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Boltzmann-Langevin Equation

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Abstract

We have studied that the Fox-Uhlenbeck Ansatz, which expresses how the correlation function of random force is related to the collision operator, can be derived from Mori theory which is a microscopic theory of the Boltzmann - Langevin equation with its random force term.

§1 Introduction

Landau and Lifshitz proposed the fundamental equations of fluctuation phenomena in fluids, using thermodynamic fluctuation theory in relation to the linearized hydrodynamic equations.[1] Fox and Uhlenbeck[2] and Bixon and Zwanzig[3] postulated a generalization of the linearized Boltzmann equation with a fluctuation term based on the theory of the Gaussian Markov process. The assumption of general statistical properties concerning this term is more or less ad hoc, and its meaning remains dark.

In this note, we present that the Fox-Uhlenbeck Ansatz,[4] which expresses how the correlation function of random force is related to the collision operator, can be derived from the Mori theory[5] which is a microscopic theory of the Boltzmann-Langevin equation with its random force term.

§2 Microscopic theory of the Boltzmann-Langevin equation

The fundamental state variables are the particle density in μ space

$$n(\boldsymbol{p},\ \boldsymbol{r};\ t)=\sum_{j=1}^{N}\delta(\boldsymbol{p}_j(t)-\boldsymbol{p})\delta(\boldsymbol{r}_j(t)-\boldsymbol{r}), \tag{1}$$

where $\boldsymbol{p}_j(t)$amd $\boldsymbol{r}_j(t)$ are the momentum and position of the $j-$th particle at time t, respectively. Mori has introduced a coarse grained particle density $A(\boldsymbol{p},\ \boldsymbol{r};\ t)$ by replacing $\delta(\boldsymbol{r}_j-\boldsymbol{r})$ in (1) by the coarse-grained δ function[5]

$$\Delta(\boldsymbol{r}_j-\boldsymbol{r})\equiv(1/V)\sum_{\boldsymbol{q}}{}'\exp[-i\boldsymbol{q}\cdot(\boldsymbol{r}_j-\boldsymbol{r})], \tag{2}$$

where V is the volume of the system. $\Sigma'\boldsymbol{q}$ is the sum over the wave vectors $\boldsymbol{q}$ whose magnetudes are smaller than $1/\lambda$, where λ is a characteristic length which is larger than the linear range r_0 of the intermolecular force but is semi-macroscopic length. Mori has been presented the fundamental equation for the kinetic description of the dilute gases, if there are no external force, as follows:[5]

$$\frac{\partial}{\partial t}A(\boldsymbol{p},\boldsymbol{r};t)+\frac{\boldsymbol{p}}{m}\cdot\partial r A(\boldsymbol{p},\boldsymbol{r};t)=C[A(\boldsymbol{p},\boldsymbol{r};t)]+R_{pr}(t), \tag{3}$$

$$C[A(\boldsymbol{p},\boldsymbol{r};t)]=\int d\boldsymbol{p}_2 g_{21}\int_0^\infty db\ \ b\int_0^{2\pi} d\phi[A(\boldsymbol{p}'_1,\boldsymbol{r};t)A(\boldsymbol{p}'_2,\boldsymbol{r};t)$$
$$-A(\boldsymbol{p}_1,\boldsymbol{r};t)A(\boldsymbol{p}_2,\boldsymbol{r};t)], \tag{4}$$

where m is the mass of a molecule and $g_{21}=|\boldsymbol{p}_2-\boldsymbol{p}_1|/m$ and b is the impact parameter and ϕ the azimuth, and $\boldsymbol{p}'_i\,(i=1,2)$ is the momentum of the molecule i in the resulting collision. The fluctuation force $R_{\boldsymbol{pr}}(t)$ is charactrized by

$$\langle R_{\boldsymbol{pr}}(t)R^*_{\boldsymbol{p}'\boldsymbol{r}'}(0)\,;a\rangle=2\gamma_{\boldsymbol{pr},\boldsymbol{p}'\boldsymbol{r}'}(a)\delta(t), \tag{5}$$

where

$$\gamma_{\boldsymbol{pr},\boldsymbol{p}'\boldsymbol{r}'}(a)=\int_0^\infty\langle R_{\boldsymbol{pr}}(s)R^*_{\boldsymbol{p}'\boldsymbol{r}'}(0)\,;a\rangle ds. \tag{6}$$

$\langle G;a\rangle=\langle G\delta(A-a)\rangle/\langle\delta(A-a)\rangle$ denotes the conditional average of G with a fixed values a of A.

When $A(\boldsymbol{p},\boldsymbol{r};t)$ is near the Maxwell equilbrium distribution

$$f_{eq}(p)=n_{eq}(2\pi mk_{\rm B}T_{eq})^{-3/2}\exp(-p^2/2mk_{\rm B}T_{eq}), \tag{7}$$

where n_{eq} is the equilibrium density, T_{eq} is the equilibrium temperature, and k_B is the Boltzmann constant, one can write

$$A(\boldsymbol{p},\boldsymbol{r};t)=f_{eq}(p)[1+h(\boldsymbol{p},\boldsymbol{r};t)]. \tag{8}$$

Thus $h(\boldsymbol{p},\boldsymbol{r};t)$ fulfills the linearized Boltzmann equation

$$\frac{\partial h}{\partial t}+\frac{\boldsymbol{p}}{m}\cdot\frac{\partial h}{\partial \boldsymbol{r}}=D[h(\boldsymbol{p},\boldsymbol{r};t)]+\tilde{R}_{\boldsymbol{pr}}(t), \tag{9}$$

where

$$D[h(\boldsymbol{p},\boldsymbol{r};t)]=C[A(\boldsymbol{p},\boldsymbol{r};t)]/f_{eq}(p)$$
$$=\iint f_{eq}(p_2)gI(g,\theta)[h(\boldsymbol{p}_1',\boldsymbol{r};t)+h(\boldsymbol{p}_2',\boldsymbol{r};t)-h(\boldsymbol{p}_1,\boldsymbol{r};t)$$
$$-h(\boldsymbol{p}_2,\boldsymbol{r};t)]d\Omega d\boldsymbol{p}_2, \tag{10}$$

and

$$\tilde{R}_{\boldsymbol{pr}}(t)=R_{\boldsymbol{pr}}(t)/f_{eq}(p). \tag{11}$$

g is the relative velocity which turns the angle θ in the solid angle $d\Omega$ during the collision and $I(g,\ \theta)$ is the differential collision cross section, which depends on the intermolecular force.

§ 3 Correlation function of random force

Now we can also express another from for $C[A(\boldsymbol{p},\boldsymbol{r};t)]$,[5]

$$C[A(\boldsymbol{p},\boldsymbol{r};t)]=\iint d\boldsymbol{p}'d\boldsymbol{r}'\ [-\beta_0\gamma_{\boldsymbol{pr},\boldsymbol{p}'\boldsymbol{r}'}(A)X_{\boldsymbol{p}'\boldsymbol{r}'}(A)+\frac{\partial}{\partial A(\boldsymbol{p}',\boldsymbol{r}';t)}\gamma_{\boldsymbol{pr},\boldsymbol{p}'\boldsymbol{r}'}(A)], \tag{12}$$

where $X_{\boldsymbol{pr}}(A)$ is the thermodynamic force for the coarse-grained density $A(\boldsymbol{p},\boldsymbol{r};t)$

$$X_{\boldsymbol{pr}}(A)=-\frac{1}{\beta_0}\frac{\partial\ln w(A)}{\partial A(\boldsymbol{p},\boldsymbol{r};t)}, \tag{13}$$

where $\beta_0 = 1/k_B T_{eq}$ and $w(a) = \langle \delta(A-a) \rangle$.

When the system is close to the complete equilibrium, the thermodynamic force takes the form

$$X_{pr}(A) = h(\boldsymbol{p}, \boldsymbol{r}; t)/\beta_0. \tag{14}$$

In the case of dilute gases we can assume that

$$\langle R_{pr}(t) R^*_{p' r'}(0); a \rangle \simeq \langle R_{pr}(t) R^*_{p' r'}(0) \rangle \simeq 2\gamma_{p,p'} \delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t). \tag{15}$$

Then we have

$$D[h(\boldsymbol{p}, \boldsymbol{r}; t)] = -\int d\boldsymbol{p}' \gamma_{p,p'} h(\boldsymbol{p}', \boldsymbol{r}; t)/f_{eq}(p) \tag{16}$$

$$= -\int d\boldsymbol{p}' \Gamma(\boldsymbol{p}; \boldsymbol{p}') f_{eq}(\mathrm{p}') h(\boldsymbol{p}' \boldsymbol{r}; t), \tag{17}$$

where

$$\Gamma(\boldsymbol{p}; \boldsymbol{p}') = \gamma_{p,p'} / f_{eq}(p) f_{eq}(p'). \tag{18}$$

One then obtains

$$\frac{\partial h}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \frac{\partial h}{\partial \boldsymbol{r}} = -\int d\boldsymbol{p}' \Gamma(\boldsymbol{p}; \boldsymbol{p}') f_{eq}(p') h(\boldsymbol{p}' \boldsymbol{r}; t) + \tilde{R}_{pr}(t), \tag{19}$$

and, for the correlation function of random force,

$$\langle \tilde{R}_{pr}(t) \tilde{R}^*_{p'r'}(0) \rangle = 2\Gamma(\boldsymbol{p}; \boldsymbol{p}')\delta(t)\delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{20}$$

$$\text{or } \langle R_{pr}(t) R^*_{p' r'}(0) \rangle = 2\gamma_{p,p'} \delta(t)\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{21}$$

The right-hand side of (1) may be written in the form[6)]

$$-\int d\boldsymbol{p}' f_{eq}(p') K(\boldsymbol{p}; \boldsymbol{p}') h(\boldsymbol{p}', \boldsymbol{r}; t). \tag{22}$$

The kernel $K(\boldsymbol{p}; \boldsymbol{p}')$ is symmetric, isotropic and has nonnegative eigenvalues. This fact was first shown by Hilbert[7)] for the case of a gas of rigit elastic spherical molecules and later by Enskog[8)] for the general case. Thus we can consider that $\Gamma(\boldsymbol{p}; \boldsymbol{p}')$ is the same as the kernel $K(\boldsymbol{p}; \boldsymbol{p}')$ and (19) is the linearized Boltzmann equation with fluctuation. In this case, the correlation function of random force is characterized by the kernel $\Gamma(\boldsymbol{p}; \boldsymbol{p}')$as (20). These equations furnish a source for a random force term introduced by Fox and Uhlenbeck in the Boltzmann equation.

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