Diagonalization of full finite temperature Green's functions by quasi-particles

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Abstract

For thermal systems, standard perturbation theory breaks down because of the absence of stable, observable asymptotic states. We show, how the introduction of statistical quasi-particles (stable, but not observable) gives rise to a consistent description. Statistical and spectral information can be cleanly separated also for interacting systems.

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1 Introduction

It is a well established fact by now, that naive perturbation theory breaks down at finite temperature, see refs. [1, 2] for a recent overview. This is due the modification of space-time symmetry in the presence of matter or a heat bath [3], i.e. to the absence of stable asymptotic states for the observable physical particles. To overcome this problem, first of all one has to employ a "doubling" of the Hilbert space, leading to two-point Green functions that are $2 \times 2$ matrices.

The Schwinger-Keldysh [4] or Closed-Time-Path method (CTP) is such a model, which has been used to derive transport equations, e.g. for nuclear phenomena, over several decades [5, 6]. However, the physical interpretation of the matrix structure of the propagator remains quite obscure in this formalism, and no justification is obtained for a perturbation expansion.

Another model is called Thermo Field Dynamics (TFD) [7, 8]. It differs from CTP in the important aspect, that the doubling of the Hilbert space is due to two disjoint, mutually (anti-) commuting representations of the canonical commutation relations. Thus, in contrast to CTP, TFD has a firm mathematical basis [9] and can be used perturbatively. To this end, one has to sacrifice either the stability aspect or the observability aspect of asymptotic states. The first leads to a perturbation expansion in terms of unstable particles [10]. It is the purpose of the present paper to demonstrate, that the second way leads to a simpler and straightforward approach.

To this end we show, that the thermal instability of observable states can be absorbed into a Bogoliubov transformation also for interacting systems. This Bogoliubov transformation then defines stable, albeit non-observable, quasi-particles which serve as basis for a perturbation expansion [11]. Throughout this paper we term them, for historical more than physical reasons, statistical quasi-particles [12].

2 Thermal Bogoliubov transformation

To establish the notation, we first discuss TFD for a single bosonic quantum state. We introduce creation and annihilation operators $a^\dagger$, $a$, $\tilde{a}^\dagger$, $\tilde{a}$ for the two representations, with canonical commutation relations

$$[a, a^\dagger] = 1 \quad [\tilde{a}, \tilde{a}^\dagger] = 1 \quad [a, \tilde{a}^\dagger] = 0 \quad (1)$$
The \(a, \tilde{a}\) operators annihilate the physical vacuum \(\langle 0, 0 \rangle\) and the two sets are transformed into another by means of an anti-unitary mapping, called the \textit{tilde} conjugation (see [13] for the tilde conjugation rules). For brevity, we work in the \(\alpha = 1\) representation, i.e., the thermal equilibrium state at inverse temperature \(\beta\) and chemical potential \(\mu\) is described by two state vectors

\[
\|O(\beta)\rangle = \exp\left(fa^\dagger \tilde{a}^\dagger\right) \langle 0, 0 \rangle, \quad f = e^{-\beta(\omega - \mu)}
\]

(2)

\[
\langle O(\beta) \| = \langle 0, 0 \| \exp(a\tilde{a})
\]

Within this framework, the ensemble average of an observable \(E[a, a^\dagger]\) is calculated as the expectation value

\[
\langle E \rangle = \frac{\langle O(\beta)\| E \| O(\beta) \rangle}{\langle O(\beta)\| O(\beta) \rangle}.
\]

(3)

Obviously then the state vectors \(\langle O(\beta) \|\) and \(\| O(\beta) \rangle\) are annihilated by certain linear combinations of the above operators,

\[
\xi\|O(\beta)\rangle = 0 \quad \tilde{\xi}\|O(\beta)\rangle = 0 \quad \langle O(\beta)\|\xi^\dagger = 0 \quad \langle O(\beta)\|\tilde{\xi}^\dagger = 0,
\]

(4)

obtained as

\[
\begin{pmatrix}
\xi \\
\tilde{\xi}^\dagger
\end{pmatrix} = \mathcal{B}
\begin{pmatrix}
a \\
a^\dagger
\end{pmatrix}, \quad
\begin{pmatrix}
\xi^\dagger \\
\tilde{\xi}^\dagger
\end{pmatrix}^T = \begin{pmatrix}
a^\dagger \\
-\tilde{a}
\end{pmatrix}^T \mathcal{B}^{-1}.
\]

(5)

\(\mathcal{B}\) is a \(2 \times 2\) matrix with determinant 1. Since the \(\xi\)-operators obey similar commutation relations as do the \(a\)-operators, they define our quasi-particles. It is crucial to realize, that these entities have nothing in common with the ”usual” definition of quasi-particles, which refers to physical states with an almost pointlike mass spectrum.

Eqn. (5) is essentially a Bogoliubov transformation [14]. The most general form for the Bogoliubov matrix compatible with our choice of state vectors is then

\[
\mathcal{B} = \frac{1}{\sqrt{1 - f}} \exp(s\tau_3) \begin{pmatrix}
1 & -f \\
-1 & 1
\end{pmatrix},
\]

(6)
where $\tau_3 = \text{diag}(1, -1)$ is a Pauli matrix, $s$ is free parameter and $f$ is the statistical weight of a physical single particle state within the ensemble. Therefore the number density of the physical particles is

$$n = \frac{f}{1 - f}.$$  

(7)

We find, that the following considerations are extremely simplified by choosing $s = 1/2 \log(1 + n) = -1/2 \log(1 - f)$, since then the Bogoliubov transformation is linear in the density parameter

$$B = \begin{pmatrix} 1 + n & -n \\ -1 & 1 \end{pmatrix}.$$  

(8)

3 Interacting Boson field

We now consider a fully interacting bosonic quantum field. At finite temperature the irreducible representations of the space-time symmetry group are characterized by two rather than one continuous parameter \[3, 10\]. Hence, the interacting field can be expand into modes with definite energy and momentum as

$$\phi(x) = \int_0^\infty dE \int \frac{d^3k}{\sqrt{(2\pi)^3}} \rho^{1/2}(E, k) \phi_{E, k}(x)$$  

(9)

The commutation relation of these fields are, in general, not known. However, we want to calculate only the two-point Green function of the interacting field, i.e. it is sufficient to know the expectation value of the commutator of these fields.

This expectation value in turn can be absorbed in the definition of the weight function $\rho(E, k)$, i.e. for the field operators we can define

$$\bigg\langle [\phi_{E, k}(t, x), \partial_t \phi_{E', k'}(t', x')] \bigg\rangle = e^{i(k(x - x'))} 2E \delta(E - E') \delta(k - k').$$  

(10)

In other words, for the calculation of bilinear expectation values of interacting fields it is sufficient to consider the $\phi_{E, k}(x)$ as generalized free fields \[10\]. The full information about the single-particle spectrum of the theory is contained in the weight function $\rho(E, k)$, and we require the normalization

$$\int dE^2 \rho(E, k) = 1.$$  

(11)
Note, that the existence of this spectral decomposition is only guaranteed in case the system is space-time translation invariant, i.e., if it is in a thermal equilibrium state.

We now apply the thermal quasi-particle concept to each energy-momentum eigenmode of the system, i.e. we define quasi-particle operators \( \xi_{E,k} \) associated with energy-momentum eigenstates and annihilating the statistical state vectors as in (4). These are then Bogoliubov transformed into physical particle operators for definite energy and momentum, and those are summed with the above weight function to operators \( a_k(t) \) such that the interacting field is

\[
\phi(x) = \int \frac{d^3k}{\sqrt{(2\pi)^3}} \left( a_k^\dagger(t) e^{-ikx} + a_k(t) e^{ikx} \right)
\]  

(12)

(note the absorption of the usual energy normalization factor into the operators). In this expansion of course, the ”creation” and ”annihilation” operators are quite complex objects. From the above reasoning, i.e. their decomposition into the modes of definite energy and momentum, we then obtain

\[
\langle \langle O(\beta) \| a_k^{(a)}(t) \ a_k^{(b)}(t') \| O(\beta) \rangle \rangle = \delta^3(k - k') \int dE \rho(E, k) \left( \tau_3 B^T(n_{E,k}) \tau_3 \right)^{-1} e^{-iE(t-t')}
\]

\[
\langle \langle O(\beta) \| a_k^{(a)}(t) \ a_k^{(b)}(t') \| O(\beta) \rangle \rangle = \delta^3(k - k') \int dE \rho(E, k) \left( B(n_{E,k}) \right)^{-1} \left( \tau_3 B(n_{E,k}) \tau_3 \right) e^{-iE(t-t')}.
\]

(13)

The parameter \( n_{E,k} \) defining the individual Bogoliubov transformations thus appears under the energy integral. While this result can be understood intuitively, i.e. every mode is in thermal equilibrium with the rest of the system, it can also be understood in a more formal way.

To this end one has to look at the time evolution of initially free particle operators: it is highly nonlinear. Therefore the Bogoliubov transformation in interacting systems is non-linear, and this non-linearity is reflected in the above...
energy integral. It is indeed possible to derive the above equation without ever touching the concept of generalized free fields [11].

Note, that in our notation the weight function $\rho$ has only support for positive energy arguments. The retarded and advanced propagator are in momentum space

$$D^{R,A}(E, k) = \int dE' \rho(E', k) \left( \frac{1}{E - E' \pm i\epsilon} - \frac{1}{E + E' \pm i\epsilon} \right), \quad (14)$$

and the limit of free particles is recovered when

$$\rho(E, k) \rightarrow \delta(E^2 - \omega_k^2)\Theta(E). \quad (15)$$

We then obtain for the propagator matrix

$$D^{(ab)}(t, t'; k) = -i \int dE \rho(E, k) \times \left( (B(n_{Ek}))^{-1} \begin{pmatrix} \Theta(t - t') & -\Theta(t' - t) \\ -\Theta(t - t') & \Theta(t' - t) \end{pmatrix} B(n_{Ek}) \tau_3 e^{-iE(t-t')} + \tau_3 B^T(n_{Ek}) \begin{pmatrix} \Theta(t' - t) & -\Theta(t - t') \\ -\Theta(t' - t) & \Theta(t - t') \end{pmatrix} (B^T(n_{Ek}))^{-1} e^{iE(t-t')} \right). \quad (16)$$

This is a straightforward generalization of the result from ref. [15]. In the free-particle limit, the textbook result for the finite temperature boson propagator is recovered.

The above expression is still somewhat unsatisfactory, since the $B$-matrices are subject to an energy integration. However, because of the special form (8) we chose for the parametrization, the integrand is linear in the parameter $n_{Ek}$. Thus the integration can be carried out if one defines

$$\bar{N}(t, t') = \frac{1}{Z(t, t')} \int dE \rho(E, k) n_{Ek} \left( e^{-iE(t-t')} + e^{iE(t-t')} \right) \quad (17)$$

$$Z(t, t') = \int dE \rho(E, k) \left( e^{-iE(t-t')} + e^{iE(t-t')} \right).$$
Some elementary matrix operations then lead to the result for the propagator

\[ D^{(ab)}(t, t'; k) \]

\[ = -i Z(t, t') (B(\bar{N}(t, t')))^{-1} \begin{pmatrix} \Theta(t - t') & -\Theta(t' - t) \\ -\Theta(t' - t) & \Theta(t - t') \end{pmatrix} B(\bar{N}(t, t')) \tau_3 \]

\[-i Z^*(t, t') \tau_3 B^T(\bar{N}(t, t')) \begin{pmatrix} \Theta(t' - t) & -\Theta(t - t') \\ -\Theta(t - t') & \Theta(t' - t) \end{pmatrix} (B^T(\bar{N}(t, t')))^{-1}.\]

(18)

Here we have kept positive and negative energy states separate: the inner propagator matrices are diagonal in this case. One can, however, also combine the two parts into one triangular inner matrix, sandwiched between two Bogoliubov matrices:

\[ D^{(ab)}(t, t'; k) \]

\[ = (B(\bar{N}(t, t')))^{-1} \times \]

\[ \begin{pmatrix} -i \Theta(t - t') (Z(t, t') - Z^*(t, t')) & i (1 + 2 \bar{N}(t, t')) Z^*(t, t') \\ i \Theta(t' - t) (Z(t, t') - Z^*(t, t')) & -i \Theta(t' - t) (Z(t, t') - Z^*(t, t')) \end{pmatrix} \]

\[ \times B(\bar{N}(t, t')) \tau_3. \]

(19)

The physical relevance of the function \( \bar{N}(t, t') \) diagonalizing the propagator becomes obvious, when we consider its equal time limit. It approaches a constant then,

\[ \lim_{t' \to t} \bar{N}(t, t') = N^H_k \quad \lim_{t' \to t} \frac{\partial}{\partial t} \bar{N}(t, t') = 0. \]

(20)
Comparison to (13) gives
\[ N_k^H = \frac{\int dE \rho(E, \mathbf{k}) n_{Ek}}{\int dE \rho(E, \mathbf{k})} = \lim_{t'-t\to0} \frac{\int d^3\mathbf{k} \langle \langle O(\beta) | a_k^\dagger(t) a_{k'}(t') | O(\beta) \rangle \rangle}{\int dE \rho(E, \mathbf{k})}. \] (21)

In other terms, \( N_k^H \) is the time-independent equilibrium Heisenberg density of the physical particles with momentum \( \mathbf{k} \). The quantity \( \bar{N}(t, t') \) therefore is the observable fluctuating particle number of these modes.

The separate diagonality of the inner matrices of the propagator, i.e. the requirement of unperturbed statistical quasi-particle propagation, is therefore equivalent to choosing the correct physical Bogoliubov parameter.

4 Conclusions

The concept of quasi-particles in statistical physics is known for some time [12], and it is also known that a linear relation between the matrix elements of an interacting propagator can be used to bring it to a triangular \( 2 \times 2 \) matrix form [17]. We have put these two things together and introduced statistical quasi-particles into Thermo Field Dynamics. This leads to a diagonal propagator for nonrelativistic models [16].

When negative energy states are taken into account, the full propagator can also be written as diagonal matrix sandwiched among Bogoliubov matrices, but separately so for particle and anti-particle states [11]. Their combination then gives a triangular inner propagator matrix, see eqn. (19). We find, that the Bogoliubov transformation necessary for this diagonalization is given in terms of a physical parameter, the observable fluctuating particle density \( \bar{N}(t, t') \). This diagonalization also defines stable physical modes with fixed momentum and an average energy [18].

While this is clearly a conceptual advantage, the diagonalization of the full propagator at finite temperature also has a tremendous technical advantage over the CTP formalism. In effect our method separates the statistical information about the system (boundary conditions, thermal particle-hole excitation etc.) from the purely spectral information contained in the weight function \( \rho(E, \mathbf{k}) \). Let us note, that the same separation can be achieved for non-equilibrium systems.
The application of the quasi-particle concept to a given system not only demonstrates this technical advantage, but lends a physical interpretation of the $2 \times 2$ matrix structure of thermal quantum theories \[1, 3\]. For brevity we only state the results: Requiring, that the triangular propagator \[13\] solves the diagonal components of a Schwinger-Dyson equation gives \(\rho(E, k)\) as function of real and imaginary part of a retarded self energy function.

The off-diagonal component of the Schwinger-Dyson equation contains the statistical information, i.e. it is a consistency criterion for the function \(\tilde{N}(t, t')\). For the time-independent case considered here, we were able to derive this consistency criterion as the condition of global thermal equilibrium. For non-equilibrium systems, where a similar separation of statistical and "spectral" information can be obtained, the diagonalization condition for the propagator is nothing but a transport equation \[11\].

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