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Mean Field Theories and Dual Variation

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Preface

In general, systems of nonlinear partial differential equations are formulated and studied individually according to specific physical or biological models of interest. There are, however, certain classes of Lagrangian systems for which the asymptotic behavior of the non-stationary solutions, including the blowup mechanism, is controlled by their total sets of stationary solutions. In this book, we will show that these equations have their origin in mean field theory and that the associated elliptic problems are provided with mass and energy quantizations because of their scaling properties.

Mean field approximation has been adopted to describe macroscopic phenomena from microscopic overviews, with some success, though still in progress, in many areas of science, such as the study of turbulence, gauge field, plasma physics, self-interacting fluids, kinetic theory, distribution function method in quantum chemistry, tumor growth modelling, phenomenology of critical phenomena. In this last scientific area, phase transition, phase separation, and shape memory alloys are included.

However, in spite of such a wide range of scientific areas that are concerned with the mean field theory, a unified study of its mathematical structure has not been discussed explicitly in the open literature. The benefit of this point of view on nonlinear problems should have significant impact on future research, as will be seen from the underlying features of self-assembly or bottom-up self-organization which is to be illustrated in a unified way. The aim of this book is to formulate the variational and hierarchical aspects of the equations that arise in the mean field theory from macroscopic profiles to microscopic principles, from dynamics to equilibrium, and from biological models to models that arise from chemistry and physics.

One of the key concepts to be used repeatedly in our discussion in this book is the notion of duality, which has been the origin of the extension of functions to distributions²⁷³ that provides a useful tool for the formulation of *weak solutions* in the theory of partial differential equations. In addition, Riesz' representation theorem¹⁰⁰ provides the formulation of duals for such important function spaces as $C(K)' \cong \mathcal{M}(K)$ and $L^1(\Omega)' \cong L^\infty(\Omega)$, where K and Ω are compact and open sets in $\mathbf{R}^n$, respectively. Thus if a family of continuous approximate solutions is not compact but is provided with *a priori* estimates, say, in the L^∞ or L^1 norm, then the weak solution is realized as an L^∞ function or a measure, respectively, whereby several fundamental profiles caused by the nonlinearity can be observed (e.g., interface, shock, localization, concentration, condensate, blowup, self-similar evolution, travelling and spiral waves, ...). Another concept of duality, namely, that of Hardy-BMO²⁸⁸ is reflex-

ive. It is represented by $L \log L(\Omega)' \cong \text{Exp}(\Omega)$ and $\text{Exp}(\Omega)' \cong L \log L(\Omega)$, where $\Omega \subset \mathbf{R}^n$ is a bounded domain. The Hardy-BMO duality is associated with the mean field hierarchy through the *entropy* functional and the *Gibbs measure*. Thus this duality notion can be applied to the study of phenomena between particles and fields in the microscopic level as governed by the Boltzmann principle and the zeta-function, respectively. Yet another duality concept that will be used in this book is operator theoretical. For example, for some given rectangular matrix A a column vector b , the duality of the linear model $Ax = b$ is the transposed operation that arises in the context of the Fredholm formulation concerning the existence and uniqueness of the solution. On the other hand, the linear inequality $Ax \geq b$ in convex analysis has an analogous duality formulation. For example, this formulation results from integrating a linear functional equation where the *Legendre transformation* takes on the role of the transposed operator.³⁰ This involutive operation is often referred to as the Fenchel-Moreau duality, which results in the more complicated dualities of Kuhn-Tucker and Toland. Here, the *Toland* duality is concerned with the functional represented by the difference of two convex functionals, such as the Helmholtz free energy. The field functional then is obtained in its dual form, and these two principal functionals are regarded as unfoldings of the *Lagrangian*.

This book consists of two main chapters. The first chapter is devoted to the study of variational structures, where the quantized blowup mechanism observed in the chemotaxis system³⁰⁴ is first described. Within this section, the free energy transmission, which results in the formation of self-assembly, is emphasized which means that the source of the emergence is the wedge of blowup envelope, while entropy and mass are exchanged to create a clean self with the quantized mass. The leading principle derived from this study can be summarized as follows: dual variation sealed in the mean field hierarchy and scaling that reveals this hierarchy. In fact, the phenomenon of quantization is sealed in the total set of stationary solutions, referred to as the nonlinear spectral mechanics. The structure of dual variation controls, not only the local dynamics around the stationary state, but also the formation of self-assembly realized as a global dynamics including the blowup of the solution. This duality is associated with the convexity of the functional; and thus, our description involves convex analysis as mentioned above. We will examine the phenomena and logistics of both variational and dynamical structures of several problems including phase transition, phase separation, hysteresis in shape memory alloys which review the theory of non-equilibrium thermodynamics.

Chapter 2 is devoted to the discussion of the method of scaling for revealing the mathematical principles hidden in the mean field hierarchy subject to the second law of thermodynamics. More precisely, we will describe the quantized blowup mechanism observed in self-gravitating fluid, turbulence, and self-dual gauge field. In particular, blowup analysis, one of the most important applications of the method of scaling, is used to clarify this mechanism. This analysis consists of four ingredients, namely, scaling invariance of the problem, classification of the solution of the limit problem defined on the whole space and time, control of the rescaled solution at infinity, and hierarchical arguments. Meanwhile we will also describe the method of statistical mechanics for the study of macroscopic

phenomena caused by the micro-scopic principles. In particular, we will re-formulate the simplified system of chemotaxis as a fundamental equation of the material transport, the Smoluchowski-Poisson equation.

Unfortunately, a complete overview of the topics mentioned above is beyond the scope of this book, and the list of references is far from being sufficient. Furthermore, several important related topics are missing, among which are the complex Ginzburg-Landau free energy associated with super-conductivity in low temperature,^{22,227} Arnold's variational principle for describing the MHD equilibrium,¹¹ the density function theory of quantum chemistry,⁴³ kinetic equations in fluid dynamics,²⁹ and the duality between Aleksandrov's problem in integral geometry and the optimal mass transport theory.²³⁸ There are also several stationary problems in engineering associated with duality¹¹³ which may be extended to the non-stationary problems of their own.

We take this opportunity to clarify several terminologies used in this book that are the concern of thermal phenomena associated with *dissipation*. First, we follow the classical concepts of equilibrium thermodynamics and classify thermal systems into isolated, closed, and open systems. This classification is also associated with the theory of equilibrium statistical mechanics. More precisely, these systems are provided with the microscopic structures of micro-canonical, canonical, and grand-canonical ensembles, respectively. A closed system here indicates the lack of transport of materials between the outer systems, whereby the transport of heat and that of the energy are permitted. In the open system, on the other hand, the transport of material between the outer systems is also permitted. Next, in view of the theory of non-equilibrium thermodynamics, we add one more aspect to the openness, that is the dissipation of entropy to the outer system.²²⁴ Under this agreement, closedness is re-formulated as a system provided with decreasing total free energy or that provided with increasing total entropy. Thus we have two kinds of closedness: physical closedness in terms of kinetic and/or material, and thermodynamical closedness described by two typical models discussed in details in this book. Free energy *transmission* occurs in the latter case and could be the origin of "self-assembly".

In this connection, we note that the *dissipative system* is defined by the presence of an attractor in the theory of dynamical systems. Gradient system with compact semi-orbits is a typical dissipative system in this case.¹²⁸ We believe, however, that this definition of dissipative system does not describe what were observed by.²²⁴ More precisely, decrease of the free energy or increase of the entropy means thermodynamical *closedness*. It is formulated by the gradient system in the same two models as mentioned above, and, therefore, is never provided with the dissipation in the sense of non-equilibrium thermodynamics²²⁴ in spite of the fact that these two models are typical dissipative systems in the theory of dynamical systems. To avoid this confusion, the above mentioned terminology of dissipative system in the theory of dynamical systems¹²⁸ is *not* used in this book. Actually, a recent paradigm asserts two aspects of self-organization, *far-from-equilibrium* (top-down self-organization) and *self-assembly* (bottom -up self-organization), emphasizing the role of their *hierarchical developments*, with the Hopf bifurcation casting the threshold.³⁴⁵ Dissipation occurs in a state far-from-equilibrium, which results in a spiral wave, a travelling

wave, a periodic structure, a self-similar development, and so forth; while self-assembly, we believe, is formed near-from-equilibrium of thermodynamically closed system induced by the stationary states, developing a condensate, a collapse, a blowup, a spike, and so forth. This book is concerned with the formation of self-assembly. Its profile is provided with the "triple seal," of which basic concepts have already been described. First, several features of self-assembly that is one aspect of the self-organization are sealed in thermodynamically closed systems. Secondly, the dynamics of the closed system is sealed in the total set of stationary states. Finally, the stationary states themselves are sealed in the (skew-) Lagrangian, provided with the structure of dual variation. These features of the mean field hierarchy are certainly revealed by the method of scaling derived from the microscopic principle. In summary, formation of self-assembly arises in thermodynamically closed systems, and hence this process is subject to the calculus of variation. The closed system follows the microscopic principle. This principle controls the mean field hierarchy totally, and, therefore, fundamental profiles of the macroscopic mean field equation are revealed by the method of scaling. We would like to thank Professor Tomohiko Yamaguchi for several stimulative discussions on non-equilibrium thermodynamics. Thanks are also due to Professors Biotr Biler, Fumio Kikuchi, Futoshi Takahashi, and Gershon Wolansky for careful reading over the primary version of the manuscript.

Takashi Suzuki
Osaka, Japan
June, 30, 2008

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