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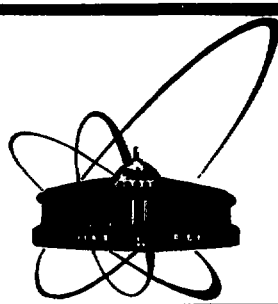

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NONEQUILIBRIUM STATISTICAL AVERAGES AND THERMO FIELD DYNAMICS

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1. INTRODUCTION

The extension of the methods of the Quantum Field Theory to Quantum Statistical Mechanics is a long-standing problem to which many works have been devoted.

The imaginary-time formalism, developed by Matsubara[1] to study systems in thermal equilibrium, has given only partial answers to the problem. In fact, it is well known that it permits the direct computation, through Feynman diagrammatic techniques, only of the imaginary-time Green functions; the real-time Green functions have to be computed by analytic continuation. Thus, the formalism applies successfully to direct computation of static quantities, but proves less useful in the analysis of time-dependent quantities.

Furthermore the Matsubara formalism does not permit one to obtaine the QFT as limit for $T \to 0$. This makes it difficult to obtain low temperature expansions and leaves completely unsolved the problems of regularization and renormalization at $T \neq 0$. To overcome the above-mentioned difficulties other methods have been introduced, in particular the Closed-Time Path (CTP) formalism[2-5] and for systems in thermal equilibrium, the Thermo Field Dynamics[6] (TFD) which work directly in terms of real-time. Both methods entail a diagrammatic perturbative theory, in terms of causal Green's functions, realized by doubling the degrees of freedom of the field.

It is worth mentioning that from the axiomatic point of view a quantum field theory of free field at finite temperature requires the doubling of the number of degrees of freedom; this fact is well known to physicists who work on the Liouville equations[7]. In recent papers[8] the relations among the Matsubara method, the CTP formalism and TFD have been analyzed. The complete equivalence between TFD and CTP formalism has been proved for systems in thermal equilibrium. Besides, TFD permits to study regularization and renormalization at $T \neq 0$, yielding temperature independent[9] counterterms. In conclusion, at present, the extension of Quantum Field Theory methods to Quantum Statistical Mechanics can be considered accomplished for what concerns systems in thermal equilibrium.

Some questions are instead still open in the study of non-equilibrium statistical Green's functions, in spite of some results obtained recently[4] with the CTP formalism.

An extension of TFD to the study of nonequilibrium systems seems therefore of interest. The aim of this work is to show, by analyzing a very simple nonequilibrium problem, how a possible extension of TFD to nonequilibrium situation can be realized. We shall analyze with the TFD formalism the classic problem of the brownian motion of a quantum oscillator.

The central idea of TFD is the introduction of the Bogolubov transformation which, once the degrees of freedom are doubled, transforms the physical vacuum at $T = 0$ in a new temperature dependent state $|\beta>$ which can be considered as the physical ground state for systems in thermal equilibrium at $T = 0$. The Bogolubov transformation works here as in super-conductivity, when used to obtain the BCS ground-state. The Cooper pairs are here substituted with thermal pairs formed by putting together each degree of freedom of the field with its doubled counterpart. In the following we shall show that in order to extend TFD to nonequilibrium systems, we have to distinguish between two different situations:

a) stationary systems out of equilibrium for which a generalized fluctuation and dissipation theorem is valid;

b) time-dependent statistical averages.

Our main results are the following:

1) The extension of TFD to stationary systems can be accomplished straight by introducing a new Bogolubov transformation, whose coefficients are fixed by the generalized fluctuation-dissipation theorem.

2) The description of time-dependent statistical averages can be accomplished by using a statistical mixture of states at different temperatures. Therefore, in order to study time-dependent averages we introduce a representation of matrix density in terms of the $|\beta>$ states.

In Part 2, reanalyzing the Bogolubov transformation for quantum oscillators in thermal equilibrium, we show how to extend the TFD to stationary systems.

In Part 3 we extend our formalism to describe a damped quantum oscillator. We show that damping does not affect the Bogolubov transformation.

Part 4 is devoted to the study of the approach to equilibrium of a damped oscillator. The correct two-point Green function is obtained by using a statistical mixture of states at different temperatures.

PART 2. The aim of this section is to rederive the Bogolubov transformation, which connects the vacuum state at $T = 0$ with the ground state at $T \neq 0$ of a quantum oscillator in thermal equilibrium by using the fluctuation-dissipation theorem. This derivation allows us a straight extension of TFD to stationary systems satisfying a generalized fluctuation-dissipation theorem. Let us recall shortly the main steps of the TFD formalism. One

considers a quantum system with one degree of freedom described by the Hamiltonian $H = \omega a^+ a$. It is assumed that the operators a, a^+ satisfy the usual commutation relations $[a, a^+] = 1$; $[a, a] = 0$; $[a^+, a^+] = 0$. The quantities of interest are the thermal equilibrium averages of any operator $O(a^+, a)$ that we denote as

$$\ll O(a^+, a) \gg = \mathrm{Tr} O(a^+, a)\, e^{-\beta(H-\mu N)} / \mathrm{Tr}\, e^{-\beta(H-\mu N)}. \qquad (1)$$

The aim of TFD is to express the average (1) as a single matrix element on a suitable temperature-dependent state $|\beta>$

$$\ll O(a^+, a) \gg = \ll \beta | O(a^+, a) | \beta >. \qquad (2)$$

To achieve this result it is necessary to double the degrees of freedom by introducing in correspondence of a and a^+ the tilde operator $\tilde{a}$ and $\tilde{a}^+$ which form thermal doublets

$$\begin{pmatrix} a \\ \tilde{a}^+ \end{pmatrix} ; \begin{pmatrix} a^+ \\ \tilde{a} \end{pmatrix} . \qquad (3)$$

The dynamics is determined by the Hamiltonian

$$\hat{H} = \omega a^+ a - \omega \tilde{a}^+ \tilde{a} . \qquad (4)$$

In general

$$\hat{H} = H(a^+, a) - H(a^+, a), \qquad (5)$$

where the $\sim$ operation means.

$$O(a^+, a) = O^*(\tilde{a}^+, \tilde{a}); \quad O_1 O_2 = \tilde{O}_1 \tilde{O}_2 ; \quad \tilde{\tilde{O}}_1 = O_1 . \qquad (6)$$

Here* denotes a complex conjugate. The operators $\tilde{a}^+, \tilde{a}$ commute with the operators a^+, a and satisfy the commutation relations

$$[\tilde{a}, \tilde{a}^+] = 1, \quad [\tilde{a}, \tilde{a}] = [\tilde{a}^+, \tilde{a}^+] = 0 . \qquad (7)$$

The Fock space is spanned by the vectors

$$|n m> = |n> \bullet |m> = \frac{(a^+)^n}{n!} \frac{(\tilde{a}^+)^m}{m!} |0, \tilde{0}> , \qquad (8)$$

a^+, $\tilde{a}^+$ and the conjugate operators a, $\tilde{a}$ are the creation and annihilation operators on the vacuum state $|0, \tilde{0}> = |0> \bullet |\tilde{0}>$. The Fock space so obtained is the physical space (in-space) for the system at $T = 0$. According to the TFD, in order to describe the

system at $T \neq 0$, we have to construct a new Fock space, which is the physical space corresponding to the new boundary conditions ($T \neq 0$). This can be accomplished in analogy with what is done in presence of quantum condensation (superconductors, superfluids,...) by a suitable Bogolubov transformation which transforms the state $|0\tilde{0}\rangle$ (physical vacuum at $T = 0$) in the new temperature-dependent state $|\beta\rangle$ and preserves the equations of the motion and the commutation relations. The state $|\beta\rangle$ is the appropriate ground state for the description of the systems at $T \neq 0$. The expectation values of any operator on this state coincide with the thermal average.

In the framework of TFD it is assumed that $|\beta\rangle$ is a condensed state of the couples $\tilde{a}a$ and $\tilde{a}^{+}a^{+}$. Set there

$$L = i\Theta(a\tilde{a} - a^{+}\tilde{a}^{+}), \tag{9}$$

where Θ is a real function of temperature, one defines:

$$|\beta\rangle = e^{iL}|0\tilde{0}\rangle, \quad e^{iL}a(t)e^{-iL} = \alpha(t), \quad e^{iL}a^{+}(t)e^{-iL} = \alpha^{+}(t). \tag{10}$$

The operators $\tilde{\alpha}, \tilde{\alpha}^{+}$ are obtained by using the $\sim$ operation. The set of operators α, α^{+}, $\tilde{\alpha}$, $\tilde{\alpha}^{+}$ satisfies the same dynamic and the same commutation relations as the set a, a^{+}, $\tilde{a}$, $\tilde{a}^{+}$. They are annihilation and creation operators on the state $|\beta\rangle$

$$\alpha|\beta\rangle = \tilde{\alpha}|\beta\rangle = 0. \tag{11}$$

We note that the equations (10) can be written as follows

$$\alpha(t) = g_1 a(t) + g_2\tilde{a}^{+}(t), \quad \alpha^{+}(t) = g_1 a^{+}(t) + g_2\tilde{a}(t). \tag{12}$$

The inverse formulas are

$$\alpha(t) = g_1\alpha(t) - g_2\tilde{a}^{+}(t), \quad a^{+}(t) = g_1\alpha^{+}(t) - g_2\tilde{\alpha}(t), \tag{13}$$

with

$$g_1 = \cosh\Theta; \quad g_2 = \sinh\Theta. \tag{14}$$

In previous works the function Θ was determined by the requirement that the equations (2) were satisfied. We observe that Θ can be fixed more generally by requiring that the fluctuation-dissipation theorem is satisfied. This implies the well-known relation between the commutator and the anticommutator of the a, a^{+} operators

$$\langle\beta|[a(t), a^{+}(t')]_{-}|\beta\rangle(2n_\beta - 1) = \langle\beta|[a(t), a^{+}(t')]_{+}|\beta\rangle, \tag{15}$$

where in the case under consideration

$$n_\beta = \frac{1}{1 - \exp[-\beta(\omega - \mu)]} \tag{16}$$

is the equilibrium distribution function for the quantum oscillator at the temperature $kT = 1/\beta$.

From (13), (14) and (15) we have

$$g_2^2 = \sinh^2\Theta = n_\beta - 1; \quad g_1^2 = \cosh^2\Theta = n_\beta. \tag{17}$$

The well-known two point Green function is obtained immediately, in fact, from (13)

$$G(t, t') = \langle\langle T(a(t)\, a^+(t'))\rangle\rangle = \langle\beta|T(a(t)\, a^+(t'))|\beta\rangle =$$

$$= [n_\beta \theta(t - t') + (n_\beta - 1)\theta(t' - t)]\, e^{i\omega(t-t')} .$$

More generally we can write the matrix which contains all the two-point functions different from zero

$$\langle\beta|T\left[\begin{pmatrix} a(t) \\ \tilde{a}^+(t) \end{pmatrix} \quad (a^+(t') \;\; \tilde{a}(t'))\right]|\beta\rangle = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}$$

with

$$G_{11} = G_{22} = G(tt'), \quad G_{12} = G_{21} = -\sqrt{n_\beta(n_\beta - 1)}\, e^{i\omega(t-t')}.$$

It is now evident that the derivation of the Bogolubov transformation here presented allows a straight-forward generalization to systems out of equilibrium for which a generalized fluctuation-dissipation theorem is valid. In fact, in this case one can apply the same procedure and fix the Θ function appearing in the Bogolubov transformation by using the appropriate distribution function instead of (16). The application to the case of the one-mode laser is immediate.

PART 3. In this Part, by analyzing a quantum oscillator loosely coupled to a thermal bath, which is essentially a macroscopic system in thermal equilibrium at temperature T, we shall show how the TFD can be generalized to describe systems which present a damping effect during the time evolution.

We write the Lagrangian of the system as

$$L(t) = L_0(a^+, a) + \lambda(a^+ + a)Q + L_{ext.}, \tag{18}$$

where

$$L_0(a^+, a) = a\frac{d}{dt}a^+ - \omega_0 a^+ a \tag{19}$$

is the Lagrangian of the free oscillator; L_{ext}, the Lagrangian of the macroscopic system; $Q(t)$ is an hermitian operator of that system; λ is the coupling constant between the oscillator and the macroscopic system. To analyze this system in the framework of TFD we introduce the tilde operators and write the Lagrangian of the doubled system as

$$\hat{L} = L_0 - \tilde{L}_0 + \lambda(a^+ + a)Q - \lambda(\tilde{a}^+ + \tilde{a})\tilde{Q} + L_{ext} - \tilde{L}_{ext} \quad . \tag{20}$$

We assume that the bath and the oscillator, both in thermal equilibrium at temperature T, are put in contact at the time t = 0.

We are interested only in the behaviour of the oscillator and assume, following Schwinger /2/, that, after performing the thermal average on the variables Q, Q^+, $\tilde{Q}$, $\tilde{Q}^+$ of the macroscopic system in the limit of weak coupling and neglecting the correlation functions of the macroscopic system with more than two points, we obtain the effective Hamiltonian.

$$\hat{H} = (\omega - i\gamma)a^+a - (\omega + i\gamma)\tilde{a}^+\tilde{a} \quad , \tag{21}$$

where

$$\gamma = \frac{\lambda}{2(2n_\beta - 1)} \int dt\, e^{i\omega t} \ll [Q(t), Q(0)]_+ \gg . \tag{22}$$

The operators a, a^+, $\tilde{a}$, $\tilde{a}^+$ satisfy the usual commutation relations; they can be used to construct the Fock space

$$|mn> = \frac{(a^+)^m}{m!} \frac{(\tilde{a}^+)^n}{n!} |0\tilde{0}> . \tag{23}$$

Then, as before, the properties of the damped oscillator in thermal equilibrium at temperature T, will be computed by transforming thermal averages into expectation values on the state $|\beta>$ obtained with the Bogolubov transformation (13) applied to the vacuum of the a fields. In particular, the two-point Green function, keeping in mind (13) and (17), becomes

$$\begin{aligned} G(tt') &= <\beta|T(a(t)\,a^+(t'))|\beta> = \\ &= [n_\beta \theta(t-t') + (n_\beta - 1)\theta(t'-t)]e^{i\omega(t-t')}\ e^{-\gamma|t-t'|} \quad . \end{aligned} \tag{24}$$

This is the correct behaviour /2/ of a quantum oscillator in thermal equilibrium with a bath at temperature T. There is, as expected, a damping in the correlation function. The bath acts as a stochastic force.

The matrix containing all the two point functions is, as before:

$$\hat{G}(t,t') = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} , \tag{25}$$

$$G_{11} = G_{22} = G(tt'), \tag{26}$$

$$G_{12} = G_{21} = -\sqrt{n_\beta (n_\beta - 1)}\, e^{i\omega(t-t')}\, e^{-\gamma|t-t'|} . \tag{27}$$

PART 4. In this Part we show how a problem of approach to equilibrium or, more generally, a time-dependent statistical averages can be treated in the framework of TFD. To describe the procedure, we analyze, as simple example the approach to equilibrium of an oscillator. The system that we consider is the same described previously, but the oscillator, in thermal equilibrium at the temperature T_0, is put at the time $t = 0$ in thermal contact with a bath, which is essentially a macroscopic system in equilibrium at the temperature T_1 different from T_0. In this case statistical averages are time-dependent and cannot be computed as expectation values on a pure state, obtained through a Bogolubov transformation, as before. The boundary conditions are such that the statistical average depends on the two temperatures T_0 and T_1, and on time.

To treat this type of situation we propose to consider the system as a statistical mixture of states at different temperatures.

Thus if we indicate with $|\beta>$ the equilibrium state at temperature $kT = 1/\beta$, the time-dependent averages are expressed as follows:

$$<< O(t_1)\, O(t_2) >>_{n.e.} = \mathrm{Tr}(O(t_1)\, O(t_2)\, \rho(t_4)) , \tag{28}$$

where

$$\rho(t) = \int_{\beta_0}^{\beta_1} |\beta> W(\beta t) <\beta| d\beta . \tag{29}$$

The time-dependent quantity $W(\beta t)$ gives the probability of finding at time t the system in the state at temperature $kT = 1/\beta$; β_0 and β_1 correspond respectively to the initial and final temperatures. The state $|\beta>$ is obtained by using the Bogolubov transformation (10)

$$|\beta> = e^{\Theta(\beta)(a\tilde{a} - a^+\tilde{a}^+)}\, |0\tilde{0}> .$$

It is worth putting into evidence the relation between $W(\beta t)$ and the distribution function; from (28) and (29) we have:

$$n(t) = << a^+(t)\, a(t) >>_{n.e.} = \int_{\beta_0}^{\beta_1} W(\beta t)\, n_\beta\, d\beta , \tag{30}$$

where n_β is the equilibrium distribution function at temperature $kT = 1/\beta$. Let us show how this procedure, when applied to approach to equilibrium of a damped oscillator, gives the correct two-point Green function. In this case it is sufficient to assume that the oscillator can be either in the state at initial temperature T_0 or in the state at the temperature of the bath T_1. Therefore

$$W(\beta t) = w(t)\,\delta(\beta - \beta_0) + (1 - w(t))\,\delta(\beta - \beta_1) \tag{31}$$

and

$$\rho(t) = |\beta_0 > w(t) < \beta_0| + |\beta_1 > w(t) < \beta_1| . \tag{32}$$

In order to fix $w(t)$ we use the equation (30)

$$w(t) = (n(t) - n_{\beta_1})/(n_{\beta_0} - n_{\beta_1}), \tag{33}$$

where n_{β_0}, n_{β_1} are respectively the equilibrium distribution functions for the oscillator at the initial and final temperature.

By remembering /2/ that for the damped oscillator $n(t) = n_{\beta_1} + (n_{\beta_0} - n_{\beta_1}) e^{-2\gamma t}$ we have

$$w(t) = \exp(-2\gamma t). \tag{34}$$

The computation of the two-point Green function is immediate; infact by using (24), (28), (32) and (34) we have:

$$G(tt') = e^{i\omega(t-t')} e^{-\gamma|t-t'|} \left[n_{\beta_1}\theta(t-t') + (n_{\beta_1} - 1)\theta(t'-t) \right] + (n_{\beta_0} - n_{\beta_1})\, e^{-\gamma(t+t')} . \tag{35}$$

The matrix, containing all the two-point Green functions different from zero, is

$$\hat{G}(tt') = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}$$

where

$$G_{11} = G_{22} = G(tt'),$$

$$G_{12} = G_{21} = -\exp[i\omega(t-t')] \cdot \left[\sqrt{n_{\beta_1}(n_{\beta_1} - 1)}\, \exp(-\gamma|t-t'|) + \left(\sqrt{n_{\beta_0}(n_{\beta_0} - 1)} - \sqrt{m_{\beta_1}(n_{\beta_1} - 1)} \right) \exp(-\gamma(t+t')) \right] .$$

In conclusion, the procedure proposed to computation of time-dependent statistical average gives the correct two-point Green function for the damped oscillator. A simple extension can be used to compute two-point Green functions of free particles. The extension to the study of interacting particles system and n-point Green functions is not trivial; work in this direction is in progress.

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