

# Self-Consistent Approximations to Non-Equilibrium Many-Body Theory

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## Abstract

Within the non-equilibrium Green's function technique on the real-time contour, the  $\Phi$ -functional method of Baym is generalized to arbitrary non-equilibrium many-particle systems. The scheme may be closed at any desired order in the number of loops or vertices of the generating functional. It defines effective theories, which provide a closed set of coupled classical-field and Dyson equations, which are self-consistent, conserving and thermodynamically consistent. The approach permits to include unstable particles and therefore unifies the description of resonances with all other particles, which obtain a mass width by collisions, decays or creation processes in dense matter. The inclusion of classical fields enables the treatment of soft modes and phase instabilities. The method can be taken as a starting point for adequate and consistent quantum improvements of the in-medium rates in transport theories. Properties of resonances are discussed within the dilute density limit in terms of scattering phase shifts.

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## 1 Introduction

Non-equilibrium Green's function technique, developed by Schwinger, Kadanoff, Baym and Keldysh [1–4], is the appropriate concept to study the space–time evolution of many-particle quantum systems. This formalism finds now applications in various fields, such as quantum chromodynamics [5], nuclear physics [6–13], astrophysics [10,14,15], cosmology [16], spin systems [17], lasers [18], physics of plasma [19,20], physics of liquid <sup>3</sup>He [21], critical phenomena, quenched random systems and disordered systems [22], normal metals and super-conductors [14,23,24], semiconductors [25], tunneling and secondary emission [26], etc. The Green's function technique provides description in terms of one- and two-point

functions. Compared to the various equal-time operator formulations of transport theories, c.f. [27], and within the path-integral formulation [28], the Green's function approach with its non-localities in time offers a convenient description of spectral information such as the damping width of particles. Such mass-width effects become increasingly important especially in the realm of high-energy nuclear collisions.

For actual calculations certain approximation steps are necessary. In many cases perturbative approaches are insufficient, as for systems with strong couplings treated in nuclear physics. In such cases, one has to re-sum certain sub-series of diagrams in order to obtain a reasonable approximation scheme. In contrast to perturbation theory for such re-summations one frequently encounters the complication that the resulting equations of motion may no longer comply with the conservation laws, e.g., of charge, energy and momentum, in particular, if the mass width of the particles is no longer negligible. This problem has first been considered in two pioneering papers by Baym and Kadanoff [29,30] discussing the response to an external perturbation of quantum systems in thermodynamic equilibrium. Baym, in particular, showed [30] that any approximation, in order to be conserving, must be so-called  $\Phi$ -derivable. He exploited the properties of a resummation technique in terms of an auxiliary functional, the  $\Phi$ -functional, introduced by Luttinger and Ward [31] for the formulation of the thermodynamic potential (see also [32]). Mean fields were included in this formalism in ref. [33]. The  $\Phi$ -functional is determined in terms of full, i.e. re-summed, Green's functions and classical fields coupled by free vertices and serves as a generating functional for the driving terms of the equations of motion.

In the non-equilibrium formalism the problem of conserving approximations is even more severe than in the case of the systems response to an external perturbation close to thermal equilibrium, since the system may exercise a rather violent evolution. Apart from transport models, mostly based on the quasi-particle approximation like Landau's Fermi liquid theory, there were only few attempts to discuss the issue of conserving approximations in the context of the non-equilibrium field theory (see, e.g., [2,6,9]), which mainly considered Hatree-Fock and T-matrix approximations. However, the general problem of constructing conserving approximations in the non-equilibrium case and, in particular, beyond the quasi-particle limit has not explicitly been addressed yet.

Alongside, the question of thermodynamic consistency is vital. If, as a result of a non-equilibrium evolution, a system arrives at an equilibrium state, the non-equilibrium Green's functions should properly describe thermodynamic quantities and potentials, such that thermodynamic relations between them are preserved. This problem is also relevant to the thermodynamic Green's function technique, as already considered by Baym [30]. Baym demonstrated that any  $\Phi$ -derivable approximation is at the same time thermodynamically consistent.

In this paper we re-address the above problems and extend the concept to the genuine non-equilibrium case formulated on the closed real-time contour and to the inclusion of classical fields, i.e. non-vanishing expectation values of the field operators. The generalized scheme permits to construct self-consistent, approximate, coupled dynamical equations of

motion for the classical fields and Green's functions of the system on the closed real-time contour. The inclusion of classical fields allows to account for the phase-transition phenomena or to describe the coherent dynamics of soft modes, much in the spirit of hard-thermal-loop re-summations [34–36,13]. In this paper we confine the presentation to the derivation of closed self-consistent approximations to the Kadanoff-Baym and classical field equations. This constitutes the basis for various further steps towards classical-type transport schemes through the gradient approximation, which will be presented in a forthcoming paper [37].

The paper is organized as follows. In sect. 2 we briefly recapitulate the general equations of motion and expressions for the conserved quantities on the operator level. The equations of motion for the corresponding expectation values within the real-time closed contour formalism are formulated in sect. 3. It is advantageous to use the concepts of generating functionals, where the special functional  $\Phi$  plays a central role (sect. 4). The latter takes the same status in the space of Green's functions (two-point functions) and classical fields (one-point functions), as the original Lagrangian on the level of field operators. Subsequently, we formulate the diagrammatic representation for  $\Phi$  (sect. 5). We show that any approximation, where all classical field sources and self-energies are  $\Phi$ -derivable in the sense of a variational principle, has the following properties: (i) it is self-consistent, i.e. the equations close, (ii) it is conserving, i.e. it provides conserved current and energy-momentum tensor, which are identical to the corresponding Noether quantities (sect. 6), and (iii) it is at the same time thermodynamically consistent (sect. 7). In sect. 8 we discuss the low density limit at the example of an interacting  $\pi N\Delta$  system [40]. It illustrates how scattering phase shifts can provide the second-order virial corrections of the thermo-dynamic potential and the self-energies in a consistent way in the sense of the  $\Phi$ -derivable scheme. In the summary, we discuss the main results and briefly prospect possible applications of the derived formalism. Appendix A contains some helpful relations for contour functions, the list of diagrammatic rules is deferred to the Appendix B.

Except for the example in sect. 8 and the appendices, the presentation of the general concept in the main part of the paper is restricted to the case of relativistic scalar bosons. This allows us to formulate the basic ideas in simple and transparent terms. Generalizations to vector mesons and relativistic fermions or to non-relativistic kinematics, as well as to multi-component systems, as discussed for the example in sect. 8, and to interactions with derivative coupling are straightforward, though in some cases technically more involved.

## 2 Prerequisites

We consider a system of relativistic scalar bosons, specified by the free Klein-Gordon Lagrangians [41]

$$\widehat{\mathcal{L}}^0 = \begin{cases} \frac{1}{2} (\partial_\mu \widehat{\phi} \cdot \partial^\mu \widehat{\phi} - m^2 \widehat{\phi}^2) & \text{for neutral bosons,} \\ \partial_\mu \widehat{\phi}^\dagger \cdot \partial^\mu \widehat{\phi} - m^2 \widehat{\phi}^\dagger \widehat{\phi} & \text{for charged bosons,} \end{cases} \quad (2.1)$$

where  $\widehat{\phi}(x)$  and  $\widehat{\phi}^\dagger(x)$  are bosonic field operators. The convention of units is such that  $\hbar = c = 1$  and symbols for field operators carry a hat. The interaction Lagrangians  $\widehat{\mathcal{L}}^{\text{int}}\{\widehat{\phi}\}$  (for neutral bosons) and  $\widehat{\mathcal{L}}^{\text{int}}\{\widehat{\phi}, \widehat{\phi}^\dagger\}$  (for charged bosons) are assumed to be local, i.e. without derivative coupling. Under these conditions the Lagrangians are charge symmetric. Charges are understood as the electric charge, strangeness, iso-spin, etc.

The variational principle of stationary action leads to the Euler–Lagrange equations of motion for the field operators

$$-S_x \widehat{\phi}(x) = \widehat{J}(x) = \frac{\partial \widehat{\mathcal{L}}^{\text{int}}}{\partial \widehat{\phi}^\dagger}, \quad \text{where} \quad S_x = -\partial_\mu \partial^\mu - m^2, \quad (2.2)$$

and similarly for the corresponding adjoint equation. Thereby, the  $\widehat{J}(x)$  operator is a local source current of the field  $\widehat{\phi}$ , while  $S_x$  is the differential operator of the free evolution with the free propagator  $\Delta^0(y, x)$  as resolvent.

Invariances of the Lagrangian provide a set of conservation laws, the most prominent of which are those for the energy–momentum and certain currents. In addition to the standard canonical energy–momentum tensor [41], different representations of this tensor both in classical case and for the operator form in quantum field theory have been considered [42,43]. Using the Euler–Lagrange equations of motion and the definition of the source current (2.2), one can show that the following form also defines a conserving energy momentum tensor

$$\widehat{\Theta}^{\mu\nu}(x) = \frac{1}{4} \kappa \left[ \left( (\widehat{p}_x^\nu)^* + \widehat{p}_y^\nu \right) \left( (\widehat{p}_x^\mu)^* + \widehat{p}_y^\mu \right) \left( \widehat{\phi}^\dagger(x) \widehat{\phi}(y) + \widehat{\phi}(y) \widehat{\phi}^\dagger(x) \right) \right]_{x=y} + g^{\mu\nu} \left( \widehat{\mathcal{E}}^{\text{int}}(x) - \widehat{\mathcal{E}}^{\text{pot}}(x) \right), \quad (2.3)$$

where

$$\widehat{p}_x^\mu = i\partial_x^\mu, \quad \text{and} \quad \kappa = \begin{cases} 1/2 & \text{for neutral bosons,} \\ 1 & \text{for charged bosons.} \end{cases} \quad (2.4)$$

We use this expression, since it represents the operator form of the energy–momentum tensor later derived at the expectation value level from the invariance of the  $\Phi$ -functional (see sect. 6). For notational simplicity, expression (2.3) and similar expressions below, which appear symmetric in  $\widehat{\phi}$  and  $\widehat{\phi}^\dagger$ , are written in such a way that they directly apply to complex fields with  $\kappa = 1$ . For real fields  $\kappa = 1/2$  and the corresponding expressions are

obtained by equating  $\hat{\phi}^\dagger = \hat{\phi}$ . Above, we have introduced the operators of the interaction energy density  $\hat{\mathcal{E}}^{\text{int}}(x)$  of the system, which accounts for the total interaction part of the energy density, and the potential energy density  $\hat{\mathcal{E}}^{\text{pot}}(x)$ , both given as

$$\begin{aligned}\hat{\mathcal{E}}^{\text{int}}(x) &= -\hat{\mathcal{L}}^{\text{int}}(x), \\ \hat{\mathcal{E}}^{\text{pot}}(x) &= -\frac{1}{2}\kappa \left( \hat{J}^\dagger(x)\hat{\phi}(x) + \hat{\phi}^\dagger(x)\hat{J}(x) \right).\end{aligned}$$

For a multi-component system, the latter defines the sum of the potential energies per volume of any particle with the current  $\hat{J}(x)$  in the field  $\hat{\phi}(x)$  induced by the other particles in the system.

For specific interactions there are simple relations between  $\hat{\mathcal{E}}^{\text{int}}(x)$  and  $\hat{\mathcal{E}}^{\text{pot}}(x)$ . E.g., if all vertices of  $\hat{\mathcal{L}}^{\text{int}}$  have the same number  $\gamma$  of field operators attached, one simply deduces

$$\hat{\mathcal{E}}^{\text{int}}(x) = \frac{2}{\gamma}\hat{\mathcal{E}}^{\text{pot}}(x), \quad \text{e.g. for } \hat{\mathcal{L}}^{\text{int}} = \text{---}\times\text{---} \Rightarrow \gamma = 4. \quad (2.5)$$

As shown, for two-body interactions or the  $\phi^4$ -theory, where  $\gamma = 4$ , the interaction energy is half of the potential energy.

If the Lagrangian is invariant under some global transformation of charged fields (with the charge  $e$ ), e.g.,

$$\hat{\phi}(x) \Rightarrow e^{-ie\Lambda}\hat{\phi}(x); \quad \hat{\phi}^\dagger(x) \Rightarrow e^{ie\Lambda}\hat{\phi}^\dagger(x), \quad (2.6)$$

there exists a Noether current defined as [41]

$$\hat{j}^\mu(x) = e\frac{1}{2} \left[ \left( (\hat{p}_x^\mu)^* + \hat{p}_y^\mu \right) \left( \hat{\phi}^\dagger(x)\hat{\phi}(y) + \hat{\phi}(y)\hat{\phi}^\dagger(x) \right) \right]_{x=y}, \quad (2.7)$$

which is conserved, i.e.  $\partial_\mu \hat{j}^\mu = 0$ . This current naturally vanishes for the neutral particles ( $e = 0$ ).

One may also define the tensor  $M^{\mu\nu\rho}$ , which is associated with the Lorentz invariance of the Lagrangian and provides the angular momentum conservation. However, we do not treat this tensor in this paper, since it is of no common use in kinetics.

### 3 Real-Time Contours

In the non-equilibrium case, one assumes that the system has been prepared at some initial time  $t_0$  described in terms of a given density operator  $\hat{\rho}_0 = \sum_a P_a |a\rangle \langle a|$ , where

the  $|a\rangle$  form a complete set of eigenstates of  $\hat{\rho}_0$ . All observables can be expressed through  $n$ -point Wightman functions of Heisenberg operators  $\hat{A}(t_1), \dots, \hat{O}(t_n)$  at some later times

$$\begin{aligned} \langle \hat{O}(t_n) \dots \hat{B}(t_2) \hat{A}(t_1) \rangle &=: \text{Tr } \hat{O}(t_n) \dots \hat{B}(t_2) \hat{A}(t_1) \hat{\rho}_0(t_0) \\ &= \sum_a P_a \langle a | \hat{O}(t_n) \dots \hat{B}(t_2) \hat{A}(t_1) | a \rangle. \end{aligned} \quad (3.1)$$

Note that due to the fixed operator ordering for Wightman functions, they are analytic and permit analytic extensions to complex-time arguments.

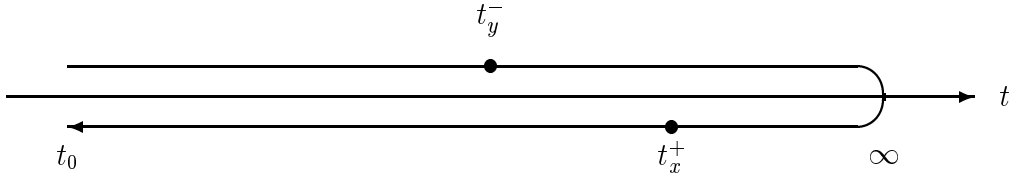


Figure 1: Closed real-time contour with two external points  $x, y$  on the contour.

The non-equilibrium theory can entirely be formulated on a *special* contour—the *closed real-time contour* (see figure 1) with the time argument running from  $t_0$  to  $\infty$  along the *time-ordered* branch and back to  $t_0$  along the *anti-time-ordered* branch. Contour-ordered multi-point functions are defined as expectation values of contour ordered products of operators

$$\langle \mathcal{T}_{\mathcal{C}} \hat{A}(x_1) \hat{B}(x_2) \dots \rangle = \left\langle \mathcal{T}_{\mathcal{C}} \hat{A}_{\text{I}}(x_1) \hat{B}_{\text{I}}(x_2) \dots \exp \left\{ i \int_{\mathcal{C}} \hat{\mathcal{L}}_{\text{I}}^{\text{int}} dx \right\} \right\rangle, \quad (3.2)$$

where  $\mathcal{T}_{\mathcal{C}}$  denotes the special time-ordering operator, which orders the operators according to a time parameter running along the time contour  $\mathcal{C}$ . The l.h.s. of eq. (3.2) is written in the Heisenberg representation, whereas the r.h.s. is given in the interaction (I) representation. Here and below, the subscript "I" indicates the *interaction* picture. Note that at this level the contour is not a contour in the complex plane, as the figure may suggest, but rather it runs along *real* time arguments. It is through the placement of external points on the contour that the contour ordering obtains its particular sense.

In certain calculations, e.g., in those that apply the Fourier and Wigner transformations, it is necessary to decompose the full contour into its two branches—the *time-ordered* and *anti-time-ordered* branches. One then has to distinguish between the physical space-time coordinates  $x, \dots$  and the corresponding contour coordinates  $x^{\mathcal{C}}$  which for a given  $x$  take two values  $x^- = (x_{\mu}^-)$  and  $x^+ = (x_{\mu}^+)$  ( $\mu \in \{0, 1, 2, 3\}$ ) on the time ordered and anti-time ordered branches, respectively (see figure 1). Closed real-time contour integrations can then be decomposed as

$$\int_{\mathcal{C}} dx^{\mathcal{C}} \dots = \int_{t_0}^{\infty} dx^- \dots + \int_{\infty}^{t_0} dx^+ \dots = \int_{t_0}^{\infty} dx^- \dots - \int_{t_0}^{\infty} dx^+ \dots, \quad (3.3)$$

where only the time limits are explicitly given. Thus, the anti-time-ordered branch acquires an extra minus sign if integrated over physical times. For any two-point function  $F$ , the contour values on the different branches define a  $e \times 2$ -matrix function

$$F^{ij}(x, y) := F(x^i, y^j), \quad i, j \in \{-, +\}, \quad (3.4)$$

depending on the physical coordinates  $(x, y)$ . The contour  $\delta$ -function is defined as

$$\delta_{\mathcal{C}}^{i,j}(x, y) = \delta_{\mathcal{C}}(x^i, y^j) = \sigma^{ij} \delta^4(x - y), \quad \sigma^{ij} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3.5)$$

where the matrix  $\sigma^{ik}$  accounts for the integration sense on the two branches. For any multi-point function, the external point  $x_{max}$ , which has the largest physical time, can be placed on either branch of the contour without changing the value, since the contour-time evolution from  $x_{max}^-$  to  $x_{max}^+$  provides unity. Therefore, one-point functions have the same value on both sides of the contour. Due to the change of operator ordering, genuine multi-point functions are discontinuous in general, when two contour coordinates become identical. The corresponding properties of two-point functions and their equilibrium relations are summarized in Appendix A.

Boson fields may take non-vanishing expectation values of the field operators  $\phi(x) = \langle \hat{\phi} \rangle$ , called *classical* fields. The corresponding equations of motion are provided by the ensemble average of the operator equations of motion (2.2)

$$S_x \phi(x) = -J(x), \quad \text{or} \quad \phi(x) = \phi^0(x) - \int_{\mathcal{C}} dy \Delta^0(x, y) J(y). \quad (3.6)$$

Here  $J(x) = \langle \hat{J}(x) \rangle$ , while  $\phi^0(x) = \langle \hat{\phi}_I(x) \rangle$  is the freely evolving classical field which starts from  $\phi^0(t_0, \mathbf{x})$  at time  $t_0$ . Thereby,  $\Delta^0(x, y)$  is the free contour Green's function

$$i\Delta^0(x, y) = \langle \mathcal{T}_{\mathcal{C}} \hat{\phi}_I(x) \hat{\phi}_I^\dagger(y) \rangle - \phi^0(x)(\phi^0(y))^* \quad (3.7)$$

which resolves the equation

$$S_x \Delta^0(x, y) = \delta_{\mathcal{C}}(x, y) \quad (3.8)$$

on the contour, where  $\delta_{\mathcal{C}}(x, y)$  is the contour  $\delta$ -function (3.5). The reader can easily verify the equivalence of the *contour* form (3.6) with the standard *retarded* classical field

equation due to eq. (A.2) and the fact that  $J(x)$  and  $\phi(x)$  are one-point functions, which have identical values on both sides of the contour.

Subtracting the classical fields via  $\hat{\phi} = \phi + \hat{\varphi}$ , the full propagator in terms of quantum-fluctuating parts  $\hat{\varphi}$  of the fields is defined as

$$i\Delta(x, y) = \langle \mathcal{T}_c \hat{\varphi}(x) \hat{\varphi}^\dagger(y) \rangle = \langle \mathcal{T}_c \hat{\phi}(x) \hat{\phi}^\dagger(y) \rangle - \phi(x) \phi^*(y) = \langle \mathcal{T}_c \hat{\phi}(x) \hat{\phi}^\dagger(y) \rangle_c. \quad (3.9)$$

Here and below, the sub-label "c" indicates that uncorrelated parts are subtracted. In terms of diagrams it implies, that the corresponding expectation values are given by sums of entirely *connected* diagrams.

Averaging the operator equations of motion (2.2) multiplied by  $\hat{\varphi}^\dagger(y)$  and subtracting classical field parts one obtains the equation of motion for the propagator

$$S_x \Delta(x, y) = \delta_c(x, y) + i \langle \mathcal{T}_c \hat{J}(x) \hat{\varphi}^\dagger(y) \rangle_c, \quad (3.10)$$

which is still exact and accounts for the full set of initial correlations contained in  $\hat{\rho}_0$ . In order to proceed further, one may suggest that the typical interaction time  $\tau_{\text{int}}$  for the change of the correlation functions is significantly shorter than the typical relaxation time  $\tau_{\text{rel}}$ , which determines the system evolution. Then, describing the system at times  $t - t_0 \gg \tau_{\text{int}}$ , one can neglect the initial correlations which are supposed to die out beyond  $\tau_{\text{int}}$  in line with the Bogolyubov's principle of weakening of initial correlations<sup>1</sup> [44]. As a result, one can apply the standard Wick decomposition dropping higher order correlations for the driving terms on the r.h.s. of both equations of motion (3.6) and (3.10). Then both driving terms can be expressed as functionals solely of classical fields and one-particle propagators rather than of higher order correlations. The so obtained description level is then irreversible in general. Thus,

$$\begin{aligned} i \langle \mathcal{T}_c \hat{J}(x) \hat{\varphi}^\dagger(y) \rangle_c &= i \left\langle \mathcal{T}_c \left[ \exp \left\{ i \int_c dz \hat{\mathcal{L}}_I^{\text{int}} \right\} \hat{J}_I(x) \hat{\varphi}_I^\dagger(y) \right] \right\rangle_c \\ &= i \int_c dz \left\langle \mathcal{T}_c \frac{\partial}{\partial \hat{\varphi}_I(z)} \left[ \exp \left\{ i \int_c dz' \hat{\mathcal{L}}_I^{\text{int}} \right\} \hat{J}_I(x) \right] \right\rangle_{c1} \langle \mathcal{T}_c \hat{\varphi}(z) \hat{\varphi}^\dagger(y) \rangle \\ &= \int_c dz \Pi(x, z) \Delta(z, y) \end{aligned} \quad (3.11)$$

one recovers Dyson's equation in the differential form

<sup>1</sup> Actually, considering a dilute gas limit, Bogolyubov suggested the weakening of all the correlations, whereas we use a weaker assumption on the weakening of only short-range ( $\sim \tau_{\text{int}}$ ) correlations.



$$S_x \Delta(x, y) = \delta_c(x, y) + \int_c dz \Pi(x, z) \Delta(z, y), \quad (3.12)$$

$$(S_y)^* \Delta(x, y) = \delta_c(x, y) + \int_c dz \Delta(x, z) \Pi(z, y). \quad (3.13)$$

The resolvent property of the free contour propagator  $\Delta^0$  permits to write down these equations also in the integral form, which then include the appropriate initial and boundary conditions through the inhomogeneous  $\Delta^0$  term in the usual manner. Thereby causality is incorporated through the contour formulation. Above  $\Pi$  denotes the *proper* self-energy of the particle. Since we have separated the *full* propagator in (3.11),  $-i\Pi$  has to be *one-particle irreducible* (label  $c1$ ), i.e. the corresponding diagram cannot be split into two pieces which separate  $x$  from  $z$  by cutting a single propagator line. Obviously,  $\Pi$  in (3.11) may have singular ( $\delta$ -functional) one-point parts and genuine two-point parts

$$-i\Pi(x, z) = \left\langle \mathcal{T}_c \frac{\partial^2 i\hat{\mathcal{L}}^{\text{int}}(x)}{\partial \hat{\phi} \partial \hat{\phi}^\dagger} \right\rangle_c \delta_c(x, y) - \left\langle \mathcal{T}_c \hat{J}(x) \hat{J}^\dagger(y) \right\rangle_{1c}. \quad (3.14)$$

here given in the Heisenberg picture.

In diagrams free and full classical fields are represented by "pins" with cross and "o-cross" as heads, c.f. (3.15), while free and full propagators are given by thin and thick long lines, respectively. Complex fields carry a sense, the arrow always pointing towards the  $\hat{\phi}$  in the contour ordered expressions. In diagrammatic representation, the classical field equations (3.6) and Dyson equations (3.12) are then given by

$$\textcircled{\times} = \times + \textcircled{iJ}, \quad (3.15)$$

$$\text{---} \leftarrow = \text{---} \leftarrow + \text{---} \leftarrow \textcircled{-i\Pi} \leftarrow \text{---} \quad (3.16)$$

with the one- and two-point functions  $iJ(x)$  and  $-i\Pi(x, y)$ , as driving terms.

The averaged values of conserved quantities can be expressed in terms of the one- and two-point functions introduced so far. Averaging the operator value of the energy-momentum tensor of eq. (2.3), we arrive at

$$\begin{aligned} \Theta^{\mu\nu}(x) =: \langle \hat{\Theta}^{\mu\nu} \rangle = & \frac{1}{2} \kappa \left[ \left( (\hat{p}_x^\nu)^* + \hat{p}_y^\nu \right) \left( (\hat{p}_x^\mu)^* + \hat{p}_y^\mu \right) \left( \phi^*(x) \phi(y) + i\Delta^{\text{sym}}(y, x) \right) \right]_{x=y} \\ & + g^{\mu\nu} \left( \mathcal{E}^{\text{int}}(x) - \mathcal{E}^{\text{pot}}(x) \right), \end{aligned} \quad (3.17)$$

where  $\mathcal{E}^{\text{int}}(x) = -\langle \hat{\mathcal{L}}^{\text{int}}(x) \rangle$ , and the potential energy density becomes

$$\mathcal{E}^{\text{pot}}(x) = \langle \widehat{\mathcal{E}}^{\text{pot}}(x) \rangle = \frac{1}{2}\kappa \left\{ - [J^*(x)\phi(x) + J(x)\phi^*(x)] \right. \\ \left. + i \int_{\mathcal{C}} dz [\Pi(x, z)\Delta(z, x) + \Delta(x, z)\Pi(z, x)] \right\}. \quad (3.18)$$

due to eqs. (2.5) and (3.11). Note that we do not prescribe any contour indices to  $x$  in the integral term of  $\mathcal{E}^{\text{pot}}$ , since actually this term is independent of the contour placement of  $x$  due to discontinuity property (A.4). The Noether current (2.7) takes the form

$$j^\mu(x) =: \langle \widehat{j}^\mu \rangle = e \left[ \left( (\widehat{p}_x^\mu)^* + \widehat{p}_y^\mu \right) \left( \phi^*(x)\phi(y) + i\Delta^{\text{sym}}(y, x) \right) \right]_{x=y}. \quad (3.19)$$

In order to keep the expressions  $\Theta^{\mu\nu}$  and  $j^\mu$  charge symmetric we have introduced the symmetric quantities

$$F^{\text{sym}}(x, y) = \frac{1}{2} \left( F(x^-, y^+) + F(x^+, y^-) \right), \quad (3.20)$$

where  $F(x, y)$  is any two-point function on the real-time contour. This is not automatically provided by the variational methods leading to the Noether energy–momentum tensor and current, as they only provide the vanishing of the corresponding divergence. The integrated form of the conserved quantities has to be adjusted such that charge symmetry is maintained, thus describing contributions of both, particles and anti-particles, on equal footing. This way one properly accounts for the modification of the vacuum polarization in the medium, since the vacuum-polarization energy coincides with the zero point energies of the field oscillations. The corresponding divergence has still to be appropriately renormalized.

#### 4 Functionals $W$ , $\Gamma$ and $\Phi$

The standard generating functional  $W$  for connected  $n$ -point functions with external one-point sources will be extended in three ways. First, it will be used on the real-time contour. Secondly, in our non-equilibrium case we also include external bilinear sources  $K(x, y)$  [31]. In addition we introduce a space-time dependent interaction scale  $\lambda(x)$  into the variational concept, which scales interaction vertices, i.e.

$$\widehat{\mathcal{L}}_\lambda^{\text{int}} = \lambda(x) \widehat{\mathcal{L}}^{\text{int}} \left\{ \widehat{\phi}^\dagger(x), \widehat{\phi}(x) \right\}. \quad (4.1)$$

The latter provides the clue to the proof of the diagrammatic representation for the auxiliary functional  $\Phi$  in terms of closed diagrams. The generating functional then reads

$$\begin{aligned}
W\{\eta, K, \lambda\} = & -i \ln \left\langle \exp \left[ -i \int_{\mathcal{C}} dx \widehat{H}_I^0 \right] \mathcal{T}_{\mathcal{C}} \exp \left\{ i \int_{\mathcal{C}} dx \left( \lambda(x) \widehat{\mathcal{L}}_I^{\text{int}} \right. \right. \right. \\
& \left. \left. \left. + \kappa \left[ \eta(x) \widehat{\phi}_I^\dagger(x) + \eta^*(x) \widehat{\phi}_I(x) + i \int_{\mathcal{C}} dy \widehat{\phi}_I(x) K(x, y) \widehat{\phi}_I^\dagger(y) \right] \right) \right\} \right\rangle, \quad (4.2)
\end{aligned}$$

with the free Hamiltonian of the system in the interaction representation  $\widehat{H}_I^0$ . As already introduced, the factor  $\kappa$  takes the value of 1/2 for real fields thereby equating  $\widehat{\phi}$  with  $\widehat{\phi}^\dagger$ , else it is 1. Since the functional dependence concerns only the external sources, the operator part can be cast into different pictures, such as the Heisenberg or interaction ones. The latter establishes the perturbation expansion. Furthermore,  $\langle \dots \rangle$  denotes the trace over all states, which includes the ensemble average over the density operator  $\widehat{\rho}_0(t_0)$  at initial time  $t_0$ . Accordingly, multi-point functions are defined as ensemble averages of field operators with  $\rho_0$  (cf. eq. (3.2)).

While  $n$ -th order functional variations of (4.2) with respect to  $\eta$  generate the *connected*  $n$ -point functions, the first functional variation with respect to  $K(x, y)$  gives the total two-point propagator including disconnected pieces

$$\begin{aligned}
\delta W\{\eta, K, \lambda\} = & \kappa \left[ \int_{\mathcal{C}} dx [\phi^*(x) \delta \eta(x) + \phi(x) \delta \eta^*(x)] \right. \\
& \left. + \int_{\mathcal{C}} dx \int_{\mathcal{C}} dy [\phi(x) \phi^*(y) + \Delta(x, y)] \delta K(y, x) \right] - \int_{\mathcal{C}} dx \mathcal{E}_\lambda^{\text{int}}(x) \delta \lambda(x) / \lambda(x). \quad (4.3)
\end{aligned}$$

Here,  $\phi$  and  $\Delta$  denote the classical fields and propagators, respectively, which now implicitly depend on  $\lambda$ . The term, resulting from the variation of the interaction scale function  $\lambda(x)$ , defines a one-point function  $\mathcal{E}_\lambda^{\text{int}}(x) = -\langle \widehat{\mathcal{L}}_\lambda^{\text{int}}(x) \rangle$ , which agrees with the corresponding expectation value of (2.5) but for the scaled Lagrangian.

The step towards a functional that depends on the classical fields  $\phi$  and propagators  $\Delta$  rather than on the external sources  $\eta$  and  $K$  is provided by the double Legendre transformation of  $W$  to  $\Gamma\{\phi, \phi^*, \Delta, \lambda\}$  given as [31]

$$\begin{aligned}
\Gamma\{\phi, \phi^*, \Delta, \lambda\} = & W\{\eta, K, \lambda\} - \kappa \left[ \int_{\mathcal{C}} dx [\eta^*(x) \phi(x) + \eta(x) \phi^*(x)] \right. \\
& \left. + \int_{\mathcal{C}} dx dy [\phi(y) \phi^*(x) + \Delta(y, x)] K(y, x) \right]. \quad (4.4)
\end{aligned}$$

Here, the sources  $\eta$  and  $K$  have to be expressed through  $\phi$  and  $\Delta$ . Apart from the  $\delta \lambda$  dependences, the functional variation

$$\begin{aligned} \delta\Gamma\{\phi, \phi^*, \Delta, \lambda\} = & -\kappa \left[ \int_c dx [\eta^*(x)\delta\phi(x) + \eta(x)\delta\phi^*(x)] \right. \\ & \left. + \int_c dx \int_c dy [\delta\phi(y)\phi^*(x) + \phi(y)\delta\phi^*(x) + \delta\Delta(y, x)] K(y, x) \right] - \int_c dx \mathcal{E}_\lambda^{\text{int}}(x) \frac{\delta\lambda(x)}{\lambda(x)} \end{aligned} \quad (4.5)$$

vanishes at vanishing external sources  $\eta$  and  $K$ . The latter together with the condition  $\lambda = 1$  determines the physical solution. Note also that for the physical solution, i.e. at  $\eta = K = 0$ , the values of the two functionals  $\Gamma$  and  $W$  are identical. Indeed, the variations

$$\delta\Gamma/\delta\phi = 0, \quad \delta\Gamma/\delta\phi^* = 0, \quad \delta\Gamma/\delta\Delta = 0 \quad (4.6)$$

provide us with equations of motion for classical fields (3.6) and the complex conjugated one, as well as Dyson's equation (3.12).

Similarly to equilibrium case treated by Luttinger, Ward [31], and later by Cornwall, Jackiw and Tomboulis [33], which included mean bosonic fields, we represent our  $\Gamma$  functional related to the real-time quantities in the form

$$\begin{aligned} \Gamma\{\phi, \phi^*, \Delta, \lambda\} = & \Gamma^0 + \int_c dx \mathcal{L}^0\{\phi, \partial_\mu\phi\} \\ & + i\kappa \left[ \ln\left(1 - \odot\Delta^0 \odot\Pi\right) + \odot\Delta \odot\Pi \right] + \Phi\{\phi, \phi^*, \Delta, \lambda\}, \end{aligned} \quad (4.7)$$

this way defining the auxiliary functional  $\Phi\{\phi, \phi^*, \Delta, \lambda\}$ <sup>2</sup>. Constructing  $\Phi$  solely in terms of the fields and one-particle propagators complies with the assumption of ignoring higher order correlations. The  $\Gamma^0$  and  $\mathcal{L}^0$  parts, where  $\mathcal{L}^0$  is the *classical* free Lagrangian function, represent the non-interacting parts of  $\Gamma$ . The  $\Gamma^0$  term solely depends on the unperturbed propagator  $\Delta^0$  and hence is treated as a constant with respect to functional variations of  $\Gamma$ . The  $\ln(\dots)$  is understood in the functional sense, i.e. by a series of  $n$ -folded contour convolutions, denoted by the  $\odot$ -symbol, formally resulting from the Taylor expansion of the  $\ln(1+x)$  at  $x=0$ . This  $\ln$ -term accounts for the change of  $\Gamma$  due to the self-energies of the particles. The  $\Gamma^0$ ,  $\mathcal{L}^0$  and  $\ln$  terms in eq. (4.7) account for the one-body components in  $\Gamma$ . The remaining  $\Delta \odot \Pi$  and  $\Phi$  terms correct for the true interaction energy part of  $\Gamma$ . As shown in the next section, the form (4.7) presents a re-summation of the corresponding perturbative expansion of the value of  $\Gamma$  (c.f. eq. (4.4)) in terms of full classical fields and full propagators.

The specific form (4.7) has important functional properties, which provide us with a number of useful relations. Functional variation of  $\Gamma\{\phi, \phi^*, \Delta, \lambda\}$  in the form of eq. (4.7)

<sup>2</sup> Note that we have placed all  $\widehat{\mathcal{L}}^{\text{int}}$ -dependent parts into  $\Phi$ , i.e. our  $\Phi$  includes zero and one-loop terms and therefore differs from the auxiliary quantity  $\Gamma_2$  defined by Cornwall et. al. [33] which is void of zero- and one-loop terms. There these terms are rather included in defining a full classical Lagrangian that depends on interacting classical field and tad-pole terms.

leads to

$$\begin{aligned} \delta \Gamma \{ \phi, \phi^*, \Delta, \lambda \} = & \kappa \left\{ \int_{\mathcal{C}} dx [\delta \phi(x) (S_x)^* \phi^*(x) + \delta \phi^*(x) S_x \phi(x)] \right. \\ & \left. - i \left( \odot \frac{1}{1 - \odot \Delta^0 \odot \Pi} \odot \Delta^0 - \odot \Delta \right) \odot \delta \Pi + i \int dx dy \Pi(x, y) \delta \Delta(y, x) \right\} + \delta \Phi \{ \phi, \phi^*, \Delta, \lambda \}. \end{aligned} \quad (4.8)$$

Here  $\delta \Pi$  is understood as a variation induced by  $\delta \Delta$ ,  $\delta \phi$ ,  $\delta \phi^*$ , and  $\delta \lambda$ , respectively. For physical solutions the variations (4.6) of  $\Gamma$  vanish. They require the round bracket term in (4.8) to vanish, which provides the Dyson equation on the contour, and from (4.5) further imply the following variational rules for the auxiliary  $\Phi$  functional

$$\begin{aligned} \delta \Phi \{ \phi, \phi^*, \Delta, \lambda \} = & \kappa \left\{ \int_{\mathcal{C}} dx [J^*(x) \delta \phi(x) + J(x) \delta \phi^*(x)] \right. \\ & \left. - i \int_{\mathcal{C}} dx dy \Pi(x, y) \delta \Delta(y, x) \right\} - \int_{\mathcal{C}} dx \mathcal{E}^{\text{int}}(x) \delta \lambda(x), \end{aligned} \quad (4.9)$$

or

$$iJ(x) = \frac{\delta i \Phi}{\delta \phi^*(x)}, \quad (4.10)$$

$$-i\Pi(x, y) = \frac{\delta i \Phi}{\delta i \Delta(y, x)} \times \begin{cases} 2 & \text{for neutral bosons,} \\ 1 & \text{for charged bosons,} \end{cases} \quad (4.11)$$

$$-\mathcal{E}^{\text{int}}(x) = \frac{\delta i \Phi}{\delta i \lambda(x)}. \quad (4.12)$$

The virtue of the functional form (4.7) is that these requirements can be met simultaneously and that there exists a unique form of  $\Phi$ , for which the three derived quantities—the one-body source current  $J(x)$ , the two-body self-energy  $-i\Pi(x, y)$  and the interaction energy density  $\mathcal{E}^{\text{int}}(x)$ —take their physical values at the physical solutions of the equations of motion (3.12) and (3.6). This will become clear in more detail in the next section, where we discuss the diagrams defining the various functionals. From (4.10) and (4.11)  $\Phi$  can be seen as a *generating* functional for the source terms  $J$  of classical fields and self-energies  $\Pi$  for the set of Dyson equations, respectively. Therefore, approximation schemes can be defined through particular approximations to  $\Phi$ . Thereby, the invariance properties of  $\Phi$  play a central role to define conservation laws for the approximate dynamics.

It is important to emphasize that we do all functional variations independently of any place on the contour. Thus, different contour times are considered as independent, even though

they may refer to the same physical time<sup>3</sup>. In principle, all variational considerations given in this section apply to any kind of time contour, even to non closed and complex ones as well as to any operator  $\hat{\rho}_0$  defining the averaging  $\langle \dots \rangle = \text{Tr} \{ \dots \hat{\rho}_0 \}$  including the unit operator, as used in Matsubara's imaginary-time formalism. For a particular choice of  $\hat{\rho}_0$  and of a contour the *physical* values of  $W$  and  $\Gamma$  are identical for the corresponding physical solutions along this contour. In the imaginary-time method the value  $\Gamma = W$  takes the meaning of the thermodynamic potential (c.f. sect. 7). In the non-equilibrium closed real-time formalism, for which  $\text{Tr} \hat{\rho}_0 = 1$ , the *physical* values of  $W$  and  $\Gamma$  trivially vanish, i.e.  $W = \Gamma = \Phi = 0$  for physical solutions of  $\Delta, \phi, \phi^*$  on the contour.

An important comment must be given at this stage. One should clearly distinguish between the *functional* form of a functional, which acquires its meaning through variational methods, and the *physical* value that functional takes once the physical solutions of the equations of motion are inserted. For instance, two functionals  $W$  and  $\Gamma$  are completely different in their functional meaning, while they take the same physical value for the physical solution. Therefore, for all functionals the functional dependences are explicitly given in braces. Our strategy below will be first to perform general variations of  $\Gamma$  and  $\Phi$ , allowing non-physical values of  $\Delta, \phi, \phi^*$  and  $\lambda$ , and only then to put them to their physical values. This way, a number of important relations between Green's functions, self-energies and mean fields will be obtained.

## 5 Diagrams for $\Gamma, \Phi$ and $\mathcal{E}_\lambda^{\text{int}}(x)$

$$-\int_c dx \mathcal{E}^{\text{int}}(x) = \left[ \lambda \frac{d}{d\lambda} \Gamma \{ \phi \{ \lambda \}, \phi^* \{ \lambda \}, \Delta \{ \lambda \}, \lambda \} \right]_{\lambda=1} = \left[ \lambda \frac{\partial}{\partial \lambda} \Phi \{ \phi, \phi^*, \Delta, \lambda \} \right]_{\lambda=1}, \quad (5.1)$$

where now  $\lambda$  is treated as a global scale parameter (note that only a partial derivative is applied to  $\Phi$ , i.e. the  $\phi, \phi^*$  and  $\Delta$  values are kept constants.). In the perturbation theory, the diagrammatic rules to calculate the one-point function  $\mathcal{E}^{\text{int}}(x)$  are straightforward

$$-i\mathcal{E}^{\text{int}}(x) = i \left\langle \mathcal{T}_c \hat{\mathcal{L}}_I^{\text{int}}(x) \exp \left[ i \int_c dx' \hat{\mathcal{L}}_I^{\text{int}}(x') \right] \right\rangle = \sum_{n_\lambda} \bullet \text{Diagram}_c. \quad (5.2)$$

Here the diagram symbolically denotes all connected (label  $c$ ) closed perturbation-theory diagrams generated by expanding the exponential function in (5.2). The full dot denotes

<sup>3</sup> The fact that for the physical solutions the components of  $\Delta$  on the different branches of the contour are not independent (cf. (A.2)), has no importance for the variational procedure. The reason is that rules (A.2) only apply to the physical  $\Delta$  and  $\phi$ , which are provided by the stationary "points" of the variational principle, i.e. solving the equations of motion (3.6), (3.12) and (3.13).

the external point  $x$  which is not integrated out. Integrating (5.1) with respect to  $\lambda$ , we define the quantity  $i\bar{\Gamma}$  given by the following perturbative diagrammatic representation

$$i\bar{\Gamma}\{\phi^0, \phi^{0*}, \Delta^0, \lambda\} = i\Gamma^0\{\Delta^0\} + i \int_c dx \mathcal{L}^0\{\phi^0, \partial_\mu \phi^0\} + \sum_{n_\lambda} \frac{1}{n_\lambda} \text{c}_c, \quad (5.3)$$

where the integration constants have been chosen such that for physical solutions  $\bar{\Gamma} = \Gamma$ . One can see that each diagram contributing to  $\bar{\Gamma}$  has to be weighted with its inverse number of vertices  $1/n_\lambda$ , due to the formal  $\lambda$ -integration of (5.2). It is important to realize that due to these global factors such a set of diagrams *is not resumable* in the standard diagrammatic sense<sup>4</sup>. Also  $\bar{\Gamma}$  in the form of eq. (5.3) is a functional of  $\phi^0, \phi^{0*}, \Delta^0, \lambda$  rather than of  $\phi, \phi^*, \Delta, \lambda$ , as required for  $\Gamma$  and  $\Phi$ . However, we can arrive at this functional dependence of  $\Gamma$  as follows. The expression (5.2) for  $-i\mathcal{E}^{\text{int}}(x)$  can be re-summed and entirely expressed in terms of full classical fields and full propagators. The re-summed diagrams are then void of any self-energy insertions and therefore have to be *two-particle irreducible*

$$-i\mathcal{E}^{\text{int}}(x) = \sum_{n_\lambda} \text{c}_{c2}. \quad (5.4)$$

Diagrams of class  $c2$  cannot be decomposed into two pieces by cutting two propagator lines. The formal integration of the last equality in (5.1) with respect to  $\lambda$  keeping  $\phi$  and  $\Delta$  constant provides the diagrammatic expression for  $\Phi$  in terms of full Green's functions and classical fields. Therefore,  $i\Gamma\{\phi, \phi^*, \Delta, \lambda\}$  can be expressed in terms of the following diagrams (c.f. eq. (4.7))

$$i\Gamma\{\phi, \phi^*, \Delta, \lambda\} = i\Gamma^0\{\Delta^0\} + i \int_c dx \mathcal{L}^0\{\phi, \partial_\mu \phi\} + \kappa \left\{ \underbrace{\sum_{n_\Pi} \frac{1}{n_\Pi} \left( \text{ring diagrams} \right)}_{-\ln(1 - \odot \Delta^0 \odot \Pi)} - \underbrace{\left( \text{closed diagrams} \right)}_{-\odot \Delta \odot \Pi} \right\} + \underbrace{\sum_{n_\lambda} \frac{1}{n_\lambda} \text{c}_{c2}}_{+i\Phi}. \quad (5.5)$$

Here  $n_\Pi$  counts the number of  $\Pi$  insertions in the ring diagrams providing the  $\ln$ -terms, while for the closed diagrams of  $\Phi$  the value  $n_\lambda$  counts the number of vertices building

<sup>4</sup> Diagrammatic re-summation implies that sub-diagrams with the same external structure (i.e. same number of external points and types of propagators to be attached at each external point) can be summed up to give a total re-summed expression that can then be embedded into more complicated diagrams, e.g. self-energy insertions can be re-summed to full Green's functions.

up the functional  $\Phi$ . Contrary to the perturbative diagrams of  $i\bar{\Gamma}$ , c.f. eq. (5.3), here the diagrams contributing to  $\Phi$  are given in terms of full propagators  $\Delta$  and full time-dependent classical fields  $\phi$ . As a consequence, these diagrams have to be *two-particle irreducible* (label  $c2$ ). The latter property is required because of the re-summations of  $\mathcal{E}^{\text{int}}(x)$ . This also matches the diagrammatic rules for the re-summed self-energy  $\Pi(x, y)$ , which results from functional variation of  $\Phi$  with respect to any propagator  $\Delta(y, x)$ . In graphical terms, this variation is realized by opening a propagator line in all diagrams of  $\Phi$ . The resulting set of thus opened diagrams must then be that of proper skeleton diagrams of  $\Pi$  in terms of *full propagators*, i.e. void of any self-energy insertion.

The diagrammatic rules for  $\Phi$ ,  $\mathcal{E}^{\text{int}}(x)$ ,  $J$  and  $\Pi$  are determined by the following steps:

- (a) For all bosonic fields in  $i\hat{\mathcal{L}}^{\text{int}}$ , replace  $\hat{\phi}$  by  $\phi + \hat{\varphi}$  in order to account for the classical fields;
- (b) consider all possible pair contractions of the field operator  $\hat{\varphi}(x)$  with  $\hat{\varphi}^\dagger(y)$  in the formal expressions (5.6)–(5.9) given below and replace them by  $i\Delta(x, y)$ ;
- (c) keep only those terms that correspond to two-particle irreducible diagrams for  $\Phi$ , i.e. which cannot be split into two pieces by cutting two different propagator lines.

Further details are given in Appendix B. The diagrams of  $i\Phi$ ,  $-i\mathcal{E}^{\text{int}}(x)$ ,  $iJ(x)$  and  $-i\Pi(x, y)$  are then generated by applying the above general rules to the following formal expressions

$$i\Phi = \left\langle \mathcal{T}_c \exp \left( i \int_c dx' \hat{\mathcal{L}}^{\text{int}}(x') \right) \right\rangle_{2c\{\Delta\}} \quad (5.6)$$

$$= \sum_n \frac{1}{n!} \int_c dx_1 \dots dx_n \left\langle \mathcal{T}_c i\hat{\mathcal{L}}^{\text{int}}(x_1) \dots i\hat{\mathcal{L}}^{\text{int}}(x_n) \right\rangle_{2c\{\Delta\}},$$

$$-i\mathcal{E}^{\text{int}}(x) = \left\langle \mathcal{T}_c i\hat{\mathcal{L}}^{\text{int}}(x) \exp \left( i \int_c dx' \hat{\mathcal{L}}^{\text{int}}(x') \right) \right\rangle_{2c\{\Delta\}}, \quad (5.7)$$

$$iJ(x) = \left\langle \mathcal{T}_c \frac{\delta}{\delta\phi^*(x)} \exp \left( i \int_c dx' \hat{\mathcal{L}}^{\text{int}}(x') \right) \right\rangle_{2c\{\Delta\}}, \quad (5.8)$$

$$-i\Pi(x, y) = \left\langle \mathcal{T}_c \frac{\delta^2}{\delta\hat{\varphi}^\dagger(x)\delta\hat{\varphi}(y)} \exp \left( i \int_c dx' \hat{\mathcal{L}}^{\text{int}}(x') \right) \right\rangle_{2c\{\Delta\}}, \quad (5.9)$$

where the sub-label  $2c\{\Delta\}$  refers to the above point (c).

As an example, we quote the diagrams in neutral scalar  $g\hat{\phi}^4/4!$  theory. The functional  $\Phi$  is given by the following expressions



$$\begin{aligned}
i\Phi &= \frac{-ig}{4!} \int_{\mathcal{C}} dx \left( \phi^4(x) + 6\phi^2(x) \langle \hat{\varphi}(x) \hat{\varphi}(x) \rangle_{\mathcal{C}} + 3 \langle \hat{\varphi}(x) \hat{\varphi}(x) \rangle_{\mathcal{C}}^2 \right) \\
&+ \frac{1}{2} \left( \frac{-ig}{4!} \right)^2 \int_{\mathcal{C}} dx \int_{\mathcal{C}} dy \left( 4 \cdot 4! \phi(x) \phi(y) \langle \hat{\varphi}(x) \hat{\varphi}(y) \rangle_{\mathcal{C}}^3 + 4! \langle \hat{\varphi}(x) \hat{\varphi}(y) \rangle_{\mathcal{C}}^4 \right) + \dots,
\end{aligned} \tag{5.10}$$

where only the terms up to two vertices are explicitly presented. In terms of diagrams (c.f. also Appendix B) we get

$$\begin{aligned}
i\Phi &= \begin{array}{c} \text{Diagram 1: Four external pins meeting at a central vertex} \\ \text{Diagram 2: A tadpole with two external pins} \\ \text{Diagram 3: A tadpole with one external pin} \end{array} + \frac{1}{2} \left\{ \begin{array}{c} \text{Diagram 4: A loop with two external pins} \\ \text{Diagram 5: A loop with one external pin} \end{array} \right\} + \frac{1}{3} \dots \\
&\quad \left[ \frac{1}{4!} \right] \quad \left[ \frac{1}{2 \cdot 2!} \right] \quad \left[ \frac{1}{2^2 \cdot 2!} \right] \quad \left[ \frac{1}{3!} \right] \quad \left[ \frac{1}{4!} \right]
\end{aligned} \tag{5.11}$$

The  $1/n_\lambda$  factors are explicitly given, while the combinatorial factors according to rule (vii) in Appendix B are given in square brackets below each diagram. Functional derivatives with respect to  $\phi$  (pins) and propagators (full lines), c.f. eq.(4.9), determine the source  $J(x)$  of the classical field and the self-energy  $\Pi(x, y)$ , respectively,

$$\begin{aligned}
iJ(x) &= \begin{array}{c} \text{Diagram 1: Three external pins meeting at a central vertex} \\ \text{Diagram 2: A tadpole with one external pin} \\ \text{Diagram 3: A loop with one external pin} \end{array} + \dots, \\
&\quad \left[ \frac{1}{3!} \right] \quad \left[ \frac{1}{2} \right] \quad \left[ \frac{1}{3!} \right] \\
-i\Pi(x, y) &= \begin{array}{c} \text{Diagram 1: Two external pins meeting at a central vertex} \\ \text{Diagram 2: A tadpole with one external pin} \\ \text{Diagram 3: A loop with two external pins} \\ \text{Diagram 4: A loop with one external pin} \end{array} + \dots \\
&\quad \left[ \frac{1}{2!} \right] \quad \left[ \frac{1}{2} \right] \quad \left[ \frac{1}{2!} \right] \quad \left[ \frac{1}{3!} \right]
\end{aligned} \tag{5.12}$$

Small full dots define vertices which are to be integrated over, while big full dots specify the external points  $x$  or  $y$ ; the first two diagrams of  $\Pi(x, y)$  give the singular  $\delta_{\mathcal{C}}(x, y)$  parts arising from classical fields and tad-poles.

## 6 $\Phi$ -Derivable Approximations and Invariances of $\Phi$

The expressions for  $W$ ,  $\Gamma$  and  $\Phi$  given so far are exact and represent a convenient formulation of the theory in terms of full propagators and self-energies. However, for any practical calculation one needs to truncate the scheme. We consider so-called  $\Phi$ -derivable

approximations, first introduced by Baym [30] within the imaginary time method. Such approximations are constructed by confining the infinite diagrammatic series for  $\Phi$  either to a set of a few diagrams or to some sub-series of diagrams. Note that the approximate  $\Phi^{(\text{appr.})}$  itself is constructed in terms of “full” Green’s functions and “full” classical fields, where “full” now implies that we have to self-consistently solve the classical-field and Dyson equations with the driving terms derived from this  $\Phi^{(\text{appr.})}$  through relations (4.10) and (4.11). It means that even restricting ourselves to a single diagram in  $\Phi^{(\text{appr.})}$ , in fact, we deal with a whole sub-series of diagrams in perturbation theory. Thereby, the term “full” takes the sense of the sum of this whole sub-series. Thus, a  $\Phi$ -derivable approximation offers a natural way of introducing closed, and therefore self-consistent approximation schemes based on summation of diagrammatic sub-series. In order to preserve the symmetry of the exact  $\Phi$  with respect to permutations among  $i\hat{\mathcal{L}}^{\text{int}}(x_1)\dots i\hat{\mathcal{L}}^{\text{int}}(x_n)$  (see eq. (5.6)), we postulate that  $\Phi$  complies with the original symmetries. As a consequence, approximate forms of  $\Phi^{(\text{appr.})}$  define *effective* theories, where  $\Phi^{(\text{appr.})}$  serves as a generating functional for the approximate source currents  $J^{(\text{appr.})}(x)$  and self-energies  $\Pi^{(\text{appr.})}(x, y)$  (see eqs. (4.10) and (4.11))

$$iJ^{(\text{appr.})}(x) = \frac{\delta i\Phi^{(\text{appr.})}}{\delta(\phi^{(\text{appr.})*}(x)} \tag{6.1}$$

$$-i\Pi^{(\text{appr.})}(x, y) = \frac{\delta i\Phi^{(\text{appr.})}}{\delta i\Delta^{(\text{appr.})}(y, x)} \times \begin{cases} 2 & \text{for neutral fields,} \\ 1 & \text{for charged fields,} \end{cases} \tag{6.2}$$

which then are the driving terms for the equations of motion for the classical fields and propagators. The approximate  $\Phi$  also provides the corresponding expression for  $\mathcal{E}^{\text{int}}$  (see eq. (4.12)). While  $\Phi$ -functionals with only one internal point lead to the standard Hartree approximation (tadpole insertions), which is entropy conserving, the approximation level with two and more internal points for  $\Phi$  generate genuine transport terms, which are entropy generating and for which an H-theorem can be derived in special cases [37]. Below, we omit the superscript “appr.”. Below, we omit the superscript “appr.”.

We now like to demonstrate that  $\Phi$ -derivable approximations possess a number of remarkable properties. For such approximations, the invariances of  $\Phi$  play as central a role as the invariances of the Lagrangian for the full theory. Thereby, the variational principle, where the interaction strength  $\lambda(x)$ , the classical fields  $\phi(x)$ , and propagators  $\Delta(x, y)$  can be varied independently, provides a set of useful identities and relations.

A general invariance of  $\Phi$  is provided by the substitution  $x \Rightarrow x + \xi(x)$  for all integration variables in the contour integrations defining  $\Phi$ . The Jakobi determinant required for each integration variable can be accommodated by a simultaneous change of the scale function  $\lambda(x)$  at each vertex. Thus, the simultaneous variation

$$\phi(x) \Rightarrow \phi(x + \xi(x)),$$

$$\begin{aligned}\Delta(x, y) &\Rightarrow \Delta(x + \xi(x), y + \xi(y)), \\ \lambda(x) = 1 &\Rightarrow \lambda(x) = \det \left( \delta_\mu^\nu + \frac{\partial \xi_\mu}{\partial x_\nu} \right), \quad \text{i.e. } \delta\lambda(x) = \frac{\partial \xi_\mu}{\partial x_\mu},\end{aligned}\tag{6.3}$$

leaves  $\Phi$  invariant. This way, one deduces

$$\begin{aligned}\delta\Phi &= \kappa \left\{ \int_{\mathcal{C}} dx \left[ J^*(x) \frac{\partial \phi(x)}{\partial x_\mu} + J(x) \frac{\partial \phi^*(x)}{\partial x_\mu} \right] \xi_\mu(x) \right. \\ &\quad \left. - i \int_{\mathcal{C}} dx dy \Pi(x, y) \left[ \frac{\partial \Delta(y, x)}{\partial x_\mu} \xi_\mu(x) + \frac{\partial \Delta(y, x)}{\partial y_\mu} \xi_\mu(y) \right] \right\} - \int_{\mathcal{C}} dx \mathcal{E}^{\text{int}}(x) \frac{\partial \xi_\mu}{\partial x_\mu} = 0.\end{aligned}\tag{6.4}$$

Interchanging  $x$  and  $y$  in the second  $\Pi$  term in squared brackets, using partial integration and that the transformation  $\xi(x)$  can be chosen arbitrarily, one obtains the following relation

$$\begin{aligned}\frac{\partial}{\partial x_\mu} \mathcal{E}^{\text{int}}(x) + \kappa \left\{ \left[ J^*(x) \frac{\partial \phi(x)}{\partial x_\mu} + J(x) \frac{\partial \phi^*(x)}{\partial x_\mu} \right] \right. \\ \left. - i \int_{\mathcal{C}} dy \left[ \Pi(x, y) \frac{\partial \Delta(y, x)}{\partial x_\mu} + \frac{\partial \Delta(x, y)}{\partial x_\mu} \Pi(y, x) \right] \right\} = 0.\end{aligned}\tag{6.5}$$

This is the key relation to prove energy–momentum conservation. It has features similar to a Ward identity, as it links derivatives of one-point functions with those of two-point functions. The two-point function contribution to this expression is of type of eq. (A.5), so that in eq. (6.5) the differentiations of the discontinuities indeed cancel out.

With the help of the equations of motion (3.6), (3.12) and (3.13), the divergence of the kinetic term of the energy–momentum tensor  $\Theta^{\mu\nu}$  (3.17) can be cast into

$$\begin{aligned}\frac{1}{2} \kappa \partial_\mu \left[ \left( (\hat{p}_x^\nu)^* + \hat{p}_y^\nu \right) \left( (\hat{p}_x^\mu)^* + \hat{p}_y^\mu \right) \left( \phi^*(x) \phi(y) + i \Delta^{\text{sym}}(y, x) \right) \right]_{x=y} \\ = \partial_\mu g^{\mu\nu} \mathcal{E}^{\text{pot}}(x) + \kappa \left\{ \left[ J(x) \partial_\nu \phi^*(x) + J^*(x) \partial_\nu \phi(x) \right] \right. \\ \left. - i \int_{\mathcal{C}} dz \left[ \Pi(x, z) \cdot \partial_\nu^x \Delta(z, x) + \partial_\nu^x \Delta(x, z) \cdot \Pi(z, x) \right] \right\} \\ = \partial_\nu \left\{ \mathcal{E}^{\text{pot}}(x) - \mathcal{E}^{\text{int}}(x) \right\}\end{aligned}\tag{6.6}$$

with the last line resulting from eq. (6.5). This is recognized as the energy–momentum conservation law  $\partial_\mu \Theta^{\mu\nu}(x) = 0$  with the energy–momentum tensor given by the Noether expression (3.17). Hence, the existence of a conserved energy–momentum tensor is proven for any  $\Phi$ -derivable approximation.

Along similar lines charge conservation can be proven, assuming that  $\Phi$  is invariant under the following simultaneous variation of classical fields and propagators

$$\phi(x) \Rightarrow e^{-ie\Lambda(x)}\phi(x), \quad \phi^*(x) \Rightarrow e^{ie\Lambda(x)}\phi^*(x), \quad \Delta(x, y) \Rightarrow e^{-ie\Lambda(x)}\Delta(x, y)e^{ie\Lambda(y)}. \quad (6.7)$$

Applying the rule (4.9) of the  $\Phi$  variation, to linear order in the phase  $\Lambda$ , one obtains

$$\delta\Phi = e \int_c dx \left\{ J^*(x)\phi(x) - J(x)\phi^*(x) + ie \int_c dy [\Pi(x, y)\Delta(y, x) - \Delta(x, y)\Pi(y, x)] \right\} [-i\Lambda(x)] = 0, \quad (6.8)$$

which implies the brace expression to vanish. Note that the integral term in the brace expression is independent of the contour placement of the  $x$  variable due to discontinuity relation (A.3) and, therefore, it is only a function of the physical value of  $x$ . By means of equations of motion (3.6), (3.12) and (3.13), the divergence of the Noether current of eq. (3.19) is seen to vanish

$$i\partial_\mu j^\mu = e \left\{ J^*(x)\phi(x) - J(x)\phi^*(x) + i \int_c dy [\Pi(x, y)\Delta(y, x) - \Delta(x, y)\Pi(y, x)] \right\} = 0, \quad (6.9)$$

according to eq. (6.8). Thus, we have arrived at the current conservation for any  $\Phi$ -derivable approximation, which is invariant under (6.7).

Similarly, one may derive the relation, resulting from the Lorentz invariance of the  $\Phi$  functional, which permits to demonstrate the conservation of the angular momentum. However, we do not consider it here, since the angular-momentum conservation is not of practical use in kinetics. Further invariances generally depend on the properties of the interaction vertices in the theory considered. An example is the invariance discussed in the context of eq. (2.5) which now transcribes to the corresponding expectation values.

## 7 Thermodynamic Consistency

In the thermal equilibrium the density matrix is explicitly known, c.f. [45],

$$\hat{\rho}^{\text{eq}} = \frac{\exp(-\beta\hat{H}\{\mu\})}{Z}, \quad (7.1)$$

where  $\beta = 1/T$  is the inverse temperature, and  $Z$  is the partition function which is directly related to the thermodynamical potential,

$$\Omega = -T \ln Z. \quad (7.2)$$

Since we deal now with thermodynamics, we have introduced the chemical potential  $\mu$  in the conventional way, i.e. by adding to the Hamiltonian the relevant term

$$\hat{H}\{\mu\} = \hat{H} - \mu \int d^3x \hat{j}^0(x), \quad (7.3)$$

where  $\hat{j}^0$  is the time-component of the charged current eq. (2.7), now with  $e = 1$ .

We can use the same trick as that in the Matsubara technique, i.e. use the fact that the equilibrium density matrix formally coincides with evolution operator in the imaginary time. In the definition of the  $W$  functional (4.2) we explicitly write  $\text{Tr} \hat{\rho}^{\text{eq}} \dots$  instead of  $\langle \dots \rangle$ . Thus, taking into account that  $\Gamma = W$  at vanishing external sources, we arrive at the following form of  $\Gamma$  functional in equilibrium

$$\Gamma^{\text{eq}}\{\phi, \phi^*, \Delta, \mu\} = -i \ln \left( \frac{1}{Z} \text{Tr} \exp \left[ -i \int_{\mathcal{C}_{\text{eq}}} dt \hat{H}_I^0\{\mu\} \right] \mathcal{T}_{\mathcal{C}} \exp \left[ i \int_{\mathcal{C}_{\text{eq}}} dx \hat{\mathcal{L}}_I^{\text{int}} \right] \right), \quad (7.4)$$

with the integration contour  $\mathcal{C}_{\text{eq}}$  now being the sum of the real-time Schwinger-Keldysh contour (see figure 1) and the imaginary-time Matsubara contour, i.e. it starts from an initial time  $t_0$  goes to infinity, then back to this initial time and after that, to  $t_0 - i\beta$ . Taking into account the fact that  $\Gamma = 0$  for the physical values of  $\phi$ ,  $\phi^*$ , and  $\Delta$ , we obtain for the value of the thermodynamic potential (7.2)

$$\Omega\{\phi, \phi^*, \Delta, \mu\} = -T \ln \left\{ \text{Tr} \left( \exp \left[ -i \int_{\mathcal{C}_{\text{eq}}} dt \hat{H}_I^0\{\mu\} \right] \mathcal{T}_{\mathcal{C}} \exp \left[ i \int_{\mathcal{C}_{\text{eq}}} dx \hat{\mathcal{L}}_I^{\text{int}} \right] \right) \right\}, \quad (7.5)$$

where the integral over the real-time section of the contour gives zero. Hence, in eq. (7.5) we can make the replacement

$$\int_{\mathcal{C}_{\text{eq}}} dt \dots = \int_0^{-i\beta} dt \dots \quad . \quad (7.6)$$

Thus, we have arrived at the proper thermodynamic representation of the thermodynamic potential originally proposed by Luttinger and Ward [31]. Indeed, since all quantities under the integral are analytically continued from the Schwinger-Keldysh contour to the Matsubara contour,  $\Omega$  is determined by the same expression as the  $\Gamma$  functional (4.7) but in terms of the Matsubara Green's functions with the thermodynamic  $\Phi_T$  functional represented by the same set of closed diagrams. Thus, in the momentum representation from eq. (7.5) we arrive at

$$\begin{aligned} \Omega \{ \phi, \phi^*, \Delta, \mu \} = & - \int d^3x \mathcal{L}^0 \{ \phi, \partial_\mu \phi \} + T\kappa \sum_{\omega_n} \int d^3x \frac{d^3p}{(2\pi)^3} \exp(i\omega_n \eta) \\ & \times \left( -\ln[-\Delta(\omega_n, \mathbf{p})] + \Pi(\omega_n, \mathbf{p})\Delta(\omega_n, \mathbf{p}) \right) + \Phi_T, \quad \eta \rightarrow 0, \end{aligned} \quad (7.7)$$

where  $\Phi_T = -iT\Phi$ ,  $\omega_n = 2\pi i n T$ , and summation runs over Matsubara frequencies. In the standard way (see, e.g., ref. [32]) by converting the  $\omega_n$ -sum in eq. (7.7) into the energy integral, this thermodynamic potential is also easily expressed in terms of the real-time quantities (A.7) and (A.8) (in the rest frame of the system)

$$\begin{aligned} \Omega \{ \phi, \phi^*, \Delta, \mu \} = & - \int d^3x \mathcal{L}^0 \{ \phi, \partial_\mu \phi \} + \kappa \int d^3x \frac{d^4p}{(2\pi)^4} n(p_0 - \mu) \\ & \times \left( -2\text{Im} \ln \left[ -\Delta^R(p_0 + i0, \mathbf{p}) \right] - \text{Re} \Delta^R \Gamma - A \text{Re} \Pi^R \right) + \Phi_T, \end{aligned} \quad (7.8)$$

where  $p = (p_0, \mathbf{p})$  is the 4-momentum,

$$n(\varepsilon) = [\exp(\varepsilon/T) - 1]^{-1} \quad (7.9)$$

is the thermal Bose–Einstein occupation number, and

$$A(p) = -2\text{Im} \Delta^R(p), \quad \Gamma(p) = -2\text{Im} \Pi^R(p) \quad (7.10)$$

are the spectral function  $A$  and spectral width<sup>5</sup>  $\Gamma$ , respectively, defined in terms of retarded quantities, c.f. eq. (A.2). Note that the exact form of equilibrium distribution (7.9) is a function of the particle energy only (which can be off-shell for particles with width), rather than a function of momenta  $\mathbf{p}$  through the on-shell energy momentum dispersion relation, as often encountered in text books which deal with the quasi-particle picture. Thus, the problem of the thermodynamic consistency can immediately be re-addressed from the Schwinger–Keldysh approach to the Matsubara one. Within the Matsubara formalism, this problem was considered by Baym [30]. He has shown that any  $\Phi$ -derivable approximation to the thermodynamic potential is thermodynamically consistent. Hence, we have proved that our  $\Phi$  derivable approximations to the  $\Gamma$ -functional are also thermodynamically consistent.

The stationary property of the  $\Gamma$  functional (and, hence, of  $\Omega$ ) with respect to variations in full Green’s functions and classical fields, eq. (4.6), is the key feature that provides the thermodynamic consistency. It implies that any derivative of the thermodynamic potential with respect to any thermodynamic parameter like  $\beta$  or  $\mu$  is determined only by the explicit dependence of  $\Omega$  on these parameters, since the implicit dependences through  $\Delta$  and  $\phi$  drop out due to the stationary property. Therefore,  $\Phi$ -derivable approximations preserve the corresponding thermodynamic relations as for the exact partition sum, and thus provide thermodynamic consistency.

<sup>5</sup> Please, do not confuse with the  $\Gamma\{\dots\}$ -functional

## 8 Virial limit

A particular simplification is obtained in the dilute density limit (virial limit). It has the advantage that the corresponding self-energies of the particles and intermediate resonances are entirely determined by two-body scattering properties, in particular, by scattering phase shifts. We illustrate this at the example of the interacting system of nucleons, pions and delta resonances, which has recently been investigated by Weinhold et al. [40]. Following their study we consider a pedagogical example, where the  $\pi NN$ -interaction is omitted. Then with a  $p$ -wave  $\pi N\Delta$ -coupling vertex among the three fields the first and only diagram of  $\Phi$  up to two vertices and the corresponding three self-energies are given by

$$\Phi = \text{diagram 1} \quad \Pi_N = \text{diagram 2} \quad \Pi_\pi = \text{diagram 3} \quad \Pi_\Delta = \text{diagram 4} \quad (8.1)$$

Here the solid, dashed and double lines denote the propagators of  $N$ ,  $\pi$  and  $\Delta$ , respectively. In non-relativistic approximation for the baryons we ignore contributions from the baryon Dirac-sea. Then the bare pion mass agrees with its vacuum value, while the nucleon and delta masses require appropriate mass counter terms. The  $\Delta$  self-energy  $\Pi_\Delta$  attains the vacuum width and position of the delta resonance due to the decay into a pion and a nucleon. The corresponding scattering diagrams are obtained by opening two propagator lines of  $\Phi$  with the prominent feature that the  $\pi N$ -scattering proceeds through the delta resonance. Since in this case a single resonance couples to a single scattering channel, the vacuum spectral function of the resonance can directly be expressed through the scattering  $T$ -matrix and hence through measured scattering phase shifts

$$|T_{33}|^2 = 4 \sin^2 \delta_{33}(p) = \Gamma_\Delta^{\text{vac}}(p) A_\Delta^{\text{vac}}(p), \quad (8.2)$$

where  $p = p_N + p_\pi$ . Thus through (8.2) the vacuum properties of the delta can almost model-independently be obtained from scattering data. Further details and extensions to multi-channel and multi-resonance cases can be found in ref. [46].

For the multi-component system the renormalized thermodynamic potential including vacuum counter terms, c.f. eq. (7.8), can be written<sup>6</sup> as

$$\Omega \{ \Delta_\pi, \Delta_N, \Delta_\Delta \} = T \sum_{a \in \{ \pi, N, \Delta \}} \mp \kappa \text{Tr} \left\{ -\ln \left[ -\Delta_a^R(p_0 + i0, \mathbf{p}) \right] + \Delta_a^R \Pi_a^R \right\}_{T, \mu} + \Phi_T. \quad (8.3)$$

<sup>6</sup> We generalize the boson expressions (7.7) and (7.8) to the case multi-component system of fermions and bosons.

Here for any function  $f(p)$  the thermodynamic trace  $\text{Tr}\{\dots\}_{T,\mu}$  is defined as

$$\begin{aligned} \text{Tr}\{f(p)\}_{T,\mu} & \quad (8.4) \\ & := dV \int \frac{d^3p}{(2\pi)^3} \sum_m \exp(i\omega_m \eta) f(\omega_m - \mu, \mathbf{p}) \quad \left| \begin{array}{l} \eta \rightarrow +0 \\ \omega_m = 2m\pi i T \quad (\text{bosons}) \\ \omega_m = (2m+1)\pi i T \quad (\text{fermions}), \end{array} \right. \\ & = \mp d \frac{V}{T} \int \frac{d^4p}{(2\pi)^4} n(p_0 - \mu) 2 \text{Im} f(p_0 + i0, \mathbf{p}) \end{aligned}$$

either expressed in terms of the Matsubara summation over frequencies  $\omega_m$ , or converted into an energy integral over thermal occupations  $n(\varepsilon) = [\exp(\varepsilon/T) \pm 1]^{-1}$ , of Fermi–Dirac/Bose–Einstein type, c.f. eqs (7.7) and (7.8) above. The upper sign appears for fermions,  $d$  is the degeneracy in that particle channel, and  $V$  denotes the volume. Eq. (8.3) still has the functional property to provide the retarded Dyson equations for the  $\Delta_a^R$  from the stationary condition which we use in order to determine the physical value of  $\Omega$ . For the particular case here one further can exploit that the value

$$\Phi_T = \pm \kappa T \text{Tr}\{\Pi_a \Delta_a\}_{T,\mu}; \quad \text{for } a \in \{N, \pi, \Delta\} \text{ and } \Phi \text{ of form (8.1),} \quad (8.5)$$

valid for this  $\Phi_T$  which linearly depends on all three propagators. Compatible with the low density limit one can expand the  $\text{Tr} \ln\{-\Delta\}$  terms for the pion and nucleon around the *free* propagators, and finally obtains

$$\begin{aligned} \Omega_{\pi N \Delta} & = \Omega \{ \Delta_\pi, \Delta_N, \Delta_\Delta \} \Big|_{\text{stationary}} \\ & = \Omega_N^{\text{free}} + \Omega_\pi^{\text{free}} + T \text{Tr} \left\{ \ln \left[ -\Delta_\Delta^R(p_0 + i0, \mathbf{p}) \right] \right\}_{T,\mu} \end{aligned} \quad (8.6)$$

$$= \Omega_N^{\text{free}} + \Omega_\pi^{\text{free}} + d_\Delta T V \int \frac{d^4p}{(2\pi)^4} 2 \frac{\partial \delta_{33}(p)}{\partial p_0} \ln [1 - n_\Delta(p_0 - \mu_\Delta)] \quad (8.7)$$

for the physical *value* of  $\Omega$ . Here the  $\Omega_a^{\text{free}}$  are the *free* single-particle thermodynamic potentials<sup>7</sup>, while  $\mu_\Delta$  and  $d_\Delta = 16$  are the chemical potential and degeneracy factor of the  $\Delta$  resonance, respectively. The last term in (8.7) obtained through (8.2), represents a famous result derived by Beth-Uhlenbeck [47,48], later generalized by Dashen, Ma and Bernstein [49] and applied to nuclear resonance matter in refs. [50,51,40,46]. It illustrates that the virial corrections of the system’s level density due to interactions are entirely given by the energy variation of the corresponding two-body scattering phase shifts  $\partial\delta/\partial p_0$ .

All thermodynamic properties can be obtained from  $\Omega$  through partial differentiations with respect to  $T$  and the  $\mu$ . The final form (8.7) may give the impression that one deals

<sup>7</sup> The appropriate cancellation of terms for the result (8.6) is only achieved, if one uses  $\Omega^{\text{free}}$ , i.e. the partition sum of free particles with the free energy–momentum dispersion relation. Within this model already on the *vacuum* level the nucleon would acquire loop corrections to its self-energy which would lead to deviations between  $\Omega^{\text{vac}}$  and  $\Omega^{\text{free}}$ , as well as between the corresponding propagators off their mass shell.



with non-interacting nucleons and pions. This is however not the case. For instance the densities of baryons and pions derived from (8.7) become

$$\rho_B = \frac{\partial \Omega_{\pi N \Delta}}{\partial \mu_N} = \rho_N^{\text{free}} + \rho_\Delta + \rho_{\text{corr}}, \quad \rho_\pi = \frac{\partial \Omega_{\pi N \Delta}}{\partial \mu_\pi} = \rho_\pi^{\text{free}} + \rho_\Delta + \rho_{\text{corr}}, \quad (8.8)$$

with

$$\rho_\Delta = d_\Delta \int \frac{d^4 p}{(2\pi)^4} n_\Delta(p_0 - \mu_\Delta) A_\Delta(p), \quad \rho_{\text{corr}} = d_\Delta \int \frac{d^4 p}{(2\pi)^4} n_\Delta(p_0 - \mu_\Delta) B_{\text{corr}}(p), \quad (8.9)$$

and  $\mu_\Delta = \mu_N + \mu_\pi$ <sup>8</sup>. Here the density of deltas  $\rho_\Delta$  is determined by the delta spectral function. The interaction contribution contained in the correlation density  $\rho_{\text{corr}}$  depends on the difference between the phase-shift variation and the spectral function

$$B_{\text{corr}} = 2 \frac{\partial \delta_{33}(p_0)}{\partial p_0} - A_\Delta(p) = 2 \text{Im} \left[ \frac{\partial \Pi_\Delta^R(p)}{\partial p_0} \Delta_\Delta^R(p) \right]. \quad (8.10)$$

Due to the fact that  $\Gamma_\Delta(p)$  grows with energy and the real part of  $\Delta_\Delta$  changes sign at the resonance energy,  $B_{\text{corr}}$  becomes positive below and negative above resonance, respectively. It leads to an enhancement of both densities at low energies, i.e. below resonance and this way to a further softening of the resulting equation of state compared to the naive spectral function treatment ignoring the  $B_{\text{corr}}$  terms. This illustrates that an interacting resonance gas *cannot* consistently be described by a set of free particles (here the pions and nucleons) plus vacuum resonances (here the delta), described by their spectral function. Rather the coupling of a bare resonance to the stable particles determines its width, and thus its spectral properties in vacuum. At the same time the stable particles are modified due to the interaction with the resonance. Only the account of all three self-energies in (8.1) provides a conserving and thermodynamically consistent approximation.

Alternatively to the picture above, the properties of the system can be discussed entirely in terms of the stable particles, i.e. the pion and the nucleon, thus eliminating the delta. The thermodynamic potential is then still given by (8.7). This form is valid even without intermediate resonances and the phase-shifts just account for the  $\pi N$  interaction properties. Also the self-energy of the lightest particle in the system, the pion, can be obtained from phase shifts by means of the optical theorem [52,53]. To linear order in the nucleon density  $\rho_N$  one determines the pion self energy

$$\Pi_\pi = 4\pi \rho_N F_{\pi N}(0) = -\frac{d_\Delta}{d_\pi} \frac{2\pi}{k} \frac{\rho_N}{d_N} 2 \sin \delta_{33} e^{i\delta_{33}}, \quad (8.11)$$

from the forward  $\pi N$ -scattering amplitude  $F_{\pi N}(0)$ . The degeneracy factors  $d_N : d_\pi : d_\Delta = 4 : 3 : 16$  just provide the proper spin/isospin counting. This self-energy, which determines

<sup>8</sup> In equilibrium  $\mu_\pi$  has to be put to zero after differentiation.

an optical potential or index of refraction, is attractive below the delta resonance energy and repulsive above. It agrees with a related effect in optics, where a resonance in the medium causes an anomalous behavior of the real part of the index of refraction, which is larger than 1 below the resonance frequency and less than 1 above the resonance. Thus, absorption, e.g. by exciting a resonance, is always accompanied by a change of the real part of the index of refraction of the scattered particle. The  $\Phi$ -derivable principle automatically takes care about these features.

As has been discussed in [54], the corrections to the system's level density (last term in (8.7)) can also be inferred from the time shifts (or time delays) induced by the scattering processes. From ergodicity arguments [54] one obtains for a single partial wave

$$\begin{aligned} \frac{\partial}{\partial p_0} \left( N_{\text{level}}(p_0) - N_{\text{level}}^{\text{free}}(p_0) \right) &= \tau_{\text{forward}} + \tau_{\text{scatt.}} = \tau_{\text{delay}} \\ &= 2 \frac{\partial}{\partial p_0} [\sin \delta_{33} \cos \delta_{33}] + 4 \sin^2 \delta_{33} \frac{\partial \delta_{33}}{\partial p_0} = 2 \frac{\partial \delta_{33}}{\partial p_0}. \end{aligned} \quad (8.12)$$

Here the forward delay time  $\tau_{\text{forward}}$  is identical to the change of the mean free propagation time in between successive scattering due to the change of the group velocity induced by the real part of the optical potential, c.f. (8.11). The scattering time  $\tau_{\text{scatt.}}$  finally results from the delayed re-emission of the pion from the intermediate resonance to angles off the forward direction.

Similar considerations as presented in this section apply for example to the interacting  $\pi\rho$ -meson system, e.g. on the basis of a renormalizable hidden gauge model [55].

## 9 Conclusion

With the aim to develop self-consistent approximations to quantum transport we investigated the  $\Phi$ -functional method introduced by Luttinger and Ward [31] and later used by Baym [30]. We have employed functional methods for Green's functions within the formalism of non-equilibrium Green's functions on the real-time contour, developed by Schwinger, Kadanoff, Baym and Keldysh [1–3].

In diagrammatic terms the main quantity, the functional  $\Phi$ , is determined by the sum of all closed (i.e. without external points) skeleton diagrams in terms of classical fields and full Green's functions on the real-time contour. It is a generating functional which allows all important quantities of a system (such as sources of classical fields, self-energies, interaction energy, etc.) to be derived by respective variations of the  $\Phi$  functional. Therefore this  $\Phi$  functional plays a central role in the space of classical fields and full Green's functions on the contour similar to that of the interaction Lagrangian on the operator level. Our treatment extends the definition of the  $\Phi$  functional to any non-equilibrium system including non-vanishing classical bosonic fields. This last generalization allows to

self-consistently describe the dynamics of both the order parameter (the classical field) and fluctuations on equal footing, e.g. in the theory of phase-transition phenomena.

The advantage of the  $\Phi$  functional is that we may formulate various approximations at the level of  $\Phi$ , thus defining so called  $\Phi$ -derivable approximations. In particular, we may construct effective theories right at the level of Green's functions and effective vertices. These approximations possess some important features: they respect exact conservation laws on the level of expectation values (with the Noether values for the conserved quantities) and have a proper thermodynamic limit. Note that other approximation schemes, e.g. at the level of self-energies, far not always possess such properties.

The question of consistency becomes especially important for a multi-component system, where the properties of one species can change due to the presence of interactions with the others and *vice versa*. The "*vice versa*" is very important and corresponds to the principle of *actio = re-actio*. This implies that the self-energy of one species cannot be changed through the interaction with other species without affecting the self-energies of the latter ones also. The  $\Phi$ -derivable scheme offers a natural and consistent way to account for this principle. Within thermodynamic considerations this has recently been considered for the interacting pion–nucleon–delta-resonance system, where the coupling to the delta resonance leads to a softening of the pion modes below the resonance mass [40], as we have discussed it in sect. 8, and for a relativistic QED plasma in [56]. We also expect a consistent description of chiral  $\sigma$ -,  $\pi$ - condensates together with fluctuations, as an immediate application of our results to multi-component systems.

For the relativistic scheme considered here we argue that a careful construction of conserved quantities requires symmetric expressions in terms of  $\Delta^{-+}$  and  $\Delta^{+-}$  Green's functions ( $\Delta^<$  and  $\Delta^>$  in the Kadanoff–Baym notation, respectively). This is in contrast to expressions only involving  $\Delta^{-+}$  Green's function, which are often used in the literature. These symmetric expressions describe contributions of both particles and anti-particles on equal footing, as well as take proper account of modifications of the vacuum polarization in the medium. Of course, these symmetric expressions still require a proper vacuum renormalization to be done in any actual calculation.

The dynamical equations of motion discussed within this paper are still on the level of Dyson's equation, i.e. they are time non-local with two time arguments for any two point function formulated on the non-equilibrium time contour. As initial condition they require the statistical operator be given at initial time  $t_0$ , a circumstance which may not be very practical, since one may like the initial conditions rather be formulated in terms of the Green's functions themselves. There are two simplifying cases where the initial conditions can be formulated easily. Both require the system to be stationary for a certain while prior to the genuine non-equilibrium dynamics. This effectively pushes the initial time  $t_0$  back to  $-\infty$ . The first case is realized in collision processes, where two complex objects in a stationary state, generally the ground state, eventually collide. This situation is relevant to the problem of heavy-ion collisions which we are mostly interested in. The initial configuration consisting of two ground-state nuclei incident on each other can be

described in terms of casual finite-density Green's functions (e.g., see [57,58]) which then should be translated into the contour Green's functions by means of relations (A.1). The second situation is realized by systems prepared in thermodynamic equilibrium within some confined volume, which in the course of time are driven out of equilibrium by an external perturbation. In this case, mostly applying to condensed matter physics, the system is no longer closed and an external perturbation has to be included in the dynamical equations of motion with corresponding explicitly time-dependent external terms for the conservation laws, while the  $\Phi$ -derivable properties discussed here still refer to the internal motion of the system. In this case the stationary initial situation can be calculated by the Matsubara formalism, which then has to be transformed to the corresponding real time form, e.g. by means of identity (8.4). The finite volume conditions have to be imposed during the entire non-equilibrium evolution. Such conditions are quite complicated already in the Boltzmann kinetics (e.g., see [59]) and have to be formulated separately in each particular case. Note that in both cases the initial stationary configuration should be calculated at the very same level of  $\Phi$ -approximation as the non-equilibrium dynamics itself.

Apart from the Hartree level, which implies truncating  $\Phi$  at the one-time-point level, the resulting contour Dyson equations of motion are not as practical yet for numerical applications. Still, the here presented scheme of constructing self-consistent approximations provides a solid basis for the derivation of suitable kinetic equations which apply beyond the limitations of the quasi-particle approximation. In that case the time non-locality is transformed into a spectral distribution in energy by means of a time Wigner transformation. Such generalized transport schemes respect parts of the quantum nature of the particles and, in particular, take due account of their finite mass-widths. The finite mass-width may be either an inherent vacuum property of the particle (e.g. resonance) or may be acquired by a stable particle in a dense environment due to frequent interactions. In the case of nuclear collisions at intermediate ( $\sim 1$  GeV/nucleon) to ultra-relativistic energies, for example, one encounters mean single-particle energies in the range of the typical temperature of  $T = 50 - 200$  MeV. Important resonances, like the delta-resonance or the rho-meson, have decay widths beyond 100 MeV, while typical collision rates estimated from presently used quasi-particle transport schemes are also in the order of  $T$ . These circumstances definitely prevent quasi-particle based transport codes from providing reliable results for such collisions. The main steps in the derivation of self-consistent and numerically tractable transport equations for particles with finite width are formulated and will be published in a forthcoming paper [37], brief accounts are given in [38,39].

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## APPENDICES

### A Contour Function Relations

For completeness we give all relations both for fermions (upper sign) and bosons (lower sign). Due to the change of operator ordering, genuine multi-point functions are discontinuous in general, when two contour coordinates become identical. In particular, two-point functions like  $iF(x, y) = \langle \mathcal{T}_c \hat{A}(x) \hat{B}(y) \rangle$  become<sup>9</sup>

$$iF(x, y) = \begin{pmatrix} iF^{--}(x, y) & iF^{-+}(x, y) \\ iF^{+-}(x, y) & iF^{++}(x, y) \end{pmatrix} = \begin{pmatrix} \langle \mathcal{T} \hat{A}(x) \hat{B}(y) \rangle & \mp \langle \hat{B}(y) \hat{A}(x) \rangle \\ \langle \hat{A}(x) \hat{B}(y) \rangle & \langle \mathcal{T}^{-1} \hat{A}(x) \hat{B}(y) \rangle \end{pmatrix}, \quad (\text{A.1})$$

where  $\mathcal{T}$  and  $\mathcal{T}^{-1}$  are the usual time and anti-time ordering operators. Since there are altogether only two possible orderings of the two operators, in fact given by the Wightman functions  $F^{-+}$  and  $F^{+-}$ , which are both continuous, not all four components of  $F$  are independent. From eq. (A.1) follow relations between non-equilibrium and the retarded and advanced functions

$$\begin{aligned} F^R(x, y) &= F^{--}(x, y) - F^{-+}(x, y) = F^{+-}(x, y) - F^{++}(x, y) \\ &:= \Theta(x_0 - y_0) (F^{+-}(x, y) - F^{-+}(x, y)), \\ F^A(x, y) &= F^{--}(x, y) - F^{+-}(x, y) = F^{-+}(x, y) - F^{++}(x, y) \\ &:= -\Theta(y_0 - x_0) (F^{+-}(x, y) - F^{-+}(x, y)), \end{aligned} \quad (\text{A.2})$$

where  $\Theta(x_0 - y_0)$  is the step function of the time difference.

Discontinuities of a two-point function may cause problems for differentiations, in particular, since they often occur simultaneously in products of two or more two-point functions. The proper procedure is, first, with the help of eq. (A.2) to represent the discontinuous parts in  $F^{--}$  and  $F^{++}$  by the continuous  $F^{-+}$  and  $F^{+-}$  times  $\Theta$ -functions, then to combine all discontinuities, e.g. with respect to  $x_0 - y_0$ , into a single term proportional to  $\Theta(x_0 - y_0)$ , and finally to apply the differentiations. One can easily check that in the following particularly relevant cases

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<sup>9</sup> Quite commonly, like in refs. [2,6], the notation  $F = \begin{pmatrix} F^c & F^< \\ F^> & F^a \end{pmatrix}$  is used for two-point functions instead of (A.1). We prefer the more flexible  $\{-+\}$  labelling of contour points.

$$\int_c dz \left( F(x^i, z)G(z, x^j) - G(x^i, z)F(z, x^j) \right), \quad (\text{A.3})$$

$$\frac{\partial}{\partial x_\mu} \int_c dz \left( F(x^i, z)G(z, x^j) + G(x^i, z)F(z, x^j) \right), \quad (\text{A.4})$$

$$\left[ \left( \frac{\partial}{\partial x_\mu} - \frac{\partial}{\partial y_\mu} \right) \int_c dz \left( F(x^i, z)G(z, y^j) - G(x^i, z)F(z, y^j) \right) \right]_{x=y} \quad (\text{A.5})$$

*all discontinuities exactly cancel.* Thereby, these values are independent of the placement of  $x^i$  and  $x^j$  on the contour, i.e. the values are only functions of the physical coordinate  $x$ .

Equilibrium relations between quantities on the real-time contour basically follow from the Kubo–Martin–Schwinger condition [60]

$$\Delta^{-+}(p) = \Delta^{+-}(p)e^{-\varepsilon/T}, \quad \Pi^{-+}(p) = \Pi^{+-}(p)e^{-\varepsilon/T}, \quad (\text{A.6})$$

where  $\varepsilon = p_\nu U^\nu - \mu$  with  $U^\nu$  and  $\mu$  being a global 4-velocity of the system and a chemical potential related to the charge, respectively. All the Green's functions can be expressed through retarded or advanced Green's functions:

$$\left( \Delta^{i,j}(p) \right) = \begin{pmatrix} [1 \mp n(\varepsilon)] \Delta^R(p) \pm n(\varepsilon) \Delta^A(p) & \pm i n(\varepsilon) A(p) \\ -i [1 \mp n(\varepsilon)] A(p) & - [1 \mp n(\varepsilon)] \Delta^A(p) \mp n(\varepsilon) \Delta^R(p) \end{pmatrix}, \quad (\text{A.7})$$

$i, j \in \{+, -\}$ , and the self-energies take a similar form

$$\left( \Pi^{i,j}(p) \right) = \begin{pmatrix} \Pi^R(p) \pm i n(\varepsilon) \Gamma(p) & \pm i n(\varepsilon) \Gamma(p) \\ -i [1 \mp n(\varepsilon)] \Gamma(p) & -\Pi^A(p) \pm i n(\varepsilon) \Gamma(p) \end{pmatrix}. \quad (\text{A.8})$$

Here  $n(\varepsilon)$  is the thermal Fermi–Dirac or Bose–Einstein occupation number (c.f. eq. (7.9) for bosons), and  $A$  and  $\Gamma$  are the spectral function and spectral width, respectively, defined in (7.10).

## B Diagram Rules for $\Phi$ , $J$ , and $\Pi$

The interaction vertex function  $V(x)$  entering the diagram is normalized in the standard way, c.f. [41], i.e. with factors  $n!$  relative to  $\hat{\mathcal{L}}^{\text{int}}(x)$  for each type of operator occurring with multiplicity  $n$  in the vertex. E.g., the vertex function simply becomes  $-iV(x_k) = -ig$

for  $\hat{\mathcal{L}}^{\text{int}} = -g\phi^4/4!$  (4 identical operators) and for  $\hat{\mathcal{L}}^{\text{int}} = -g(\phi^*\phi)^2/(2! \cdot 2!)$  (twice two identical operators). The diagrammatic rules to calculate  $i\Phi$ ,  $iJ(x)$  and  $-i\Pi$  for a given theory are as follows

- (i) Draw all topologically distinct, closed and entirely connected diagrams with  $N$  internal vertices  $x_1, x_2, \dots, x_N$ , where classical field pins and propagator lines saturate the valences of all vertices in the diagram, c.f. (5.11) above. Closed diagrams for  $i\Phi$  have no external points, while  $iJ(x)$  has one external point, and  $-i\Pi$  has two external points. For charged bosons, pins and propagator lines have an arrows sense, distinguishing  $\hat{\phi}$  from  $\hat{\phi}^\dagger$  at the vertices, the sense direction pointing towards  $\hat{\phi}$ .
- (ii) For  $i\Phi$ ,  $iJ(x)$  and  $-i\mathcal{E}^{\text{int}}(x)$  keep only those diagrams that are two-particle irreducible, i.e. which cannot be split into two pieces by cutting two different propagator lines. For  $-i\Pi$  keep only those diagrams which result from  $\Phi$  by opening one propagator line.
- (iii) To each line, connecting  $x_l \longrightarrow x_k$ , assign the factor  $i\Delta(x_k, x_l)$ .
- (iv) To each pin attached to  $x_k$ , assign the factor  $\phi(x_k)$  or  $\phi^*(x_k)$  depending on the sense.
- (v) To each vertex  $x_k$  assign the vertex factor  $-iV(x_k)$  as determined by  $\hat{\mathcal{L}}^{\text{int}}(x)$ .
- (vi) Integrate all internal  $x_1, x_2, \dots, x_N$  over the contour.
- (vii) Multiply the result by the symmetry factor  $S$ , which is calculated as follows
  - $1/N_G!$  factor for every  $N_G$  equivalent internal lines,
  - $1/N_\phi!$  factor for every  $N_\phi$  classical fields entering each vertex,
  - $1/2$  factor for every self-closed line loop (tad-poles) for *real* fields.
- (viii) Sum all diagrams. For the calculation of  $i\Phi$  (contrary to  $iJ(x)$  and  $-i\Pi$ ), an extra factor  $1/n_\lambda$  appears for each diagram, where  $n_\lambda$  counts the number of vertices in the diagram. This factor has however been given explicitly in all diagram formulae concerning  $\Phi$ !
- (ix) For fermions each closed fermion loop contributes a factor  $(-1)$ .

In many cases like in transport treatments, it is advantageous to consider the diagrams decomposed into the two contour sections at each vertex, e.g., to calculate quantities like  $\Pi^{-+}$  and  $\Pi^{+-}$  self-energies in terms of exact Green's functions. Therefore, "physical"-time diagrammatic rules in the matrix scheme are also required. Here we present only those rules which differ from the above ones on the real-time contour, bearing in mind that all other rules remain valid:

- (iii') To each internal vertex  $x_k$  first assign a sign  $i_k \in \{+, -\}$  defining the contour placement  $x_k^{i_k}$ . To each line, connecting  $x_l^{i_l} \longrightarrow x_k^{i_k}$ , assign the factor  $i\Delta^{i_k i_l}(x_k, x_l)$ ,  $i_k, i_l \in \{+, -\}$ .
- (vi') For all internal points integrate all  $x_1, x_2, \dots, x_N$  over the real-time axis and space, for each internal " + " vertex multiply by  $(-1)$  and finally sum over all internal contour placements  $i_1, i_2, \dots, i_N$  ( $i_k \in \{+, -\}$ ).

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