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CLASSICAL CANONICAL DISTRIBUTION FOR DISSIPATIVE SYSTEMS

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We derive the canonical distribution as a stationary solution of the Liouville equation for the classical dissipative system. Dissipative classical systems can have stationary states that look like canonical Gibbs distributions. The condition for non-potential forces which leads to this stationary solution is very simple: the power of the non-potential forces must be directly proportional to the velocity of the Gibbs phase (phase entropy density) change. The example of the canonical distribution for a linear oscillator with friction is considered.

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1. Introduction

The canonical distribution was defined 101 years ago in the book "Elementary principles in statistical mechanics, developed with especial reference to the rational foundation of thermodynamics"[1] published in 1902. The canonical distribution function usually can be derived as a stationary solution of the Liouville equation for non-dissipative Hamiltonian N-particle systems with a special set of potential forces.[2–6]

In general, classical systems are not Hamiltonian systems and the forces which act on particles are the sum of potential and non-potential forces. The non-potential internal forces for an N-particle system can be connected with nonelastic collisions.[7] Dissipative and non-Hamiltonian systems can have the same stationary states as Hamiltonian systems.[8] For example, dissipative quantum systems have pure stationary states of linear harmonic oscillators.[9] We can assume that canonical distribution exists for classical dissipative systems.

In this paper we consider the Liouville equation for classical dissipative and non-Hamiltonian N-particle systems. This equation is the equation of continuity in $6N$-dimensional phase space. We find that the condition for the non-potential forces which leads to the stationary solution of this equation look like the canonical distribution function. This condition is very simple: the power of non-potential forces must be directly proportional to the velocity of the Gibbs phase (phase entropy density) change. Note that the velocity of the phase entropy density change is equal to the velocity of the phase volume change.

In Sec. 2, the mathematical background and notations are considered. In this section, we formulate the main conditions for non-potential forces and derive the canonical distribution from an N-particle Liouville equation in the Hamilton picture. In Sec. 3, in the Liouville picture we substitute the canonical distribution function into the Liouville equation for a dissipative system and derive the condition for non-potential forces. In this section, we consider the Maxwell–Boltzmann distribution function for dissipative systems. In Sec. 4, the example of the canonical distribution for linear oscillators with friction is considered. Finally, a short conclusion is given in Sec. 5.

2. Canonical Distribution from the Liouville Equation in the Hamilton Picture

Let us consider the N-particle classical system in the Hamilton picture. In general, the equation of motion the ith particle, where $i = 1, \dots, N$, has the form

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i\,,$$

where $\mathbf{F}_i$ is a resulting force which acts on the ith particle. In the general case, the force is not a potential and we can write

$$\mathbf{F}_i = -\frac{\partial U}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)}\,, \tag{1}$$

where $U = U(\mathbf{r})$ is the potential energy of the system, $\mathbf{F}_i^{(n)}$ is the sum of non-potential forces (internal and external) which act on the ith particle. For any classical observable $A = A(\mathbf{r}_t, \mathbf{p}_t, t)$, where $\mathbf{r} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ and $\mathbf{p} = (\mathbf{p}_1, \dots, \mathbf{p}_N)$ in the Hamilton picture, we have

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\frac{\partial A}{\partial \mathbf{r}_i} + \sum_{i=1}^{N} \mathbf{F}_i \frac{\partial A}{\partial \mathbf{p}_i}\,. \tag{2}$$

The Hamiltonian of this system,

$$H(\mathbf{r}, \mathbf{p}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + U(r)\,, \tag{3}$$

is not a constant along the trajectory in the $6N$-dimensional phase space. From Eqs. (2) and (1) we have

$$\frac{dH}{dt} = \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\frac{\partial U}{\partial \mathbf{r}_i} + \sum_{i=1}^{N} \left(-\frac{\partial U}{\partial \mathbf{r}_i} + \mathbf{F}_i^{(n)} \right) \frac{\mathbf{p}_i}{m}\,,$$

i.e.

$$\frac{dH}{dt} = \sum_{i=1}^{N} (\mathbf{F}_i^{(n)}, \mathbf{v}_i) , \tag{4}$$

where $\mathbf{v}_i = \mathbf{p}_i/m$. Therefore, the energy change is equal to a power $\mathcal{P}$ of the non-potential forces $\mathbf{F}_i^{(n)}$:

$$\mathcal{P}(\mathbf{r}, \mathbf{p}, t) = \sum_{i=1}^{N} (\mathbf{F}_i^{(n)}, \mathbf{v}_i) . \tag{5}$$

The N-particle distribution function in the Hamilton picture is normalized using

$$\int \rho_N(\mathbf{r}_t, \mathbf{p}_t, t) d^N \mathbf{r}_t d^N \mathbf{p}_t = 1 . \tag{6}$$

The evolution equation of the function $\rho_N(\mathbf{r}_t, \mathbf{p}_t, t)$ is the Liouville equation in the Hamilton picture (for the Euler variables) which has the form:

$$\frac{d\rho_N(\mathbf{r}_t, \mathbf{p}_t, t)}{dt} = -\Omega(\mathbf{r}_t, \mathbf{p}_t, t) \rho_N(\mathbf{r}_t, \mathbf{p}_t, t) . \tag{7}$$

This equation describes the change of distribution function ρ_N along the trajectory in $6N$-dimensional phase space. Here, Ω is defined by

$$\Omega(\mathbf{r}, \mathbf{p}, t) = \sum_{i=1}^{N} \frac{\partial \mathbf{F}_i^{(n)}}{\partial \mathbf{p}_i} , \tag{8}$$

and d/dt is a total time derivative (2):

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m} \frac{\partial}{\partial \mathbf{r}_i} + \sum_{i=1}^{N} \mathbf{F}_i \frac{\partial}{\partial \mathbf{p}_i} .$$

If $\Omega < 0$, then the system is called a dissipative system. If $\Omega \neq 0$, then the system is a generalized dissipative system. In the Liouville picture the function Ω is equal to the velocity of the phase volume change.[10]

Let us define a phase density of entropy by

$$S(\mathbf{r}_t, \mathbf{p}_t, t) = -k \ln \rho_N(\mathbf{r}_t, \mathbf{p}_t, t) .$$

This function is usually called a Gibbs phase. Equation (7) leads to the equation for the Gibbs phase:

$$\frac{dS(\mathbf{r}_t, \mathbf{p}_t, t)}{dt} = k\Omega(\mathbf{r}_t, \mathbf{p}_t, t) . \tag{9}$$

Therefore, the function Ω is proportional to the velocity of the phase entropy density (Gibbs phase) change.

Let us assume that the power $\mathcal{P}(\mathbf{r}_t, \mathbf{p}_t, t)$ of the non-potential forces is directly proportional to the velocity of the Gibbs phase (phase density of entropy) change $\Omega(\mathbf{r}_t, \mathbf{p}_t, t)$:

$$\mathcal{P}(\mathbf{r}_t, \mathbf{p}_t, t) = kT\Omega(\mathbf{r}_t, \mathbf{p}_t, t) , \tag{10}$$

with some coefficient T, which is not dependent on $(\mathbf{r}_t, \mathbf{p}_t, t)$, i.e. $dT/dt = 0$.

Using Eqs. (4), (5) and (9), assumption (10) can be rewritten in the form:

$$\frac{dH(\mathbf{r}_t, \mathbf{p}_t)}{dt} = T\frac{dS(\mathbf{r}_t, \mathbf{p}_t, t)}{dt}\,.$$

Since coefficient T is constant, we have

$$\frac{d}{dt}(H(\mathbf{r}_t, \mathbf{p}_t) - TS(\mathbf{r}_t, \mathbf{p}_t, t)) = 0\,,$$

i.e. the value $(H - TS)$ is a constant along the trajectory of the system in $6N$-dimensional phase space. Let us denote this constant value by $\mathcal{F}$. Then we have

$$H(\mathbf{r}_t, \mathbf{p}_t) - TS(\mathbf{r}_t, \mathbf{p}_t, t) = \mathcal{F}\,,$$

where $d\mathcal{F}/dt = 0$, i.e.

$$\ln \rho_N(\mathbf{r}_t, \mathbf{p}_t, t) = \frac{1}{kT}(\mathcal{F} - H(\mathbf{r}_t, \mathbf{p}_t))\,.$$

As the result we have a canonical distribution function:

$$\rho_N(\mathbf{r}_t, \mathbf{p}_t, t) = \exp\frac{1}{kT}(\mathcal{F} - H(\mathbf{r}_t, \mathbf{p}_t))$$

in the Hamilton picture. The value $\mathcal{F}$ is defined by normalization condition (6).

Note that N is an arbitrary natural number since we do not use the condition $N \gg 1$ or $N \to \infty$.

3. Canonical Distribution in the Liouville Picture

Let us consider the Liouville equation for the N-particle distribution function $\rho_N = \rho_N(\mathbf{r}, \mathbf{p}, t)$ in the Liouville picture (for the Lagnangian variables):

$$\frac{\partial \rho_N}{\partial t} + \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\frac{\partial \rho_N}{\partial \mathbf{r}_i} + \sum_{i=1}^{N} \frac{\partial}{\partial \mathbf{p}_i}(\mathbf{F}_i \rho_N) = 0\,. \tag{11}$$

In general, the forces $\mathbf{F}_i$ are non-potential forces. This equation is the equation of continuity for $6N$-dimensional phase space. Substituting the canonical distribution function:

$$\rho_N(\mathbf{r}, \mathbf{p}, t) = \exp\frac{1}{kT}(\mathcal{F} - H(\mathbf{r}, \mathbf{p}, t))$$

in Eq. (11), we get

$$-\frac{1}{kT}\left(\frac{\partial H}{\partial t} + \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\frac{\partial H}{\partial \mathbf{r}_i} + \sum_{i=1}^{N} \mathbf{F}_i\frac{\partial H}{\partial \mathbf{p}_i}\right)\rho_N + \sum_{i=1}^{N}\frac{\partial \mathbf{F}_i}{\partial \mathbf{p}_i}\rho_N = 0\,.$$

Since ρ_N is not equal to zero, we have

$$\frac{\partial H}{\partial t} + \sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\frac{\partial H}{\partial \mathbf{r}_i} + \sum_{i=1}^{N} \mathbf{F}_i\frac{\partial H}{\partial \mathbf{p}_i} = kT\sum_{i=1}^{N}\frac{\partial \mathbf{F}_i}{\partial \mathbf{p}_i}\,.$$

If the Hamiltonian H has the form (3), then this equation leads to

$$\sum_{i=1}^{N} \frac{\mathbf{p}_i}{m}\left(\frac{\partial U}{\partial \mathbf{r}_i} + \mathbf{F}_i\right) = kT \sum_{i=1}^{N} \frac{\partial \mathbf{F}_i}{\partial \mathbf{p}_i} .$$

Substituting Eq. (1) in this equation, we get the following condition for non-potential forces $F_i^{(n)}$:

$$\sum_{i=1}^{N} \left(\frac{\mathbf{p}_i}{m}, \mathbf{F}_i^{(n)}\right) = kT \sum_{i=1}^{N} \frac{\partial \mathbf{F}_i^{(n)}}{\partial \mathbf{p}_i} .$$

Using notations (5) and (8), we can rewritte this condition in the form:

$$\mathcal{P}(\mathbf{r}, \mathbf{p}, t) = kT\Omega(\mathbf{r}, \mathbf{p}, t) .$$

As a result we have that the canonical distribution function is a solution of the Liouville equation for dissipative and non-Hamiltonian systems if the power of the non-potential forces is proportional to the velocity of the phase volume change.

Let us consider a chain of Bogoliubov equations[11,6] for the Liouville equation of the dissipative systems (11) in approximation:

$$\rho_2(\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2, t) = \rho_1(\mathbf{r}_1, \mathbf{p}_1, t)\rho_1(\mathbf{r}_2, \mathbf{p}_2, t) . \tag{12}$$

The non-potential forces $\mathbf{F}_i^{(n)}$ in Eq. (1) is a sum of external forces $F_i^{(n,e)}$ and internal forces $\mathbf{F}_i^{(n,i)}$. For example, in the case of binary interactions we have

$$\mathbf{F}_i^{(n)} = \mathbf{F}_i^{(n,e)}(\mathbf{r}_i, \mathbf{p}_i, t) + \sum_{j=1, j\neq i}^{N} \mathbf{F}_{ij}^{(n,i)}(\mathbf{r}_i, \mathbf{p}_i, \mathbf{r}_j, \mathbf{p}_j, t) .$$

In approximation (12) we can define the force

$$\mathbf{F}_1 = -\frac{\partial(U + U_{\text{eff}})}{\partial \mathbf{r}_1} + \mathbf{F}_1^{(n)} + \mathbf{F}_{1,\text{eff}}^{(n)} ,$$

where

$$\mathbf{F}_{1,\text{eff}}^{(n)}(\mathbf{r}_1, \mathbf{p}_1, t) = \int d\mathbf{r}_2 d\mathbf{p}_2 \rho_1(\mathbf{r}_2, \mathbf{p}_2, t)\mathbf{F}_{12}^{(n,i)}(\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2, t) ,$$

$$U_{\text{eff}}(\mathbf{r}_1, \mathbf{p}_1, t) = \int d\mathbf{r}_2 d\mathbf{p}_2 \rho_1(\mathbf{r}_2, \mathbf{p}_2, t) U(|\mathbf{r}_2 - \mathbf{r}_1|) .$$

If we consider the 1-particle distribution then Liouville equation (11) in approximation (12) has the form:

$$\frac{\partial \rho_1}{\partial t} + \frac{\mathbf{p}_1}{m}\frac{\partial \rho_1}{\partial \mathbf{r}_1} + \frac{\partial}{\partial \mathbf{p}_1}(\mathbf{F}_1 \rho_1) = 0 , \tag{13}$$

where $\rho_1 = \rho_1(\mathbf{r}_1, \mathbf{p}_1, t)$. Let us consider a condition for the non-potential forces

$$(\mathbf{p}_1, \mathbf{F}_1^{(n)} + \mathbf{F}_{1,\text{eff}}^{(n)}) = mkT \frac{\partial(\mathbf{F}_1^{(n)} + \mathbf{F}_{1,\text{eff}}^{(n)})}{\partial \mathbf{p}_1} .$$

In this case, we can derive the 1-particle distribution function (as in Sec. 3) in the form:

$$\rho_1(\mathbf{r},\mathbf{p},t) = A\exp -\frac{1}{kT}\left(\frac{\mathbf{p}^2}{2m} + U(\mathbf{r}) + U_{\text{eff}}(\mathbf{r})\right).$$

This is a Maxwell–Bolztmann distribution function.

4. Canonical Distribution for Harmonic Oscillator with Friction

Let us consider the N-particle system with a linear friction defined by non-potential forces

$$\mathbf{F}_i^{(n)} = -\gamma\mathbf{p}_i, \tag{14}$$

where $i = 1,\dots,N$. Note that N is an arbitrary natural number. Substituting Eq. (14) into Eqs. (5) and (8), we get the power $\mathcal{P}$ and the Gibbs phase Ω:

$$\mathcal{P} = -\frac{\gamma}{m}\sum_{i=1}^{N} p_i^2, \quad \Omega = -\gamma\,.$$

Condition (10) has the form:

$$\sum_{i=1}^{N}\frac{p_i^2}{m} = kT\,, \tag{15}$$

i.e. the kinetic energy of the system must be a constant. Note that Eq. (15) has no friction parameter γ. Condition (15) is a non-holonomic (non-integrable) constraint.[12]

Let us consider the N-particle system with friction (14) and non-holonomic constraint (17). The equations of motion for this system have the form:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = -\gamma\mathbf{p}_i - \frac{\partial U}{\partial\mathbf{r}_i} + \lambda\frac{\partial G}{\partial\mathbf{p}_i}\,, \tag{16}$$

where the function G is defined by

$$G(\mathbf{r},\mathbf{p}) = \frac{1}{2}\left(\sum_{i=1}^{N} p_i^2 - mkT\right), \quad G(\mathbf{r},\mathbf{p}) = 0\,. \tag{17}$$

Equations (16) with condition (17) define $6N+1$ variables $(\mathbf{r},\mathbf{p},\lambda)$.

Let us find the Lagrange multiplier λ. Substituting Eq. (17) into Eq. (16), we get

$$\frac{d\mathbf{p}_i}{dt} = -(\gamma-\lambda)\mathbf{p}_i - \frac{\partial U}{\partial\mathbf{r}_i}\,. \tag{18}$$

Multiplying both sides of Eq. (18) by $\mathbf{p}_i/m$ and summing over index i, we obtain

$$\frac{d}{dt}\left(\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}\right) = -(\gamma-\lambda)\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{m} - \sum_{i=1}^{N}\left(\frac{\mathbf{p}_i}{m},\frac{\partial U}{\partial\mathbf{r}_i}\right). \tag{19}$$

Using $dG/dt = 0$ and substituting Eq. (15) into Eq. (19), we get

$$0 = -(\gamma - \lambda)kT - \sum_{j=1}^{N} \left(\frac{\mathbf{p}_j}{m}, \frac{\partial U}{\partial \mathbf{r}_j} \right).$$

Therefore, the Lagrange multiplier λ is equal to

$$\lambda = \frac{1}{mkT} \sum_{j=1}^{N} \left(\mathbf{p}_j, \frac{\partial U}{\partial \mathbf{r}_j} \right) + \gamma \,.$$

As the result, we have the holonomic system which is equivalent to the non-holonomic system (16) and (17) and defined by

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}, \quad \frac{d\mathbf{p}_i}{dt} = \frac{1}{mkT} \sum_{j=1}^{N} \left(\mathbf{p}_j, \frac{\partial U}{\partial \mathbf{r}_j} \right) \mathbf{p}_i - \frac{\partial U}{\partial \mathbf{r}_i} \,. \tag{20}$$

Condition (10) or (15) for the classical N-particle system (20) is satisfied. If the time evolution of the N-particle system (16) has non-holonomic constraints (17) or the evolution is defined by Eq. (20), then we have the canonical distribution function in the form:

$$\rho(\mathbf{r}, \mathbf{p}) = \exp \frac{1}{kT} \left(\mathcal{F} - \sum_{i=1}^{N} \frac{p_i^2}{2m} - U \right).$$

For example, the N-particle system with the forces

$$\mathbf{F}_i = \frac{\omega^2}{kT} \mathbf{p}_i \sum_{j=1}^{N} (\mathbf{p}_j, \mathbf{r}_j) - m\omega^2 \mathbf{r}_i$$

can have a canonical distribution that look likes the canonical distribution of the linear harmonic oscillator:

$$\rho(\mathbf{r}, \mathbf{p}) = \exp \frac{1}{kT} (\mathcal{F} - H(\mathbf{r}, \mathbf{p})) \,,$$

where

$$H(\mathbf{r}, \mathbf{p}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N} \frac{m\omega^2 r_i^2}{2} \,.$$

5. Conclusion

Dissipative and non-Hamiltonian classical systems can have stationary states that look like canonical distributions. The condition for non-potential forces which leads to the canonical distribution function for dissipative systems is very simple: the power of all non-potential forces must be directly proportional to the velocity of the Gibbs phase (phase entropy density) change.

In Refs. 13 and 14, the quantization of evolution equations for dissipative and non-Hamiltonian systems was suggested. Using this quantization it is easy to derive quantum Liouville–von Neumann equations for the N-particle matrix density operator of the dissipative quantum system. The condition which leads to the canonical matrix density solution of the Liouville–von Neumann equation can be generalized for the quantum case by the quantization method suggested in Refs. 13 and 14.

The canonical distribution for dissipative quantum systems allows one to consider stationary states of dissipative quantum states as an unusual quantum computer. In general, we can consider dissipative quantum systems as quantum computers with mixed states.[15] The quantum gates of this computer are general quantum operations, not necessarily unitary.

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