh loop:

$$\mathbf{G} = \begin{vmatrix} G^R & G^< \\ 0 & G^A \end{vmatrix}, \quad \mathbf{\Sigma} = \begin{vmatrix} \Sigma^R & \Sigma^< \\ 0 & \Sigma^A \end{vmatrix}. \quad (2)$$

They satisfy the Dyson equation

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0 \mathbf{\Sigma} \mathbf{G}, \quad (3)$$

The self-energy matrix is, in the self-consistent theory, expressed as a functional, exact or approximate, of the Green's function. All quantities are double-time operator functions.²¹ The Dyson equation has a simple structure free of the correlated initial condition terms,^{17,18} because we restrict our study to the switch-on processes governed by the Keldysh initial condition by definition.

For an arbitrary external time-local disturbance $U(t)$, the field dependent GF and self-energy satisfy

$$\mathbf{G}_U = \mathbf{G}_{0U} + \mathbf{G}_{0U} \mathbf{\Sigma}_U \mathbf{G}_U,$$

$$\mathbf{G}_{0U}^{-1} = \mathbf{G}_0^{-1} - \mathbf{U}, \quad \mathbf{U}(t, t') = \delta(t - t') \begin{vmatrix} U(t) & 0 \\ 0 & U(t) \end{vmatrix}. \quad (4)$$

The vertex corrections appear, in an integral form, as $\delta_U \mathbf{\Sigma}$ in the linear response of the one-electron GF to a small variation $\delta \mathbf{U}$ of the external field. By Eq. (4),

$$\delta_U \mathbf{G} = \mathbf{G} \delta_U [-\mathbf{G}^{-1}] \mathbf{G} = \mathbf{G} [\delta \mathbf{U} + \delta_U \mathbf{\Sigma}] \mathbf{G}. \quad (5)$$

The gauge invariance of the first kind [in other words, the global U(1) symmetry] is invoked as follows: a time variable shift $\mathcal{U}(t)$ is added to the one-particle energy in the free GF. This is obtained by a particular external disturbance,

$$\mathbf{G}_{0U}^{-1} = \mathbf{G}_0^{-1} - \mathcal{U}(t) \delta(t - t') \mathbf{1}, \quad \mathbf{1} \equiv \begin{vmatrix} I & 0 \\ 0 & I \end{vmatrix}, \quad (6)$$

with the spatially homogeneous potential energy $\mathcal{U}(t)$ being an arbitrary real function of time, but not of canonical variables, and I the operator unity.

The field dependence of the Dyson equation is then expressed by explicit relations

$$\mathbf{X}_U(t, t') = \mathbf{X}(t, t') \exp\left(-i \int_{t'}^t d\tau \mathcal{U}(\tau)\right), \quad (7)$$

where $\mathbf{X} = \mathbf{G}, \mathbf{G}_0, \mathbf{\Sigma}$. For \mathbf{G} and \mathbf{G}_0 , Eq. (7) follows from definition and fermion number conservation (1). The self-energy $\mathbf{\Sigma}$ must transform according to Eq. (7) to keep the Dyson equation (gauge) invariant. This nontrivial requirement leads to the Ward identity.

From the gauge transformation (7), the vertex correction $\delta_U \mathbf{\Sigma}$ follows as

$$\delta_U \mathbf{\Sigma}(t, t') = \mathbf{\Sigma}(t, t') \left(-i \int_{t'}^t d\tau \delta \mathcal{U}(\tau)\right). \quad (8)$$

We define an operator vertex correction having three *time* terminals. By Eq. (8), it has the explicit form

$$\Lambda(t, t'; t_\times) \equiv \frac{\delta}{\delta \mathcal{U}(t_\times)} \mathbf{\Sigma}(t, t') = -i \mathbf{\Sigma}(t, t') \eta(t, t'; t_\times),$$

$$\eta(t, t'; t_\times) = \vartheta(t - t_\times) \vartheta(t_\times - t') - \vartheta(t' - t_\times) \vartheta(t_\times - t). \quad (9)$$

This is our central result, and we will call it for obvious reasons the nonequilibrium Ward identity. It was obtained, as expected, in a nonperturbative fashion by executing the functional derivative of the Dyson equation with respect to \mathcal{U} and letting $\mathcal{U} \rightarrow 0$.

We first compare Eq. (9) with the Ward identities in equilibrium. Λ then depends only on two time differences—say, $\tau = t - t_\times$ and $\tau' = t' - t_\times$ —and its Fourier transform has the well known form^{5,11,13}

$$\begin{aligned} \tilde{\Lambda}(\omega, \omega') &= \int \int d\tau d\tau' \Lambda(\tau, \tau'; 0) e^{i(\omega\tau - \omega'\tau')} \\ &= - \frac{\mathbf{\Sigma}(\omega) - \mathbf{\Sigma}(\omega')}{\omega - \omega'}. \end{aligned} \quad (10)$$

The interpretation of the ω, ω' arguments depends on the matrix element. In the $\Lambda^{R,A}$ elements, $\Sigma^{R,A}(\omega) = \Sigma(\omega \pm i0)$ correspond to the one-particle renormalization; in the transport component $\Lambda^<$, the fluctuation-dissipation theorem yields $\Sigma^<(\omega) = [\Sigma(\omega + i0) - \Sigma(\omega - i0)] f_{\text{FD}}(\omega)$, so that the vertex correction connects both rims of the cut. The original Ward identity $\tilde{\Lambda}(\omega, \omega) = -\partial \mathbf{\Sigma}(\omega) / \partial \omega$ concerns the limit $\omega' \rightarrow \omega$ of Eq. (10). Our WI corresponding to a finite energy transfer could well be termed the Ward-Takahashi identity.

The more common form of the Ward identity in the coordinate representation involves a local external field $\mathbf{U}(1, 2) = \mathbf{U}(1) \delta(1 - 2)$, $\mathbf{1} \equiv \{\mathbf{r}_1, t_1\}$ and the three-point vertex correction $\mathbf{\Gamma}$ introduced as⁶

$$\mathbf{\Gamma}(1, 1'; 2) \equiv \frac{\delta}{\delta \mathbf{U}(2)} \mathbf{\Sigma}(1, 1'; \mathbf{U}). \quad (11)$$

For $\mathbf{U}(1) = \mathcal{U}(t_1)$, the gauge field of Eq. (6) is recovered and the Ward identity of Eq. (9) assumes the form of a sum rule for the vertex correction $\mathbf{\Gamma}$,

$$\begin{aligned}\Lambda(1,1';t_\times) &= \frac{\delta}{\delta\mathcal{M}(t_\times)}\Sigma(1,1') \\ &= \int d\bar{\mathbf{r}} \Gamma(1,1';\bar{\mathbf{r}}t_\times) \\ &= -i\Sigma(1,1')\eta(t,t';t_\times).\end{aligned}\quad (12)$$

Integration over the splitting time t_\times yields

$$\int dt_\times \Lambda(1,1';t_\times) = \int d\bar{3} \Gamma(1,1';\bar{3}) = -i(t-t')\Sigma(1,1').\quad (13)$$

This equation extends the WI for inhomogeneous systems⁶ [Eq. (7.22)] to nonequilibrium.

To explore the meaning and usefulness of the nonequilibrium WI, we will consider (9) for two widely known and rather transparent approximations of the NGF, SCBA, and GKBA, extended beyond equilibrium.

First, we consider the SCBA for disorder scattering on a weak static random potential D .^{5,12,20} This single-particle problem is turned to a field-theoretic one by configuration averaging $\langle \cdots \rangle_c$ over the ensemble of D fields. The SCBA self-energy for Σ ,

$$\Sigma = \langle \mathbf{D}\mathbf{G}\mathbf{D} \rangle_c, \quad \langle \mathbf{D} \rangle_c = \mathbf{0}, \quad \mathbf{D} = \begin{vmatrix} D & 0 \\ 0 & D \end{vmatrix}, \quad (14)$$

is an ultimately a simple functional of \mathbf{G} . From this, we get the Bethe-Salpeter equation for the vertex correction (11) if we differentiate (14) at $U(2)$, $2 \equiv \{\mathbf{r}_\times, t_\times\}$, use Eq. (5), and define $\Gamma^{(0)}(1,1';2) = \delta(1-2)\delta(1'-2)\mathbf{1}$:

$$\begin{aligned}\Gamma(1,1';2) &= \int \int d3 d4 \langle \mathbf{D}\mathbf{G}(1,3)\{\Gamma^{(0)}(3,4;2) \\ &\quad + \Gamma(3,4;2)\}\mathbf{G}(4,1')\mathbf{D} \rangle_c.\end{aligned}\quad (15)$$

Integrating over \mathbf{r}_\times , we get an integral equation for the contracted vertex $\Lambda(1,1';t_\times)$. We verify, in analogy to the equilibrium consistency check,⁵ that this equation is satisfied by the WI expression (12) for Λ . This procedure leads to the following condition:

$$\begin{aligned}\mathbf{G}(t,t')\eta(t,t';t_\times) &= i\mathbf{G}(t,t_\times)\mathbf{G}(t_\times,t')\eta(t,t';t_\times) \\ &\quad + \int \int d\bar{t} d\bar{t}' \mathbf{G}(t,\bar{t})\Sigma(\bar{t},\bar{t}')\eta(\bar{t},\bar{t}';t_\times)\mathbf{G}(\bar{t}',t').\end{aligned}\quad (16)$$

We shall give two different proofs of (16) shortly, but first it should be noted that (i) this relation has a general character, disassociated from *any* specific approximation, and (ii) it provides a sufficient condition for the WI to hold in a given physical situation, when combined with a self-consistent approximation for Σ —as shown here on the archetypal example of SCBA.

Equation (16) is, next to Eq. (9), the second basic result of this paper. It is a purely single-particle equation for \mathbf{G} and Σ . It is easily derived from Eq. (9) [introduce (8) \Leftrightarrow (9) and the analog of (8) for \mathbf{G} into the identity (5)]. Hence, it serves as

a necessary condition for the WI. On the other hand, Eq. (16) combined with a self-consistent approximation implies the WI as a relation between the simpler single-particle Σ and the two-particle transport vertex Λ . It is then very important that Eq. (16), unlike the Ward identity proper, can also be derived without invoking the gauge symmetry. Only the related Dyson equation is needed, with any reasonable approximation for the self-energy. To outline this second derivation, we first write Eq. (16) by components.

A nonzero result is obtained only for two arrangements of times. First, for $t > t_\times > t'$, two equations are obtained from Eq. (16), one for the retarded propagator, the other for the particle correlation function:

$$\begin{aligned}G^R(t,t') &= iG^R(t,t_\times)G^R(t_\times,t') \\ &\quad + \int_{t_\times}^t d\bar{t} \int_{t'}^{t_\times} d\bar{t}' G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{t}')G^R(\bar{t}',t'),\end{aligned}\quad (17)$$

$$\begin{aligned}G^<(t,t') &= iG^R(t,t_\times)G^<(t_\times,t') \\ &\quad + \int_{t_\times}^t d\bar{t} \int_{-\infty}^{t_\times} d\bar{t}' G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{t}')G^<(\bar{t}',t') \\ &\quad + \int_{t_\times}^t d\bar{t} \int_{-\infty}^{t_\times} d\bar{t}' G^R(t,\bar{t})\Sigma^<(\bar{t},\bar{t}')G^A(\bar{t}',t').\end{aligned}\quad (18)$$

Note the structure of these equations which follows the Langreth-Wilkins rules.^{17,18}

For the reverse order of times, $t < t_\times < t'$, another two relations result from Eq. (16). One is the analog of Eq. (17) for the advanced propagator G^A . The other one, for $G^<$, is symmetric to Eq. (18); we will refer to them as Eqs. (17') and (18') without writing them down explicitly.

The direct way from the Dyson equation (3) to Eq. (17) starts from the “semigroup composition rule” (SGR) for the free GF, $G_0^R(t,t') = iG_0^R(t,t_\times)G_0^R(t_\times,t')$ for $t > t_\times > t'$. Introduced into the retarded component of the Dyson equation (3), it leads to

$$\begin{aligned}\vartheta(t-t_\times)G^R(t,t') - \int_{t_\times}^t d\bar{t} \int_{t_\times}^{\bar{t}} d\bar{t}' G_0^R(t,\bar{t}) \\ \times \Sigma^R(\bar{t},\bar{t}')\vartheta(\bar{t}-t_\times)G^R(\bar{t}',t') \\ = iG_0^R(t,t_\times)G^R(t_\times,t') \\ + \int_{t_\times}^t d\bar{t} \int_{t'}^{t_\times} d\bar{t}' G_0^R(t,\bar{t})\Sigma^R(\bar{t},\bar{t}')G^R(\bar{t}',t').\end{aligned}\quad (19)$$

Employing $(1-G_0^R\Sigma^R)^{-1}G_0^R = G^R$, we arrive at Eq. (17). Equations (17) and (18) are then derived in a similar fashion and this completes the proof of Eq. (16).

In Eq. (16), the first term represents the NGF split at an intermediate “splitting time” t_\times into two factors: propagation in the past and in the future. This sharp factorization (“NE SGR”) is blurred in time by the vertex correction (“NE RSGR”), reflecting coherence past-future—i.e., memory of the system—except if retardations are negligible (free GF, mean-field approximation.) Thus, Eqs. (17) and (17') are a renormalized SGR for nonequilibrium propagators; the time

blurring is on the order of the quasiparticle formation time τ_Q ,²² if it exists. Equations (18) and (18') for $G^<$ are similar, only there are two vertex corrections now and two characteristic times τ_Q for Σ^R and a collision duration time τ_c related to the time spread of $\Sigma^<(t, t')$.²²

Now we are ready to continue with the link between the NE WI and some approximations, in particular with the generalized Kadanoff-Baym ansatz (Refs. 17–19).

$$G_{\text{GKBA}}^<(t, t') = -G^R(t, t')\rho(t') + \rho(t)G^A(t, t'). \quad (20)$$

In the NGF theory of quantum transport equations,^{17–19} it serves to build up the whole $G^<(t, t')$ from its time diagonal $\rho(t') = -iG^<(t', t')$, the one-particle density matrix, by means of the propagators. The GKBA is closely related to the NE SGR: Eqs. (18) and (18') go over to the renormalized counterparts of the GKBA, known as reconstruction equations, in the respective limits $t_x \rightarrow t'$, $t_x \rightarrow t$. While the latter are consistent with the Ward identity, the bare GKBA itself clearly is not.²³ Yet the GKBA has been widely used with success in the NE quantum transport practice. A partial explanation may be as follows. Let $t > t_x > t'$. Eq. (17), $G_{\text{GKBA}}^<$ satisfies the relation (schematically) $G_{\text{GKBA}}^< = iG^R G_{\text{GKBA}}^< + \iint G^R \Sigma^R G_{\text{GKBA}}^<$ for any t_x . This is different from Eq. (18) indeed, as the “dynamical” vertex part $\iint G^R \Sigma^< G^A$ is missing. This term, however, is zero for $t_x > t'' \equiv t' + 2\tau_Q + \tau_c$ and $G_{\text{GKBA}}^<$ then obeys the complete equation (18). In the long time asymptotics, $t - t' \gg \tau_Q, \tau_c$, which is decisive for the use of quantum transport equations,^{17–19} $G_{\text{GKBA}}^<$ is governed by this exact functional relation everywhere, except in the presumably narrow interval $t'' > t_x > t'$.

In conclusion, we have derived a Ward identity for Fermi systems far from equilibrium. The general derivation is based on only two assumptions: the global U(1) symmetry (the Fermion number conservation) and the Keldysh initial condition for the nonequilibrium process. Second, a renormalized multiplicative law for the NGF—NE RSGR—has been derived and linked with the Ward identity on the common physical basis of reducing two-particle vertex functions to single particle self-energies. These results are shown to have an important bearing on the NE WI based consistency checks, but mainly on the theory of quantum transport equations.

Two directions for further work can be singled out. On the formal end, one goal is the Ward identity for general non-equilibrium processes with a correlated initial condition. Another goal is an exact reduction of NE RSGR to a multiplicative form by absorbing the vertex corrections into the NE quasiparticle propagators: $G^R(i+\Lambda)G^< \rightarrow iG_{\text{QP}}^R G^<$, etc. As concerns applications, the universal nature of the NE WI hints at two areas: (i) the presently topical NE dynamical mean-field theory for strongly correlated systems,^{24,25} and (ii) nanostructures under strong and/or transient bias.²⁶

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²³ $G_{\text{GKBA}}^<$ is gauge invariant just like $G^<$ if the propagators $G^{R,A}$ are the following: The U(1) does not allow one to distinguish between them. The difference discussed in the text stems from the second condition for the Ward identity to hold: The ansatz $G_{\text{GKBA}}^<$ violating the reconstruction equations is not associated with a self-energy which would allow one to write down a meaningful Dyson equation for it.

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