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Non-Equilibrium Thermo Field Dynamics

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A fundamental framework for the construction of a quantum field theory for open systems, which will be called *non-equilibrium thermo field dynamics* (NETFD), is built upon two concepts. One is *the thermal state* in *the thermal-Liouville space*, by which *the quasi-particle superoperator* is introduced generally from *the thermal state condition*. The other is *the coarse graining* which is realized by projecting out some partial space from the complete thermal-Liouville space, and by which the dissipation is introduced. Most 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.) are preserved in NETFD. The entropy for the nonequilibrium state can be also introduced in NETFD.

§ 1. Introduction

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)~9)] we find the projection operator method of the damping theory,[1)~7)] especially *the time-convolution-less* (TCL) formulation of the damping theory,[4)~7)] quite suitable to our purpose of constructing a field theoretical framework for open systems.[10)]

As for the equilibrium situation, the so-called thermo field dynamics (TFD)[11)~17)] 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 is *the thermal state* which describes the themal equilibrium state and forms a linear vector space. This space is built on a vacuum state which is called *the thermal vacuum state.* The statistical average is given by the thermal vacuum state expectation value.

In this and the following papers, we present a general framework for the construction of a quantum field theory for open systems by combining the concepts of *the coarse graining* and *the thermal state,* which will be called *the non-equilibrium thermo field dynamics* (NETFD).[10)] We introduce *the thermal-Liouville space* in which *superoperators* are defined. In the thermal-Liouville space, the "Schrödinger equation" for the thermal state is reduced to a "master equation" by eliminating the reservoir thermal-Liouville subspace in terms of the TCL projection operator method which is reformulated in terminology of NETFD. The thermal state condition at time t is determined by the thermal state condition at the initial time together with the "master

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equation". The thermal state condition at time t for unperturbed system determines *the quasi-particle annihilation- and creation-superoperators* and *the thermal vacuum state* for the non-stationary and nonequilibrium situation, and leads to a quantum field theory for open systems.

In § 2, the thermal-Liouville space and superoperators are introduced and their basic properties are investigated. This somewhat mathematical preparation of the space and operators makes us possible to unite quantum field theoretical and statistical mechanical arguments. In § 3, using the thermal state condition in NETFD, we introduce thermal vacuum state and quasi-particle superoperators, which provide us with the representation space of the theory. We see that the methods of canonical formalism in the ordinary quantum field theory can be extended to the perturbative calculation in NETFD. In § 4, we discuss the coarse graining in the thermal-Liouville space. The method is applied, in § 5, to eliminate reservoir variables in order to introduce dissipation. This shows explicitly that, within the framework of NETFD, we can treat dissipation effects quantum-field-theoretically, which have been treated statistical-mechanically. Section 6 is devoted to discussion. In Appendix A, the characteristics of *the mirror space* is given with the definition of *mirror superoperators*. In Appendix B, the TCL formulation of the damping theory is applied to obtain the "master equation" in the thermal-Liouville space. The time-convolution (TC) formulation of the damping theory[1)~3)] is also reviewed. These considerations are to be compared with the one in §§ 4 and 5. In Appendix C, another derivation of the "master equation" is shown.

§ 2. Thermal-Liouville space and superoperators

After giving the general properties of *the Liouville space* and introducing *superoperators*, we build a linear vector space which will be called *the themal-Liouville space*.

2.1. *Liouville space*

The Liouville space[18),19)] can be spanned by a complete orthonormal basis

$$|mn\rangle\!\rangle = ||m\rangle\langle n|\rangle\!\rangle\,, \tag{2·1}$$

$$\langle\!\langle mn| = |mn\rangle\!\rangle^\dagger = \langle\!\langle(|m\rangle\langle n|)^\dagger| = \langle\!\langle|n\rangle\langle m||\,, \tag{2·2}$$

which satisfies

$$\langle\!\langle mn|m'n'\rangle\!\rangle = \delta_{mm'}\delta_{nn'}\,, \tag{2·3}$$

$$\sum_{mn}|mn\rangle\!\rangle\langle\!\langle mn| = \hat{1}\,, \tag{2·4}$$

where $\{|n\rangle = |n_1, n_2, \cdots\rangle\}$ is a complete orthonormal basis of the Hilbert space which is generated by cyclic operations of the creation operators $a_i^\dagger$ on the vaccum $|0\rangle$. These operators obey the commutation relations:

$$[a_i, a_j^\dagger]_\sigma = \delta_{ij}\,, \tag{2·5}$$

$$[a_i, a_j]_\sigma = [a_i^\dagger, a_j^\dagger]_\sigma = 0\,, \tag{2·6}$$

where the σ-commutator is defined by

$$[A, B]_\sigma = AB - \sigma BA \tag{2·7}$$

with

$$\sigma = \begin{cases} +1 & \text{for boson} \\ -1 & \text{for fermion} \end{cases}. \tag{2·8}$$

When A consists of a_i and $a_i^\dagger$, we define

$$|A\rangle\!\rangle = \sum_{mn} |mn\rangle\!\rangle \langle m|A|n\rangle\,, \tag{2·9a}$$

$$\langle\!\langle A| = \sum_{mn} \langle n|A|m\rangle \langle\!\langle mn|\,. \tag{2·9b}$$

We then have

$$\langle\!\langle mn|A\rangle\!\rangle = \langle m|A|n\rangle\,, \tag{2·10a}$$

$$\langle\!\langle A|mn\rangle\!\rangle = \langle n|A|m\rangle\,. \tag{2·10b}$$

It is obvious that $|A\rangle\!\rangle$ and $\langle\!\langle A|$ belong to the Liouville space. They are related to each other through

$$\langle\!\langle A| = |A^\dagger\rangle\!\rangle^\dagger\,. \tag{2·11}$$

We have also

$$\langle\!\langle A|B\rangle\!\rangle = \sum_n \langle n|AB|n\rangle = \mathrm{Tr}\, AB\,. \tag{2·12}$$

When A in (2·9) is the unit operator, we have

$$|1\rangle\!\rangle = \sum_n |nn\rangle\!\rangle\,, \tag{2·13a}$$

$$\langle\!\langle 1| = \sum_n \langle\!\langle nn|\,. \tag{2·13b}$$

2.2. *Superoperators*

The operators which induce linear transformations among the vectors in the Liouville space are called *superoperators.*[20] Any superoperator is a linear sum of operators, each being a product of four kinds of basic operations; $m_i \to m_i \pm 1$ or $n_i \to n_i \pm 1$.

Following Schmutz,[21] we thus define a special set of the superoperators a_i and $\tilde{a}_i$ by

$$a_i|mn\rangle\!\rangle = |a_i|m\rangle\langle n|\rangle\!\rangle\,, \tag{2·14a}$$

$$\tilde{a}_i|mn\rangle\!\rangle = \sigma^{\mu+1} ||m\rangle\langle n|a_i^\dagger\rangle\!\rangle \tag{2·14b}$$

with $\mu = \sum_i (m_i - n_i)$, where we used the particle-number eigenstates for $\{|n\rangle\}$:

$$a_i^\dagger a_i|n\rangle = n_i|n\rangle\,. \tag{2·15}$$

In the mapping rule (2·14), we used the same notation for the superoperator a_i as the ordinary operator a_i.

By analysing the Hermitian conjugate of the matrix elements of the superoperators a_i and $\tilde{a}_i$, we find

$$a_i^\dagger|mn\rangle\!\rangle = |a_i^\dagger|m\rangle\langle n|\rangle\!\rangle\,, \tag{2·16a}$$

$$\tilde{a}_i^\dagger|mn\rangle\!\rangle = \sigma^{\mu}||m\rangle\langle n|a_i\rangle\!\rangle\,. \tag{2·16b}$$

For example, (2·16b) is derived from (2·14b) as

$$\begin{aligned}\langle\!\langle m'n'|\tilde{a}_i^\dagger|mn\rangle\!\rangle &= \langle\!\langle mn|\tilde{a}_i|m'n'\rangle\!\rangle^* \\ &= \sigma^{\mu'+1}\langle\!\langle mn||m'\rangle\langle n'|a_i^\dagger\rangle\!\rangle^* \\ &= \sigma^{\mu'+1}\langle m|m'\rangle^*\langle n'|a_i^\dagger|n\rangle^* \\ &= \sigma^{\mu'+1}\langle m'|m\rangle\langle n|a_i|n'\rangle \\ &= \sigma^{\mu}\langle\!\langle m'n'||m\rangle\langle n|a_i\rangle\!\rangle\,,\end{aligned} \tag{2·17}$$

where $\mu' = \sum_i (m_i' - n_i')$ and we used the fact that $m = m'$ and $n = n' - 1$ in the last equality.

It is obvious that the four superoperators $(a_i, a_i^\dagger, \tilde{a}_i, \tilde{a}_i^\dagger)$ form a basic set of superoperators in the sense that any superoperator is a linear sum of products of them. As a matter of fact, this set is the smallest among the basic sets.

From (2·14) and (2·16) follow the commutation relations among the superoperators, i.e.,

$$[a_i, a_j^\dagger]_\sigma = [\tilde{a}_i, \tilde{a}_j^\dagger]_\sigma = \delta_{ij}\,, \tag{2·18}$$

while the other commutation relations vanish. We also obtain

$$a_i^\dagger a_i|mn\rangle\!\rangle = m_i|mn\rangle\!\rangle\,, \tag{2·19a}$$

$$\tilde{a}_i^\dagger \tilde{a}_i|mn\rangle\!\rangle = n_i|mn\rangle\!\rangle \tag{2·19b}$$

and

$$a_i|00\rangle\!\rangle = \tilde{a}_i|00\rangle\!\rangle = 0\,, \tag{2·20}$$

where

$$|00\rangle\!\rangle = ||0\rangle\langle 0|\rangle\!\rangle\,, \tag{2·21}$$

which is called the supervacuum.[21]

From (2·13), we have

$$|1\rangle\!\rangle = \sum_n |nn\rangle\!\rangle = \exp(\sum_i a_i^\dagger \tilde{a}_i^\dagger)|00\rangle\!\rangle\,, \tag{2·22a}$$

$$\langle\!\langle 1| = \sum_n \langle\!\langle nn| = \langle\!\langle 00|\exp(\sum_i \tilde{a}_i a_i)\,. \tag{2·22b}$$

It follows from (2·22) that

$$a_i|1\rangle\!\rangle=\tilde{a}_i{}^\dagger|1\rangle\!\rangle\,, \tag{2·23a}$$

$$a_i{}^\dagger|1\rangle\!\rangle=\sigma\tilde{a}_i|1\rangle\!\rangle\,. \tag{2·23b}$$

According to the definition (2·2), we have

$$\langle\!\langle mn|a_i{}^\dagger=\langle\!\langle|n\rangle\langle m|a_i{}^\dagger|\,, \tag{2·24a}$$

$$\langle\!\langle mn|\,\tilde{a}_i{}^\dagger=\langle\!\langle a_i|n\rangle\langle m||\sigma^{\mu+1}\,, \tag{2·24b}$$

$$\langle\!\langle mn|a_i=\langle\!\langle|n\rangle\langle m|a_i|\,, \tag{2·25a}$$

$$\langle\!\langle mn|\,\tilde{a}_i=\langle\!\langle a_i{}^\dagger|n\rangle\langle m||\sigma^{\mu} \tag{2·25b}$$

and

$$\langle\!\langle 1|a_i{}^\dagger=\langle\!\langle 1|\,\tilde{a}_i\,, \tag{2·26a}$$

$$\langle\!\langle 1|a_i=\langle\!\langle 1|\,\tilde{a}_i{}^\dagger\sigma\,. \tag{2·26b}$$

It is obvious from (2·9a), (2·14a) and (2·16a) that when A and B consist only of a and $a^\dagger$,

$$A|1\rangle\!\rangle=|A\rangle\!\rangle\,, \tag{2·27a}$$

$$BA|1\rangle\!\rangle=B|A\rangle\!\rangle=|BA\rangle\!\rangle\,, \tag{2·27b}$$

and from (2·9b), (2·24a) and (2·25a)

$$\langle\!\langle 1|A=\langle\!\langle A|\,, \tag{2·28a}$$

$$\langle\!\langle 1|AB=\langle\!\langle A|B=\langle\!\langle AB|\,. \tag{2·28b}$$

These relations satisfy the self-consistency condition

$$\langle\!\langle A|B|C\rangle\!\rangle=\langle\!\langle A|BC\rangle\!\rangle=\langle\!\langle AB|C\rangle\!\rangle\,. \tag{2·29}$$

Then we also have, using (2·12)

$$\langle\!\langle 1|A\rangle\!\rangle=\langle\!\langle A|1\rangle\!\rangle=\langle\!\langle 1|A|1\rangle\!\rangle=\mathrm{Tr}A\,. \tag{2·30}$$

We now set up the rule for *the tilde conjugation.* We first note that (2·14b) gives

$$c(\tilde{a}_i{}^\dagger\cdots\tilde{a}_j{}^\dagger)(\tilde{a}_k\cdots\tilde{a}_l)|mn\rangle\!\rangle=\bar{\sigma}\,||m\rangle\langle n|[c^*(a_i{}^\dagger\cdots a_j{}^\dagger)(a_k\cdots a_l)]^\dagger\rangle\!\rangle\,, \tag{2·31}$$

where c is a complex c-number and $\bar{\sigma}$ is the product of $\sigma^{\mu+1}$ which comes from (2·14b). This relation indicates the following rule for the tilde conjugation:

$$(AB)^{\sim}=\tilde{A}\tilde{B}\,, \tag{2·32a}$$

$$(c_1A+c_2B)^{\sim}=c_1{}^*\tilde{A}+c_2{}^*\tilde{B}\,, \tag{2·32b}$$

because this rule puts (2·31) in the form

$$\tilde{A}|mn\rangle\!\rangle=\bar{\sigma}\,||m\rangle\langle n|A^\dagger\rangle\!\rangle\,. \tag{2·33}$$

We generalize the definition (2·32) to any operators (A, B) consisting of a and $a^\dagger$ (although the simple form of (2·33) does not always hold when A is a linear sum of more than two product terms).

When A has the form $c(a_{i1}^\dagger \cdots a_{im}^\dagger)(a_{k_1} \cdots a_{kn})$ with a c-number c, (2·23) leads to

$$A|1\rangle\rangle = \sigma^{\nu_A(\nu_A+1)/2}\tilde{A}^\dagger|1\rangle\rangle\,, \tag{2·34a}$$

$$A^\dagger|1\rangle\rangle = \sigma^{\nu_A(\nu_A-1)/2}\tilde{A}|1\rangle\rangle\,, \tag{2·34b}$$

where $\nu_A \equiv m-n$. Here it was considered that the total number of permutations needed in reversing the order of the operator elements in A is $(m+n)(m+n-1)/2$ which is equal to $[\nu_A(\nu_A+1)/2+m+\text{an even number}]$, and that each $a^\dagger$ in A contributes to the phase factor on the right-hand side of (2·34a) by an amount σ, according to (2·23b). In a similar manner, (2·26) leads to

$$\langle\langle 1|A^\dagger = \langle\langle 1|\tilde{A}\sigma^{\nu_A(\nu_A+1)/2}\,, \tag{2·35a}$$

$$\langle\langle 1|A = \langle\langle 1|\tilde{A}^\dagger\sigma^{\nu_A(\nu_A-1)/2}\,. \tag{2·35b}$$

Now (2·27b) gives

$$\begin{aligned}|BA\rangle\rangle = BA|1\rangle\rangle &= \sigma^{\nu_A(\nu_A+1)/2}B\tilde{A}^\dagger|1\rangle\rangle \\ &= \sigma^{\nu_A(\nu_A+1)/2+\nu_A\nu_B}\tilde{A}^\dagger|B\rangle\rangle\,,\end{aligned} \tag{2·36}$$

where $\sigma^{\nu_A\nu_B}$ is created by the commutation among B and $\tilde{A}^\dagger$. Here ν_B is related to B in the same way as ν_A to A. Thus ν_A and ν_B are the fermion numbers of A and B, respectively. The relations (2·34)~(2·36) hold true even if A is the linear sum of the products of the above form with common $m-n$ and when B has the same structure, because, then ν_A and ν_B can be assigned to A and B, respectively. When B has an inverse, (2·36), gives

$$BAB^{-1}|B\rangle\rangle = \sigma^{\nu_A(\nu_A+1)/2+\nu_A\nu_B}\tilde{A}^\dagger|B\rangle\rangle\,. \tag{2·37}$$

Finally, we note that, comparing the tilde conjugate of the both sides of (2·34a) [or (2·35a)] with (2·34b) [(2·35b)] gives

$$\tilde{\tilde{A}} = \sigma_A A\,, \tag{2·38}$$

where σ_A is the fermion number of A, i.e., $\sigma_A = \sigma^{\nu_A}$. A similar argument holds for A consisting of $\tilde{a}$ and $\tilde{a}^\dagger$. Note that we can modify[14),22)] the phase factor in the definition of the superoperators in (2·14) in such a manner that $\tilde{\tilde{A}} = A$. However, in this paper we use (2·14) which leads to (2·38).

As particular cases for (2·38), we have

$$\tilde{\tilde{a}}_i = \sigma a_i\,, \qquad \tilde{\tilde{a}}_i{}^\dagger = \sigma a_i{}^\dagger\,. \tag{2·39}$$

2.3. *Thermal-Liouville space*

We now formulate NETFD in terms of the Liouville space and the superoperators. We assume that each thermal state is represented by a vector in the Liouville space. Thus our basic set of operators are the superoperators $(a, a^\dagger, \tilde{a}, \tilde{a}^\dagger)$. The ket-basic vectors are constructed by cyclic actions of "creation superoperators" on *the thermal vacuum ket-vector* which in the Schrödinger representation will be denoted by $|W(t)\rangle\rangle$. The change of thermal states in time is generated by a "Hamiltonian" $\hat{H}$

which is a superoperator consisting of a, $a^\dagger$, $\tilde{a}$, $\tilde{a}^\dagger$. Thus, we have the "Schrödinger equation"

$$\partial_t | W(t)\rangle\!\rangle = -i\hat{H} | W(t)\rangle\!\rangle . \tag{2·40}$$

When we write $| W(t)\rangle\!\rangle = W(t)|1\rangle\!\rangle$, $W(t)$ will be called *the density superoperator.*

We see from (2·40) that

$$| W(t)\rangle\!\rangle = \hat{S}(t-s)| W(s)\rangle\!\rangle , \tag{2·41}$$

where

$$\hat{S}(t) = \exp[-i\hat{H}t] . \tag{2·42}$$

Note that we did not require that $\hat{H}$ is Hermitian. Thus $\hat{S}$ is not necessarily unitary.

The thermal average is given by $\langle\!\langle 1|\hat{A}| W(t)\rangle\!\rangle$ when $| W(t)\rangle\!\rangle$ is normalized according to

$$\langle\!\langle 1| W(t)\rangle\!\rangle = 1 . \tag{2·43}$$

In order for this to be satisfied by all kinds of nonequilibrium situations, we may expect that

$$\langle\!\langle 1|\hat{H} = 0 . \tag{2·44}$$

Indeed, a derivation of this condition is presented in Appendix C. We then have

$$\langle\!\langle 1|\hat{A}| W(t)\rangle\!\rangle = \langle\!\langle 1|\hat{A}(t)| W(t_0)\rangle\!\rangle , \tag{2·45}$$

where

$$\hat{A}(t) = \hat{S}^{-1}(t-t_0)\hat{A}\hat{S}(t-t_0) . \tag{2·46}$$

The superoperator $\hat{A}(t)$ will be called the Heisenberg representation of the superoperator $\hat{A}$.

The state $| W(t_0)\rangle\!\rangle$ is called *the thermal vacuum ket-vector* in the Heisenberg representation. This state is determined by the initial condition for the system at $t = t_0$ (i.e., by the experimental setup of the system at the initial time t_0).

The Heisenberg equation of motion for the superoperators is

$$\partial_t \hat{A}(t) = i[\hat{H}, \hat{A}(t)] . \tag{2·47}$$

As particular cases of (2·46), we have

$$a(t) = \hat{S}^{-1}(t-t_0)a\ \hat{S}(t-t_0) , \tag{2·48a}$$

$$a^{\dagger\dagger}(t) = \hat{S}^{-1}(t-t_0)a^\dagger \hat{S}(t-t_0) , \tag{2·48b}$$

$$\tilde{a}(t) = \hat{S}^{-1}(t-t_0)\tilde{a}\hat{S}(t-t_0) , \tag{2·48c}$$

$$\tilde{a}^{\dagger\dagger}(t) = \hat{S}^{-1}(t-t_0)\tilde{a}^\dagger \hat{S}(t-t_0) . \tag{2·48d}$$

It should be noted that $a^{\dagger\dagger}(t)$ and $\tilde{a}^{\dagger\dagger}(t)$ are not Hermitian conjugation to $a(t)$ and $\tilde{a}(t)$, respectively, when $\hat{S}$ is not unitary, although they satisfy the "canonical" relations:

$$[a_i(t),\ a_j^{\dagger\dagger}(t)]_\sigma=[\tilde{a}_i(t),\ \tilde{a}_j^{\dagger\dagger}(t)]_\sigma=\delta_{ij}\,. \tag{2·49}$$

The basic bra-vectors are created by cyclic actions of annihilation operators on *the themal vacuum bra-vector* which is $\langle\langle 1|$.

Thus, $\langle\langle 1|$ and $|W(t_0)\rangle\rangle$ are considered to be *thermal vacuum states* (in the Heisenberg representation) for the bra- and ket-vectors, respectively. The thermal average $\langle\langle 1|\hat{A}(t)|W(t_0)\rangle\rangle$ is the vacuum expectation value of $\hat{A}(t)$ in this space. The thermal-Liouville space is a linear vector space constructed on these thermal vacuum states (see § 3 for detailed discussion). We will build a quantum field theory for open systems in this thermal-Liouville space.

It is worthwhile to note here that there is a space similar to the thermal-Liouville space, which will be called *the mirror space* of the thermal-Liouville space, the bra and ket state vectors of which are constructed on *the mirror thermal vacuum states* $\langle\langle W(t_0)|$ and $|1\rangle\rangle$, respectively. In the mirror space, we can define the Heisenberg representation of *the mirror superoperator* which is nothing but the mirror operator introduced in Ref. 7). Some investigation of the mirror space is given in Appendix A.

§ 3. Thermal state condition

In this section we extend the thermal state condition of the equilibrium TFD[11)~17)] to nonequilibrium situation.[10)] We do this by using the interaction representation (i.e., the perturbative expansion). The unperturbed Hamiltonian is of a bilinear form consisting of the superoperators a, $a^\dagger$, $\tilde{a}$ and $\tilde{a}^\dagger$. The superoperators a, $a^\dagger$, $\tilde{a}$ and $\tilde{a}^\dagger$ in this representation will be said to be *semi-free*.

For simplicity, in this paper (except § 4) we restrict our consideration to a translationally invariant case. It is straightforward to extend the discussion to cases in which the condition of the translationally invariance is broken.[23)]

In a translationally invariant case, the superoperator a_k is a linear sum of

$$a_k(t)=\hat{S}_0^{-1}(t-t_0)a_k\hat{S}_0(t-t_0)\,, \tag{3·1a}$$

$$\tilde{a}_k^{\dagger\dagger}(t)=\hat{S}_0^{-1}(t-t_0)\tilde{a}_k^{\dagger}\hat{S}_0(t-t_0)\,, \tag{3·1b}$$

where the subscript k describes the wave number, and $\hat{S}_0(t)$ is defined by (2·42) in which $\hat{H}$ is replaced by the unperturbed "Hamiltonian".

The *unperturbed* thermal state condition in the translationally invariant case is given by

$$a_k|W(t_0)\rangle\rangle=f_k\tilde{a}_k^\dagger|W(t_0)\rangle\rangle\,, \tag{3·2a}$$

$$\tilde{a}_k|W(t_0)\rangle\rangle=\sigma f_k a_k^\dagger|W(t_0)\rangle\rangle \tag{3·2b}$$

with a c-number function f_k, the form of which is determined by the knowledge of the initial density matrix $W(t_0)$. In writing (3·2), we considered the fact that the density opertor is a boson-like operator in general. The condition (3·2) is satisfied, for example, when the initial state is in thermal equilibrium.

Both the deviation of $\hat{H}$ from the unperturbed bilinear "Hamiltonian" and the deviation of the thermal state condition from its unperturbed linear form [i.e., (3·2)] are considered as perturbative effects.

Let us show how the thermal state condition (3·2) determines the "canonical" annihilation and creation superoperators of quasi-particles. Since (3·2a) is linear in the superoperators a_k and $\tilde{a}_k{}^\dagger$, and since these operators are linear combinations of $a_k(t)$ and $\tilde{a}_k{}^{\dagger\dagger}(t)$, (3·2a) becomes a linear relation among $a_k(t)$ and $\tilde{a}_k{}^{\dagger\dagger}(t)$ acting on $|W(t_0)\rangle\rangle$. This can be written as $\gamma_k(t)|W(t_0)\rangle\rangle=0$, where $\gamma_k(t)$ is a linear sum of $a_k(t)$ and $\tilde{a}_k{}^{\dagger\dagger}(t)$. Similarly the thermal state condition (2·26a) for $\langle\langle 1|$ leads to $\langle\langle 1|\tilde{\gamma}_k{}^{\dagger}(t)=0$ where $\tilde{\gamma}_k{}^{\dagger}(t)$ is a linear sum of $a_k{}^{\dagger\dagger}(t)$ and $\tilde{a}_k(t)$. Summarizing; the thermal state conditions (3·2a) and (2·26a) determine the annihilation and creation quasi-particle superoperators as

$$\gamma_k(t)=Z_k{}^{1/2}(t-t_0)[a_k(t)-f_k(t-t_0)\tilde{a}_k{}^{\dagger\dagger}(t)]\,, \tag{3·3a}$$

$$\tilde{\gamma}_k{}^{\dagger}(t)=Z_k{}^{1/2}(t-t_0)[\tilde{a}_k{}^{\dagger\dagger}(t)-\sigma a_k(t)]\,, \tag{3·3b}$$

and *in terms of which the thermal state condition at time t reads as*

$$\gamma_k(t)|W(t_0)\rangle\rangle=0\,, \qquad \langle\langle 1|\tilde{\gamma}_k{}^{\dagger}(t)=0\,. \tag{3·4a}$$

The tilde conjugation of (3·4a) leads to

$$\tilde{\gamma}_k(t)|W(t_0)\rangle\rangle=0\,, \qquad \langle\langle 1|\gamma_k{}^{\dagger}(t)=0\,. \tag{3·4b}$$

The c-number function $f_k(t)$ in (3·3a) is determined by f_k and $\hat{S}_0(t)$. The normalization factor $Z_k{}^{1/2}(t)$ is determined by the "canonical" commutation relation

$$[\gamma_k(t),\ \gamma_l{}^{\dagger}(t)]_\sigma=\delta_{kl}\,, \tag{3·5}$$

$$[\tilde{\gamma}_k(t),\ \tilde{\gamma}_l{}^{\dagger}(t)]_\sigma=\delta_{kl}\,, \tag{3·6}$$

while the other commutation relations vanish. The result is

$$Z_k(t)=1+n_{\sigma k}(t)\,, \tag{3·7}$$

where

$$n_{\sigma k}(t)=\sigma f_k(t)/[1-\sigma\, f_k(t)]\,. \tag{3·8}$$

Using the relations (3·3) and (3·4), we obtain

$$n_{\sigma k}(t-t_0)=\sigma\langle\langle 1|a_k{}^{\dagger\dagger}(t)a_k(t)|W(t_0)\rangle\rangle\,. \tag{3·9}$$

The above argument shows one of the most significant roles played by the thermal state condition; *the latter condition specifies the thermal vacuum and creation and annihilation superopertors for the quasi-particles.*

We are now ready to present a precise definition of the thermal-Liouville space. The thermal-Liouville space is nothing but the linear vector space spanned by the set of bra and ket state vectors which are generated, respectively, by cyclic operations of the annihilation superoperators $\gamma(t)$ and $\tilde{\gamma}(t)$ on the thermal vacuum $\langle\langle 1|$ and of the creation superoperators $\gamma^{\dagger}(t)$ and $\tilde{\gamma}^{\dagger}(t)$ on the thermal vacuum $|W(t_0)\rangle\rangle$.

We now adopt the usual definition of the normal product; when a product has a form in which all the creation superoperators ($\gamma^{\dagger}$and $\tilde{\gamma}^{\dagger}$) stand left to the annihilation superoperators (γ and $\tilde{\gamma}$), it is called a normal product.

When we rewrite $a(t)$ and $\tilde{a}^{\dagger\dagger}(t)$ in terms of the quasi-particle superoperators $\gamma(t)$ and $\tilde{\gamma}^{\dagger}(t)$, any product can be rewritten as a sum of normal products, leading us to a Wick-type formula for nonequilibrium systems. This Wick-type formula leads to Feynman-type diagrams for multi-time Green's functions in the interaction representation. We then obtain a Feynman-type diagram method for perturbative calculations for non-stationary and nonequilibrium statistical mechanical problems when a perturbative interaction is introduced in $\hat{H}$. 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 the dynamical map in the usual quantum field theory to nonequilibrium situations.

§ 4. Coarse graining

We divide the system into two parts A and B as

$$\hat{H}=\hat{H}_0+g\hat{H}_1\,, \qquad \hat{H}_0=\hat{H}_{\mathrm{A}}+\hat{H}_{\mathrm{B}}\,, \tag{4·1}$$

where $\hat{H}_1$ describes the interaction between two subsystems A and B. In the interaction representation with the interaction "Hamiltonian" $g\hat{H}_1$, (2·40) becomes

$$\partial_t|W(t)\rangle\!\rangle_I=-ig\hat{H}_1(t)|W(t)\rangle\!\rangle_I\,, \tag{4·2}$$

where

$$|W(t)\rangle\!\rangle_I=e^{i\hat{H}_0(t-t_0)}|W(t)\rangle\!\rangle\,, \tag{4·3}$$

$$\hat{H}_1(t)=e^{i\hat{H}_0(t-t_0)}\hat{H}_1e^{-i\hat{H}_0(t-t_0)}\,. \tag{4·4}$$

The formal solution of (4·2) is given by

$$|W(t)\rangle\!\rangle_I=\hat{Z}(t,t_0)|W(t_0)\rangle\!\rangle\,, \tag{4·5}$$

where

$$\hat{Z}(t,\tau)=T\,\exp[-ig\int_{\tau}^{t}ds\;\hat{H}_1(s)]\,, \tag{4·6}$$

and T is the well-known time ordering operator.

We now calculate

$$|W_{\mathrm{A}}(t)\rangle\!\rangle_I=\langle\!\langle 1_{\mathrm{B}}|W(t)\rangle\!\rangle_I \tag{4·7}$$

by assuming that, at the initial time $t=t_0$, the thermal vacuum ket-vector is factorizable,

$$|W(t_0)\rangle\!\rangle=|W_{\mathrm{A}}(t_0)\rangle\!\rangle|W_{\mathrm{B}}(t_0)\rangle\!\rangle\,. \tag{4·8}$$

We specified that ($\langle\!\langle 1_{\mathrm{A}}|, |W_{\mathrm{A}}(t_0)\rangle\!\rangle$) and ($\langle\!\langle 1_{\mathrm{B}}|, |W_{\mathrm{B}}(t_0)\rangle\!\rangle$) are the thermal vacuum states associated with the relevant A subsystem and the irrelevant B subsystem, respectively. By substituting (4·5) into (4·7), we obtain

$$|W_A(t)\rangle\rangle_I = T\ \exp[\int_{t_0}^{t} ds\ \hat{K}_I(s)]|W_A(t_0)\rangle\rangle \tag{4·9}$$

with

$$\hat{K}_I(t) = \partial_t T \ln\langle\langle 1_B|\hat{Z}(t, t_0)|W_B(t_0)\rangle\rangle$$
$$\equiv [\partial_t\langle\langle 1_B|\hat{Z}(t, t_0)|W_B(t_0)\rangle\rangle][\langle\langle 1_B|\hat{Z}(t, t_0)|W_B(t_0)\rangle\rangle^{-1}. \tag{4·10}$$

The right-hand side of (4·10) is given by connected diagrams without any external B-lines which are nothing but *ordered cumulants*[24)~26),6),7)] in the TCL formulation of the damping theory. The superoperator $\hat{K}_I(t)$ in (4·10) was introduced in the TCL projection operator method.[7)] The TCL formulation of the damping theory is given in Appendix B with the TC formulation of the damping theory.[1)~3)] An interesting argument related to (4·10) is found in Ref. 27).

In the Schrödinger representation,

$$|W_A(t)\rangle\rangle = e^{-i\hat{H}_A(t-t_0)}|W_A(t)\rangle\rangle_I, \tag{4·11}$$

we obtain a "master equation" for the relevant A subsystem as

$$\partial_t|W_A(t)\rangle\rangle = -i[\hat{H}_A + i\hat{K}(t)]|W_A(t)\rangle\rangle, \tag{4·12}$$

where

$$\hat{K}(t) = e^{-i\hat{H}_A(t-t_0)}\hat{K}_I(t)e^{i\hat{H}_A(t-t_0)}. \tag{4·13}$$

§ 5. Elimination of reservoir variables

In order to introduce dissipation, we eliminate the partial space in the thermal-Liouville space, which is related to the thermal reservoir, by use of the coarse graining method given in the previous section. The characteristics of the thermal reservoir will be specified in the following argument.

We divide total closed system into two parts, i.e., the system (S) which we are interested in and the reservoir (R), so that

$$\hat{H}_0 = \hat{H}_S + \hat{H}_R. \tag{5·1}$$

As for the interaction between the system and reservoir, we take a linear dissipative interaction[27),28),8)]

$$\hat{H}_1 = H_1 - \tilde{H}_1 \tag{5·2}$$

with

$$gH_1 = \sum_{kl}\lambda_{kl}(a_k R_{kl}^{\dagger} + R_{kl}a_k^{\dagger}), \tag{5·3}$$

where the reservoir superoperator R_{kl} is assumed to be a boson (fermion)-like operator when a_k is a boson (fermion) superoperator. We do not assume the canonical commutation relation for R_{kl} and $R_{kl}^{\dagger}$.

In the van Hove limit,[29)] which corresponds to the coarse graining in the time axis, (4·13) with (4·10) or equivalently (B·11) reduces to

$$\hat{K}(\infty)=\lim_{t-t_0\to\infty}(-ig)^2 e^{-i\hat{H}_A(t-t_0)}\hat{K}_I^{(2)}(t)e^{i\hat{H}_A(t-t_0)}$$

$$=-\lim_{t-t_0\to\infty} g^2\int_{t_0}^{t} dt_1 \langle\!\langle 1_R|\hat{H}_1(t_0)\hat{H}_1(t_1-t+t_0)|W_R\rangle\!\rangle\,, \tag{5·4}$$

where $\langle\!\langle 1_R|$ and $|W_R\rangle\!\rangle$ are the thermal vacuum states for the reservoir thermal-Liouville subspace. We assumed that

$$\langle\!\langle 1_R|g\hat{H}_1|W_R\rangle\!\rangle=0\,, \tag{5·5}$$

is satisfied, and used the fact

$$\langle\!\langle 1_R|e^{i\hat{H}_R(t-t_0)}=\langle\!\langle 1_R|\,, \tag{5·6a}$$

$$e^{-i\hat{H}_R(t-t_0)}|W_R\rangle\!\rangle=|W_R\rangle\!\rangle\,. \tag{5·6b}$$

By substituting (5·2) with (5·3) into (5·4), and using thermal state conditions

$$\langle\!\langle 1_R|R_{kl}^{\dagger}(t)=\langle\!\langle 1_R|\tilde{R}_{kl}(t)\,, \tag{5·7}$$

and its tilde conjugate, (5·4) becomes

$$\hat{K}(\infty)=-\sum_{kl}\lambda_{kl}^2\int_0^{\infty} dt(a_k-\sigma\tilde{a}_k^{\dagger})[\langle\!\langle 1_R|R_{kl}^{\dagger}(t)R_{kl}(0)|W_R\rangle\!\rangle a_k^{\dagger}(t_0-t)$$

$$-\sigma\langle\!\langle 1_R|R_{kl}(0)R_{kl}^{\dagger}(t)|W_R\rangle\!\rangle\tilde{a}_k(t_0-t)]+(\text{tilde conjugate})\,, \tag{5·8}$$

where we used (5·6) again. Note that e.g., $a_k(t_0)=a_k$. In deriving (5·8), we assumed that reservoirs for each mode are mutually independent and that

$$\langle\!\langle 1_R|R_{kl}(t_1)R_{kl}(t_2)|W_R\rangle\!\rangle=0 \tag{5·9}$$

and its tilde conjugate are satisfied. The time evolution, such as $a_k(t)$ is determined by (2·48) in which $\hat{H}$ in $\hat{S}(t)$ is replaced by $\hat{H}_S$ that generally contains interactions within the system S. We note that †† is equal to † since the time evolutions of $a(t)$'s and $R(t)$'s are generated by unitary superoperators [see (4·4)]. This comes from the fact that the total system is closed, i.e., $\hat{H}_0=H_0-\tilde{H}_0$ does not contain cross terms between tilde and non-tilde superoperators [see (5·23b) below].

Substituting (5·8) into (4·12), we obtain a "master equation" for the system S as

$$\partial_t|W_S(t)\rangle\!\rangle=-i\hat{H}|W_S(t)\rangle\!\rangle \tag{5·10}$$

with

$$|W_S(t)\rangle\!\rangle=\langle\!\langle 1_R|W(t)\rangle\!\rangle\,, \tag{5·11}$$

$$\hat{H}=\hat{H}_S+i\hat{K}(\infty)\,. \tag{5·12}$$

It should be noted that $\hat{H}$ satisfies the relations

$$i\hat{H}=(i\hat{H})^{\sim}\,, \tag{5·13}$$

$$\langle\!\langle 1|\hat{H}=0\,, \tag{5·14}$$

where $\langle\!\langle 1|$ describes the thermal vacuum bra-vector of the system S.

In the interaction representation with respect to the interactions within the system S, the unperturbative part of (5·8) reduces to

$$\hat{K}_0(\infty)=-\sum_k\{(a_k-\sigma\tilde{a}_k{}^\dagger)[a_k{}^\dagger\phi_k{}^{+-}(\varepsilon_k)-\sigma\tilde{a}_k\phi_k{}^{-+}(\varepsilon_k)^*]$$

$$+(\text{tilde conjugate})\}\,, \tag{5·15}$$

where ε_k describes the quasi-particle energy including the chemical potential of the reservoir self-consistently, and

$$\phi_k{}^{+-}(\varepsilon)=\sum_l\lambda_{kl}{}^2\int_0^\infty dt\langle\!\langle 1_R|R_{kl}{}^\dagger(t)R_{kl}(0)|W_R\rangle\!\rangle e^{-i\varepsilon t}\,, \tag{5·16a}$$

$$\phi_k{}^{-+}(\varepsilon)=\sum_l\lambda_k{}^2\int_0^\infty dt\langle\!\langle 1_R|R_{kl}(t)R_{kl}{}^\dagger(0)|W_R\rangle\!\rangle e^{i\varepsilon t}\,. \tag{5·16b}$$

By introducing a non-negative real valued function $\Lambda_k(u)$,

$$\sum_l\lambda_{kl}{}^2\langle\!\langle 1_R|R_{kl}{}^\dagger(t)R_{kl}(0)|W_R\rangle\!\rangle=\frac{1}{\pi}\int_{-\infty}^\infty du\; e^{iut}\Lambda_k(u)\,, \tag{5·17a}$$

we can obtain

$$\sum_l\lambda_{kl}{}^2\langle\!\langle 1_R|R_{kl}(t)R_{kl}{}^\dagger(0)|W_R\rangle\!\rangle=\frac{1}{\pi}\int_{-\infty}^\infty du\; e^{-iut}\Lambda_k(u)e^{\beta u}\,. \tag{5·17b}$$

In deriving (5·17b), we used the thermal state condition, i.e., the tilde conjugate of (5·7) together with (2·37), in such a way as

$$\begin{aligned}\langle\!\langle 1_R|R_{kl}(t)R_{kl}{}^\dagger(0)|W_R\rangle\!\rangle&=\sigma\langle\!\langle 1_R|\tilde{R}_{kl}{}^\dagger(t)R_{kl}{}^\dagger(0)|W_R\rangle\!\rangle\\&=\langle\!\langle 1_R|R_{kl}{}^\dagger(0)\tilde{R}_{kl}{}^\dagger(t)|W_R\rangle\!\rangle\\&=\langle\!\langle 1_R|R_{kl}{}^\dagger(0)\hat{W}_R R_{kl}(t)\hat{W}_R{}^{-1}|W_R\rangle\!\rangle\\&=\langle\!\langle 1_R|R_{kl}{}^\dagger(0)R_{kl}(t+i\beta)|W_R\rangle\!\rangle\end{aligned} \tag{5·18}$$

with

$$\hat{W}_R=W_R\tilde{W}_R{}^{-1}\,, \tag{5·19}$$

since the thermal vacuum state $|W_R\rangle\!\rangle$ is constructed by the grand canonical density superoperator $W_R\sim\exp[-\beta H_R]$ with the temperature $T=\beta^{-1}(k_B=1)$. The relation (5·18) is nothing but the Kubo-Martin-Schwinger relation.[30),31)]

If we define new quantities $\chi_k(\varepsilon)$ and $\Delta_k(\varepsilon)$ through the relation

$$\begin{aligned}\chi_k(\varepsilon)+i\Delta_k(\varepsilon)&=\phi_k{}^{-+}(\varepsilon)-\sigma\phi_k{}^{+-}(\varepsilon)^*\\&=\sum_l\lambda_{kl}{}^2\int_0^\infty dt\langle\!\langle 1_R|R_{kl}(t)[R_{kl}{}^\dagger(0)-\tilde{R}_{kl}(0)]|W_R\rangle\!\rangle e^{i\varepsilon t}\,,\end{aligned} \tag{5·20}$$

they are written in terms of $\Lambda_k(u)$ as

$$\chi_k(\varepsilon)=(e^{\beta\varepsilon}-\sigma)\Lambda_k(\varepsilon)\,, \tag{5·21a}$$

$$\Delta_k(\varepsilon)=\frac{1}{\pi}\int_{-\infty}^{\infty}du\frac{P}{\varepsilon-u}\chi_k(u)\,. \tag{5·21b}$$

Equation (5·21a) indicates that $\chi_k(\varepsilon)\geq 0$ for $\varepsilon\geq 0$. Equation (5·21b) is nothing but the Kramers-Kronig relation.

By using $\chi_k(\varepsilon)$ and $\Delta_k(\varepsilon)$ and their properties, (5·15) finally reduces to

$$\hat{K}_0(\infty)=-i\Delta\hat{H}_S+\hat{\Pi} \tag{5·22}$$

with

$$\Delta\hat{H}_S=\sum_k\Delta_k(a_k{}^\dagger a_k-\tilde{a}_k{}^\dagger\tilde{a}_k)\,, \tag{5·23a}$$

$$\hat{\Pi}=-\sum_k\chi_k[(1+2\bar{n}_{\sigma k})(a_k{}^\dagger a_k+\tilde{a}_k{}^\dagger\tilde{a}_k)-2(1+\bar{n}_{\sigma k})\tilde{a}_k a_k$$
$$-2\bar{n}_{\sigma k}\tilde{a}_k{}^\dagger a_k{}^\dagger]-2\sigma\sum_k\chi_k\bar{n}_{\sigma k}\,, \tag{5·23b}$$

where

$$\chi_k=\chi_k(\varepsilon_k)\,,\qquad \Delta_k=\Delta_k(\varepsilon_k)$$

and

$$\bar{n}_{\sigma k}=\bar{n}(\varepsilon_k)=\sigma(e^{\beta\varepsilon_k}-\sigma)^{-1}\,. \tag{5·24}$$

It may be worthwhile to note that in the above argument we do not need to specify the explicit form of H_R as far as the values of $\chi_k(\varepsilon)$ and $\Delta_k(\varepsilon)$, defined by (5·20), are left undetermined. They depend on the structure of H_R and can be calculated systematically by TFD[32] within the conventional linear response theory.[30]

The "master equation" (5·10) with (5·12) is equivalent to the one derived from the rigorous treatment of the damping theory.[7),33)~36)] In the convenional treatment of the damping theory, in which the effect of the interactions in the system S on the relaxation of the system is ignored, one considers only $\hat{K}_0(\infty)$ instead of $\hat{K}(\infty)$ in (5·12).

§ 6. Discussion

We presented a fundamental framework for the construction of a quantum field theory for open systems by means of the thermal-Liouville space of thermal states.

Although, for simplicity, we assumed the translational invariance for the reservoir and also for the thermal state condition, we can extend straightforwardly the consideration to the case where the translationally invariance is broken. We formulated a coarse graining method with which we project out the reservoir to obtain a "master equation" from the "Schrödinger equation" in the themal-Liouville space. This method is equivalent to the TCL formulation of the projection operator method[4)~7)] when the thermal vacuum ket-vector in the Heisenberg representation is factorizable. When we are interested in a smaller subsystem, we can further apply the projection method to this "master equation" to eliminate more partial subsystems in order to obtain a "master equation" for the subsystem in which we are interested.[7]

However, in this paper we restricted the discussion only to the first step, i.e., the reduction of the reservoir variables. A formulation of the second step (i.e., further reduction of partial subsystems, in terms of the superoperators) is required in the applications of this formalism to some practical problems such as the parametric amplifier,[33] the microscopic laser theory,[34),37),38] the transient nonlinear optical problems related to the dephasing,[39)~44] a localized electron-phonon system,[45),46] etc. Introduction of the time-dependent projection operator method[47),48] into the thermal-Liouville space will be interesting in view of its relation to the local equilibrium state.

As in equilibrium TFD,[11)~17] most 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.) are preserved in NETFD. We expect that our formalism for nonequilibrium systems may easily accommodate the Ward-Takahashi relations, the renormalization method and the renormalization group. The general quantization procedures of the free field[49)~52] can be extended to the cases of semi-free field (i.e., $\hat{\Pi}\neq 0$). We can formulate NETFD by the generating functional method.[53] The relation of NETFD to the real time-path methods[54)~56] is an interesting problem.

The entropy for the nonequilibrium state,[18),57] in the thermal-Liouville space can be given by

$$S(t)=-\frac{1}{2}\ln\Omega(t)/\Omega(\infty) \tag{6·1}$$

with

$$\Omega(t)=\langle\!\langle 1|W_S{}^\dagger(t)|W_S(t)\rangle\!\rangle \tag{6·2a}$$

$$=\langle\!\langle W_S{}^\dagger(t)|W_S(t)\rangle\!\rangle\,. \tag{6·2b}$$

Operations, ~, †† and M in the thermal-Liouville space are closely related[58] to the three conjugations of Prigogine's.[57]

With the general framework presented in this paper, the linear response theory proposed by Kubo[30] can be made to include the effect of reservoir on the response of the system under consideration.[7] A systematic calculation method for the response function can be formulated in terms of NETFD.

In the following paper, we will show that NETFD can be formulated in an extremely compact form on several basic requirements (axioms) *without referring to the existence of the reservoir*. The determination of $\hat{H}$ in NETFD becomes completely simple especially for the first step of the coarse graining. The whole structure of NETFD will be constructed upon the basic requirements.

We close this paper by noting that a "matrix element" in terms of the complete orthonormal basis of the Liouville space has the property:

$$\langle\!\langle m'n'|\hat{A}\hat{B},|mn\rangle\!\rangle=\langle\!\langle m'n'|,\hat{A}\hat{B}|mn\rangle\!\rangle$$

$$=\langle\!\langle m'n'|\hat{A},\hat{B}|mn\rangle\!\rangle\,, \tag{6·3}$$

where $\hat{A}$ and $\hat{B}$ consist of a, $a^\dagger$, $\tilde{a}$ and $\tilde{a}^\dagger$.

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Appendix A
—— *Mirror Space* ——

In the mirror space, all of the equations of motion in the Schrödinger representation are written in terms of the bra state vector. Thus the "Schrödinger equation" becomes

$$\langle\!\langle W(t)|\overleftarrow{\partial}_t=\langle\!\langle W(t)|(-i\hat{H})^M, \tag{A·1}$$

where the mapping rules (2·24) and (2·25) were considered (see also Appendix C). Here the superscript M indicates the superoperator in the mirror space.

The Heisenberg representation of a mirror superoperator $\hat{A}^M$ is defined by

$$\begin{aligned}\hat{A}^M(t)&=\hat{S}^M(t-t_0)\hat{A}^M\hat{S}^M(t-t_0)^{-1}\\&=\hat{A}[a^M(t)^{\dagger\dagger}, a^M(t), \tilde{a}^M(t)^{\dagger\dagger}, \tilde{a}^M(t)]\end{aligned} \tag{A·2}$$

with

$$\hat{S}^M(t)=\exp[(-i\hat{H})^M t], \tag{A·3}$$

because this together with

$$\langle\!\langle W(t)|=\langle\!\langle W(t_0)|\hat{S}^M(t-t_0), \tag{A·4}$$

leads to

$$\langle\!\langle W(t)|\hat{A}^M|1\rangle\!\rangle=\langle\!\langle W(t_0)|\hat{A}^M(t)|1\rangle\!\rangle \tag{A·5}$$

by using

$$\hat{H}^M|1\rangle\!\rangle=0, \tag{A·6}$$

where the definition of $|1\rangle\!\rangle$ is given by (2·22a). The Heisenberg equation of motion of the mirror superoperator is given by

$$\hat{A}^M(t)\overleftarrow{\partial}_t=[\hat{A}^M(t), (i\hat{H})^M]. \tag{A·7}$$

For the superoperator

$$\begin{aligned}\hat{A}=\sum_{\substack{kl\\mn}}\sum_{\substack{pq\\rs}}&C(p_1\cdots p_k, q_1\cdots q_l, r_1\cdots r_m, s_1\cdots s_n)\\&\times(a^\dagger_{p_1}\cdots a^\dagger_{p_k})(a_{q_1}\cdots a_{q_l})(\tilde{a}^\dagger_{r_1}\cdots a^\dagger_{r_m})(\tilde{a}_{s_1}\cdots\tilde{a}_{s_n}),\end{aligned} \tag{A·8}$$

the mirror superoperator is given by

$$\hat{A}^M=\sigma^y\tilde{\hat{A}}^\dagger \tag{A·9}$$

with $y=(\eta-\nu)(\eta-\nu-1)/2$, $\eta=k-l$ and $\nu=m-n$, where we have assumed that y is common to all the terms in (A·8). Note that the mirror superoperator $\hat{A}^M$ is defined through the relation

$$\langle\!\langle W(t)|\hat{A}^M=\langle\!\langle A_1W(t)A_2|\,,\quad \hat{A}|W(t)\rangle\!\rangle=|A_1W(t)A_2\rangle\!\rangle\,, \tag{A·10}$$

because of the original definition (A·1). If the fermion number is conserved, i.e., $\eta=\nu$, then (A·9) reduces to

$$\hat{A}^M=\tilde{\hat{A}}^\dagger\,. \tag{A·11}$$

It is worthwhile to note that the relation

$$(i\hat{H})^M=(i\hat{H})^\dagger\,, \tag{A·12}$$

is satisfied because of the relation (5·13).

As particular cases of (A·9), we have

$$a^M=\sigma\tilde{a}^\dagger,\quad (a^\dagger)^M=\tilde{a}\,, \tag{A·13a}$$

$$(\tilde{a}^\dagger)^M=a,\quad \tilde{a}^M=\sigma a^\dagger\,. \tag{A·13b}$$

Note that

$$(\hat{A}\hat{B})^M=\sigma^{\mu_A\mu_B}\hat{B}^M\hat{A}^M\,, \tag{A·14}$$

where μ_A and μ_B describe the fermion numbers of the superoperators $\hat{A}$ and $\hat{B}$, respectively, i.e., $\mu_A=\eta-\nu$, etc.

Appendix B
—— *Projection Operator Methods* ——

An alternative derivation of the "master equation" (4·12) for the relevant subsystem is given by the TCL formulation of the damping theory[4)~7)] with the assumption (4·8). In this Appendix, we review the general structure of the TCL projection operator method[4)~7)] which is more suitable, compared with the TC projection operator method,[1)~3)] to construct a quantum field theory for open systems in which we deal with real time explicitly. The TC method is also reviewed.

We introduce a projection operator

$$P=|W_B(t_0)\rangle\!\rangle\langle\!\langle 1_B|\,, \tag{B·1}$$

which projects out the irrelevant part in the thermal-Liouville space that corresponds to the irrelevant subsystem B. We divide (4·2) into two equations by applying P and $Q=1-P$ as

$$\partial_t P|W(t)\rangle\!\rangle_I=-igP\hat{H}_1(t)P|W(t)\rangle\!\rangle_I-igP\hat{H}_1(t)Q|W(t)\rangle\!\rangle_I\,, \tag{B·2a}$$

$$\partial_t Q|W(t)\rangle\!\rangle_I=-igQ\hat{H}_1(t)P|W(t)\rangle\!\rangle_I-igQ\hat{H}_1(t)Q|W(t)\rangle\!\rangle_I\,. \tag{B·2b}$$

We can solve (B·2b) formally as

$$Q|W(t)\rangle\!\rangle_I=\hat{G}(t,t_0)Q|W(t_0)\rangle\!\rangle-ig\int_{t_0}^{t}d\tau\hat{G}(t,\tau)Q\hat{H}_1(\tau)P|W(\tau)\rangle\!\rangle_I \tag{B·3a}$$

$$=\hat{G}(t,t_0)Q|W(t_0)\rangle\!\rangle+\hat{\Sigma}(t)|W(t)\rangle\!\rangle_I \tag{B·3b}$$

with

$$\hat{\Sigma}(t)=-ig\int_{t_0}^{t}d\tau\hat{G}(t,\tau)Q\hat{H}_1(\tau)P\hat{Z}^{-1}(t,\tau), \tag{B·4}$$

$$\hat{G}(t,\tau)=T\exp\left[-ig\int_{\tau}^{t}ds\ Q\hat{H}_1(s)Q\right], \tag{B·5}$$

where to obtain (B·3b) we used (4·5) with (4·6). Equation (B·3b) can be solved as

$$Q|W(t)\rangle\!\rangle_I=[1-\hat{\Sigma}(t)^{-1}]\{\hat{G}(t,t_0)Q|W(t_0)\rangle\!\rangle+\hat{\Sigma}(t)P|W(t)\rangle\!\rangle_I\}. \tag{B·6}$$

By substituting (B·6) into (B·2a), we obtain a "master equation" in the TCL formulation of the damping theory[4)~7)] as

$$\partial_t|W_A(t)\rangle\!\rangle_I=\hat{K}_I(t)|W_A(t)\rangle\!\rangle_I+|I_A(t)\rangle\!\rangle_I, \tag{B·7}$$

where $|W_A(t)\rangle\!\rangle_I$ is defined by (4·7),

$$\hat{K}_I(t)=-ig\langle\!\langle 1_B|\hat{H}_1(t)[1-\hat{\Sigma}(t)]^{-1}|W_B(t_0)\rangle\!\rangle, \tag{B·8}$$

$$|I_A(t)\rangle\!\rangle_I=-ig\langle\!\langle 1_B|\hat{H}_1(t)[1-\hat{\Sigma}(t)]^{-1}\hat{G}(t,t_0)\delta|W(t_0)\rangle\!\rangle \tag{B·9}$$

with

$$\delta|W(t_0)\rangle\!\rangle=Q|W(t_0)\rangle\!\rangle$$
$$=|W(t_0)\rangle\!\rangle-|W_A(t_0)\rangle\!\rangle|W_B(t_0)\rangle\!\rangle. \tag{B·10}$$

The right-hand side of (B·8) can be expanded as[6)]

$$\hat{K}_I(t)=\sum_{n=1}^{\infty}(-ig)^n\hat{K}_I^{(n)}(t) \tag{B·11}$$

with

$$\hat{K}_I^{(n)}(t)=\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-2}}dt_{n-1}$$
$$\langle\!\langle 1_B|\hat{H}_1(t)\hat{H}_1(t_1)\cdots\hat{H}_1(t_{n-1})|W(t_0)\rangle\!\rangle_{oc}, \tag{B·12}$$

where the integrand of (B·12) is the n-th order *ordered cumulant*,[24)~26),6),7)] and can be expressed by (4·10).[7)]

In the Schrödinger representation, (B·7) reduces to

$$\partial_t|W_A(t)\rangle\!\rangle=-i[\hat{H}_A+i\hat{K}(t)]|W_A(t)\rangle\!\rangle+|I_A(t)\rangle\!\rangle, \tag{B·13}$$

where $|W_A(t)\rangle\!\rangle$ and $\hat{K}(t)$ are defined by (4·11) and (4·13), respectively, and

$$|I_A(t)\rangle\!\rangle=e^{-i\hat{H}_A(t-t_0)}|I_A(t)\rangle\!\rangle_I. \tag{B·14}$$

If the condition (4·8) is satisfied, (B·13) reduces to (4·12) because in this case $|I_A(t)\rangle\rangle=0$.

By substituting (B·3a) into (B·2a), we obtain a "master equation" in the TC formulation of the damping theory[1)~3)] as

$$\partial_t|W_A(t)\rangle\rangle=-i[\hat{H}_A+g\langle\langle 1_B|\hat{H}_1|W_B(t_0)\rangle\rangle]|W_A(t)\rangle\rangle + \int_{t_0}^{t} d\tau\hat{\Phi}(t,\tau)|W_A(\tau)\rangle\rangle+|\mathcal{J}_A(t)\rangle\rangle, \tag{B·15}$$

in the Schrödinger representation, where

$$\hat{\Phi}(t,\tau)=e^{-i\hat{H}_A(t-t_0)}\hat{\Phi}_I(t,\tau)e^{i\hat{H}_A(\tau-t_0)} \tag{B·16}$$

with

$$\hat{\Phi}_I(t,\tau)=-g^2\langle\langle 1_B|\hat{H}_1(t)Q\hat{G}(t,\tau)Q\hat{H}_1(\tau)|W_B(t_0)\rangle\rangle, \tag{B·17}$$

and

$$|\mathcal{J}_A(t)\rangle\rangle=e^{-i\hat{H}_A(t-t_0)}|\mathcal{J}_A(t)\rangle\rangle_I \tag{B·18}$$

with

$$|\mathcal{J}_A(t)\rangle\rangle_I=-ig\langle\langle 1_B|\hat{H}_1(t)\hat{G}(t,t_0)\delta|W(t_0)\rangle\rangle. \tag{B·19}$$

The second term of the right-hand side of (B·15) can be expanded[6)] as

$$\int_{t_0}^{t} d\tau\ \hat{\Phi}_I(t,\tau)|W_A(\tau)\rangle\rangle_I=\sum_{n=2}^{\infty}(-ig)^n\int_{t_0}^{t} d\tau\ \hat{\Phi}_I^{(n)}(t,\tau)|W_A(\tau)\rangle\rangle_I \tag{B·20}$$

with

$$\int_{t_0}^{t} d\tau\hat{\Phi}_I^{(n)}(t,\tau)|W_A(\tau)\rangle\rangle_I=\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-2}}dt_{n-1} \langle\langle 1_B|\hat{H}_1(t)\hat{H}_1(t_1)\cdots\hat{H}_1(t_{n-1})|W_B(t_0)\rangle\rangle_{PC}|W_A(t_{n-1})\rangle\rangle_I, \tag{B·21}$$

where the integral kernel of the right-hand side of (B·21) is the n-th order *partial cumulant*.[6)]

For convenience, we write down several lower terms of ordered cumulants and partial cumulants for the case

$$\langle\langle 1_B|\hat{H}_1(t)|W_B(t_0)\rangle\rangle=0. \tag{B·22}$$

They are

$$\langle 01\rangle_{OC}=\langle 01\rangle_{PC}=\langle 01\rangle, \tag{B·23}$$

$$\langle 0123\rangle_{OC}=\langle 0123\rangle-\langle 01\rangle\langle 23\rangle-\langle 02\rangle\langle 13\rangle-\langle 03\rangle\langle 12\rangle, \tag{B·24a}$$

$$\langle 0123\rangle_{PC}=\langle 0123\rangle-\langle 01\rangle\langle 23\rangle, \tag{B·24b}$$

where we have introduced notations like

$$\langle ij\cdots k\rangle=\langle\langle 1_B|\hat{H}_1(t_i)\hat{H}_1(t_j)\cdots\hat{H}_1(t_k)|W_B(t_0)\rangle\rangle, \tag{B·25}$$

in which zero refers to t, and the subscripts OC and PC indicate the ordered cumulant and the partial cumulant, respectively.

Appendix C

—— *A Different Derivation of the "Master Equation"* ——

By applying the TCL formulation of the damping theory[4)~7)] to the Liouville equation

$$\partial_t W(t) = -i[H, W(t)], \qquad (\text{C}\cdot 1)$$

to eliminate reservoir variables, we obtain a master equation for the relevant system S in the van Hove limit as

$$\partial_t W_S(t) = -i[H_S, W_S(t)] + \Pi W_S(t), \qquad (\text{C}\cdot 2)$$

where $W_S(t)$ is the density operator of the system and

$$\Pi X = \sum_k \{\chi_k([a_k X, a_k^\dagger] + [a_k, X a_k^\dagger]) + 2\chi_k \bar{n}_{\sigma k}[a_k, [X, a_k^\dagger]_\sigma]\} \qquad (\text{C}\cdot 3)$$

with definitions (5·31) for $\bar{n}_{\sigma k}$ and (5·20) for χ_k. The energy shift Δ_k is included in H_S. In deriving (C·2), we used the same linear dissipative interaction gH_1 of (5·3). Here operators a and R should be interpreted as ordinary operators. We also used the conventional treatment of damping theory in which the effect of the interaction within the system S on the relaxation operator is ignored.

By putting (C·2) into the ket-vector $|\rangle\!\rangle$, and by using the mapping rules from the ordinary operator to the superoperator given in § 2.2, we obtain the "master equation" (5·10) in which $\hat{K}(\infty)$ is replaced by $\hat{K}_0(\infty)$, (5·22).

The property

$$\text{Tr}\{[H_S, X] + i\Pi X\} = 0 \qquad (\text{C}\cdot 4)$$

for an arbitrary operator X reduces to the condition (2·44) in the thermal-Liouville space.

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