Onsager's Variational Principle in Soft Matter Dynamics

Masao Doi
The University of Tokyo, Japan

In soft matter, many equations have been proposed to describe the complex behavior of the system in non-equilibrium state. Examples are (i) the phase separation kinetics (model H) : the coupled equations for the component diffusion and the fluid flow, (ii) the gel dynamics: the coupled equation for the permeation of solvent and the deformation of gel, (iii) nemato-hydrodynamics: the equations describing the director field and the velocity field, and (iv) kinetic equation for electrolyte solutions which describe the time evolution of ion-concentration, electric field, and solvent flow etc. These equations were originally proposed as a phenomenological equations or a generalization of the existing equations, have been tested, and are now forming a common base the soft matter physics. Here I would like to show that these equations can be derived from a variational principle which I shall call Onsager's variational principle.

The variational principle is a simple rewriting of the conventional thermodynamics of irreversible processes. For the iso-thermal system, the phenomenological time evolution equation can be written as

$$\frac{dX_i}{dt} = -\mu_{ij}\frac{\partial A}{\partial X_j} \qquad (1)$$

Where X_i is the set of the variable describing the non-equilibrium state, A(X) is the free energy of the system and $\mu_{ij}(X)$ is the kinetic coefficients. Due to Onsager's reciprocal relation $\mu_{ij} = \mu_{ji}$ equation(1) can be stated in the following variational principle. The time evolution of the system is determined by $\dot{X}_i$ which minimize the following quadratic function

$$R = \frac{1}{2}\sum \zeta_{ij}\dot{X}_i\dot{X}_j + \sum \frac{\partial A}{\partial X_i}\dot{X}_i \qquad (2)$$

where ζ_{ij} is the inverse matrix of μ_{ij}.

Here I will show (i) the above equations for soft matter dynamics can be derived from this variational principle, (ii) the variational principle is convenient since it allows a great flexibility in choosing the state variable and guarantees the Onsager's reciprocal relation in the final equation.

ACKNOWLEDGEMENT
This work was supported by KAKENHI (Grant-in-Aid for Scientific Research) on Priority Area "Soft Matter Physics" from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

REFERENCES

1. S.R. de Groot and P. Mazur "Non-Equilibrium Thermodynamics", North-Holland, Amsterdam (1962)
2. H. C. Ottinger "Beyond Equilibrium Thermodynamics" Wiley (2005)
3. S. Kjelstrup and D. Bedeaux "Non-Equilibrium Thermodynamics of Heterogeneous Systems" World Scientific (2008)
4. M. Doi in "Dynamics and Patterns in Complex Fluids" ed by A.Onuki and K. Kawasaki, Springer (1990) p 100-112
5. M. Doi, J. Phys. Soc. Jpn 78 052001 (2009)