

A Note on Description of Hydrodynamic Fluctuation by a Master Equation

Kazuo KITAHARA

The hydrodynamic equations describe evolution of local density, local momentum density and local energy density. For example, Fick's law for local temperature $T(\vec{r}, t)$,

$$\frac{\partial}{\partial t} T(\vec{r}, t) = \kappa \nabla^2 T(\vec{r}, t) \quad (1)$$

describes the diffusion of internal energy. This local temperature $T(\vec{r}, t)$ is a coarse-grained quantity. If we make finer measurement of the local temperature, it is fluctuating and we may look upon Eq. (1) as an equation for the averaged quantity $\langle T(\vec{r}, t) \rangle$. In this note, we discuss how to estimate the temperature fluctuation $\langle \delta T(\vec{r}, t) \delta T(\vec{r}', t) \rangle$ in non-equilibrium conditions.

First, we review works done in this direction by van Kampen(1972), and by Nicolis & Malek-Mansour(1983). We divide the system into many local cells. Internal energy of a local cell, which is located at \vec{r} , is denoted by $E_{\vec{r}}$. We consider the probability

$$P(\{E\}, t) = P(E_{\vec{r}_1}, E_{\vec{r}_2}, \dots, t) \quad (2)$$

of having internal energy $E_{\vec{r}_1}, E_{\vec{r}_2}, \dots$, in cells at $\vec{r}_1, \vec{r}_2, \dots$, at time t . Assuming Markovian process for change of internal energy, we write the master equation

$$\begin{aligned} \frac{\partial}{\partial t} P(\{E\}, t) = & \int d\varepsilon \sum_{\vec{r}, \vec{r}'} W_{\vec{r}}(E_{\vec{r}} + \varepsilon, E_{\vec{r}'} - \varepsilon \rightarrow E_{\vec{r}}, E_{\vec{r}'}) \\ & \times P(\dots, E_{\vec{r}} + \varepsilon, E_{\vec{r}'} - \varepsilon, \dots, t) \\ & - \int d\varepsilon \sum_{\vec{r}, \vec{r}'} W_{\vec{r}'}(E_{\vec{r}}, E_{\vec{r}'} \rightarrow E_{\vec{r}} - \varepsilon, E_{\vec{r}'} + \varepsilon) \\ & \times P(\dots, E_{\vec{r}}, E_{\vec{r}'}, \dots, t). \end{aligned} \quad (3)$$

The transition probability $W_{\vec{r}}(E_{\vec{r}}+\varepsilon, E_{\vec{r}+\vec{i}}-\varepsilon \rightarrow E_{\vec{r}}, E_{\vec{r}+\vec{i}})$ should satisfy the following conditions,

1) Detailed balance at equilibrium

$$\begin{aligned} & W_{\vec{r}}(E_{\vec{r}}+\varepsilon, E_{\vec{r}+\vec{i}}-\varepsilon \rightarrow E_{\vec{r}}, E_{\vec{r}+\vec{i}}) P_{\text{eq}}(\dots, E_{\vec{r}}+\varepsilon, E_{\vec{r}+\vec{i}}-\varepsilon) \\ &= W_{\vec{r}+\vec{i}}(E_{\vec{r}}, E_{\vec{r}+\vec{i}} \rightarrow E_{\vec{r}}+\varepsilon, E_{\vec{r}+\vec{i}}-\varepsilon) P_{\text{eq}}(E_{\vec{r}}, E_{\vec{r}+\vec{i}}, \dots) \end{aligned} \quad (4)$$

2) Equilibrium probability distribution is related to local entropy

$$P_{\text{eq}}(\{E\}) = \exp \left\{ \frac{1}{k_B} \sum_{\vec{r}} S_{\vec{r}}(E_{\vec{r}}) \right\}. \quad (5)$$

We choose the transition probability of the following form,

$$\begin{aligned} & W_{\vec{r}}(E_{\vec{r}}+\varepsilon, E_{\vec{r}+\vec{i}}-\varepsilon \rightarrow E_{\vec{r}}, E_{\vec{r}+\vec{i}}) \\ & \cong \phi(\varepsilon) \exp \left\{ -\frac{1}{k_B} [S_{\vec{r}}(E_{\vec{r}}+\varepsilon) - S_{\vec{r}}(E_{\vec{r}})] \right\}. \end{aligned} \quad (6)$$

Then, expanding the expression in ε , we obtain

$$\begin{aligned} & W_{\vec{r}}(E_{\vec{r}}+\varepsilon, E_{\vec{r}+\vec{i}}-\varepsilon \rightarrow E_{\vec{r}}, E_{\vec{r}+\vec{i}}) \\ & \cong \phi(\varepsilon) \exp(-\varepsilon/k_B T_{\vec{r}}), \end{aligned} \quad (7)$$

where $T_{\vec{r}}$ is local temperature

$$\frac{\partial S_{\vec{r}}}{\partial E_{\vec{r}}} = \frac{1}{T_{\vec{r}}} \quad (8)$$

Expanding the master equation in ε , we obtain

$$\begin{aligned} \frac{\partial}{\partial t} P(\{E\}, t) &= \sum_{\vec{r}, \vec{i}} \left(\frac{\partial}{\partial E_{\vec{r}}} - \frac{\partial}{\partial E_{\vec{r}+\vec{i}}} \right) f(E_{\vec{r}}) P(\{E\}, t) \\ &+ \frac{1}{2} \sum_{\vec{r}, \vec{i}} \left(\frac{\partial}{\partial E_{\vec{r}}} - \frac{\partial}{\partial E_{\vec{r}+\vec{i}}} \right)^2 Q(E_{\vec{r}}) P(\{E\}, t), \end{aligned} \quad (9)$$

where

$$f(E_{\vec{r}}) \equiv \int d\varepsilon \phi(\varepsilon) \varepsilon \exp(-\varepsilon/k_{\text{B}}T_{\vec{r}}) \quad (10)$$

$$Q(E_{\vec{r}}) \equiv \int d\varepsilon \phi(\varepsilon) \varepsilon^2 \exp(-\varepsilon/k_{\text{B}}T_{\vec{r}}). \quad (11)$$

Hence

$$Q(E_{\vec{r}}) = - \frac{\partial f(E_{\vec{r}})}{\partial(1/k_{\text{B}}T_{\vec{r}})}. \quad (12)$$

For small fluctuation, we may derive from the drift term of Eq. (9), the average evolution,

$$\begin{aligned} \frac{\partial}{\partial t} \langle E_{\vec{r}} \rangle &\cong - \sum_{\vec{i}} [f(\langle E_{\vec{r}} \rangle) - f(\langle E_{\vec{r}+\vec{i}} \rangle)] \\ &\cong l^2 \nabla^2 f(\langle E_{\vec{r}} \rangle), \end{aligned} \quad (13)$$

where l is the size of cells (the mean free path). Since the size of the cell is fixed, we may write $d\langle E_{\vec{r}} \rangle = C_{\text{v}} d\langle T_{\vec{r}} \rangle$ from thermodynamics. By comparing Eq. (13) with the Fick's law (1), we obtain

$$f(E_{\vec{r}}) = \frac{C_{\text{v}}k}{l^2} \cdot k_{\text{B}}T_{\vec{r}}. \quad (14)$$

This determines $Q(E_{\vec{r}})$ by the relation (12), namely

$$Q(E_{\vec{r}}) = \frac{C_{\text{v}}k}{l^2} k_{\text{B}}T_{\vec{r}}^2. \quad (15)$$

When there is convection, the description is more complicated because we cannot fix each cell at a given position. Cells are moving by the convection. We assign a vector \vec{a} to a cell. The position of a cell \vec{a} at time t is denoted by $\vec{x}(\vec{a}, t)$. Then

$$\left\{ \begin{array}{l} \dot{\vec{x}}(\vec{a}, t) = \vec{u}(\vec{x}(\vec{a}, t), t) \\ \vec{x}(\vec{a}, 0) = \vec{a} \end{array} \right. \quad (16)$$

where $\vec{u}(\vec{x}, t)$ is velocity field at \vec{x} at time t . Let us denote internal energy and momentum of a cell by $E_{\vec{a}}$ and $\vec{G}_{\vec{a}}$ and consider the master equation for the probability $P(\{E\}, \{\vec{G}\}, t)$, which is written as

$$\begin{aligned}
 & \frac{\partial}{\partial t} P(\{E\}, \{\vec{G}\}, t) + \sum_{\vec{a}} \frac{\partial}{\partial G_{\vec{a}}} \cdot \vec{F}_{\vec{a}} P(\{E\}, \{\vec{G}\}, t) \\
 &= \sum_{\vec{a}, \vec{a}'} \left\{ W_{\vec{a}}^E(E_{\vec{a}} + \varepsilon, E_{\vec{a}'} - \varepsilon \rightarrow E_{\vec{a}}, E_{\vec{a}'}) P(\dots E_{\vec{a}} + \varepsilon, E_{\vec{a}'} - \varepsilon, \{\vec{G}\}, t) \right. \\
 & \quad \left. - W_{\vec{a}'}^E(E_{\vec{a}}, E_{\vec{a}'} \rightarrow E_{\vec{a}} + \varepsilon, E_{\vec{a}'} - \varepsilon) P(\dots E_{\vec{a}}, E_{\vec{a}'}, \dots \{\vec{G}\}, t) \right\} \\
 & + \sum_{\vec{a}, \vec{a}'} \left\{ W_{\vec{a}}^G(\vec{G}_{\vec{a}} + \vec{g}, \vec{G}_{\vec{a}'} - \vec{g} \rightarrow \vec{G}_{\vec{a}}, \vec{G}_{\vec{a}'}) P(\{E\}, \dots \vec{G}_{\vec{a}} + \vec{g}, \vec{G}_{\vec{a}'} - \vec{g}, \dots, t) \right. \\
 & \quad \left. - W_{\vec{a}'}^G(\vec{G}_{\vec{a}}, \vec{G}_{\vec{a}'} \rightarrow \vec{G}_{\vec{a}} + \vec{g}, \vec{G}_{\vec{a}'} - \vec{g}) P(\{E\}, \dots \vec{G}_{\vec{a}}, \vec{G}_{\vec{a}'}, \dots, t) \right\} \tag{17}
 \end{aligned}$$

where $\vec{F}_{\vec{a}}$ is the conservative force (non-dissipative). The transition probability for the momentum change is chosen to be

$$\begin{aligned}
 & W_{\vec{a}}^G(\vec{G}_{\vec{a}} + \vec{g}, \vec{G}_{\vec{a}'} - \vec{g} \rightarrow \vec{G}_{\vec{a}}, \vec{G}_{\vec{a}'}) \\
 &= \phi(\vec{g}) \exp \left[- \frac{1}{k_B} \{ S_{\vec{a}}(\vec{G}_{\vec{a}} + \vec{g}) - S_{\vec{a}}(\vec{G}_{\vec{a}}) \} \right]. \tag{18}
 \end{aligned}$$

Entropy of a system with convective velocity is given by (Martin et al (1972)),

$$TdS = dE - \mu d\rho - \vec{u} \cdot d\vec{G}. \tag{19}$$

Hence

$$\begin{aligned}
 & W_{\vec{a}}^G(\vec{G}_{\vec{a}} + \vec{g}, \vec{G}_{\vec{a}'} - \vec{g} \rightarrow \vec{G}_{\vec{a}}, \vec{G}_{\vec{a}'}) \\
 & \simeq \phi(\vec{g}) \exp(\vec{u} \cdot \vec{g} / k_B T_{\vec{a}}). \tag{20}
 \end{aligned}$$

We define

$$f_{\alpha}(\vec{G}_{\vec{a}}) = \int d^3 \vec{g} \phi(\vec{g}) g_{\alpha} \exp(\vec{u} \cdot \vec{g} / k_B T_{\vec{a}}) \quad (21)$$

and

$$Q_{\alpha\beta}(\vec{G}_{\vec{a}}) = \int d^3 \vec{g} \phi(\vec{g}) g_{\alpha} g_{\beta} \exp(\vec{u} \cdot \vec{g} / k_B T_{\vec{a}}), \quad (22)$$

which appear in the expansion of the master equation (17) in the power of \vec{g} . These two quantities are related by

$$Q_{\alpha\beta}(\vec{G}_{\vec{a}}) = k_B T_{\vec{a}} \frac{\partial}{\partial u_{\alpha}} f_{\beta}(\vec{G}_{\vec{a}}). \quad (23)$$

For small fluctuation of momentum, we find

$$\begin{aligned} \frac{d}{dt} \langle G_{\vec{a}\alpha} \rangle &= F_{\vec{a}\alpha} - \sum_{\vec{a}'} [f_{\alpha}(\langle \vec{G}_{\vec{a}} \rangle) - f_{\alpha}(\langle \vec{G}_{\vec{a}'} \rangle)] \\ &\simeq \vec{F}_{\vec{a}\alpha} + l^2 \nabla^2 f_{\alpha}(\langle \vec{G}_{\vec{a}} \rangle). \end{aligned} \quad (24)$$

On the other hand, from the Navier-Stokes equation

$$l^2 \nabla^2 f_{\alpha}(\langle \vec{G}_{\vec{a}} \rangle) = \eta \nabla^2 u_{\alpha} \quad (25)$$

Hence

$$f_{\alpha}(\vec{G}_{\vec{a}}) = \frac{\eta}{l^2} u_{\alpha}. \quad (26)$$

Therefore by the relation (23), we find

$$Q_{\alpha\beta}(\vec{G}_{\vec{a}}) = k_B T_{\vec{a}} \delta_{\alpha\beta} \cdot \eta / l^2. \quad (27)$$

Thus all coefficients of the Kramers-Moyal expansion of the master equation up to the second derivatives are determined by the thermodynamic relations. So it would be interesting to discuss the fluctuation of hydrodynamic quantities in non-equilibrium conditions in the framework discussed above.