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Comment on the Microscopic Derivation of the Langevin Equation

— From the New Aspect of Non-Equilibrium Thermo Field Dynamics —

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1 Introduction

Shibata and Hashitsume [1] tried to derive the quantum Langevin equation starting from the microscopic Heisenberg equation by making use of the formula [2] which decomposes a time-evolution generator into two parts, i.e., one describing the time-evolution of a relevant system and the other describing that of a irrelevant one (a system producing random forces). In the derivation, they used the formula of differentiation for multiples of analytic functions or operators even after the operators become stochastic ones. Note that the operators appearing in the microscopic Heisenberg equation should be represented by stochastic operators (a kind of the dynamical mapping), before the equation reduces to the Langevin equation [3, 4]. Since the Stratonovich multiplication [5] of stochastic variables gives us the same formula of the differentiation for multiples of analytic variables, one may presume that the Langevin equation derived by Shibata and Hashitsume should be of the Stratonovich type instead of Ito one [6]. In any case, physicists apt to regard the Langevin equations derived from some microscopic equations as of the Stratonovich type.

In this paper, we will review the derivation proposed by Shibata and Hashitsume [1] in terms of Non-Equilibrium Thermo Field Dynamics (NETFD) [7]-[14] which is one of the canonical operator formalism for dissipative quantum fields, and will claim that, in fact, the derived Langevin equation is of the Ito type instead of the Stratonovich one by comparing it with the one derived within NETFD upon some actiomatic consideration.

2 Shibata-Hashitsume's Proposal

2.1 Heisenberg Equation

Shibata and Hashitsume [1] started their consideration with the Heisenberg equation which is written within NETFD in the form

$$\frac{d}{dt}A(t) = i[\hat{H}(t),\ A(t)], \tag{1}$$

with

$$\hat{H}(t) = \mathrm{e}^{i\hat{H}t}\hat{H}\mathrm{e}^{-i\hat{H}t}, \qquad \hat{H} = H - \tilde{H}. \tag{2}$$

The Hamiltonian H can be divided into two parts:

$$H = H_0 + H_1, \qquad H_0 = H_S + H_R, \tag{3}$$

where H_S and H_R are, respectively, the free Hamiltonians of the relevant and of the irrelevant sub-systems, and H_1 represents the interaction Hamiltonian between the relevant and the irrelevant subsystems.

For later convenience, let us introduce the time-evolution operator $\hat{U}(t,0)$ through the relation:

$$\mathrm{e}^{-i\hat{H}t} = \mathrm{e}^{-i\hat{H}_0 t}\hat{U}(t,0). \tag{4}$$

Then, $\hat{U}(t,s)$ satisfies the differential equation

$$\frac{d}{dt}\hat{U}(t,s) = -i\hat{H}_1^I(t)\hat{U}(t,s), \tag{5}$$

with the initial condition $\hat{U}(s,s) = 1$.

2.2 Projector Method

Introducing a projector P which satisfies $P^2 = P$ and $P^\dagger = P$, it is straightforward to get the formula

$$\begin{aligned}\frac{d}{dt}\hat{U}(t,s) &= -i\hat{H}_1^I(t)P\hat{U}(t,s) \\ &\quad - \int_s^t dt'\hat{H}_1^I(t)\hat{U}_{QQ}(t,t')\hat{H}_{1,QP}^I(t')P\hat{U}(t',s) \\ &\quad -i\hat{H}_1^I(t)\hat{U}_{QQ}(t,s)Q,\end{aligned} \tag{6}$$

where Q is defined by $Q = 1 - P$, and $\hat{U}_{QQ}(t,s)$ is introduced by the differential equation

$$\frac{d}{dt}\hat{U}_{QQ}(t,s) = -i\hat{H}_{1,QQ}^I(t)\hat{U}_{QQ}(t,s), \tag{7}$$

with the initial condition $\hat{U}_{QQ}(s,s) = 1$. Here, we have introduced notations

$$\hat{H}^I_{1,QQ}(t) = Q\hat{H}^I_1(t)Q, \qquad \hat{H}^I_{1,QP}(t) = Q\hat{H}^I_1(t)P. \tag{8}$$

The operator $A(t)$ in the Heisenberg representation is related to the operator $A^I(t)$ in the interaction representation by

$$A(t) = \hat{U}^{-1}(t,0)A^I(t)\hat{U}(t,0). \tag{9}$$

Applying the vacuum, $\langle\!\langle 1| = \langle|\langle 1|$, to (9) from the right, we have

$$\begin{aligned}\langle\!\langle 1|A(t) &= \langle\!\langle 1|\hat{U}^{-1}(t,0)A^I(t)\hat{U}(t,0)\\ &= \langle\!\langle 1|A^I(t)\hat{U}(t,0),\end{aligned} \tag{10}$$

where we used the properties

$$\langle\!\langle 1|\hat{H} = 0, \qquad \langle\!\langle 1|\hat{H}_0 = 0, \tag{11}$$

which guarantee the conservation of provability. $\langle 1|$ is the bra-vacuum of the relevant sub-system, and $\langle|$ is the one of the irrelevant sub-system.

Differentiating the vector $\langle\!\langle 1|A(t)$ for observable operator $A(t)$ which consists of non-tilde operators, we have

$$\frac{d}{dt}\langle\!\langle 1|A(t) = i\langle\!\langle 1|[\hat{H}_0(t),\ A^I(t)]\hat{U}(t,0) + \langle\!\langle 1|A^I(t)\frac{d}{dt}\hat{U}(t,0), \tag{12}$$

which reduces to

$$\begin{aligned}\frac{d}{dt}\langle\!\langle 1|A(t) &= -i\langle\!\langle 1|A^I(t)\left(\hat{H}_0 + \hat{H}^I_1(t)P\right)\hat{U}(t,0)\\ &- \int_0^t dt'\langle\!\langle 1|A^I(t)\hat{H}^I_1(t)\hat{U}_{QQ}(t,t')\hat{H}^I_{1,QP}(t')P\hat{U}(t',0)\\ &-i\langle\!\langle 1|A^I(t)\hat{H}^I_1(t)\hat{U}_{QQ}(t,0)Q,\end{aligned} \tag{13}$$

by the substitution of (6).

2.3 Recipe

In order to put (13) into the Langevin equation, Shibata and Hashitsume [1] made the following recipe:

1. Adopt $P = |\rangle\langle|$ for the projector.
2. Retain the non-trivial lowest terms with respect to $\hat{H}^I_1(t)$ in each line in the right-hand side of (13).
3. In the last term depending on the random force operators, replace the relevant operators in the interaction representation by those in the Heisenberg representation.

2.4 Langevin Equation

With the help of the first and the second items of the recipe, we have

$$\begin{aligned}
\frac{d}{dt}\langle\!\langle 1|A(t) &= -i\langle\!\langle 1|A^I(t)\left(\hat{H}_S + \langle\hat{H}_1^I(t)\rangle\right)\hat{U}(t,0) \\
&\quad - \int_0^t dt' \langle\!\langle 1|A^I(t)\langle\hat{H}_1^I(t)\hat{H}_{1,QP}^I(t')\rangle\hat{U}(t',0) \\
&\quad -i\langle\!\langle 1|A^I(t)\hat{H}_1^I(t) \\
&= -i\langle\!\langle 1|A(t)\hat{H}_S(t) \\
&\quad - \int_0^t dt' \langle\!\langle 1|A(t)\hat{U}^{-1}(t,0)\langle\hat{H}_1^I(t)\hat{H}_1^I(t')\rangle\hat{U}(t',0) \\
&\quad -i\langle\!\langle 1|A^I(t)\hat{H}_1^I(t),
\end{aligned} \tag{14}$$

where we assumed that

$$\langle\hat{H}_1^I(t)\rangle = 0. \tag{15}$$

For convenience, we introduced the abbreviation for the vacuum expectation with respect to the vacuums of the irrelevant sub-system: $\langle\cdots\rangle = \langle|\cdots|\rangle$.

Consulting the third item of the recipe and taking the long-time limit (the van Hove limit), we finally get

$$\begin{aligned}
d\langle\!\langle 1|A(t) &= i\langle\!\langle 1|[H_S(t),\ A(t)]dt \\
&\quad +\kappa\langle\!\langle 1|\{a^\dagger(t)[A(t),\ a(t)] + [a^\dagger(t),\ A(t)]a(t)\}dt \\
&\qquad +2\kappa\bar{n}\langle\!\langle 1|[a^\dagger(t),\ [A(t),\ a(t)]]dt \\
&\quad +\langle\!\langle 1|[A(t),\ a^\dagger(t)]\sqrt{2\kappa}\, dB_t + \langle\!\langle 1|[a(t),\ A(t)]\sqrt{2\kappa}\, dB_t^\dagger,
\end{aligned} \tag{16}$$

where

$$\kappa = \Re\mathrm{e}\ g^2\int_0^\infty dt\ \langle b_t\ b^\dagger\rangle e^{i\omega t}, \qquad \bar{n} = \left(e^{\omega/T} - 1\right), \tag{17}$$

with T being the temperature of the irrelevant system. In deriving (16), we put

$$H_S = \omega a^\dagger a, \qquad H_1 = g\left(ab^\dagger + \text{h.c.}\right), \tag{18}$$

for the relevant and the interaction Hamiltonians, respectively. The operators of the relevant system satisfy the canonical commutation relation:

$$[a,\ a^\dagger] = 1. \tag{19}$$

2.5 Quantum Brownian Motion

The operators dB_t and $dB_t^\dagger$ representing the quantum Brownian motion are defined by

$$dB_t = b_t dt, \qquad dB_t^\dagger = b_t^\dagger dt, \tag{20}$$

where the operators b_t and $b_t^\dagger$ satisfy the canonical commutation operator

$$[b_t,\ b_t^\dagger] = 1, \tag{21}$$

and are defined in the sense introduced within the white noise analysis [15]-[17]. The quantum Brownian operators satisfy

$$\langle dB_t \rangle = \langle dB_t^\dagger \rangle = 0, \tag{22}$$

$$\langle dB_t^\dagger dB_t \rangle = \bar{n} dt, \qquad \langle dB_t dB_t^\dagger \rangle = (\bar{n}+1)\, dt. \tag{23}$$

2.6 Comment

In the derivation, Shibata and Hashitsume never specified the stochastic calculus nor the representation space (the Fock space) for the stochastic operators [18]-[20], but performed the same calculation as the one for analytic function which is compatible with the Stratonovich calculus.

3 Langevin Equations within NETFD

3.1 Introduction

With the help of NETFD, we succeeded to construct a unified framework of the *canonical operator formalism* for quantum stochastic differential equations where the stochastic Liouville equation and the Langevin equation are, respectively, equivalent to a Schrödinger equation and a Heisenberg equation in quantum mechanics.

In the course of the construction, it is found that there are at least two physically attractive formulations, i.e.,

(P) Based on a Non-Hermitian Martingale
Employed is the characteristics of the classical stochastic Liouville equation where *the stochastic distribution function satisfies the conservation of probability within the phase space of a relevant system.*

(N) Based on a Hermitian Martingale
Employed is the characteristics of the Schrödinger equation where *the norm of the stochastic wave function preserves itself in time.*

The latter is intimately related to the approach investigated by mathematicians in order to extend the Ito formula to non-commutative stochastic quantities [21, 22].

3.2 Stochastic Liouville Equation

Let us start the consideration with the stochastic Liouville equation of the Ito type:

$$d|0_f(t)\rangle = -i\hat{\mathcal{H}}_{f,t}dt\ |0_f(t)\rangle. \tag{24}$$

The generator $\hat{V}_f(t)$, defined by $|0_f(t)\rangle = \hat{V}_f(t)|0\rangle$ satisfies

$$d\hat{V}_f(t) = -i\hat{\mathcal{H}}_{f,t}dt\ \hat{V}_f(t), \tag{25}$$

with $\hat{V}_f(0) = 1$. The hat-Hamiltonian is a tildian operator satisfying

$$\left(i\hat{\mathcal{H}}_{f,t}dt\right)^{\sim} = i\hat{\mathcal{H}}_{f,t}dt. \tag{26}$$

Any operator A of NETFD is accompanied by its partner (tilde) operator $\tilde{A}$, which enables us treat non-equilibrium and dissipative system by the method similar to the usual quantum mechanics.

From the knowledge of the stochastic integral, we know that the required form of the hat-Hamiltonian should be

$$\hat{\mathcal{H}}_{f,t}dt = \hat{H}dt + d\hat{M}_t, \tag{27}$$

where the martingale $d\hat{M}_t$ is the term containing the operators representing the quantum Brownian motion dB_t, $d\tilde{B}_t^\dagger$ and their tilde conjugates. $\hat{H}$ is given by

$$\hat{H} = \hat{H}_S + i\hat{\Pi}, \tag{28}$$

with

$$\hat{H}_S = H_S - \tilde{H}_S, \qquad \hat{\Pi} = \hat{\Pi}_R + \hat{\Pi}_D, \tag{29}$$

where $\hat{\Pi}_R$ and $\hat{\Pi}_D$ are, respectively, the ***relaxational*** and the ***diffusive*** parts of the damping operator $\hat{\Pi}$.

Here, it is assumed that, at $t = 0$, the relevant system starts to contact with the irrelevant system representing the stochastic process included in the martingale $d\hat{M}_t$.[1]

3.3 Specification of the Martingale

Now, we need something which specifies the structure of the martingale. For the case (P), it is the conservation of probability within the relevant subsystem:

$$\langle 1|d\hat{M}_t = 0. \tag{30}$$

[1]Within the formalism, the random force operators dB_t and $dB_t^\dagger$ are assumed to commute with any relevant system operator A in the Schrödinger representation: $[A,\ dB_t] = [A,\ dB_t^\dagger] = 0$ for $t \geq 0$.

On the other hand, for the case (N), it is the conservation of norm:

$$d\hat{M}_t^\dagger = d\hat{M}_t. \tag{31}$$

The Hermitian martingale is intimately related to the approach started with the stochastic Schrödinger equation where the norm of the wave function preserves itself in time.

3.4 Fluctuation-Dissipation Theorem of the Second Kind

In order to specify the martingale, we need another condition which gives us the relation between multiple of the martingale and the damping operator. For (P), it is

$$d\hat{M}_t \; d\hat{M}_t = -2\hat{\Pi}_D dt, \tag{32}$$

whereas, for (N), it is

$$d\hat{M}_t \; d\hat{M}_t = -2\left(\hat{\Pi}_R + \hat{\Pi}_D\right) dt. \tag{33}$$

This operator relation for each case may be called a generalized fluctuation dissipation theorem of the second kind, which should be interpreted within the weak relation.

3.5 Quantum Langevin Equations

The dynamical quantity $A(t)$ is defined by

$$A(t) = \hat{V}_f^{-1}(t) \; A \; \hat{V}_f(t), \tag{34}$$

where $\hat{V}_f^{-1}(t)$ satisfies

$$d\hat{V}_f^{-1}(t) = \hat{V}_f^{-1}(t) \; i\hat{\mathcal{H}}_{\tilde{f},t}^{-} dt, \tag{35}$$

with

$$\hat{\mathcal{H}}_{\tilde{f},t}^{-} dt = \hat{\mathcal{H}}_{f,t} dt + i d\hat{M}_t \; d\hat{M}_t, \tag{36}$$

which are given, respectively, by

$$\hat{\mathcal{H}}_{\tilde{f},t}^{-} dt = \hat{H}_S dt + i\left(\hat{\Pi}_R - \hat{\Pi}_D\right) dt + d\hat{M}_t, \tag{37}$$

for (P), and by

$$\hat{\mathcal{H}}_{\tilde{f},t}^{-} dt = \hat{H}_S dt - i\left(\hat{\Pi}_R + \hat{\Pi}_D\right) dt + d\hat{M}_t, \tag{38}$$

for (N).

In NETFD, the Heisenberg equation for $A(t)$ within the Ito calculus is the quantum Langevin equation in the form

$$\begin{aligned} dA(t) &= d\hat{V}_f^{-1}(t) \; A \; \hat{V}_f(t) + \hat{V}_f^{-1}(t) \; A \; d\hat{V}_f(t) + d\hat{V}_f^{-1}(t) \; A \; d\hat{V}_f(t) \\ &= i[\hat{\mathcal{H}}_f(t) dt, \; A(t)] - d\hat{M}(t) \; [d\hat{M}(t), \; A(t)], \end{aligned} \tag{39}$$

with

$$\hat{\mathcal{H}}_f(t)dt = \hat{V}_f^{-1}(t)\ \hat{\mathcal{H}}_{f,t}dt\ \hat{V}_f(t), \qquad d\hat{M}(t) = \hat{V}_f^{-1}(t)\ d\hat{M}_t\ \hat{V}_f(t). \tag{40}$$

Since $A(t)$ is an arbitrary observable operator in the relevant system, (39) can be the Ito's formula generalized to quantum systems.

3.6 Langevin Equation for the Bra-Vector

Applying the bra-vacuum $\langle\!\langle 1|$ to (39) from the left, we obtain the Langevin equation for the bra-vector $\langle\!\langle 1|A(t)$ in the form

$$d\langle\!\langle 1|A(t) = i\langle\!\langle 1|[H_S(t),\ A(t)]dt + \langle\!\langle 1|A(t)\hat{\Pi}(t)dt - i\langle\!\langle 1|A(t)d\hat{M}(t). \tag{41}$$

In the derivation, use had been made of the properties

$$\langle 1|\tilde{A}^\dagger(t) = \langle 1|A(t), \qquad \langle|d\tilde{B}^\dagger(t) = \langle|dB(t), \qquad \langle\!\langle 1|d\hat{M}(t) = 0. \tag{42}$$

Note that (41) has the same form both for (P) and (N).

3.7 Quantum Master Equation

Taking the random average by applying the bra-vacuum $\langle|$ of the irrelevant sub-system to the stochastic Liouville equation (24), we can obtain the quantum master equation as

$$\frac{\partial}{\partial t}|0(t)\rangle = -i\hat{H}|0(t)\rangle, \tag{43}$$

with $\hat{H}dt = \langle|\hat{\mathcal{H}}_{f,t}dt|\rangle$ and $|0(t)\rangle = \langle|0_f(t)\rangle$.

3.8 An Example

We will apply the above formula to the model described by (18). We are now confining ourselves to the case where the stochastic hat-Hamiltonian $\hat{\mathcal{H}}_t$ is bi-linear in a, $a^\dagger$, dB_t, $dB_t^\dagger$ and their tilde conjugates, and is invariant under the phase transformation $a \longrightarrow a\mathrm{e}^{i\theta}$, and $dB_t \rightarrow dB_t\ \mathrm{e}^{i\theta}$. Then, we have

$$\hat{\Pi}_R = -\kappa\left(\alpha^{\scriptsize ?}\alpha + \text{t.c.}\right), \qquad \hat{\Pi}_D = 2\kappa\,[\bar{n}+\nu]\,\alpha^{\scriptsize ?}\tilde{\alpha}^{\scriptsize ?}, \tag{44}$$

where we introduced a set of canonical stochastic operators

$$\alpha = \mu a + \nu\tilde{a}^\dagger, \qquad \alpha^{\scriptsize ?} = a^\dagger - \tilde{a}, \tag{45}$$

with $\mu+\nu = 1$, which satisfy the commutation relation $[\alpha,\ \alpha^{\scriptsize ?}] = 1$. The tilde and non-tilde operators are related with each other by the relation $\langle 1|a^\dagger = \langle 1|\tilde{a}$.

The martingale operator for the case (P) is given by

$$d\hat{M}_t = i\left[\alpha^{♀} dW_t + \text{t.c.}\right], \tag{46}$$

and the one for the case (N) has the form

$$d\hat{M}_t = i\left[\alpha^{♀} dW_t + \text{t.c.}\right] - i\left[\alpha\, dW_t^{♀} + \text{t.c.}\right]. \tag{47}$$

Here, the random force operators dW_t and $dW_t^{♀}$ are defined, respectively, by

$$dW_t = \sqrt{2\kappa}\left(\mu dB_t + \nu d\tilde{B}_t^{\dagger}\right), \qquad dW_t^{♀} = \sqrt{2\kappa}\left(dB_t^{\dagger} - d\tilde{B}_t\right). \tag{48}$$

The latter annihilates the bra-vacuum $\langle|$ of the irrelevant system:

$$\langle| dW_t^{♀} = 0, \qquad \langle| d\tilde{W}_t^{♀} = 0. \tag{49}$$

The quantum Langevin equation for the case (P) is given by

$$\begin{aligned} dA(t) = {} & i[\hat{H}_S(t),\ A(t)]dt \\ & +\kappa\left\{[\alpha^{♀}(t)\alpha(t),\ A(t)] + [\tilde{\alpha}^{♀}(t)\tilde{\alpha}(t),\ A(t)]\right\} dt \\ & +2\kappa(\bar{n}+\nu)[\tilde{\alpha}^{♀}(t),\ [\alpha^{♀}(t),\ A(t)]]dt \\ & -\left\{[\alpha^{♀}(t),\ A(t)]dW_t + [\tilde{\alpha}^{♀}(t),\ A(t)]d\tilde{W}_t\right\}, \end{aligned} \tag{50}$$

and the one for (N) is given by

$$\begin{aligned} dA(t) = {} & i[\hat{H}_S(t),\ A(t)]dt \\ & +\kappa\left\{[\alpha^{♀}(t),\ A(t)]\alpha(t) - \alpha^{♀}[\alpha(t),\ A(t)]\right. \\ & \left. +[\tilde{\alpha}^{♀}(t),\ A(t)]\tilde{\alpha}^{♀}(t) - \tilde{\alpha}^{♀}(t)[\tilde{\alpha}(t),\ A(t)]\right\} dt \\ & +2\kappa\,(\bar{n}+\nu)\,[\tilde{\alpha}^{♀}(t),\ [\alpha^{♀}(t),\ A(t)]]dt \\ & -\left\{[\alpha^{♀}(t),\ A(t)]dW_t + [\tilde{\alpha}^{♀}(t),\ A(t)]d\tilde{W}_t\right\} \\ & +\left\{dW_t^{♀}[\alpha(t),\ A(t)] + d\tilde{W}_t^{♀}[\tilde{\alpha}(t),\ A(t)]\right\}, \end{aligned} \tag{51}$$

with $\hat{H}_S(t) = \hat{V}_f^{-1}(t)\hat{H}_S\hat{V}_f(t)$.

The Langevin equation for the bra-vector state, $\langle\!\langle 1|A(t)$, reduces to

$$\begin{aligned} d\langle\!\langle 1|A(t) = {} & i\langle\!\langle 1|[H_S(t),\ A(t)]dt \\ & +\kappa\left\{\langle\!\langle 1|[a^{\dagger}(t),\ A(t)]a(t) + \langle\!\langle 1|a^{\dagger}(t)[A(t),\ a(t)]\right\} dt \\ & +2\kappa\bar{n}\langle\!\langle 1|[a(t),\ [A(t),\ a^{\dagger}(t)]]dt \\ & +\langle\!\langle 1|[A(t),\ a^{\dagger}(t)]\sqrt{2\kappa}\, dB_t + \langle\!\langle 1|[a(t),\ A(t)]\sqrt{2\kappa}\, dB_t^{\dagger}, \end{aligned} \tag{52}$$

both for the cases (P) and (N).

3.9 Comment

We showed that both of the two formulations within NETFD, i.e., one is based on the density operator formalism and the other on the wave function formalism, give the same results in the weak relation (a relation between matrix elements in certain representation space) but with different equations in the strong relation (a relation between operators), while each formulation provides us with a consistent and unified system of quantum stochastic differential equations.

4 Discussion

We showed that the Langevin equation (16) is, in fact, of the Ito type by comparing it with (52) derived with the help of the unified formulation of the stochastic differential equations within NETFD. Some investigation of the Shibata-Hashitsume Langevin equation in its original formulation will be given elsewhere [23]. There, it is checked for several systems that the Langevin equations are indeed of the Ito type from the view points of physical consistencies.

The derivation of stochastic differential equations from a microscopic stage is an old problem in statistical mechanics. It may be necessary to think it over again after knowing the unified formulations within NETFD.

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