Prog. Theor. Phys. Vol. 74, No, 2, August 1985, Progress Letters

# A General Formulation of Nonequilibrium Thermo Field Dynamics

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(Received April 22, 1985)

A fundamental framework for construction of a quantum field theory for open systems is built on two basic concepts; *the coarse graining* realized by the projection operator method of the damping theory, and of *the thermal state*, a fundamental concept in the thermo field dynamics.

*Coarse graining* is a fundamental concept in a microscopic theory of open systems, especially in non-stationary and nonequilibrium situations in which certain dissipation process takes place or need of projecting out some irrelevant subsystems arises. Among many formulations available,[1)~5)] we find the projection operator method of the damping theory[1)~3)] quite suitable to our purpose of constructing a field theoretical framework for open systems. As it has been shown by several examples,[6)] the coarse graining of irrelevant subsystems in addition to that of reservoir systems can be well formulated in terms of the *time-convolution-less* (TCL) formulation of the damping theory.[2),3)]

As for the equilibrium situation, the so-called thermo field dynamics (TFD)[7),8)] extends the usual quantum field theory to the one at finite temperature, preserving many properties of the usual quantum field theory, e.g., the operator formalism, the time-ordered formulation of the Green's functions, the Feynman diagram method in real time, etc. A central concept in TFD[7),8)] is *the thermal states* which describe equilibrium states and form a linear vector space. This space is built on a vacuum state which will be called *the thermal vacuum state.* The statistical average is given by the thermal vacuum state expectation value.

In this note we will present a framework for construction of a quantum field theory for open systems by combining the concepts of *the coarse graining* and *the thermal state.* The Liouville equation is mapped on the Liouville space[9)] through a use of the superoperator method,[10)] and the reservoir variables are projected out by the damping theory.[1)~3)] The thermal state condition at time $t$ determines *the quasi-particle superoperators* and *the thermal vacuum state* for the non-stationary and nonequibrium situation, and leads to a quantum field theory for open systems. Only a brief outline of fundamental framework of the theory will be presented here; a detailed account will be published elsewhere.[11)]

The Liouville space[9)] can be spanned by a complete orthonormal basis $\{|mn\rangle\rangle = \| m\rangle\langle n|\rangle\rangle\}$, which satisfies

$$\langle\langle mn|m'n'\rangle\rangle = \delta_{mm'}\delta_{nn'}, \quad \sum_{mn}|mn\rangle\rangle\langle\langle mn| = \hat{1}\,, \tag{1}$$

where $\langle\langle mn| = |mn\rangle\rangle^\dagger = \langle\langle(|m\rangle\langle n|)^\dagger| = \langle\langle |n\rangle\langle m\||$, and $\{|n\rangle = |n_1, n_2\cdots\rangle\}$ is a complete orthonormal basis of the Hilbert space which is generated by cyclic operations of the creation operators $a_i^\dagger$ on the vacuum $|0\rangle$. These operators obey the commutation relations $[a_i, a_j^\dagger]_\sigma = \delta_{ij}$, and $[a_i, a_j]_\sigma = [a_i^\dagger, a_j^\dagger]_\sigma = 0$, where $[A, B]_\sigma = AB - \sigma BA$, and $\sigma = +1(-1)$ for boson (fermion). An element $|A\rangle\rangle$ of the Liouville space can be expanded as

$$|A\rangle\rangle = \sum_{mn}|mn\rangle\rangle\langle\langle mn|A\rangle\rangle,$$
$$\langle\langle mn|A\rangle\rangle = \langle m|A|n\rangle\,, \tag{2}$$

and the scalar product in the Liouville space reduces to

$$\langle\langle A|B\rangle\rangle = \mathrm{Tr}AB, \quad \langle\langle A| \equiv (|A^\dagger\rangle\rangle)^\dagger\,. \tag{3}$$

Following Schmutz,[10)] we define a special set of the superoperators $a_i$, $\tilde{a}_i$ (in the following we use the same notation for the superoperator $a_i$ as the ordinary operator $a_i$) by

$$a_i|mn\rangle\rangle = |a_i|m\rangle\langle n|\rangle\rangle,$$
$$\tilde{a}_i|mn\rangle\rangle = \sigma^{\mu+1}\| m\rangle\langle n|a_i^\dagger\rangle\rangle \tag{4}$$

with $\mu = \sum_i(m_i - n_i)$, where we have used the particle-number eigenstates for $\{|n\rangle : a_i^\dagger a_i|n\rangle = n_i|n\rangle$. By using (3) we get

$$a_i^\dagger|mn\rangle\rangle = |a_i^\dagger|m\rangle\langle n|\rangle\rangle,$$
$$\tilde{a}_i^\dagger|mn\rangle\rangle = \sigma^\mu\| m\rangle\langle n|a_i\rangle\rangle\,. \tag{5}$$

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From (4) and (5), we obtain the commutation relations between the superoperators as $[a_i, a_j^\dagger]_\sigma = [\tilde{a}_i, \tilde{a}_j^\dagger]_\sigma = \delta_{ij}$, while the other commutation relations vanish.

From (4) and (5), we obtain

$$|a_i\rangle\rangle = a_i|1\rangle\rangle = \tilde{a}_i^\dagger|1\rangle\rangle,$$
$$|a_i^\dagger\rangle\rangle = a_i^\dagger|1\rangle\rangle = \sigma\tilde{a}|1\rangle\rangle, \qquad (6)$$

where $|1\rangle\rangle = \Sigma_n|nn\rangle\rangle = \exp(\Sigma_i a_i^\dagger \tilde{a}_i^\dagger)|00\rangle\rangle$, by using the completeness relation $\Sigma_n|n\rangle\langle n| = 1$.

The double-tilde conjugation rule follows from (4) and (5) as $\tilde{\tilde{a}}_i = \sigma a_i$, $\tilde{\tilde{a}}_i^{\dagger\prime\prime} = \sigma a_i^\dagger$. It should be noted that we can modify the choice of phase factors in (4) and (5) in such a manner that $\tilde{\tilde{a}}_i = a_i$, etc. hold.[12),8)] However, in this note we proceed with the choice in (4) and (5).

By applying the mapping rules (4) and (5) to the Liouville equation for a system with a reservoir, we obtain a "Schrödinger equation" in the Liouville space. Then we apply the TCL formulation of the damping theory[2),3)] (which is more suitable to the treatment of non-stationary and nonequilibrium states than the time-convolution (TC) formulation of the damping theory[1)] to this "Schrödinger equation" in order to project out the reservoir variables; the result is a "master equation" in the Liouville space. When we are interested in a still smaller subsystem, we can further apply the TCL formulation of the damping theory to this "master equation" to eliminate still more partial subsystems in order to obtain a "master equation" for the subsystem which we are interested in.[3)] However, in this paper we confine ourselves to the first step, i.e., reduction of the reservoir variables only. A formulation of the second step[3)] (i.e., further reduction of partial subsystems, in terms of the superoperators) and its application to some practical problems[6)] will be given in separate publications.

After projecting out the reservoir variables, we obtain the "master equation" in the form ($\hbar=1$, $k_B=1$)

$$\partial_t|W_S(t)\rangle\rangle = -i\hat{H}|W_S(t)\rangle\rangle, \quad \hat{H} = \hat{H}_S + i\hat{\Pi}, \qquad (7)$$

$$\hat{\Pi} = i\Delta\hat{H}_S - \int_0^\infty dt\langle\langle 1_R|\hat{H}_{SR}(t)\hat{H}_{SR}(0)|W_R\rangle\rangle$$
$$= -\sum_k \chi_k[(1+2\bar{n}_{\sigma k})(a_k^\dagger a_k + \tilde{a}_k^\dagger\tilde{a}_k)$$
$$-2(1+\bar{n}_{\sigma k})\tilde{a}_k a_k - 2\bar{n}_{\sigma k}\tilde{a}_k^\dagger a_k^\dagger] - 2\sum_k \chi_k\bar{n}_{\sigma k}, \qquad (8)$$

where $H_S$ describes the Hamiltonian of the system, $H_{SR}$ the interaction between the reservoir and the system, and

$$\chi_k = \mathrm{Re}\ \lambda_k^2\int_0^\infty dt\langle\langle 1_R|R_k(t)$$
$$\times[R_k^\dagger(0) - \tilde{R}_k(0)]|W_R\rangle\rangle e^{i\varepsilon_k t}, \qquad (9a)$$
$$\bar{n}_{\sigma k} = \sigma[\exp(\beta\varepsilon_k) - \sigma]^{-1}, \quad \beta = 1/T \qquad (9b)$$

with $T$ being the temperature of the reservoir and $\varepsilon_k$ the quasi-particle energy including the chemical potential of the reservoir. Recall the rule in the equilibrium TFD that $\hat{H}$ has the form $(H\text{-}\tilde{H})$. This rule does not hold in the nonequilibrium TFD as is seen from (8). We have put $\hat{H}_{SR} = \Sigma_k\lambda_k(a_kR_k^\dagger + R_ka_k^\dagger - \tilde{a}_k\tilde{R}_k^\dagger - \tilde{R}_k\tilde{a}_k^\dagger)$, where the reservoir operator $R_k$ is assumed to be a boson (fermion)-like operator when $a_k$ is a boson (fermion). The time evolution of the reservoir operator $R_k(t)$ is generated by the Hamiltonian, $H_R$, of the reservoir, the explicit form of which does not need to be specified in the following formulation. It is worth while to note that the reservoir correlation functions, which determine $\chi_k$ in (9a), can be calculated systematically by TFD[13)] within the conventional linear response theory[14)] when $H_R$ is specified. The state $|W_S(t)\rangle\rangle$ is constructed by the density operator $W_S(t)$ of the system which is an ordinary operator, and the state $|W_R\rangle\rangle$ is constructed by the grand canonical density operator $W_R$ of the reservoir with temperature $T$. The state $\langle\langle 1_R|$ is spanned only in the Liouville space of the reservoir. We have used the fact that the density operator is a boson-like operator in general. It should be noted that $\hat{H}$ satisfies the relation $i\hat{H} = (i\hat{H})^\sim$ which relates to the hermitisity of $W_S(t)$.

In deriving (7) we have assumed that the reservoirs of different modes are independent, that $\langle\langle 1_R|\hat{H}_{SR}|W_R\rangle\rangle = 0$, that the density operator of the total system is factorized as $W_S(t_0)W_R$ at $t = t_0$, and that the correlation time of the reservoir is much shorter than the time we are interested in. Furthermore, for simplicity we have considered a translationally invariant reservoir.

The Heisenberg representation of a superoperator $\hat{A}$ is defined by $\hat{A}(t) = \hat{S}^{-1}(t-t_0)\hat{A}\hat{S}(t-t_0)$, $\hat{S}(t) = \exp(-i\hat{H}t)$, because this together with $|W_S(t)\rangle\rangle = \hat{S}(t-t_0)|W_S(t_0)\rangle\rangle$ leads to $\langle\langle 1|\hat{A}|W_S(t)\rangle\rangle = \langle\langle 1|\hat{A}(t)|W_S(t_0)\rangle\rangle$. Here use has been made of the relation $\langle\langle 1|\hat{H} = 0$ which follows from explicit computation uning (8) and implies the conservation of the probability. It should be noted that the time evolution of the mirror operator[3] is generated by $\hat{S}^\dagger(t)$. A further investigation of the relation between the mirror operation and the superoperator will be given in a forthcoming paper.

Let us now extend the thermal state condition of the equilibrium TFD[7),8)] to nonequilibrium situation. We do this by using the interaction representation (i.e., the perturbative expansion). Then, $\hat{H}_S$ in the unperturbed Hamiltonian becomes the free Hamiltonian although $\hat{\Pi}$ *remains as it is in* (8). The operators $a$ and $\tilde{a}$ in this representation will be said to be *semi-free.* In this case $a_k$ is a linear sum of $a_k(t) \equiv \hat{S}^{-1}(t-t_0)a_k\hat{S}(t-t_0)$ and $\tilde{a}_k{}^{\dagger\dagger}(t) \equiv \hat{S}^{-1}(t-t_0)\tilde{a}_k{}^\dagger\hat{S}(t-t_0)$. The thermal state condition requires the knowledge of the initial density matrix $W_S(t_0)$. In this note we consider a simple case in which $a|W_S(t_0)\rangle\!\rangle = f\tilde{a}^\dagger|W_S(t_0)\rangle\!\rangle$ with a $c$-number $f$. This condition is satisfied, for example, when the initial state is in equilibrium. Then the thermal state condition at time $t$ reads as

$$\gamma_k(t)|W_S(t_0)\rangle\!\rangle = 0, \quad \langle\!\langle 1|\tilde{\gamma}_k{}^{\dagger\dagger}(t) = 0, \tag{10}$$

where

$$\gamma_k(t) = z_k{}^{1/2}(t-t_0)[a_k(t) - f_k(t-t_0)\tilde{a}_k{}^{\dagger\dagger}(t)], \tag{11a}$$

$$\tilde{\gamma}_k{}^{\dagger\dagger}(t) = z_k{}^{1/2}(t-t_0)[\tilde{a}_k{}^{\dagger\dagger}(t) - \sigma a_k(t)] \tag{11b}$$

with a $c$-number function $f_k(t-t_0)$. The superoperators $\gamma_k{}^{\dagger\dagger}(t)$ and $\tilde{\gamma}_k(t)$ are given by the tilde conjugation of (11). The normalization factor $z_k{}^{1/2}(t-t_0)$ is determined by the "canonical commutation relation" $[\gamma_k(t), \gamma_l{}^{\dagger\dagger}(t)]_\sigma = [\tilde{\gamma}_k(t), \tilde{\gamma}_l{}^{\dagger\dagger}(t)]_\sigma = \delta_{kl'}$, etc. The result is $Z_k(t) = 1 + n_{\sigma k}(t)$ with the definition $n_{\sigma k}(t) = \sigma f_k(t)/[1-\sigma f_k(t)]$. The operators $\gamma_k(t)$, $\tilde{\gamma}_k{}^{\dagger\dagger}(t)$, etc., will be called *the quasi-particle superoperators.* As is seen from (10), in our formulation, $|W_S(t_0)\rangle\!\rangle$ and $\langle\!\langle 1|$ can be interpreted as *the thermal vacuum state.*

When we rewrite $a(t)$ and $\tilde{a}^{\dagger\dagger}(t)$ in terms of the quasi-particle superoperators $\gamma(t)$ and $\tilde{\gamma}^{\dagger\dagger}(t)$, the Wick-type formula for nonequilibrium system immediately follows from (10). This Wick-type formula leads to the Feynman-type diagrams for multi-time Green's functions in the interaction representation. We then obtain the Feynman-type diagram method for perturbative calculations for non-stationary and non-equilibrium statistical mechanical problems when a perturbative interaction is istroduced in $\hat{H}_S$. The perturbative calculation leads us to an expression of the Heisenberg operators in terms of product of quasi-particle superoperators. This is an extension of the concept of dynamical map in the usual quantum field theory to non-equilibrium situations.

The two-point Green's function of the semi-free field is the basic element of the Feynman diagram. It can be given by the Wick formula. The result is

$$\begin{aligned} G_k{}^{\alpha\beta}(t,s) &= -i\langle\!\langle 1|T[a_k{}^\alpha(t)\bar{a}_k{}^\beta(s)]W_S(t_0)\rangle\!\rangle \\ &= [I_{\bar{\sigma}}W_K(t-t_0)\mathcal{G}_k(t,s) \\ &\quad \times W_K{}^{-1}(s-t_0)I_\sigma]^{\alpha\beta}, \end{aligned} \tag{12}$$

where $a_k{}^1(t) = a_k(t)$, $a_k{}^2(t) = \bar{a}_k{}^{\dagger\dagger}(t)$, $\bar{a}_k{}^1(t) = a_k{}^{\dagger\dagger}(t)$, $\bar{a}_k{}^2(t) = -\sigma\tilde{a}_k(t)$ and

$$\mathcal{G}_k{}^{\alpha\beta}(t,s) = \begin{pmatrix} Z_k{}^{1/2}(s-t_0)Z_k{}^{-1/2}(t-t_0)G_k{}^r(t-s), & 0 \\ 0, & Z_k{}^{1/2}(t-t_0)Z_k{}^{-1/2}(s-t_0)G_k{}^a(t-s) \end{pmatrix} \tag{13}$$

with

$$G_k{}^r(t) = -i\theta(t)\exp[-i(\varepsilon_k - i\chi_k)t], \tag{14a}$$

$$G_k{}^a(t) = i\theta(-t)\exp[-i(\varepsilon_k + i\chi_k)t]; \tag{14b}$$

$$W_k{}^{\alpha\beta}(t) = Z_k{}^{1/2}(t)\begin{pmatrix} 1, & n_{\sigma k}(t)Z_k{}^{-1}(t) \\ 1, & 1 \end{pmatrix}, \quad I_\sigma^{\alpha\beta} = \begin{pmatrix} 1 & 0 \\ 0 & \sigma \end{pmatrix}. \tag{15}$$

Especially in the case where the initial state is of the grand canonical distribution with temperature $T_0 = \beta_0{}^{-1}$, $n_{\sigma k}(t)$ is given by $n_{\sigma k}(t) = \bar{n}_{\sigma k} + (\bar{n}^0_{\sigma k} - \bar{n}_{\sigma k})\exp(-2\chi_k t)$, where $\bar{n}^0_{\sigma k}$ is defined by putting $\beta_0$ instead of $\beta$ in (9b). It should be noted that, for this choice of the initial state, the Green's function (12) reduces to that derived by Schwinger[4] when $\sigma = 1$, i.e., boson field. The relation between his method and our formulation will be given in a forthcoming paper in which the other real time-path methods[15] will also be discussed.

With the general framework presented above, the linear response theory, which was proposed by Kubo,[14] can be made to include the effect of reservoir on the response of the system under consideration.[3] A systematic calculation method of the response function can be formulated in terms of the diagram method presented in this paper. This will be discussed in a separate paper.

We expect also that our formalism for non-equilibrium systems may easily accommodate the Ward-Takahashi relations, the renomalization method, and the renormalization group. A study in this direction is currently in progress. We close this paper by noting that the general quantization procedures of the free field[16] can be extended to the cases of semi-free field (i.e., $\hat{\Pi} \neq 0$).[17]

One of the authors (T.A.) would like to express his sincere thanks to Professor Y. Takahashi for his invitation to and hospitality at The University of Alberta.

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