Thermal field theory to all orders in gradient expansion

Peter Millington$^1$ and Apostolos Pilaftsis$^2$

$^1$Consortium for Fundamental Physics, School of Mathematics and Statistics, University of Sheffield, Sheffield S3 7RH, United Kingdom
$^2$Consortium for Fundamental Physics, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom
E-mail: p.w.millington@sheffield.ac.uk, apostolos.pilaftsis@manchester.ac.uk

Abstract. We present a new perturbative formulation of non-equilibrium thermal field theory, based upon non-homogeneous free propagators and time-dependent vertices. The resulting time-dependent diagrammatic perturbation series are free of pinch singularities without the need for quasi-particle approximation or effective resummation of finite widths. After arriving at a physically meaningful definition of particle number densities, we derive master time evolution equations for statistical distribution functions, which are valid to all orders in perturbation theory and all orders in a gradient expansion. For a scalar model, we make a loopwise truncation of these evolution equations, whilst still capturing fast transient behaviour, which is found to be dominated by energy-violating processes, leading to non-Markovian evolution of memory effects.

1. Introduction

The description of out-of-equilibrium many-body field-theoretic systems is of increasing relevance in theoretical and experimental physics at the density frontier. Examples range from the early Universe to the deconfined phase of QCD, the quark-gluon plasma, relevant at heavy-ion colliders, such as RHIC and the LHC; as well as the internal dynamics of compact astro-physical phenomena, such as neutron stars, and condensed matter systems.

In [1], the present authors introduce a new perturbative approach to non-equilibrium thermal quantum field theory and an alternative framework in which to derive master time evolution equations for macroscopic observables. In contrast to existing semi-classical approaches based upon the Boltzmann equation, this new approach allows the systematic incorporation of finite-width and off-shell effects without the need for effective resummations. Furthermore, having a well-defined underlying perturbation theory that is free of pinch singularities, these time evolution equations may be truncated in a loopwise sense whilst retaining all orders of the time behaviour. Existing frameworks, based upon systems of Kadanoff–Baym equations [2], whilst retaining all orders in perturbation theory, often rely upon the truncation of a gradient expansion in time derivatives in order to obtain calculable expressions. In this case, one necessarily makes assumptions as to the separation of various time-scales in these systems. In addition, one must generally assume a quasi-particle ansatz for the form of the propagators appearing in these gradient expansions. On the other hand, the loopwise-truncated evolution equations of this new perturbative formalism are built from non-homogeneous free propagators and time-dependent vertices, which together encode spatial and temporal inhomogeneity from tree-level without any of the aforementioned approximations.
2. Canonical quantization

We begin by highlighting the details of the canonical quantization of a scalar field pertinent to a perturbative treatment of non-equilibrium thermal field theory.

The time-independent Schrödinger-picture field operator, denoted by a subscript S, may be written in the familiar plane-wave decomposition

$$\Phi_S(x; \tilde{t}_i) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E(p)} \left( a_S(p; \tilde{t}_i)e^{ip\cdot x} + a_S^\dagger(p; \tilde{t}_i)e^{-ip\cdot x} \right),$$

where $E(p) = \sqrt{p^2 + M^2}$ and $a_S^\dagger(p; \tilde{t}_i)$ and $a_S(p; \tilde{t}_i)$ are the usual single-particle creation and annihilation operators. It is essential to emphasize that we define the Schrödinger-, Heisenberg- and Interaction (Dirac)-pictures to be coincident at the finite microscopic boundary time $\tilde{t}_i$, i.e.

$$\Phi_S(x; \tilde{t}_i) = \Phi_H(\tilde{t}_i, x; \tilde{t}_i) = \Phi_I(\tilde{t}_i, x; \tilde{t}_i).$$

It is at this picture-independent boundary time $\tilde{t}_i$ that initial conditions must be specified. Implicit dependence on $\tilde{t}_i$ is marked by separation from explicit arguments with a semi-colon.

The time-dependent interaction-picture operator $\Phi_I(x; \tilde{t}_i)$ is obtained via the unitary transformation $\Phi_I(x; \tilde{t}_i) = e^{iH^S[x_0 - \tilde{t}_i]}\Phi_S(x; \tilde{t}_i)e^{-iH^S[x_0 - \tilde{t}_i]}$, where $H^S$ is the free part of the Hamiltonian in the Schrödinger picture. This yields

$$\Phi_I(x; \tilde{t}_i) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E(p)} \left( a_I(p, 0; \tilde{t}_i)e^{-iE(p)x_0}e^{ip\cdot x} + a_I^\dagger(p, 0; \tilde{t}_i)e^{iE(p)x_0}e^{-ip\cdot x} \right).$$

Notice that in (3) the time-dependent interaction-picture operators $a_I^\dagger(p, \tilde{t}; \tilde{t}_i)$ and $a_I(p, \tilde{t}; \tilde{t}_i)$ are evaluated at the microscopic time $\tilde{t} = 0$. These operators satisfy the commutation relation

$$[a_I(p, \tilde{t}; \tilde{t}_i), a_I^\dagger(p', \tilde{t}; \tilde{t}_i')] = (2\pi)^32E(p)\delta^{(3)}(p - p')e^{-iE(p)(\tilde{t} - \tilde{t}')},$$

with all other commutators vanishing, where we obtain an overall phase $e^{-iE(p)(\tilde{t} - \tilde{t}')}$ for $\tilde{t} \neq \tilde{t}'$.

In quantum statistical mechanics, we are interested in the calculation of Ensemble Expectation Values (EEVs) of operators at a fixed microscopic time of observation $\tilde{t}_f$. Such EEVs are obtained by taking the trace with the density operator $\rho(\tilde{f}; \tilde{t}_i)$, i.e.

$$\langle \bullet \rangle_{\tilde{t}_f} = \mathcal{Z}^{-1}(t) \text{Tr} \rho(\tilde{f}; \tilde{t}_i) \bullet,$$

where $\mathcal{Z}(t) = \text{Tr} \rho(\tilde{f}; \tilde{t}_i)$ is the partition function. Here, we have introduced the macroscopic time $t = \tilde{t}_f - \tilde{t}_i$, which is simply the interval of microscopic time between the specification of the boundary conditions and the subsequent observation of the system.

Consider the following observable, which is the EEV of a two-point product of field operators:

$$O(x, y, \tilde{f}; \tilde{t}_i) = \mathcal{Z}^{-1}(t) \text{Tr} \rho(\tilde{f}; \tilde{t}_i)\Phi(\tilde{f}, x; \tilde{t}_i)\Phi(\tilde{f}, y; \tilde{t}_i).$$

It has not been necessary to specify the picture in which the operators of the RHS of (6) are to be interpreted. This is because these operators are evaluated at equal times. Potential observables built from operators evaluated at different times are picture-dependent and therefore unphysical. In addition, the observable $O$ should be invariant under simultaneous time translations of the boundary and observation times, depending only on the macroscopic time $t$, i.e. $O(x, y, \tilde{f}; \tilde{t}_i) \equiv O(x, y, \tilde{f} - \tilde{t}_i; 0) \equiv O(x, y, t)$. Notice also that there are 7 independent coordinates: the spatial coordinates $x$ and $y$ and the macroscopic time $t$. It will later be convenient to work in terms of the central spatial coordinate $X = (x + y)/2$ and the three-momentum $q_i$ conjugate to the relative spatial coordinate $R = x - y$. 


The density operator of a time-dependent and spatially inhomogeneous background will in general be an intractable incoherent sum of all possible \( n \) to \( m \) multi-particle correlations, non-diagonal in the Fock space. We may account for our ignorance of this density operator by appealing to the remaining freedom in the commutation relation in (4). In particular, we define

\[
\langle a_l(p, \tilde{t}; \tilde{t}_l) a_l^\dagger(p', \tilde{t}; \tilde{t}_l) \rangle_t = (2\pi)^3 2E(p) \delta^{(3)}(p-p') + 2E^{1/2}(p) E^{1/2}(p') f(p, p', t), \quad (7a)
\]

\[
\langle a_l^\dagger(p', \tilde{t}; \tilde{t}_l) a_l(p, \tilde{t}; \tilde{t}_l) \rangle_t = 2E^{1/2}(p) E^{1/2}(p') f(p, p', t), \quad (7b)
\]

where \( f(p, p', t) = f^*(p', p, t) \). The statistical distribution function \( f(p, p', t) \) is related to the particle number density \( n(q, X, t) \) via the Wigner transform

\[
n(q, X, t) = \int \frac{d^3Q}{(2\pi)^3} e^{iQ \cdot X} f(q + Q/2, q - Q/2, t). \quad (8)
\]

Notice that spatial homogeneity is broken by the explicit dependence of \( f(p, p', t) \) on the two three-momenta \( p \) and \( p' \). In the thermodynamic equilibrium limit, we have the correspondence: \( f(p, p', t) \rightarrow f_{\text{eq}}(p, p') = (2\pi)^3 \delta^{(3)}(p-p') f_B(E(p)) \), where \( f_B(x) = (e^{\beta x} - 1)^{-1} \) is the Bose–Einstein distribution function and \( \beta \) is the inverse thermodynamic temperature.

### 3. Schwinger–Keldysh CTP formalism

We require a path-integral approach to generating EEVs of products of field operators. Such an approach is provided by the Schwinger–Keldysh CTP formalism [3, 4].

In order to obtain the generating functional of EEVs, we insert unitary evolution operators to the left and the right of the density operator in the partition function \( Z \), yielding

\[
Z[\rho, J_x, t] = \text{Tr} \left[ T e^{i \int_{t_0}^t d^4x J_x(x) \Phi_H(x)} \rho_H(\tilde{t}_f; \tilde{t}_i) T e^{i \int_{t_0}^t d^4x J_x(x) \Phi_H(x)} \right], \quad (9)
\]

where the spacetime hypervolume \( \Omega_t \simeq [-t/2, t/2] \times \mathbb{R}^3 \) is temporally bounded.

We may interpret this evolution as defining a closed contour \( C = C_+ \cup C_- \) in the complex-time plane (t-plane, \( t \in \mathbb{C} \)), as shown in figure 1, which is the union of two anti-parallel branches: \( C_+ \),\( C_− \).
running from \( \tilde{t}_i \) to \( \tilde{t}_f - \i/2 \); and \( C_- \), running from \( \tilde{t}_f - \i/2 \) back to \( \tilde{t}_i - \i \). A small imaginary part \( \epsilon = 0^+ \) is added to separate the two, essentially coincident, branches. We may introduce a parametrization of this contour \( \tilde{z}(u) \), where \( u \) increases monotonically along \( C \), which allows the definition of a path-ordering operator \( T_C \). Notice that, in contrast to other interpretations of the CTP formalism, this contour evolves in time, with each branch having length \( t \).

Following the notation of \([5, 6]\), we denote by \( \Phi_\pm(x) \equiv \Phi(x^0 \in C_\pm, \chi) \) fields confined to the positive and negative branches of the CTP contour. We then define the doublets

\[
\Phi^a(x) = \left( \Phi_+(x), \Phi_-(x) \right), \quad \Phi_a(x) = \eta_{ab}\Phi^b(x) = \left( \Phi_+, -\Phi_-(x) \right),
\]

where the CTP indices \( a, b = 1, 2 \) and \( \eta_{ab} = \text{diag}(1, -1) \) is an \( \mathbb{SO}(1, 1) \) 'metric.'

Inserting into (9) complete sets of eigenstates of the Heisenberg field operator, we derive a path-integral representation of the CTP generating functional, which depends on the path-ordered CTP propagator \( i\Delta^{ab}(x, y; \tilde{t}_f; \tilde{t}_i) \), written as the \( 2 \times 2 \) matrix

\[
i\Delta^{ab}(x, y; \tilde{t}_f; \tilde{t}_i) \equiv \langle T_C \left[ \Phi^a(x; \tilde{t}_i)\Phi^b(y; \tilde{t}_i) \right] \rangle_t = i \left[ \Delta_F(x, y; \tilde{t}_f; \tilde{t}_i) \quad \Delta_C(x, y; \tilde{t}_f; \tilde{t}_i) \right] \left[ \Delta_C(x, y; \tilde{t}_f; \tilde{t}_i) \quad \Delta_D(x, y; \tilde{t}_f; \tilde{t}_i) \right].
\]

For \( x^0, y^0 \in C_+ \), the path-ordering \( T_C \) is equivalent to the standard time-ordering \( T \) and we obtain the time-ordered Feynman propagator \( i\Delta_F(x, y; \tilde{t}_f; \tilde{t}_i) \). On the other hand, for \( x^0, y^0 \in C_- \), \( T_C \) is equivalent to anti-time-ordering \( T \) and we obtain the anti-time-ordered Dyson propagator \( i\Delta_D(x, y; \tilde{t}_f; \tilde{t}_i) \). For \( x^0 \in C_+ \) and \( y^0 \in C_- \), \( x^0 \) is always 'earlier' than \( y^0 \), yielding the absolutely-ordered negative-frequency Wightman propagator \( i\Delta_< (x, y; \tilde{t}_f; \tilde{t}_i) \). Conversely, for \( y^0 \in C_+ \) and \( x^0 \in C_- \), we obtain the positive-frequency Wightman propagator \( i\Delta_> (x, y; \tilde{t}_f; \tilde{t}_i) \).

From a Legendre transform of the CTP generating functional, we derive the Cornwall–Jackiw–Tomboulis effective action \([7]\). We may then obtain the CTP Schwinger–Dyson equation

\[
\Delta^{-1}_{ab}(x, y; \tilde{t}_f; \tilde{t}_i) = \Delta^{0, -1}_{ab}(x, y) + \Pi_{ab}(x, y; \tilde{t}_f; \tilde{t}_i),
\]

where \( \Delta^{-1}_{ab}(x, y; \tilde{t}_f; \tilde{t}_i) \) and \( \Delta^{0, -1}_{ab}(x, y) \) are the resummed and free inverse CTP propagators and \( \Pi_{ab}(x, y; \tilde{t}_f; \tilde{t}_i) \) is the CTP self-energy, analogous to (11).

4. Non-homogeneous diagrammatics

We consider a simple scalar theory, which comprises one heavy real scalar field \( \Phi \) and one light pair of complex scalar fields \( (\chi^\dagger, \chi) \), described by the Lagrangian

\[
\mathcal{L} = \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} M^2 \Phi^2 + \partial_\mu \chi^\dagger \partial^\mu \chi - m^2 \chi^\dagger \chi - g \Phi \chi^\dagger \chi - \cdots,
\]

where \( M = 1 \) GeV and \( m = 0.01 \) GeV. The ellipsis contains omitted self-interactions and the spacetime dependence of the fields has been suppressed. We prepare two isolated but coincident subsystems \( \mathcal{S}_\Phi \) and \( \mathcal{S}_\chi \), both separately in thermodynamic equilibrium at the same temperature \( T = 10 \) GeV with the interactions switched off. The subsystem \( \mathcal{S}_\Phi \) contains only the field \( \Phi \) and \( \mathcal{S}_\chi \), only \( \chi \). At \( t = 0 \), we turn on the interactions and the system \( \mathcal{S} = \mathcal{S}_\Phi \cup \mathcal{S}_\chi \) re-thermalizes. The subsystem \( \mathcal{S}_\chi \) is taken to be infinite so that it is unperturbed by interactions with \( \mathcal{S}_\Phi \).

The one-loop non-local \( \Phi \) self-energy is shown in figure 2. In particular, we draw attention to two features of the modified Feynman rules. Firstly, with the vertices, we associate a term

\[
-ig e^{iq0\tilde{t}_f}(2\pi)^3 \int \frac{1}{2\pi} \text{sinc} \left[ \left( \sum \rho_{0,i} \right) \frac{1}{2} \right] \delta^{(3)} \left( \sum \rho_i \right),
\]

where the \( \rho_i = q, k_1, k_2 \) are the four-momenta flowing into the vertex. The phase \( e^{iq0\tilde{t}_f} \), where \( q_0 \) is the energy flow external to the loop, results from the proper consideration of the
Wick contraction and field-particle duality relations. Due to the finite upper and lower bounds on time integrals appearing in the CTP generating functional, the familiar energy-conserving Dirac delta function has been replaced by a sinc function in (14). This violation of energy conservation is shown diagrammatically by the dotted line terminated in a cross and results from the uncertainty principle, since the observation of the system is made over a finite time interval. Furthermore, by virtue of this energy violation, the perturbation series remains free of the pinch singularities that would otherwise result from products of delta functions with identical arguments at early times. Secondly, the double lines occurring in the CTP propagators of the loop reflect the violation of three-momentum due to the dependence on the inhomogeneous statistical distribution function \( f(p, p', t) \). The full set of non-homogeneous free propagators is listed in table 1. Together, these modified Feynman rules encode the time-dependence and spatial inhomogeneity of the system from tree-level. All four-momenta internal to the loop are integrated over and the usual combinatorial factors apply. The CTP indices \( a, b = 1, 2 \) indicate the location of a vertex on either the positive or negative branch of the CTP contour.

For the system \( \mathcal{S} \), the one-loop time-dependent \( \Phi \) width is given by the following integral:

\[
\Gamma_{\Phi}^{(1)}(q,t) = \frac{g^2 t}{64\pi^3 M} \sum_{\alpha_1, \alpha_2} \int \frac{d^3 k}{E_1 E_2} \text{sinc} \left( (q_0 - \alpha_1 E_1 - \alpha_2 E_2) t \right) (1 + f_B(\alpha_1 E_1) + f_B(\alpha_2 E_2)) ,
\]

where \( \alpha_1, \alpha_2 = \pm 1 \), \( E_1 \equiv E_\chi(k) = \sqrt{k^2 + m^2} \) and \( E_2 \equiv E_\chi(q - k) \). The violation of energy conservation, due to the sinc function in (15), leads to otherwise-forbidden contributions from for \( \alpha_1, \alpha_2 = -1 \) (total annihilation) and \( \alpha_1 = -\alpha_2 \) (Landau damping). In addition, the kinematically-allowed phase space for normal \( 1 \to 2 \) decays is expanded. These evanescent processes are shown in figure 3. For \( t \to \infty \), we recover the known equilibrium result, since

\[
\lim_{t \to \infty} \frac{t}{\pi} \text{sinc} \left( (q_0 - \alpha_1 E_1 - \alpha_2 E_2) t \right) = \delta(q_0 - \alpha_1 E_1 - \alpha_2 E_2) .
\]
Table 1: The full complement of non-homogeneous free propagators for the scalar field \( \Phi \), where \( \tilde{f}(p,p',t) = \theta(p_0)\theta(p_0')\tilde{f}(p,p',t) + \theta(-p_0)\theta(-p_0')f^\ast(-p,-p',t) \).

In figure 4, we plot the ratio \( \Gamma^{(1)}_\Phi(\{q\},t) = \Gamma^{(1)}_\Phi(\{|q|\},t) / \Gamma^{(1)}_\Phi(\{|q|\},t \to \infty) \) of the time-dependent width to its late-time equilibrium value as a function of \( Mt \) for \( q^2 = M^2 \). In addition, we show the separate contributions of the four processes in figure 3. We note that the oscillations in the width have time-dependent frequencies. This non-Markovian behaviour is inherent to truly out-of-equilibrium systems exhibiting so-called memory effects.

5. Master time evolution equations for particle number densities

In order to count both on-shell and off-shell contributions systematically, we ‘measure’ the number of charges, rather than quanta of energy. This avoids any need to identify ‘single-particle’ energies by a quasi-particle approximation. We begin by relating the Noether charge

\[
Q(x_0;\tilde{t}_i) = i \int d^3x \left( \Phi^\dagger_H(x;\tilde{t}_i) \pi^\dagger_H(x;\tilde{t}_i) - \pi_H(x;\tilde{t}_i)\Phi_H(x;\tilde{t}_i) \right)
\]

(17)

to a charge density operator \( Q(q,X,X_0;\tilde{t}_i) \) via

\[
Q(X_0;\tilde{t}_i) = \int d^3X \int \frac{d^3q}{(2\pi)^3} Q(q,X,X_0;\tilde{t}_i) .
\]

(18)

By taking the equal-time EEV of \( Q(q,X,X_0;\tilde{t}_i) \) and extracting the positive- and negative-frequency particle components, we arrive at the following definition of the particle number density in terms of off-shell Green’s functions:

\[
n(q,X,t) = \lim_{X_0 \to t} 2 \int \frac{d^4q_0}{2\pi} \int \frac{d^4Q}{(2\pi)^3} e^{-iQ \cdot X} \theta(q_0)q_0i\Delta_c(q + \frac{Q}{2},q - \frac{Q}{2};t;0) ,
\]

(19)

where we have used the translational invariance of the CTP contour.
It is important to stress here that (20) provides a self-consistent time evolution equation for the LHS of (20) may be associated with the total derivative in the phase space (X, p), which appears in the classical Boltzmann transport equation. The $F$ terms on the LHS of (20) are the force terms, generated by the potential due to the dispersive part of the self-energy, and the $C$ terms on the RHS of (20) are the collision terms.
Truncating (20) to leading order in a loopwise sense, we obtain, for our simple scalar theory, the following time evolution equation for the $\Phi$ statistical distribution function:

$$
\partial_t f_\Phi(|q|, t) = -\frac{g^2}{2} \sum_{\alpha, \alpha_1, \alpha_2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{2E_\Phi(q)} \frac{1}{2E_\chi(k)} \frac{1}{2E_\chi(q-k)} 
\times \frac{t}{2\pi} \text{sinc}\left[\left(\alpha E_\Phi(q) - \alpha_1 E_\chi(k) - \alpha_2 E_\chi(q-k)\right)t/2\right] 
\times \left\{ \pi + 2\text{Si}\left[\left(\alpha E_\Phi(q) + \alpha_1 E_\chi(k) + \alpha_2 E_\chi(q-k)\right)t/2\right]\right\} 
\times \left[ \theta(-\alpha) + f_\Phi(|q|, t) \right] \left[ \theta(\alpha_1)(1 + f_\chi(|k|, t)) + \theta(-\alpha) f_\chi(|k|, t) \right] 
\times \left[ \theta(\alpha_2)(1 + f_\chi(|q-k|, t)) + \theta(-\alpha_2) f_\chi(|q-k|, t) \right] 
- \left[ \theta(\alpha) + f_\Phi(|q|, t) \right] \left[ \theta(\alpha_1)f_\chi(|k|, t) + \theta(-\alpha_1)(1 + f_\chi(|k|, t)) \right] 
\times \left[ \theta(\alpha_2)f_\chi(|q-k|, t) + \theta(-\alpha_2)(1 + f_\chi(|q-k|, t)) \right], \tag{22}
$$

where $\alpha, \alpha_1, \alpha_2 = \pm 1$. The second and third lines of (22) encode the early-time violation of energy conservation. This leads to the non-Markovian evolution of memory effects and evanescent contributions from otherwise kinematically-disallowed processes. Replacing these lines by an energy-conserving delta function, we recover the semi-classical Boltzmann transport equation. However, given the equilibrium initial conditions of our model, the artificial imposition of energy conservation along with the properties of the Bose–Einstein distribution ensure that the RHS of (22) is zero for all times. Thus, the semi-classical Boltzmann equation cannot describe the re-thermalization of our simple model. This is true also for gradient expansions of Kadanoff–Baym equations when truncated to zeroth order in time derivatives. Hence, it is only when energy-violating effects are systematically included, as in this new perturbative approach, that the dynamics of this re-thermalization are captured.

6. Conclusions

We have obtained master time evolution equations for particle number densities that are valid to all orders in perturbation theory and to all orders in gradient expansion. The loopwise truncation of these time evolution equations remains valid to all orders in gradient expansion, capturing the evolution on all time scales, including the transient dynamics. This prompt behaviour is dominated by energy-violating processes that lead to non-Markovian evolution of memory effects. The underlying perturbation series are built from non-homogeneous free propagators and explicitly time-dependent vertices. Due to the systematic treatment of finite boundary and observation times, these diagrammatic series remain free of pinch singularities.

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