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Feynman Rule of the Non-Equilibrium Process

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Abstract:

Complete rule of the Feynman diagram expansion of the non- equilibrium process is given by using the path integral technique. At initial time t_I, the system is in the equilibrium and it is brought into the non-equilibrium state by a time dependent Hamiltonian. All the interactions, including the initial correlation, are taken into account by the diagrammatic expansion. Besides the well-known equilibrium propagators and the conventional 2×2 non-equilibrium propagator matrix, the propagator becomes a 3×3 matrix which contains extra elements depending explicitly on t_I.

Both the Feynman rule of the co-ordinate representation and the coherent state representation are presented. It is shown that propagator matrix is expressed compactly by the contour representation. The classical limit is also discussed.

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§1. Introduction

The diagrammatic technique of the non-equilibrium thermodynamics for any quantum system has been widely discussed and applied to various phenomena. Matsubara's Green function[1] is defined for the equilibrium system but it contains the informations on the real time process in the sense of the analytic continuation. The use of the real time from the start is known as the double path method and it has been developed by Schwinger[2] and Keldysh.[3] The operator version of this double path method has extensively been studied by Umezawa et.al.[4] and Niemi- Semenoff[5] presented the path integral form.

Let us assume that the system is initially in the equilibrium under the Hamiltonian H_I. It is brought into the non-equilibrium state by the time dependent Hamiltonian $H(t)$ starting from some time $t = t_I$. Both H_I and $H(t)$ contains the same interaction part inherent in the system and it is required to discuss both Hamiltonians on the same footing. We take this attitude in this paper and study the Feynman rule of the non-equilibrium process by expanding both H_I and $H(t)$ in powers of the unharmonicity. This type of formalism enables us to discuss the equilibrium and the non-equilibrium phenomenon in a unified way.

There is another important aspects of our paper that has to be stressed. In the usual Feynman diagram approach, the initial time $t = t_I$ when the state is prepared is taken to be $-\infty$. But once this is done we cannot answer such a fundamental question as how the system looks like at the time t when we know the system at the time t_I. To know the system for finite value of $t - t_I$ is the real interest in the non-equilibrium mechanics. Usually the detailed knowledge of the whole system is not necessary but the expectation value $< O >_t$ of some operator O at t is our concern. Let ρ be the initial density matrix and $H(t)$ is the Hamiltonian of our system, then what we are interested in is given by

$$< O >_t = Tr(\rho K^\dagger O K), \tag{1.1}$$

$$K = T \exp(-\frac{i}{\hbar}\int_{t_I}^{t} H(t')dt') \tag{1.2}$$

where T is the time ordering operator.

The purpose of this paper is to give the precise form of the Feynman rule for the diagrammatic expansion of Eq.(1.1). We assume that the system is in the equilibrium state at $t = t_I$. The Hamiltonian becomes time dependent after t_I. This will be the situation of the usual experiment where t_I corresponds to the time when the system is brought into the non-equilibrium state. We then follow $< O >_t$ as a function of the time.

We will see that the propagator of the diagram becomes 3×3 matrix and that off-diagonal ((13) and (23) see below), elements depend explicitly on t_I. Conventional approach takes

$t_I = -\infty$ and neglects these off-diagonal terms thus the propagator matrix becoming 2×2. Also the time integration appearing in our Feynman rule starts from t_I, not from $-\infty$.

In §2, we take the coordinate representation and examine the Feynman rule. The 3×3 propagator matrix is shown to be compactly written by using the contour integral. After discussing the classical limit of our formulas, we notice the natural mechanism of the appearance of the dissipative term. It utilizes the inversion between the source and the expectation value — equivalent to the Legendre transformation.

The coherent state representation is studied in §3, which is another convenient form for the physical problems. The contour expression takes a compact form and its explicit representation is also given.

The formula presented here can be a basis for the exact treatment of the non-equilibrium problem and the applications to the real systems will be published in a forthcoming paper.

§2. Co-ordinate Representation

Let us take a quantum mechanical system whose Hamiltonian is given by $H(p, q)$. In order to make our formula as simple as possible, we first consider a system of one degree of freedom, q or p denoting the co-ordinate or the canonical momentum respectively. The Hamiltonian is initially assumed to be time independent with the unharmonic potential part $V_I(q)$ (the initial correlation);

$$H_I = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 + V_I(q). \tag{2.1}$$

Here m is the mass of the particle and we assume $\omega > 0$. It is straightforward to generalize the following discussions to the case where the potential V_I includes the momentum variable p.

Initially the system is supposed to be in the equilibrium with the temperature T and the time dependent external force is applied at some time $t = t_I$ which brings the system to the non-equilibrium state. The Hamiltonian for $t \geq t_I$ is therefore written as

$$H(t) = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 + V(q, t). \tag{2.2}$$

The relation $V_I(q) = V(q, t_I)$ or $H_I = H(t_I)$ holds but the following discussions do not rely on this equality. The initial density matrix is therefore,

$$\rho = \exp(-\beta H_I)/Tr\exp(-\beta H_I), \tag{2.3}$$

$$\beta = 1/kT. \tag{2.4}$$

The Feynman rule for $< O >_t$ given in (1.1) is most easily studied by adding tentatively the source term to the Hamiltonian which couples linearly to the co-ordinate q:

$$H_I \to H_I^j(\tau) = H_I - j(\tau)q, \tag{2.5a}$$

$$H(t) \to H(t)^j = H(t) - j(t)q. \tag{2.5b}$$

As we will see later, the surce term $j(\tau)$ or $j(t)$ enables us to extract the unharmonic part $V_I(q)$ or $V(q,t)$ from the integrand. Introducing independent source in K, $K^\dagger$ and ρ, the following expression is the object of the following discussions;

$$\exp \frac{i}{\hbar} W[j_1, j_2, j_3] \equiv Tr(\rho^{j_3} K^{\dagger j_2} K^{j_1}). \tag{2.6}$$

Here $K^{j_{1,2}}$ is the time ordered product from t_I to t_F where t_F is taken to be sufficiently large.

$$K^{j_{1,2}} = T \exp\{-\frac{i}{\hbar} \int_{t_I}^{t_F} dt' H(t')^{j_{1,2}}\}. \tag{2.7}$$

We consider the range $t_I \le t \le t_F$. ρ^{j_3} is given by

$$\rho^{j_3} = T_\tau \exp\{-\frac{1}{\hbar} \int_{\tau_I}^{\tau_F} d\tau H_I^{j_3}(\tau)\}, \qquad \tau_F - \tau_I = \beta\hbar. \tag{2.8}$$

In (2.8), T_τ is the τ-ordering operator. Recall that the results depend only on the difference $\tau_F - \tau_I$.

W is the generating functional in the following sense ($j = 0$ implies $j_1 = j_2 = j_3 = 0$),

$$\frac{\partial W}{\partial j_1(t)}|_{j=0} = -\frac{\partial W}{\partial j_2(t)}|_{j=0} =< q >_t, \qquad (t_I \le t \le t_F), \tag{2.9a}$$

$$\frac{\partial W}{i\partial j_3(t)}|_{j=0} =< q >_{t=t_I} . \tag{2.9b}$$

Note that in (2.9a), the parts of $K^{\dagger j_2}$ and K^{j_1} corresponding to the region from t to t_F cancel each other. The right hand side of (2.9b) is independent of τ. General correlation functions of q are obtained by further differentiations with respect to j. The expectation value of the operator involving the momentum p is calculated by introducing another source term $\tilde{j}(t)p$ but let us leave this case aside for simplicity (See Section 2-4).

Now we evaluate (2.6) as follows;

$$\exp \frac{i}{\hbar} W[j_1, j_2, j_3] = \int dq \int dq' < q|\rho^{j_3}|q' >< q'|K^{\dagger j_2} K^{j_1}|q > . \tag{2.10}$$

Since

$$< q'|K^{\dagger j_2} K^{j_1}|q >= \int dq'' < q'|K^{\dagger j_2}|q'' >< q''|K^{j_1}|q >, \tag{2.11}$$

we first write the path integral formula for $< q''|K^{j_1}|q >$ as[6)]

$$< q''|K^{j_1}|q >= \int [dq] \exp\{\frac{i}{\hbar}\int_{t_I}^{t_F} dt L^{j_1}(t)\}, \tag{2.12}$$

where L^{j_1} is the Lagrangian corresponding to the Hamiltonian (2.6b) and the path integral is performed under the boundary conditions $q(t_F) = q''$, $q(t_I) = q$. Now the unharmonic part is extracted as

$$< q''|K^{j_1}|q >= \exp\{-\frac{i}{\hbar}\int_{t_I}^{t_F} dt V(\frac{\hbar}{i}\frac{\partial}{\partial j_1(t)}, t)\} \times < q''|K_0^{j_1}|q > \tag{2.13}$$

where

$$< q''|K_0^{j_1}|q >= \int [dq] \exp\{\frac{i}{\hbar}\int_{t_I}^{t_F} L_0^{j_1}(t)dt\}.$$

Here $L_0^{j_1}$ is the free part of L^{j_1}. The following expression is well-known[6)] and with $T \equiv t_F - t_I$ it can be written as

$$< q''|K_0^{j_1}|q >= \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega T}} \exp\frac{i}{\hbar}S_1, \tag{2.14}$$

$$\begin{aligned} S_1 &= \frac{m\omega}{2\sin\omega T}\{(q^2 + q''^2)\cos\omega T - 2qq''\} \\ &+ \frac{1}{\sin\omega T}\int_{t_I}^{t_F}\{q \sin\omega(t_F - t) + q''\sin\omega(t - t_I)\}j_1(t)dt \\ &+ \frac{1}{2}\iint_{t_I}^{t_F} j_1(t)G(t,t')j_1(t')dtdt', \end{aligned}$$

$$G(t,t') = -\frac{1}{m\omega}[\theta(t-t')\frac{\sin\omega(t_F - t)\sin\omega(t' - t_I)}{\sin\omega T} + (t \leftrightarrow t')]. \tag{2.16}$$

Equation (2.11) is calculated by writing a similar expression for $< q'|K^{\dagger j_2}|q'' >$ and integrating over q''. Since S_1 is bilinear in q and q'', this is simple. The result is compactly written by introducing

$$\begin{aligned} j^{(+)} &= \frac{j_1 + j_2}{2}, \qquad j^{(-)} = j_1 - j_2 \\ q^{(+)} &= \frac{q + q'}{2}, \qquad q^{(-)} = q - q'. \end{aligned} \tag{2.17}$$

We get[7)]

$$\begin{aligned} < q'|K_0^{\dagger j_2}K_0^{j_1}|q >&= \delta(q^{(-)} - \int_{t_I}^{t_F} dt\Delta_R(t - t_I)j^{(-)}(t)dt) \\ &\times \exp[\frac{i}{\hbar}\int_{t_I}^{t_F} dt j^{(-)}(t)\{q^{(+)}\cos\omega(t - t_I) + \int_{t_I}^{t_F}\Delta_R(t - s)j^{(+)}(s)ds\}] \end{aligned} \tag{2.18}$$

where $\delta(\cdots)$ is the Dirac δ-function and Δ_R is the usual retarded function given by,

$$\Delta_R(t-s) = \theta(t-s)\frac{\sin\omega(t-s)}{m\omega}. \tag{2.19}$$

We notice here that (2.18) becomes $\delta(q^{(-)})$ when $j^{(-)} = 0$ as it should.

The expression for $< q|\rho^{j_3}|q' >$ in (2.10) is easily obtained by replacing $t \to -i\tau$, $T \to -i\beta\hbar$ in the formulae (2.14) $\sim$ (2.16). For definiteness we cite the explicit form,

$$\begin{aligned}
&< q|\rho^{j_3}|q' > \\
&= \exp(-\frac{1}{\hbar}\int_{\tau_I}^{\tau_F} V_I(\hbar\frac{\partial}{\partial j_3(\tau)})d\tau) \times \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega\beta\hbar}}\exp\frac{S_3}{\hbar}
\end{aligned}$$

$$\begin{aligned}
S_3 \quad &= \frac{m\omega}{2\sinh\omega\beta\hbar}[-(q^2+q'^2)\cosh\omega\beta\hbar + 2qq'] \\
&+\frac{1}{\sinh\omega\beta\hbar}\int_{\tau_I}^{\tau_F}\{q'\sinh\omega(\tau_F-\tau) + q\sinh\omega(\tau-\tau_I)\}j_3(\tau)d\tau \\
&+\frac{1}{2}\iint_{\tau_I}^{\tau_F} d\tau d\tau' j_3(\tau)G(\tau,\tau')j_3(\tau'),
\end{aligned}$$

$$G(\tau,\tau') = \frac{1}{m\omega}\{\theta(\tau-\tau')\frac{\sinh\omega(\tau_F-\tau)\sinh\omega(\tau'-\tau_I)}{\sinh\omega\beta\hbar} + (\tau\leftrightarrow\tau')\}. \tag{2.22}$$

The remaining integration $\int dq \int dq' = \int dq^{(+)} \int dq^{(-)}$ has to be done. The integration over $q^{(-)}$ is trivial because of the δ-function in (2.18) while $q^{(+)}$ integration is Gaussian. The final expression is written in φ-representation instead of the formula involving j. It is obtained by multiplying the following identity to the above expression of $\exp\frac{i}{\hbar}W$;

$$1 = \exp\frac{1}{\hbar}\{\int_{\tau_I}^{\tau_F} d\tau j_3(t)\varphi_3(\tau) + i\int_{t_I}^{t_F} dt(j_1(t)\varphi_1(t) - j_2(t)\varphi_2(t))\}|_{\varphi=0}. \tag{2.23}$$

In the presence of this factor we can replace $(j_1(t), j_2(t), j_3(\tau)) \equiv \mathrm{j}(t) \to (\frac{\hbar}{i}\frac{\partial}{\partial\varphi_1(t)}, -\frac{\hbar}{i}\frac{\partial}{\partial\varphi_2(t)}, \hbar\frac{\partial}{\partial\varphi_3(\tau)})$, $(\frac{\hbar}{i}\frac{\partial}{\partial j_1(t)}, -\frac{\hbar}{i}\frac{\partial}{\partial j_2(t)}, \hbar\frac{\partial}{\partial j_3(\tau)}) \to (\varphi_1(t), \varphi_2(t), \varphi_3(\tau)) \equiv \varphi(t)$.

Now we present the result in several forms. They all have the form

$$\begin{aligned}
\exp\frac{i}{\hbar}W[j_1,j_2,j_3] \quad &= \frac{1}{2\sinh\frac{\omega\beta\hbar}{2}}(\exp\frac{S}{\hbar}) \\
&\times\exp[-\frac{1}{\hbar}\int_{\tau_I}^{\tau_F} V_I(\varphi_3(\tau))d\tau - \frac{i}{\hbar}\int_{t_I}^{t_F}\{V(\varphi_1(t),t) - V(\varphi_2(t),t)\}dt]|_{\varphi=0}.
\end{aligned} \tag{2.24}$$

Here S is a functional of j and $\partial/\partial\varphi$. We have to differentiate with respect to j_1(or equivalently j_2) in order to extract the desired operator $O(t)$ whose expectation value is to be taken at the time t and then we set $\mathrm{j} = 0$. The essential point is the presence of $j^{(-)}$. Since $\frac{\partial}{\partial j_1}|_{j_2} = \frac{\partial}{\partial j^{(-)}}|_{j^{(+)}}$, the differentiation by j_1 can be taken in terms of $j^{(-)}$. We can set $j^{(+)} = 0$

from the start but if the physical Hamiltonian contains the linear term $-J(t)q$, $j^{(+)}(t)$ is fixed to be $J(t)$. Including this case, let us consider

$$W[j^{(-)}] \equiv W[\, j_1 = J + \frac{j^{(-)}}{2},\ j_2 = J - \frac{j^{(-)}}{2},\ j_3 = 0\,] \tag{2.25}$$

as the generating functional without loss of generality. We use $W[j^{(-)}]$ below instead of $W[j_1, j_2, j_3]$.

In the following various expressions of $W[j^{(-)}]$ are given. The different representaitons have different forms of the propagators which are the co-efficients of the quadratic term of $\partial/\partial\varphi$ appearing in S. This operator has the same effect as in the Wick's contraction theorem.

2-1. $\varphi^{(\pm)}$ representation

The most convenient form for the calculational purpose is the one written in terms of $\varphi^{(\pm)}$ and φ_3. We use the notation $\varphi_3 \equiv \varphi$ and

$$\frac{\partial}{\partial\varphi^{(\pm)}} \equiv \begin{cases} \frac{\partial}{\partial\varphi_1} + \frac{\partial}{\partial\varphi_2} \\ \frac{1}{2}\{\frac{\partial}{\partial\varphi_1} - \frac{\partial}{\partial\varphi_2}\} \end{cases} \tag{2.26}$$

S has four different propagators and is given, instead of explicit 3×3 matrix form, as follows,

$$S \;= i \iint dtds(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\varphi^{(+)}(t)} + j^{(-)}(t))\Delta_R(t-s)(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\varphi^{(-)}(s)} + J(s)) \tag{2.27a}$$

$$+\tfrac{1}{2}\iint dtds(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\varphi^{(+)}(t)} + j^{(-)}(t))\bar{\Delta}(t-s)(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\varphi^{(+)}(s)} + j^{(-)}(s)) \tag{2.27b}$$

$$+\iint dxd\tau(\tfrac{\hbar}{i}\tfrac{\partial}{\partial\varphi^{(+)}(t)} + j^{(-)}(t))\bar{G}(t,\tau)\hbar\tfrac{\partial}{\partial\varphi(\tau)} \tag{2.27c}$$

$$+\tfrac{1}{2}\iint d\tau d\tau'\hbar\tfrac{\partial}{\partial\varphi(\tau)}G(\tau,\tau')\hbar\tfrac{\partial}{\partial\varphi(\tau)}. \tag{2.27d}$$

Here the integration regions are $t_I \le t, s \le t_F$, $\tau_I \le \tau, \tau' \le \tau_F$ and Δ_R is given in (2.19). Other propagators are as follows.

$$\bar{\Delta}(t-s) \;= -\frac{\coth\frac{\omega\beta\hbar}{2}}{2m\omega}\cos\omega(t-s), \tag{2.28a}$$

$$\begin{aligned}\bar{G}(t,\tau) \;&= \frac{1}{2m\omega\sinh\frac{\omega\beta\hbar}{2}}\{\sin\omega(t-t_I)\sinh\omega(\tau - \tfrac{\tau_I+\tau_F}{2}) \\ &+ i\cos\omega(t-t_I)\cosh\omega(\tau - \tfrac{\tau_I+\tau_F}{2})\},\end{aligned} \tag{2.28b}$$

$$G(\tau,\tau') \;= \frac{1}{2m\omega\sinh\frac{\omega\beta\hbar}{2}}\{\theta(\tau'-\tau)\cosh\omega(\tau-\tau'+\tfrac{\beta\hbar}{2}) + (\tau \leftrightarrow \tau')\}. \tag{2.28c}$$

The diagrammatic expansion is given by the above propagators and by the vertices determined by $V_I(\varphi(\tau))$ and $V(\varphi_1(t),t) - V(\varphi_2(t),t))$ which is odd in $\varphi^{(-)}$. If we write an arrow $\overset{s}{\longrightarrow}{}^{t}$ for $\Delta_R(t-s)$ then from (2.27a) we see that the line with the arrow starts from the vertex $V(\varphi_1(t),t) - V(\varphi_2(t),t)$ and propagates in the future direction. This can be used to prove the non-relativistic causality in any Hamiltonian system.

We have not discussed the denominator of ρ given in (2.3). It has the following effects in the diagrammatic expansion of $W[j_1, j_2, j_3]$ given in (2.24),

- eliminate the factor $(2\sinh\frac{\omega\beta\hbar}{2})^{-1}$.
- eliminate all the diagrams having $V_I(\varphi(\tau))$ vertices only.

These exhaust our Feynman rule. $G(\tau,\tau')$ is the Matsubara Green's function.[1)] The characteristic feature of the finite time interval theory is the appearance of the mixed propagator $\bar{G}$ which explicitly involves the initial time t_I. In the conventional approach of the infinite time interval, t_I is taken to be $-\infty$ and $\bar{G}$ is neglected. If this is done our expression coincides with the existing formula. This is clearly seen in the $\varphi_1\varphi_2\varphi_3$ representation which is discussed in the next subsection.

2-2. φ_i representation

It is straightforward to rewrite S in the original variables $\varphi_i (i = 1,2,3)$. The result is given in the 3×3 matrix form. For the off-diagonal terms, there are various ways of writing them but we choose those which agree with the conventional expressions. With $\mathbf{j} = (j_1, -j_2, j_3) = (J + \frac{j^{(-)}}{2}, -J + \frac{j^{(-)}}{2}, 0)$, $\frac{S}{\hbar}$ is given by

$$\frac{S}{\hbar} = \frac{1}{2}\iint (\frac{\partial}{\partial\varphi(t)} + \frac{i}{\hbar}\mathbf{j}(t)) \cdot \mathbf{G}(t,s) \cdot (\frac{\partial}{\partial\varphi(s)} + \frac{i}{\hbar}\mathbf{j}(s)) dt ds \tag{2.29}$$

where $\partial/\partial\varphi = (\partial/\partial\varphi_1, \partial/\partial\varphi_2, \partial/\partial\varphi_3)$ and

$$G_{11}(t,s) = \Delta_F(t,s), \quad G_{22}(t,s) = \bar{\Delta}_F(t,s) \tag{2.30}$$

$$G_{12}(t,s) = \Delta^{(+)}(t,s), \quad G_{21}(t,s) = \Delta^{(-)}(t,s) = \Delta^{(+)}(s,t)$$

$$G_{33}(\tau,\tau') = \hbar G(\tau,\tau') \tag{2.31}$$

$$G_{13}(t,\tau) = G_{23}(t,\tau) = \frac{\hbar}{i}\bar{G}(t,\tau)$$

$$G_{31}(\tau,t) = G_{32}(\tau,t) = \frac{\hbar}{i}\bar{G}(\tau,t). \tag{2.32}$$

We have used in (2.29) the same notation t or s for τ or τ'; if t or s corresponds to the index 3, it referrs to τ or τ'. The functions Δ_F, $\bar{\Delta}_F$ and $\Delta^{(\pm)}$ are the usual free propagators given by

$$\begin{aligned}\Delta^{(+)}(t,s) &= Tr\rho_0 q(t)q(s)\\ &= \frac{\hbar}{2m\omega}[-i\sin\omega(t-s)+\coth\frac{\omega\beta\hbar}{2}\cos\omega(t-s)]\\ &= \frac{\hbar}{2m\omega\sinh\frac{\omega\beta\hbar}{2}}[\cos\omega(t-s+i\frac{\beta\hbar}{2})]\end{aligned} \tag{2.33}$$

$$\begin{aligned}\Delta^{(-)}(t,s) &= \Delta^{(+)}(s,t)\\ \Delta_F(t,s) &= \theta(t-s)\Delta^{(+)}(t,s)+\theta(s-t)\Delta^{(-)}(t,s) = Tr\rho_0 Tq(t)q(s),\\ \tilde{\Delta}_F(t,s) &= \theta(t-s)\Delta^{(-)}(t,s)+\theta(s-t)\Delta^{(+)}(t,s) = Tr\rho_0 \tilde{T}q(t)q(s),\end{aligned}$$

where ρ_0 is the harmonic density matrix and $\tilde{T}$ is the anti-time ordering operator. Thus the small matrix $G = \begin{pmatrix} G_{11}G_{12} \\ G_{21}G_{22} \end{pmatrix}$ agrees with the conventional one. The remaining propagators have the following representations.

$$G_{13}(t,\tau) = \frac{\hbar}{2m\omega\sinh\frac{\omega\beta\hbar}{2}}\cos\omega(t-t_I+i(\tau-\frac{\tau_I+\tau_F}{2})) \tag{2.34}$$

$$\begin{aligned}G_{33}(\tau,\tau') &= \frac{\hbar}{2m\omega\sinh\frac{\omega\beta\hbar}{2}}\{\theta(\tau'-\tau)\cos\omega i(\tau-\tau'+\frac{\beta\hbar}{2})+(\tau\leftrightarrow\tau')\}\\ &= Tr\rho_0 T_\tau q(\tau)q(\tau').\end{aligned} \tag{2.35}$$

Equations (2.33) $\sim$ (2.35) suggest that S can be written by a single cosine propagator in a complex t-plane. We show in the next subsection that this is indeed the case through the introduction of the contour integral.

2-3. The contour integral

The notion of the contur integral helps us to rewrite our formula in a compact form. In this subsection, we make for convenience the following substitution without losing the generality.

$$t_i = \tau_I = 0, \quad t_f = T, \quad \tau_F = \beta\hbar. \tag{2.36}$$

Following the method of Keldysh[3] or Niemi-Semenoff,[5] let us introduce the contour C in the complex time plane (Fig.1), which starts at $t_I = 0$ and runs along the real time axis to $t_F = T$ (the segment C_1).

Fig. 1

From T the contour returns along the real time axis to zero (the segment C_2) and finally continues parallel with the imaginary time axis to $-i\tau_F = -i\beta\hbar$ (the segment C_3). The time ordering operator is extended to an operator T_C which orders the operators from right to left according to the occurrence of their time arguments on the contour. The operators T and

T_τ are of course the special cases of T_C. On the contour, the contour δ-function is defined by

$$\int_C dt\delta_C(t-t')f(t) = f(t'). \tag{2.37a}$$

With this definition, we introduce the contour θ-function and the functional differentiation by

$$\theta_C(t-t') = \int_C^t dt''\delta_C(t''-t'), \tag{2.37b}$$

$$\frac{\delta j(t)}{\delta j(t')} = \delta_C(t-t') \tag{2.37c}$$

respectively. Here the following notation is implied,

$$j(t) = j_i(t) \quad \text{if} \quad t \in C_i \quad (i=1,2,3). \tag{2.38}$$

One can also extend other algebraic operations to the contour in a obvious way if necessary.

Then the generating functional can be written as

$$\exp\frac{i}{\hbar}W[j_1,j_2,j_3] = Tr[Tc\exp(-\frac{i}{\hbar}\int_C dtH^j(t))], \tag{2.39}$$

where

$$H^j(t) = \begin{cases} H^{j_i}(t) & t \in C_i \ (i=1,2), \\ H_0^{j_3}(t) & t \in C_3. \end{cases}$$

Going through the same procedure we used to derive the expression of (2.29) and using the above contour notations, we can rewrite (2.29) in terms of single contour propagator G_C as

$$\frac{S}{\hbar} = \frac{1}{2}\int_C\int_C dtds(\frac{\partial}{\partial\varphi(t)} + \frac{i}{\hbar}j(t))G_C(t-s)(\frac{\partial}{\partial\varphi(s)} + \frac{i}{\hbar}j(s)), \tag{2.40}$$

where the functional differentiation $\partial/\partial\varphi(t)$ is defined by

$$\frac{\partial}{\partial\varphi(t)} = \frac{\partial}{\partial\varphi_i(t)}, \qquad t \in C_i \quad (i=1,2,3)$$

and the contour propagator $G_C(t-s)$ is the cosine propagator given by,

$$G_C(t-s) = \frac{\hbar}{2m\omega}\frac{1}{\sinh\frac{\omega\beta\hbar}{2}}[\cos\omega(s-t-\frac{i\beta\hbar}{2})\theta_C(s-t) + (t \leftrightarrow s)].$$

If we recover the suffix of $j(t)$ and $\varphi(t)$, the results (2.40) is reduced to the expression (2.29).

2-4. Expectation value of the arbitrary operator

The expectation value of q or that of any function of q at the time t can be obtained by the expression like (2.9a).[8] If the operator includes the momentum p, the expectation value of the Hamiltonian for example, the propagator of the momentum has to be calculated, which can be done by slightly generalizing the studies given above. The result is that we have only to replace $p(t) \longrightarrow m\dot{q}(t)$ and use the propagator for $q(t)$.[8]

For arbitrary operator O, we have

$$< O >_t = Tr\{\exp(-\beta H_I) K^{\dagger j_2} O(q) K^{j_1}\} / Tr \exp(-\beta H_I) \tag{2.41}$$

where we set $j_1 = j_2 = J$ — the physical source if it is not zero. For $K^{j_{1,2}}$ of (2.41), the time ordered product extends from t_I to t, with the part corresponding to the region from t to t_F omitted. The path integral representation of (2.41) and the resulting Feynman rule is given in the way as above; the propagators, for example, are the same. The operator $O(q)$ can be replaced by $O(\varphi_1(t))$ or $O(\varphi_2(t))$ or by $O(\varphi^{(+)}(t))$. They all give the same results. This method is easier than the multiple differentiation with respect $j^{(-)}$.

The role of the denominator in (2.41) is to eliminate the graphs which are disconnected with the operator O — the "vacuum diagrams". This fact makes it clear that in the limit $t_I \longrightarrow -\infty$ our formalism coincides with the conventional one. The original 3×3 operator matrix G becomes block diagonal[5] for $t_I \rightarrow -\infty$ but because of the denominator of (2.41) this can further be reduced to 2×2 matrix:

$$(3 \times 3) \quad {}_{t_I \rightarrow -\infty} \quad \left(\begin{array}{c|c} 2 \times 2 & 0 \\ \hline 0 & G_{33} \end{array} \right) \simeq (2 \times 2)$$

2-5. The classical limit

It is interesting to see how our formalism reduces to the classical non-equilibrium statistical formula in the limit $\hbar \longrightarrow 0$,[9] where we know that the expectation value of any function of p and q at the time t is given by

$$< O >_t = \frac{\int dpdq O(p(t), q(t)) \exp\{-\beta H(p, q, t)\}}{\int dpdq \exp\{-\beta H_I(p, q)\}} \tag{2.42}$$

where $p(t)$, $q(t)$ is the solution of the classical equation of motion $\dot{p} = -\partial H(p, q, t)/\partial q$, $\dot{q} = \partial H(p, q, t)/\partial p$, with the boundary conditions $p(t_I) = p$, $q(t_I) = q$. Using (2.2) they are given by

$$\begin{aligned} q(t) &= q \cos\omega(t - t_I) + \tfrac{p}{m\omega} \sin\omega(t - t_I) - \textstyle\int_{t_I}^{t_F} \Delta_R(t - s) V'(q(s), s) ds. \\ p(t) &= p \cos\omega(t - t_I) - mq\omega \sin\omega(t - t_I) - m \textstyle\int_{t_I}^{t_F} \dot{\Delta}_R(t - s) V'(q(s), s) ds. \end{aligned} \tag{2.43}$$

The iterative solution of (2.43) is represented by the tree graphs with the propagator Δ_R. We consider for simplicity the case $O = O(q)$. Other case can be discussed in a similar way.

Let us examine the limit $\hbar \to 0$ of the propagators G_{ij}. The region of the τ-integration vanishes since $\tau_F - \tau_I = \beta\hbar \to 0$. Therefore we set $\tau, \tau' = 0$ in the $\varphi^{(\pm)}$ representation which is the convenient one for the discussion of the classical limit. Using eqs.(2.28a $\sim$ c) we get,

$$\bar{\Delta}(t-s) \quad \to -\tfrac{1}{m\omega^2\beta\hbar}\cos\omega(t-s) \tag{2.44a}$$

$$\tfrac{1}{i}\bar{G}(t,\tau) \quad \to \tfrac{1}{m\omega^2\beta\hbar}\cos\omega(t-t_I) \tag{2.44b}$$

$$G(\tau,\tau') \quad \to \tfrac{1}{m\omega^2\beta\hbar} \tag{2.44c}$$

while $\Delta_R(t-s)$ is independent of $\hbar$. Therefore for a given order of the perturbation in $V_I(\varphi(\tau))$ or $V(\varphi(t),t)$, the graphs with the smallest number of Δ_R become dominant in the limit $\hbar \to 0$. These are the "tree graphs" which are constructed by Δ_R. Since Δ_R is the only propagator involving $\varphi^{(-)}(t)$, we can approximate in (2.24) as,

$$-\frac{i}{\hbar}\{V(\varphi_1(t),t)) - V(\varphi_2(t),t)\} \simeq -\frac{i}{\hbar}\varphi^{(-)}(t)V'(\varphi^{(+)}(t),t). \tag{2.45}$$

Since the range of the τ-integration vanishes as $\hbar \to 0$, the following replacement is allowed;

$$\int d\tau \frac{\partial}{\partial\varphi(\tau)} \to \frac{\partial}{\partial\varphi}, \quad \exp\{-\frac{1}{\hbar}\int d\tau V(\varphi(\tau))\} \to \exp(-\beta V(\varphi)\}, \tag{2.46a, b}$$

where $\partial/\partial\varphi$ is the ordinary (not the functional) derivative. Introducing further $\tilde{\varphi}(t) = \frac{i}{\hbar}\varphi^{(-)}(t)$, $\varphi(t) \equiv \varphi^{(+)}(t)$, we can rewrite (2.27a $\sim$ d) in the limit $\hbar \to 0$ as,

$$\frac{S}{\hbar} = -\int dtds(\frac{\partial}{\partial\varphi(t)} + \frac{i}{\hbar}j^{(-)}(t))\Delta_R(t-s)(\frac{\partial}{\partial\tilde{\varphi}(s)} + J(s)) \tag{2.47a}$$

$$+\frac{1}{2}\iint dtds(\frac{\partial}{\partial\varphi(t)} + \frac{i}{\hbar}j^{(-)}(t))\frac{\cos\omega(t-s)}{m\omega^2\beta}(\frac{\partial}{\partial\varphi(s)} + \frac{i}{\hbar}j^{(-)}(s)) \tag{2.47b}$$

$$+\int dt(\frac{\partial}{\partial\varphi(t)} + \frac{i}{\hbar}j^{(-)}(t))\frac{\cos\omega(t-t_I)}{m\omega^2\beta}\frac{\partial}{\partial\varphi} \tag{2.47c}$$

$$+\frac{1}{2}\frac{1}{m\omega^2\beta}(\frac{\partial}{\partial\varphi})^2. \tag{2.47d}$$

With (2.45), (2.46b) and (2.47) inserted into (2.24) where $W[j_1, j_2, j_3]$ is replaced by $W[j^{(-)}]$ defined in (2.25), it is convenient to introduce

$$\tilde{W}[\tilde{j}^{(-)}] = \frac{i}{\hbar}W[j^{(-)} = \frac{\hbar}{i}\tilde{j}^{(-)}]. \tag{2.48}$$

Then $\tilde{W}[\tilde{j}^{(-)}]$ is the generating functional which is finite for $\hbar \to 0$. The resulting graphical rule is equivalent to that appearing in the evaluation of (2.42). Here we notice that the classical averages over the initial value of the solution given in (2.43), which are necessary for the diagrammatic expansion of (2.42), are the following two quantities. Let us define

$$< O >_I = \frac{\int dpdqO \exp(-\beta H_I(p,q))}{\int dpdq \exp(-\beta H_I(p,q))}, \tag{2.49}$$

then what we need are

$$< (q\cos\omega(t-t_I) + \frac{p}{m\omega}\sin\omega(t-t_I))(q\cos\omega(s-t_I) + \frac{p}{m\omega}\sin\omega(s-t_I)) >_I = \frac{1}{m\omega^2\beta}\cos\omega(t-s), \tag{2.50a}$$

$$< q^2 >_I = \frac{1}{m\omega^2\beta}. \tag{2.50b}$$

These are just the propagators appearing in (2.47).

There is an interesting correlation between the cancellation of the power of $\hbar$ and the power of β^{-1} of the resulting expression in the limit of $\hbar \to 0$. Consider (2.24) and (2.27a $\sim$ d) and take any diagram corresponding to any quantity $< O >_t$. If we regard the propagators $\Delta_R, \bar{\Delta}, \bar{G}, G$ as order 1 then it is of the order $(\hbar)^L$ where L is the number of loops in the diagram. However there are two other factors of $\hbar$, the one coming from the region of the τ-integration and the other from $\bar{\Delta}, \bar{G}$ and G. The former gives $(\beta\hbar)^{V_\tau}$ where V_τ is the number of vertices $V_I(\varphi(\tau))$ and the latter contributes $(\beta\hbar)^{-N_P}$ where N_P is the sum of the number of the propagators $\bar{\Delta}, \bar{G}, G$ as is seen by (2.44a $\sim$ c). For the graphs which look like tree with respect to Δ_R, which are the only graphs that survive for $\hbar \to 0$, there is a topological relation

$$V_\tau + L - N_P = 0.$$

Therefore the total factor is a finite quantity,

$$(\hbar)^L(\beta\hbar)^{V_\tau}(\beta\hbar)^{-N_P} = \beta^{-L}.$$

The theorem is thus derived for the classical statistical mechanics;

<u>any diagram is of the order $(kT)^L$</u>

We conclude this subsection by stating that the high temperature limit ($\beta \to 0$) of our formula is easily seen to be equivalent to the classical limit.

2-6. Dissipasion — continuous distribution of ω

In our formalism, the dissipative term arises in an interesting (and natural) way. In order to make the discussion clear, let us consider the expectation value of q and assume that

$$V_I(q) = 0 \qquad V(q,t) = j(t)q.$$

Here we have, for convenience, included the physical linear coupling term in the potential. Using (2.24) with $W[j^{(-)}]$ of (2.25) for W in the left hand side, we get, by differentiating with respect to $j^{(-)}(t)$,

$$q(t) \equiv < q >_t = -\int_{t_I}^{t_F} \Delta_R(t-s) j(s) ds. \tag{2.51}$$

The adiabatic expansion of the solution q is made by expanding $j(s) = j(t) + (s-t)\frac{dj(t)}{dt} + \cdots$. Integration over s' in (2.51) is performed by putting the adiabatic factor $e^{\epsilon s}$ and sending t_I to $-\infty$. Here ϵ is the infinitesimal positive parameter. Then

$$q(t) = -\frac{1}{m\omega^2} j(t) - \frac{\pi}{m\omega}\delta'(\omega)\frac{d}{dt} j(t) + \cdots. \tag{2.52}$$

The equation of motion of $q(t)$ is obtained by solving $j(t)$ in terms of $q(t)$, i.e. by inverting (2.52). Since the time dependence is small the inversion can be done by writing $j(t) = -m\omega^2 q(t) + \Delta j$ where Δj is of the order of $\dot{q} \equiv \frac{dq}{dt}$. Δj is easily obtained and we arrive at

$$\eta \dot{q}(t) + q(t) + \frac{1}{m\omega^2} j(t) = 0 \tag{2.53}$$

$$\eta = -\pi m\omega^2 \frac{\delta'(\omega)}{m\omega}. \tag{2.54}$$

The damping constant η is zero as long as $\omega > 0$. But Caldeira and Leggett[10)] considered the model where Δ_R receives the contribution from various ω_i with the distribution

$$\rho(\Omega) = \frac{1}{m}\sum_i \frac{\delta(\Omega - \omega_i)}{\omega_i}, \tag{2.55}$$

so that Δ_R is changed into

$$\Delta_R^{\Omega}(t-s) = \theta(t-s)\int_0^{\infty} d\Omega \rho(\Omega) \sin\Omega(t-s). \tag{2.56}$$

Then the non-vanishing η is obtained if $\rho(\Omega)$ behaves as $\eta\Omega$ for small Ω since η is proportional to $\rho'(\Omega = 0)$. However it requires the mode with the zero frequency and we believe that such a situation is an artificial one and cannot be a general mechanism of the dissipative phenomenon.

In our case, however, the dissipation comes from the loop diagrams which represents the scattering of the particle with those present in the heat bath. This is the case even if the system has the finite lower bound of ω. But ω is required to have a continuous distribution in our case also, which is realized by taking any field theoretical model. Let us replace q by the field variable $\varphi(\mathrm{x})$ and consider for example,

$$\begin{aligned} H_0[\varphi] &= \frac{m}{2}\int \{\dot{\varphi}(\mathrm{x})^2 + \varphi(\mathrm{x})\omega^2(-\nabla^2)\varphi(\mathrm{x})\} d^3\mathrm{x} + \lambda \int \varphi^3(\mathrm{x}) d^3\mathrm{x}. \\ H(\varphi, t) &= H_0[\varphi] + \int j(\mathrm{x}, t)\varphi(\mathrm{x}) d^3\mathrm{x}. \end{aligned}$$

Here $\omega(\mathbf{k}^2) \equiv \omega_k$ in Fourier space represents the dispersion of the φ-field. The expectation value $\varphi_{\mathbf{k}}(t) \equiv <\varphi(\mathbf{k})>_t$ satisfies the adiabatic relation, up to the order λ^2,

$$\eta\dot{\varphi}_{\mathbf{k}}(t) + \varphi_{\mathbf{k}}(t) + \frac{j(\mathbf{k},t)}{m\omega(\mathbf{k}^w)} = 0. \tag{2.57}$$

η receives the non-vanishing contribution from the diagram shown in Fig.2. Recall that the propagator $\bar{\Delta}$ represents the correlation of the two particles which are in the heat bath. Indeed cutting off the $\bar{\Delta}$ line, the self-energy part of Fig.2 looks like the scattering of φ-field with that in the thermal environment.

Fig. 2

The explicit representation of η is

$$\eta = C\lambda^2\frac{\hbar}{V}\sum_{\mathbf{k}'}\frac{\pi\delta'(\omega_{k'}-\omega_{k''})}{\omega_{k'}\omega_{k''}}\{\coth\frac{\omega_{k'}\beta\hbar}{2} - \coth\frac{\omega_{k''}\beta\hbar}{2}\} \tag{2.58}$$

where $\mathbf{k}'' = \mathbf{k} - \mathbf{k}'$ and C is some positive numerical constant. Since $\coth x$ is a decreasing function of x, η is positive. Recall that $\omega_{k'} - \omega_{k''}$ vanishes even if ω_k has the non-zero lower bound. This is in sharp contrast with the Caldeira-Leggett case of ref.10). Our mechanism can explain the universal character of the dissipative phenomenon. Note that η survives in the classical limit since (2.58) is finite for $\hbar \to 0$.

The detailed study of the mechanism of the dissipation including the explicit calculations is published in a separate paper.

§3. Coherent state representation

For some problems, the coherent state representation is more convenient. Consider the Hamiltonian

$$\begin{aligned} H_I(c^+,c) &= \hbar\omega c^+c + V_I(c^+,c) && t < t_I \\ H(c^+,c,t) &= \hbar\omega c^+c + V(c^+,c,t) && t \geq t_I \end{aligned}$$

where c^+ or c is the creation and annihilation operator satisfying

$$[c,c^+]_{-\kappa} = cc^+ - \kappa c^+c = 1. \tag{3.1}$$

Here we discuss the Boson and Fermion simultaneously so that we assume $\kappa = +1$ for Bosons and $\kappa = -1$ for Fermions. The potential V_I and V are assumed to be in the normal ordered form. The followings are the list of the well-known formulas necessary for our discussions below. Recall that the coherent states are the eigen-state of the annihilation operator c and they are not orthogonal each other but form the complete set:

$$\begin{aligned} c|z> &= z|z>, \\ |z> &= e^{\kappa z c^+}|0> \quad \text{where} \quad c|0>=0 \\ <z|z'> &= e^{z^* z'} \end{aligned}$$

$$\int d\mu(z)\exp(-z^*z)|z><z| = 1$$

$$d\mu(z) = \begin{cases} dRezdImz/\pi & \cdots \kappa = +1 \\ dz^*dz & \cdots \kappa = -1. \end{cases} \tag{3.2}$$

For Bosons, z is a complex number but for Fermions it is a Grassman number. In (3.2) $Rez(Imz)$ implies the real (imaginary) part of z. The Gaussian integral is performed by the following formula, where we introduce two sets of Grassman variables z_i, z_i^*, ξ_i and ξ_i^*.

$$\int \Pi_i d\mu(z_i)\exp[-\sum_{ij} z_i^* A_{ij} z_j + \sum_i \xi_i^* z_i + \sum_i z_i^* \xi_i] = (detA)^{-\kappa}\exp[\sum_{ij}\xi_i^*(A^{-1})_{ij}\xi_J]. \tag{3.3}$$

The special care has to be paid to the trace formula;

$$TrO = \int d\mu(z)e^{-z^*z} <\kappa z|O|z>. \tag{3.4}$$

Now we introduce the source term as

$$\begin{aligned} H_I &\rightarrow H_I - j_3^*(t)c - c^+ j_3(t) \equiv H_I^{j_3} \\ H &\rightarrow H - j_{1,2}^*(t)c - c^+ j_{1,2}(t) \equiv H^{j_{1,2}}. \end{aligned} \tag{3.5}$$

Here $j_i, j_i^*((i = 1,2,3)$ is the complex (Grassman) number source for the Bosons (Fermions). Introducing the time evolution kernel $K^{j_{1,2}}$ just as in (2.7), the generating functional is defined as

$$\begin{aligned} \exp\tfrac{i}{\hbar}W[j_1,j_2,j_3] &= Tr\rho K^{\dagger j_2}K^{j_1} \\ &= \int d\mu(z)d\mu(z')d\mu(z'')\exp(-z^*z - z'^*z' - z''^*z'') \\ &\times <\kappa z|\rho|z'><z'|K^{*j_2}|z''><z''|K^{j_1}|z>. \end{aligned} \tag{3.6}$$

The coherent state representation $<z'|K^{j_1}|z>$ is known[11] and the result is the following;

$$<z''|K^{j_1}|z> = \exp\{-\frac{i}{\hbar}\int_{t_I}^{t_F} dtV(\kappa\frac{\hbar}{i}\frac{\partial}{\partial j_1(t)}, \frac{\hbar}{i}\frac{\partial}{\partial j_1^*(t)}, t)\}\exp S, \tag{3.7}$$

$$\begin{aligned} S &= z''^* e^{-i\omega(t_I - t)} z \\ &+ \int_{t_I}^{t_F} dt \frac{i}{\hbar} j_1^*(t) e^{-i\omega(t-t_I)} z \\ &+ z''^* \int_{t_I}^{t_F} dt e^{-i\omega(t_F - t)} \frac{i}{\hbar} j_1(t) \\ &+ \iint_{t_I}^{t_F} dtds \frac{i}{\hbar} j_1^*(t) e^{-i\omega(t-s)}\theta(t-s)\frac{i}{\hbar} j_1(s). \end{aligned} \tag{3.8}$$

Here the derivative $\partial/\partial j$ is defined to be left-derivative for the Grassman variable. The similar expressions for $< \kappa z|\rho|z' >$ and $< z'|K^{\dagger j_2}|z'' >$ together with (3.7) are inserted into (3.6). Three integrals over z, z', z'' are all Gaussian which can be evaluated by (3.3). The results are written in φ-representation by using the identity (2.23) with the replacement

$$\begin{array}{lll} j_i\varphi_i & \rightarrow & j_i^*\varphi_i + \varphi_i^* j_i, \quad (i = 1,2,3) \\ \varphi = 0 & \rightarrow & \varphi = \varphi^* = 0. \end{array} \tag{3.9}$$

The final expression is given by choosing $j_1 = -j_2 \equiv \frac{j^{(-)}}{2}$, $j_1^* = -j_2^* \equiv \frac{j^{(-)*}}{2}$, and introducing $W[j^{(-)}, j^{(-)*}] \equiv W[j_1 = -j_2 = \frac{j^{(-)}}{2}, j_1^* = -j_2^* = \frac{j^{(-)*}}{2}, j_3 = 0]$. It is easy to recover non-vanishing $j^{(+)}$.

$$\begin{aligned} \exp\frac{i}{\hbar}W[j^{(-)}, j^{(-)*}] &= (f_\beta(\omega)e^{\omega\beta\hbar})^\kappa \exp S \times \exp[-\frac{1}{\hbar}\int_{\tau_I}^{\tau_F} d\tau V_I(\varphi_3^*(\tau), \varphi_3(\tau)) \\ &\quad -\frac{i}{\hbar}\int_{t_I}^{t_F} dt\{V(\varphi_1^*(t), \varphi_1(t), t) - V(\varphi_2^*(t), \varphi_2(t), t)\}] \end{aligned} \tag{3.10}$$

where

$$f_\beta(\omega) = \frac{1}{e^{\omega\beta\hbar} - \kappa}. \tag{3.11}$$

3-1. $\varphi^{(\pm)}$ representation

Using the variable $\varphi^{(\pm)}$ and $\varphi^{(\pm)*}$ defined in (2.26) together with the notations $\varphi_3 \equiv \varphi$, $\varphi_3^* \equiv \varphi^*$, S is given as κS_0 where

$$\begin{aligned} S_0 &= \iint_{t_I}^{t_F} dtds(\frac{\partial}{\partial\varphi^{(+)}(t)} + \frac{i}{\hbar}j^{(-)*}(t))\Delta_R^{c.s.}(t-s)\frac{\partial}{\partial\varphi^{(-)*}(s)} \\ &+ \iint_{t_I}^{t_F} dtds\frac{\partial}{\partial\varphi^{(-)}(t)}\Delta_A^{c.s.}(t-s)(\frac{\partial}{\partial\varphi^{(+)*}(s)} + \frac{i}{\hbar}j^{(-)}(s)) \\ &+ \iint_{t_I}^{t_F} dtds(\frac{\partial}{\partial\varphi^{(+)}(t)} + \frac{i}{\hbar}j^{(-)*}(t))\bar{\Delta}^{c.s.}(t-s)(\frac{\partial}{\partial\varphi^{(+)*}(s)} + \frac{i}{\hbar}j^{(-)}(s)) \\ &+ \int_{t_I}^{t_F}\int_{\tau_I}^{\tau_F} dtd\tau\frac{\partial}{\partial\varphi(\tau)}\bar{G}^{(+)}(\tau,t)(\frac{\partial}{\partial\varphi^{(+)*}(t)} + \frac{i}{\hbar}j^{(-)}(t)) \\ &+ \int_{t_I}^{t_F}\int_{\tau_I}^{\tau_F} dtd\tau(\frac{\partial}{\partial\varphi^{(+)}(t)} + \frac{i}{\hbar}j^{(-)*}(t))\bar{G}^{(-)}(t,\tau)\frac{\partial}{\partial\varphi^*(\tau)} \\ &+ \iint_{\tau_I}^{\tau_F} d\tau' d\tau\frac{\partial}{\partial\varphi(\tau)}D(\tau,\tau')\frac{\partial}{\partial\varphi^*(\tau')} \end{aligned}$$

where

$$\Delta_R^{c.s.}(t-s) = e^{-i\omega(t-s)}\theta(t-s),$$

$$\begin{aligned}
\Delta_A^{c.s.}(t-s) &= -e^{-i\omega(t-s)}\theta(s-t),\\
\bar{\Delta}^{c.s.}(t-s) &= (\kappa f_\beta(\omega)+\frac{1}{2})e^{-i\omega(t-s)},\\
\bar{G}^{(+)}(\tau,t) &= f_\beta(\omega)e^{\frac{\omega\beta\hbar}{2}}e^{-i\omega T},\\
\bar{G}^{(-)}(t,\tau) &= \kappa f_\beta(\omega)e^{\frac{\omega\beta\hbar}{2}}e^{i\omega T},\\
D(\tau,\tau') &= f_\beta(\omega)e^{-\omega(\tau-\tau'-\frac{\beta\hbar}{2})}\times\{\theta(\tau-\tau')e^{\frac{\omega\beta\hbar}{2}}+\theta(\tau'-\tau)\kappa e^{-\frac{\omega\beta\hbar}{2}}\}.
\end{aligned}$$

Here the definition $T=-i(\tau-\frac{\tau_I+\tau_F}{2})-(t-t_I)$ is introduced. All the propagators are expressed by the exponential form. This is the formula corresponding to (2.27a $\sim$ d) of the coordinate representation.

The expectation value of an arbitrary normal ordered operator $O(c^+,c)$ is calculated either by the appropriate differentiation of (3.10) in terms of $j^{(-)}, j^{(-)*}$ or by using the relation $<O>_t=Tr\rho K^*OK/Tr\rho$. This is calculated through inserting the factor $O(\varphi^{(+)*}(t),\varphi^{(+)}(t))$ into the end of (3.10). The division by $Tr\rho$ is accomplished by discarding the diagrams which are not connected with the inserted operator O.

3-2. φ_i representation and the contour integral

As was done in the subsection 2-2, one can rewrite $S=\kappa S_0$ by the variables φ_i(i=1,2,3) and by choosing (2.36). The result is

$$S_0=\iint dtds(\frac{\partial}{\partial\varphi(t)}+\frac{i}{\hbar}\mathbf{j}^*(t))\mathbf{D}(t,s)(\frac{\partial}{\partial\varphi^{(*)}(s)}+\frac{i}{\hbar}\mathbf{j}(s))$$

where $\partial/\partial\varphi^{(*)}=(\partial/\partial\varphi_1^{(*)},\partial/\partial\varphi_2^{(*)},\partial/\partial\varphi_3^{(*)})$ and $\mathbf{j}^{(*)}=(j_1^{(*)},-j_2^{(*)},j_3^{(*)})$. $\mathbf{D}(t,s)$ is the 3×3 propagator matrix, which has the following elements,

$$\begin{aligned}
D_{21}(t,s) &= \Delta_{(+)}^{c.s.}(t-s)=f_\beta(\omega)e^{-i\omega(t-s+\frac{i\beta\hbar}{2})}e^{\frac{\beta\hbar\omega}{2}}\\
D_{12}(t,s) &= \Delta_{(-)}^{c.s.}(t-s)=f_\beta(\omega)e^{-i\omega(t-s+\frac{i\beta\hbar}{2})}\kappa e^{-\frac{\beta\hbar\omega}{2}}\\
D_{11}(t,s) &= \Delta^{c.s.}(t-s)=\theta(t-s)\Delta_{(+)}^{c.s.}(t-s)+\theta(s-t)\Delta_{(-)}^{c.s.}(t-s)\\
D_{22}(t,s) &= \tilde{\Delta}^{c.s.}(t-s)=\theta(t-s)\Delta_{(-)}^{c.s.}(t-s)+\theta(s-t)\Delta_{(+)}^{c.s.}(t-s)\\
D_{33}(\tau,\tau') &= D(\tau,\tau')\\
D_{13}(t,\tau) &= D_{23}(t,\tau)=\bar{G}^{(-)}(t,\tau)\\
D_{31}(\tau,t) &= D_{32}(\tau,t)=\bar{G}^{(+)}(\tau,t)
\end{aligned}$$

Here for τ and τ' we have used the same notations as (2.28) and (2.29).

If we introduce the contour C as in the Section 2-3, the matrix $\mathbf{D}(t,s)$ can finally be reduced to the contour propagator in the following way.

$$S_0=\int_C\int_C dtds(\frac{\partial}{\partial\varphi(t)}+\frac{i}{\hbar}j^*(t))D_C(t-s)(\frac{\partial}{\partial\varphi^*(s)}+\frac{i}{\hbar}j(s)),$$

where $D_C(t-s)$ is the contour propagator given by

$$D_C(t-s) = f_\beta(\omega) e^{-i\omega(t-s+\frac{i\beta\hbar}{2})} \times [\theta_C(t-s) e^{\frac{\beta\hbar\omega}{2}} + \theta_C(s-t)\kappa e^{-\frac{\beta\hbar\omega}{2}}].$$

§4. Discussions

We have presented the complete diagrammatical rule of the non-equilibrium process at finite time interal assuming the initial equilibrium state. The interaction part of both H_I and $H(t)$ is expanded to produce the diagrams. We always keep track of the initial time t_I and look at the system or some operator at $t > t_I$. The time interval we have to study is limited just from t_I to t. Our formalism is convenient for the study of the non-equilibrium process in general since we can continuously follow the data starting from t_I. It is also easily unified with the equilibrium phenomenon.

The several subjects related to this formalism are presented below.

1) The effective action at finite time interval

Since the source $j_i (i = 1,2,3)$ is introduced, the Legendre transformation of $W[j_1, j_2] \equiv W[j_1, j_2, j_3 = 0]$ can be done and it is known as the effective action Γ. In our case it is actually the effective action at finite time interval. Γ is defined as

$$\Gamma[\varphi_1, \varphi_2] = W[j_1, j_2] - \int dt [j_1(t) \frac{\partial W}{\partial j_1(t)} + j_2(t) \frac{\partial W}{\partial j_2(t)}] \tag{4.1}$$

$$\varphi_1(t) = \frac{\partial W}{\partial j_1(t)}, \quad \varphi_2(t) = -\frac{\partial W}{\partial j_2(t)}. \tag{4.2}$$

Since

$$\frac{\partial \Gamma}{\partial \varphi_1(t)} = -j_1(t), \quad \frac{\partial \Gamma}{\partial \varphi_2(t)} = j_2(t) \tag{4.3}$$

and since the physical quantity is obtained by setting $j_1 = j_2 = 0$, the equation of motion of $\varphi \equiv \varphi_1 = \varphi_2$ is given by

$$\frac{\partial \Gamma[\varphi_1, \varphi_2]}{\partial \varphi_1(t)} |_{\varphi_1 = \varphi_2 = \varphi} = 0. \tag{4.4}$$

The above is the generalization of the effective action defined by Niemi and Semenoff [5] for the infinite time interval. Equation (4.4) will play a fundamental role in the non-equilibrium mechanics.

2) Field theory

As pointed out in Section 2-6, our formulas can straightforwardly be extended to the field theoretical system. Since the macroscopic system is best described by the second quantized field theory, we are particulay interested in this theory. The only change that should be made is that the summation is replaced by the integration over the independent degrees of freedom specified by that the wave vector $\mathbf{k}$ or the space point $\mathbf{x}$. We have not presented the explicit formula for the field theoretical case because these transformations are rather trivial.

3) Arbitrary initial state

If one wants the arbitrary initial density matrix ρ, what we can do is to derive the rule of

$$< q'|K^{\dagger j_2}K^{j_1}|q > \quad \text{or} \quad < z'|K^{\dagger j_2}K^{j_1}|z > \tag{4.5}$$

and then perform the integration over q, q' or z, z' multiplying $< q|\rho|q' >$ or $< z|\rho|z' >$. The explicit form of (4.5) can be given and for the co-ordinate representation we have shown it in (2.11), (2.13) and (2.18). They are characterized by the rule which has the dependence on q', q or z', z in the external line appearing in the diagram. This rule has to be used when ρ does not correspond to the equilibrium state.

4) Comparison with other approaches

In case the potential $V(q)$ is linear in q, the diagrammatical technique is unnecessary since the exact expression is obtained[12] for the expectation value of any operator. As has been pointed out in Sec.2-6, however, the unharmonic part of $V(q)$ is essential for the dissipative effects. Note that the unharmonicity represents the scattering among the harmonic modes which is of course the origin of the various non-trivial phenomenon in the non-equilibrium dynamics. This is most clearly seen in the field theoretical formulation.

Another comment is on the method of the analytic continuation.[13] It is well-known that the real time results are recovered from the imaginary time formulation through the analytic continuation in the time variable. Needless to say our method utilizes the real time from the beginning and avoids the rather intricate method of the continuation process.

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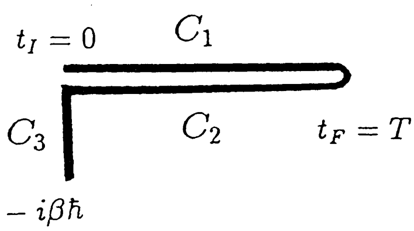

Fig.1

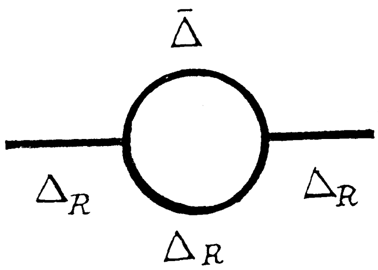

Fig.2