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LETTER TO THE EDITOR

Thermal processes in the hydrodynamic stage in terms of non-equilibrium thermofield dynamics

Toshihico Arimitsu

Institute of Physics, University of Tsukuba, Ibaraki 305, Japan

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Abstract. The thermal processes in the hydrodynamic stage are investigated within the formalism of non-equilibrium thermofield dynamics (NETFD) where the concepts in non-equilibrium thermodynamics are implanted. The treatment gives us a good indication for an understanding of the new concept, *the spontaneous creation of dissipation*, in conjunction with the realization of the representation space within NETFD.

The framework of non-equilibrium thermofield dynamics (NETFD) was firstly constructed [1, 2] by, so to speak, a *principle of correspondence* (mapping rules) based upon the damping theoretical argument within the density operator formalism [3, 4]. It was shown that the framework is constructed upon the seven axioms [5]. Then the most general expression of the renormalized time-evolution generator in the interaction representation was derived together with an equation for the one-particle distribution function [6, 7]. Within these aspects, the canonical formalism of dissipative quantum fields in NETFD was formulated, and the close structural resemblance between NETFD and usual quantum field theories was revealed [8, 9]. Furthermore, the generating functional within NETFD was derived [10], and the relation between NETFD and the closed time-path methods [11-13] was shown [14] mainly in the *kinetic stage*. Recently, it was shown that the framework of NETFD is wide and general enough to include the quantum Langevin equation and the quantum stochastic Liouville equation approach as well [15-18].

The structural resemblance of NETFD with usual quantum field theories showed us vividly the dual structure, i.e. the *operator algebra* and the *representation space*, of the dissipative quantum field theory for far-from-equilibrium states NETFD. The strong analogy between the mechanism of the *spontaneous (dynamical) breakdown of symmetry* within usual quantum field theories and that of the appearance of the dissipative time-evolution generator within NETFD made us to propose a new concept named the *spontaneous (dynamical) creation of dissipation* [6, 7, 19-22] which is still to be clarified.

In this letter, we will implant the concepts of non-equilibrium thermodynamics [23], which have not been introduced in usual quantum field theories, into NETFD in order to understand and/or to extend the formalism further, standing on the reliable basis of thermodynamics. We confine ourselves to investigation in the *hydrodynamic stage* as it should be, and consult the treatment proposed by Kubo [24] and by Zubarev [25]. We will present the formalism in its most general form; however we will bear an ℓ -component liquid system in mind for clarity.

Heisenberg fields, $\psi(\mathbf{x}, t)$ and $\psi^\dagger(\mathbf{x}, t)$, within the formalism NETFD have their partner fields, $\tilde{\psi}(\mathbf{x}, t)$ and $\tilde{\psi}^\dagger(\mathbf{x}, t)$, respectively. The tilde conjugation \sim is defined by $(A_1 A_2)^\sim = \tilde{A}_1 \tilde{A}_2$, $(c_1 A_1 + c_2 A_2)^\sim = c_1^* \tilde{A}_1 + c_2^* \tilde{A}_2$, $(\tilde{A})^\sim = \sigma A$, and $(A^\dagger)^\sim = \tilde{A}^\dagger$, with arbitrary operators A_i and c-numbers c_i , where $\sigma = 1(-1)$ for bosonic (fermionic) operator. The tilde and non-tilde Heisenberg fields are related with each other through the relations $[\tilde{\psi}(\mathbf{x}, t)]^\sim = \sigma \psi(\mathbf{x}, t)$, $[\tilde{\psi}^\dagger(\mathbf{x}, t)]^\sim = \sigma \psi^\dagger(\mathbf{x}, t)$, and $\langle 1 | \tilde{\psi}^\dagger(\mathbf{x}, t) = \langle 1 | \psi^\dagger(\mathbf{x}, t)$. The thermal vacuums $\langle 1 |$ and $|0\rangle$ are tilde invariant: $\langle 1 |^\sim = \langle 1 |$, $|0\rangle^\sim = |0\rangle$. The time-evolution generator within NETFD is $\hat{H} = H - \tilde{H}$, where H is a Hamiltonian of a system. It has the property called *Tildian*: $(i\hat{H})^\sim = i\hat{H}$, and satisfies $\langle 1 | \hat{H} = 0$ [1, 2].

One of the most important concepts in non-equilibrium thermodynamics is the concept of the *local equilibrium state* [23] which can be specified by the generalized Block equation:

$$\frac{\delta}{\delta F_m(\mathbf{x}, t)} |0_S(t)\rangle_\ell = -\hat{P}_m(\mathbf{x}) |0_S(t)\rangle_\ell \quad (1)$$

with

$$\hat{P}_m(\mathbf{x}) = \frac{1}{2} [P_m(\mathbf{x}) + \tilde{P}_m^\dagger(\mathbf{x})] \quad (2)$$

where $P_m(\mathbf{x})$ are Hermite operators corresponding to a set of *gross variables*. The Heisenberg operators $P_m(\mathbf{x}, t) = e^{iHt} P_m(\mathbf{x}) e^{-iHt}$ can be the total energy density operator, the total momentum density operator and the number density operator $n_i(\mathbf{x}, t)$ of the i th component in the case of an ℓ -component system, for example, and satisfy a set of equations of the form

$$\frac{\partial}{\partial t} P_m(\mathbf{x}, t) + \nabla j_m(\mathbf{x}, t) = J_m(\mathbf{x}, t). \quad (3)$$

The currents $j_m(\mathbf{x}, t)$ should be the operator of the total energy flux density, of the total stress tensor and of the number flux density $j_i(\mathbf{x}, t)$ of the i th component. The operators $J_m(\mathbf{x}, t)$ describe some possible sources. The real valued c-number functions $F_m(\mathbf{x}, t)$ in (1) are the conjugate to the corresponding operators $P_m(\mathbf{x}, t)$. They can be the inverse of the local temperature $\beta(\mathbf{x}, t)$, the local average velocity $-\beta(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t)$ with $\mathbf{v}(\mathbf{x}, t) = \langle \sum_{i=1}^\ell j_i(\mathbf{x}, t) \rangle_{i,\ell} / \langle \sum_{i=1}^\ell n_i(\mathbf{x}, t) \rangle_{i,\ell}$, where $\langle \dots \rangle_{i,\ell}$ is defined by (6) below, and the local chemical potential of the i th component $-\beta(\mathbf{x}, t) [\mu_i(\mathbf{x}, t) - m_i v^2(\mathbf{x}, t)/2]$ with m_i being the mass of a i th component molecule. The functional derivative in (1) should be interpreted in the sense that $\delta F_n(\mathbf{x}', t) / \delta F_m(\mathbf{x}, t) = \delta_{n,m}(\mathbf{x} - \mathbf{x}')$. The inner product of the local equilibrium thermal bra- and ket-vacuum is the partition function: $\langle 1 |_S(t)\rangle_\ell = Q_\ell(t)$.

According to the mapping rules given in [1, 2], the local equilibrium thermal vacuum defined by (1) can be expressed as

$$|0_S(t)\rangle_\ell = \left| \exp \left[-\sum_m \int d\mathbf{x} B_{m,t}^\ell(\mathbf{x}) \right] \right\rangle \quad (4)$$

with

$$B_{m,t}^\ell(\mathbf{x}) = F_m(\mathbf{x}, t) P_m(\mathbf{x}) \quad (5)$$

The local equilibrium state is specified under the condition that the information entropy be a maximum at given values of the gross variables $\langle P_m(\mathbf{x}, t) \rangle_{i,\ell}$, which depend on the macroscopic space and time coordinates, where

$$\langle \dots \rangle_{i,\ell} = Q_\ell(t)^{-1} \langle 1 | \dots |0_H(t)\rangle_\ell \quad (6)$$

with the local equilibrium thermal vacuum in the Heisenberg representation:

$$|0_H(t)\rangle_\ell = e^{i\hat{H}t}|0_S(t)\rangle_\ell = \left| \exp \left[-\sum_m \int dx B_m^\ell(x, t) \right] \right\rangle \quad (7)$$

with

$$B_m^\ell(x, t) = e^{i\hat{H}t} B_{m,t}^\ell(x) e^{-i\hat{H}t} = F_m(x, t) P_m(x, t). \quad (8)$$

Therefore there is arbitrariness in the specification of these quantities. Following Kubo [24] and Zubarev [25], we shall specify them in such a way that they satisfy the hydrodynamic equations of an ideal liquid:

$$\frac{\partial}{\partial t} \langle P_m(x, t) \rangle_{t,\ell} + \nabla \langle j_m(x, t) \rangle_{t,\ell} = 0. \quad (9)$$

Note that the local equilibrium thermal vacuum (7) can be expressed as $|0_H(t)\rangle_\ell = \Pi_x |0_H(x, t)\rangle_\ell$, with $|0_H(x, t)\rangle_\ell = \left| \exp \left[-\sum_m B_m^\ell(x, t) \right] \right\rangle$. The hydrodynamic equations (9) may be interpreted in the way that they determine the connection among the local thermal vacuums $|0_H(x, t)\rangle_\ell$.

For the local equilibrium state, we have

$$\langle P_m(x, t) \rangle_{t,\ell} = \frac{\delta \ln Q_\ell(t)}{\delta F_m(x, t)}. \quad (10)$$

Furthermore we have the thermodynamic relation of the form

$$S(x, t) = \sum_m F_m(x, t) \langle P_m(x, t) \rangle_{t,\ell} + \beta(x, t) p(x, t), \quad (11)$$

where $S(x, t)$ is the entropy density, and $p(x, t)$ is the local pressure which is related to the partition function $Q_\ell(t)$ by the relation

$$\ln Q_\ell(t) = \int dx \beta(x, t) p(x, t). \quad (12)$$

We see from (11) that the thermodynamic parameters $F_m(x, t)$ are determined by

$$F_m(x, t) = \frac{\delta S(t)}{\delta \langle P_m(x, t) \rangle_{t,\ell}} \quad S(t) = \int dx S(x, t). \quad (13)$$

Now, following Kubo [24] and Zubarev [25], let us introduce a thermal vacuum state in the Schrödinger representation, for non-equilibrium systems in the hydrodynamic stage, by the generalized Bloch equation

$$\frac{\delta}{\delta F_m(x, t')} |0_S(t)\rangle_\epsilon = -\epsilon e^{\epsilon(t'-t)} \hat{P}_m(x, t'-t) |0_S(t)\rangle_\epsilon \quad (14)$$

with $t \geq t'$, where

$$\hat{P}_m(x, t) = e^{i\hat{H}t} \hat{P}_m(x) e^{-i\hat{H}t}. \quad (15)$$

The generalized Bloch equation (14) satisfies causality in the sense that the thermal vacuum $|0_S(t)\rangle_\epsilon$ is determined by the thermodynamic parameters $F_m(x, t')$ in past time t' ($t \geq t'$). The functional derivative here in (14) should be interpreted in the sense that $\delta F_n(x', t') / \delta F_m(x, t) = \delta_{nm} \delta(x-x') \delta(t-t')$. The inner product of the thermal bra- and ket-vacuum is the partition function: $\langle 1_S(t) \rangle_\epsilon = Q(t)$.

Using to the mapping rules given in [1, 2], the thermal vacuum defined by (14) can be expressed as

$$|0_S(t)\rangle_\varepsilon = \left| \exp \left[-\sum_m \int dx B_{m,t}(x) \right] \right\rangle \tag{16}$$

where

$$B_{m,t}(x) = \varepsilon \int_{-\infty}^0 dt' e^{\varepsilon t'} F_m(x, t+t') P_m(x, t') = B_{m,t}^\ell(x) + \Pi_{m,t}(x) \tag{17}$$

with

$$\Pi_{m,t}(x) = -\int_{-\infty}^0 dt' e^{\varepsilon t'} \left[F_m(x, t+t') \dot{P}_m(x, t') + \frac{\partial F_m(x, t+t')}{\partial t} P_m(x, t') \right] \tag{18}$$

$$= -\int_{-\infty}^0 dt' e^{\varepsilon t'} j^m(x, t') X_m(x, t+t'). \tag{19}$$

The thermal vacuum (16) is specified by the condition that

$$\langle P_m(x, t) \rangle = \langle P_m(x, t) \rangle_{t,t} \tag{20}$$

where the average $\langle \dots \rangle$ with respect to the non-equilibrium thermal vacuum is defined by

$$\langle A(t) \rangle = \lim_{\varepsilon \rightarrow 0} Q^{-1}(t) \langle 1 | A(t) | 0_H(t) \rangle_\varepsilon \tag{21}$$

with the thermal vacuum in the Heisenberg representation:

$$|0_H(t)\rangle_\varepsilon = e^{i\hat{H}t} |0_S(t)\rangle_\varepsilon. \tag{22}$$

The Heisenberg operator $A(t) = e^{i\hat{H}t} A e^{-i\hat{H}t}$, satisfies the Heisenberg equation of motion within NETFD [1, 2]: $dA(t)/dt = i[\hat{H}, A(t)]$.

In the derivation of the expression (19) from (18), one needs a long and cumbersome calculation with a knowledge of thermodynamics. The thermodynamic current operators $j^m(x, t)$ reduce to the thermal flux, the viscous flux and the diffusional flux in the case of the ℓ -component system, for example. On the other hand, the thermodynamic forces $X_m(x, t)$ represent $\nabla\beta(x, t)$, $-\beta(x, t)\nabla \cdot v(x, t)$, and $-\nabla[\beta(x, t)\mu_i(x, t)]$.

We see that the thermal vacuum (16) satisfies the Shrödinger equation:

$$\frac{\partial}{\partial t} |0_S(t)\rangle_\varepsilon + i\hat{H} |0_S(t)\rangle_\varepsilon = \varepsilon(\hat{\Pi}_t + \delta\hat{\Pi}_t) |0_S(t)\rangle_\varepsilon \tag{23}$$

with

$$\hat{\Pi}_t = \sum_m \int dx \hat{\Pi}_{m,t}(x) \tag{24}$$

where $\hat{\Pi}_{m,t}(x)$ is given by taking \wedge of (18) or (19) with

$$\hat{j}^m(x, t) = \frac{1}{2}[j^m(x, t) + \tilde{j}^{m\dagger}(x, t)] \tag{25}$$

and

$$\begin{aligned} \delta\hat{\Pi}_t = & \frac{-1}{2^4 \times 3} \sum_{m_1} \sum_{m_2} \sum_{m_3} \int dx_1 \int dx_2 \int dx_3 \{ [\hat{B}_1 B_2 B_3 + \hat{B}_1 B_2 \hat{B}_3^\dagger + \hat{B}_1 \hat{B}_2^\dagger \tilde{B}_3^\dagger + \hat{B}_1^\dagger \hat{B}_2^\dagger \tilde{B}_3^\dagger] + \text{TC} \\ & - 2[(B_1 \hat{B}_2 B_3 + B_1 \hat{B}_2 \tilde{B}_3^\dagger) + \text{TC}] \} \\ & + [\text{higher order terms with respect to } B]. \end{aligned} \tag{26}$$

The symbol TC indicates to take a tilde conjugation. We have introduced an abbreviation like $B_1 = B_{m,1}(\mathbf{x}_1)$ in (26). The right-hand side of (23) represents a *symmetry breaking* effect due to the thermal processes. It may be much more vivid if we write down the time-evolution equation of the thermal vacuum in the Heisenberg representation:

$$\frac{\partial}{\partial t} |0_H(t)\rangle_\epsilon = \epsilon [\hat{\Pi}(t) + \delta\hat{\Pi}(t)] |0_H(t)\rangle_\epsilon \tag{27}$$

with

$$\hat{\Pi}(t) = \sum_m \int d\mathbf{x} \hat{\Pi}_m(\mathbf{x}, t) \quad \delta\hat{\Pi}(t) = e^{i\hat{H}t} \delta\hat{H} e^{-i\hat{H}t} \tag{28}$$

where

$$\hat{\Pi}_m(\mathbf{x}, t) = e^{i\hat{H}t} \hat{\Pi}_{m,t}(\mathbf{x}) e^{-i\hat{H}t} = - \int_{-\infty}^t dt' e^{\epsilon(t'-t)} \hat{j}^m(\mathbf{x}, t') X'_m(\mathbf{x}, t'). \tag{29}$$

Because of the existence of thermal processes, the Heisenberg thermal vacuum (22) changes in time due to the right-hand side of (27), a symmetry breaking term.

With the help of the mapping rules [1, 2], the thermal vacuum (22) can be expressed as

$$|0_H(t)\rangle_\epsilon = \left\langle \exp \left[- \sum_m \int d\mathbf{x} B_m(\mathbf{x}, t) \right] \right\rangle \tag{30}$$

with

$$B_m(\mathbf{x}, t) = e^{i\hat{H}t} B_{m,t}(\mathbf{x}) e^{-i\hat{H}t} = B_m^\ell(\mathbf{x}, t) + \Pi_m(\mathbf{x}, t) \tag{31}$$

where $\Pi_m(\mathbf{x}, t)$ is given by (29) by replacing $\hat{j}^m(\mathbf{x}, t)$ with $j^m(\mathbf{x}, t)$.

The kinetic coefficients for the thermal processes can be obtained by considering a linear response to the thermodynamic forces $X_m(\mathbf{x}, t)$. Up to the first order terms with respect to $X_m(\mathbf{x}, t)$, we have

$$|0_H(t)\rangle_\epsilon = \left[1 + \sum_m \int d\mathbf{x} \int_{-\infty}^t dt' \int_0^1 d\tau \hat{j}^m(\mathbf{x}, t'; i\tau) X_m(\mathbf{x}, t') \right] |0_H(t)\rangle_{\epsilon, \ell} \tag{32}$$

with

$$\hat{j}^m(\mathbf{x}, t'; i\tau) = \exp \left[-\tau \sum_k \int d\mathbf{x} \hat{B}_k^\ell(\mathbf{x}, t) \right] \hat{j}^m(\mathbf{x}, t') \exp \left[\tau \sum_k \int d\mathbf{x} \hat{B}_k^\ell(\mathbf{x}, t) \right] \tag{33}$$

where

$$\hat{B}_m^\ell(\mathbf{x}, t) = B_m^\ell(\mathbf{x}, t) - \tilde{B}_m^{\ell\dagger}(\mathbf{x}, t). \tag{34}$$

Then we obtain the linear response formula for the thermal current in the form

$$\langle \delta j^n(\mathbf{x}, t) \rangle = \lim_{\epsilon \rightarrow 0} \sum_m \int d\mathbf{x}' \int_{-\infty}^t dt' e^{\epsilon(t'-t)} (j^n(\mathbf{x}, t), \hat{j}^m(\mathbf{x}', t')) X_m(\mathbf{x}', t') \tag{35}$$

with

$$\begin{aligned} (j^n(\mathbf{x}, t), \hat{j}^m(\mathbf{x}', t')) &= \int_0^1 d\tau (j^n(\mathbf{x}, t) [\hat{j}^m(\mathbf{x}', t'; i\tau) - \langle \hat{j}^m(\mathbf{x}', t'; i\tau) \rangle_{\epsilon, \ell}])_{\epsilon, \ell} \\ &= \frac{1}{2} \int_0^1 d\tau \langle \{ \delta j^n(\mathbf{x}, t), \delta j^m(\mathbf{x}', t'; i\tau) \} \rangle_{\epsilon, \ell} \end{aligned} \tag{36}$$

where we have introduced

$$\delta j^m(\mathbf{x}, t) = j^m(\mathbf{x}, t) - \langle j^m(\mathbf{x}, t) \rangle_{i,\ell} \quad (37)$$

$$\delta j^m(\mathbf{x}, t'; i\tau) = j^m(\mathbf{x}, t'; i\tau) - \langle j^m(\mathbf{x}, t') \rangle_{i,\ell}. \quad (38)$$

The correlation function (36) is the symmetrized one [26]. In deriving the formula, we used the properties

$$\langle 1 | \hat{B}_m^\ell(\mathbf{x}, t) = 0 \quad \hat{B}_m^\ell(\mathbf{x}, t) | 0_H(t) \rangle_{i,\ell} = 0. \quad (39)$$

Irreversibility reveals itself as the positivity of the *local entropy production rate*

$$\sigma(\mathbf{x}, t) = \sum_m \langle \delta j^m(\mathbf{x}, t) \rangle X_m(\mathbf{x}, t) \quad (40)$$

which is introduced through the balance equation for the entropy:

$$\frac{\partial}{\partial t} S(\mathbf{x}, t) + \nabla j_S(\mathbf{x}, t) = \sigma(\mathbf{x}, t). \quad (41)$$

The entropy current density $j_S(\mathbf{x}, t)$ is given by

$$j_S(\mathbf{x}, t) = \sum_m F_m(\mathbf{x}, t) \langle j_m(\mathbf{x}, t) \rangle + \beta(\mathbf{x}, t) p(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t). \quad (42)$$

The positivity of $\sigma(\mathbf{x}, t)$ is nothing but the second law of thermodynamics.

In summarizing, we have introduced the fundamental concepts of non-equilibrium thermodynamics into NETFD in its most general way. The choice of a set of gross variables may be related to that of the representation space [27]. Once we have a set of gross variables, we can extract the dynamical motion which is in resonance with the local equilibrium state constituted by the gross variables as has been shown in this letter explicitly. The cross terms between tilde and non-tilde operators in $\delta \hat{\Pi}_i$, (26), which is constituted of nonlinear terms with respect to the thermodynamic forces, may have an important role in the description of non-equilibrium dissipative dynamics [1, 2]. A detailed version of the formalism introduced in this letter will be given in separate papers with some applications and with a further investigation of the concepts, such as the *minimum entropy production*, the *excess entropy*, the *general criterion of time-evolution* and so on [23, 28], in terms of NETFD.

Before closing this letter, it should be mentioned that the response to a mechanical disturbance [26] can be taken into account by introducing the effect of the disturbance in the form of a Hamiltonian, i.e. the form of \hat{H} .

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