Synergetics and Phase Transitions: Mounting the Quantum Ladder of Nature

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The problem of relationships between two approaches to living systems — synergetics and quantum mechanics — is discussed. Special attention is paid to the common methodological aspects of these approaches based on the fundamental ideas of the modern phase transition theory.

(Received August 29, 1994)

The problem of entire stability of macroscopic systems is one of the crucial points in natural science, being a subject of unremitting attention (see, for example, [1—9]). Stability of solids as an evidence, was starting point in constructing of classical mechanics, both in justifying its measurements (rigid rods) and in establishing the applicability limits of its theoretical principles (reference systems). However, due to the high sensitivity of dynamical systems to variability of the initial conditions, classical physics by itself was not able to substantiate the observed stability of solids. That circumstance was recognized by the creators of quantum mechanics. At the same time, the possibility of explaining (within the quantum mechanics framework) stability of solids, at least on their elements' level, was discovered.

Weisskopf [10] was probably the first who noticed that most of the authors of quantum mechanics books treating the methodological problems concentrated mainly upon the probabilistic character of quantum-mechanical results. That could be justified at the stage of forming the probabilistic way of scientific thinking to comprehend the micro-cosm processes. However, emphasizing the statistical nature of the quantum-mechanical laws often grew into the idea of uncertainty of the quantum mechanics results, in contrast, for example, to the exact ones of classical mechanics. This is incorrect. As a matter of fact, just the objects which the quantum-mechanical principles of identity and discreteness can be applied to are the truly integrable systems whereas the conventional mechanics, as a rule, describes ergodic systems whose infinitesimal uncertainty of their initial conditions results in homogeneous filling the phase space (regime of the strange attractor type). This circumstance has been completely cleared up only in the course of modern revolution in natural science when applying to physics the results of elaboration of the nonlinear dynamics mathematical basis. However, in this new context the problem of solids stability looks somewhat different from what could be considered before. It is important to emphasize that in this case it could be preserved the meaning of idea that namely the applicability of quantum-mechanical principles to such microobjects as nuclei, atoms and molecules determines their stable existence in the capacity of subjects of corresponding sections of physics as a fundamental science. It is these objects that form the three steps of the Weisskopf "quantum ladder" [10]. In terms of physics of the alive [9], the fourth step of this ladder is the alive.

As a product of nonlinear thinking, the modern evolutionary outlook shifts the stress from the statement of the stable systems existence to the problem of their formation and dynamical self-sustention. In the passage of such systems through the critical (bifurcation) points, owing to an anomalously high sensivity to the external factors (even of extremely weak intensity) at this instant, the fluctuation effects give rise to a new ordered phase, often having qualitatively new properties.

It is especially important to consider the quantum systems which form the quantum ladder steps from the viewpoint of self-organization. The necessity of such treatment of the alive is obvious. Considering self-organization of quantum systems of nuclei, atoms and molecules offers basic scope for uniting physics as a science on a new nonlinear basis. For the time being, there exist two parallel worldviews in physics, namely the quantum-relativistic and nonlinear (or synergetical) ones. Such a condition is maintained by the linearity of quantum-mechanical equations and the fact that the dynamical chaos propagation described within nonlinear dynamics is confined by the applicability limits of quantum mechanics [11]. However, this situation cannot be accepted as satisfactory one, since the conceptions of reality within the abovementioned worldviews are quite different and cannot consistently coexist. Besides, dynamical chaos does not exhaust all the diversity of nonlinear phenomena. Among these, as the most important ones can be considered self-organization and self-reproduction of relatively stable structures, hierarchy of dissipative structures in living organisms in particular. Thus, initiated by physics of the alive, studying the relationships between synergetics and quantum mechanics is of great importance for the whole physics.

The present paper is aimed to a considerable degree at the methodological problems of physics, physics of the alive as well. Our main purpose is to show the connection between the modern theory of phase transitions and i) the theory of formation of ordered structures (synergetics) and ii) the quantum theory of dynamically stable systems beyond the self-organization threshold.

In spite of the fact that the connection between nonequilibrium phase transitions and dissipative structures is a subject of numerous investigations [3, 5], we believe that there are new ideas and results based upon applying the fluctuation models to the processes of self-organization. In the first section of the paper we show how the fluctuation models of self-organization processes and formation of stable ordered structures can be constructed in accordance with the modern theory of phase transitions. We briefly discuss the main results of studying of these models.

In the second section we examine an analogy between the renormalization group method and quantum mechanics. The analogy originates from solving virtually the same Sturm-Liouville problem of seeking eigenfunctions and eigenvalues [12]. In that way the theory of phase transitions forms a basis on which it is possible to consider in a new fashion the problem of formation of stable ordered structures in its connection with the basic principles of quantum mechanics.

SYNERGETICS AND PHASE TRANSITIONS: FLUCTUATION MODELS OF SELF-ORGANIZATION PROCESSES

In papers [13—16] and monograph [17] new models of the self-organization processes were proposed and studied. The main idea of the models was to coordinate the initial principles of model construction and the corresponding equations of motion (kinetic equations) with the fundamentals of modern physics of phase transitions. Let us note that the known kinetic models of self-organization (such as "brussellator", "oregonator", Girer-Meinhardt's model, etc.) do not satisfy this requirement, since they cannot be obtained by making use of the Landau-Ginsburg Hamiltonian for several interacting order parameters, whereas the new models can. The structure of the fluctuation models obtained in [13—17] is directly connected with the following form of the free energy fluctuation part:

$$\Delta F_{\text{fluc}} = \sum_i H_{\text{LG}}[\varphi_i] + H_{\text{int}}[\varphi_1, \varphi_2, \ldots] \tag{1}$$

Here

$$H_{\text{LG}}[\varphi_i] = \frac{1}{2}\int\left\{a_i\varphi_i^2(x) + \frac{1}{2}b_i\varphi_i^4(x) + c_i[\nabla\varphi_i(x)]^2\right\}d^d x \tag{2}$$

is the Landau-Ginsburg Hamiltonian for the order parameter $\varphi_i(x)$; a_i, b_i, c_i are coefficients, given that $a_i \sim T - T_{ic}$ (T_{ic} is critical temperature for the i-th order parameter), d is the space dimensionality, and H_{int} is the Hamiltonian (free energy) of interaction between two (several) order parameters.

According to (1-2), the motion equations have the form of the known kinetic equations of Landau-Ginsburg's time-dependent theory:

$$\frac{\partial \varphi_i}{\partial t} = -\Gamma_i \left(a_i \varphi_i + b_i \varphi_i^3 + \frac{\delta H_{int}}{\delta \varphi_i} \right) + D_i \Delta \varphi_i \tag{3}$$

One can easily see that motion equations (3) coincide in their form with the kinetic equations of reaction-diffusion models widely used in synergetics [5]. Indeed, the nonlinear terms (those containing φ^3 and H_{int}) assure the feedback (interaction) among the order parameters, whereas the nonlocal (Ornstein-Zernike) contribution (containing $\Delta\varphi_I$) is responsible for the diffusion processes ($\Gamma_i C_i = D_i$ are diffusion coefficients). Moreover, beyond the phase transition threshold, when self-organization causes the formation of dynamically stable structures, $D \approx 0$ [17], and, therefore, Eq.(3) does not differ in its form from motion equations in standard synergetic models

$$\dot{q} = -k_1 q - k_2 k^3, \tag{3a}$$

associated (at $k_1 < 0$ and $k_2 > 0$) with the Landau-Haken potential and having the limit-cycle solutions in phase plane [9] (one should bear in mind that in general the interaction Hamiltonian can be explicitly taken into account during the standard procedure of proceeding from (1) to (3) by using the methods of calculus of variation.

For definiteness, let us consider a fluctuation model with two interacting order parameters and nonlinear coupling of the general form

$$\begin{aligned} \frac{\partial \varphi_1}{\partial t} &= \Psi(\varphi_1, \varphi_2) + D_1 \Delta \varphi_1, \\ \frac{\partial \varphi_2}{\partial t} &= \Theta(\varphi_1, \varphi_2) + D_2 \Delta \varphi_2, \end{aligned} \tag{4}$$

where $\Psi(\varphi_1, \varphi_2)$ and $\Theta(\varphi_1, \varphi_2)$ are arbitrary nonlinear functions. Analyzing the type of singular points according to Poincare's classification and the stability of stationary solutions $\varphi_{io}(x, t)$ with respect to small perturbations

$$\delta\varphi_i(x,t) = \varphi_i(x,t) - \varphi_{io}(x,t) = \int \sum_k \delta\varphi_i(k,\lambda) e^{ikx - \lambda t} dt \tag{5}$$

implies examining the characteristic equation

$$\mathrm{Det}\left[\hat{U} - \hat{D}k^2 - \hat{I}\lambda\right] = 0 \tag{6}$$

which gives the dispersion law and relates the damping coefficient λ to the wave vector k. Here

$$\hat{U} = \begin{pmatrix} \frac{\partial \psi}{\partial \varphi_1} & \frac{\partial \psi}{\partial \varphi_2} \\ \frac{\partial \theta}{\partial \varphi_1} & \frac{\partial \theta}{\partial \varphi_2} \end{pmatrix}, \quad \hat{D} = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}$$

and $\hat{I}$ is 2×2 unit matrix.

In [14—17] a series of statements (theorems) determining the conditions of the emergence of Hopf's and Turing's bifurcations was formulated for fluctuation model (4). For example, the necessary condition of the emergence of uniform-in-volume temporal oscillations reads as the following inequality for the coefficients of dispersion equation (6):

$$(E_1 - E_2)^2 + 4E_3 < 0,$$

where

$$E_1 = D_1 k^2 - \partial\Psi/\partial\varphi_1,$$
$$E_2 = D_2 k^2 - \partial\Theta/\partial\varphi_2,$$
$$E_3 = \partial\Psi/\partial\varphi_2 \cdot \partial\Theta/\partial\varphi_1.$$

In the specific case $E_1 = E_2 = 0$ the periodic limit-cycle solution of model (4) exists for $E_3 < 0$ only.

In [18] a numerical modelling of ordered structures was made for the fluctuation model with quadruple interaction, i.e., with $H_{\text{int}} = a_4 \int \varphi_1^2(x)\varphi_2^2(x)\,d^d x$.

Special attention should be paid to the fact (confirmed by both analytical and numerical calculations) that the ordering and self-organization within the framework of the considered models take place beyond the boundary of system's stability, that is on the nonthermodynamic branch of states, where the determinant of inverse susceptibilities Det $\hat{U}$ and/or the determinant of diffusion coefficients det $\hat{D}$ change their signs.

Concluding this Section, we should note that in the vicinity of bifurcation points the diffusion coefficients D_i (in the general case — all kinetic coefficients) and the inverse relaxation times $\tau_i^{-1} = \Gamma_i a_i \sim \chi_i^{-1}$ (related to system's susceptibilities χ_i's) included in motion equation (3) cease to be the local functions of spatial coordinates and time. Consistent taking into account this basic fact needs using the results of papers [19—21] in which the following long-range (in the vicinity of critical, or bifurcation, points) effects were simultaneously taken into account: i) spatial nonlocality and "memory" in the equation of state which are related to the value of the system anomalous susceptibility $\chi(\vec{r}, t)$ to the external factors; ii) spatio-temporal dispersion of the kinetic coefficients, such as diffusion coefficients D_i's.

Applying the results of papers [19—21] to examining the fluctuation models of self-organization processes leads to the following equations linearized for quantities $\delta\varphi_i(k, t)$ from (5):

$$\frac{\partial\delta\varphi_i(k,t)}{\partial t} = -\sum_j \hat{M}_{ij}^{(0)}(k)\delta\varphi_j(k,t) - \sum_j \int_0^t \hat{N}_{ij}(k,t-t')\delta\varphi_j(k,t')dt' \qquad (7)$$

Here the complete matrix of inverse relaxation times

$$\hat{M}_{ij}(k,t-t') = \hat{M}_{ij}^{(0)}(k)\delta(t-t') + \hat{N}_{ij}(k,t-t')$$

is decomposed into the following matrices: a) $\hat{M}_{ij}^{(0)}$ which corresponds to hydrodynamical equations describing only the nonlocality of the equation of state in the Ornstein-Zernike approximation; b) $\hat{N}(k,t-t')$ which describes the effects of nonlocality and memory in the kinetic coefficients.

In view of the similarity of Eqs.(7) and the time-dependent Schrödinger equation it is convenient to introduce the new variables

$$\varphi_i(k,t) = \left[e^{\hat{M}^{(0)}(k)t}\right]_{ij}\delta\varphi_j(k,t),$$

which are the linear combinations of Fourier transforms $\delta\varphi_i(k, t)$'s. This procedure is equivalent to proceeding to the interaction representation in the quantum field theory and enables us to use the technique of the perturbation theory to calculate the quantities $\varphi_i(k, t)$'s and, consequently, the corresponding pair correlation functions G_2.

As noted in [22] when considering the theoretical basis of morphogenesis, such nonlocal effects can initiate the break of symmetry and instabilities of Hopf's and Turing's types.

PHASE TRANSITIONS AND QUANTUM MECHANICS

The latest advance in physics of phase transitions and critical phenomena has resulted from employing the concepts and methods of scaling theory [23], with the renormalization group approach being its macroscopic justification [24]. The renormalization group (RG) transformation is complex nonlinear transformation, usually applied to the "seed", or "effective" Landau-Ginsburg Hamiltonian H_{LG} (see Eq.(1)). The coefficients a_i, b_i, c_i subjected to the RG-transformation are described as the point μ in so-called parametric space, that is $\mu = \{a_i, b_i, c_i\}$.

Within the RG-method framework the pair correlation function of the order parameter

$$G_2(r, \mu) = \left\langle \left[\varphi(\vec{r}_1) - \langle\varphi(\vec{r}_1)\rangle\right]\left[\varphi(\vec{r}_2) - \langle\varphi(\vec{r}_2)\rangle\right]\right\rangle,$$

$$r = |\vec{r}_1 - \vec{r}_2| \tag{8}$$

(in terms of which, by virtue of the known relations of the condensed matter statistical theory most of the equilibrium and kinetic properties of substance can be expressed) satisfies the following equation

$$G_2(k, \mu) = s^{2-\eta} G_2(sk, \hat{R}_s \mu) \tag{9}$$

Here $\hat{R}_s$ is the RG-transformation operator, s is a certain great parameter which is usually related to the fluctuation correlation radius, η is the critical index of anomalous dimensionality of the correlation function G_2. If the point μ of parametric space is close to the fixed (immovable) point μ^* which is invariant under the RG-transformation ($\hat{R}_s\mu^* = \mu^*$) and plays the role of a critical (bifurcation) point, then the following relation takes place:

$$\hat{R}_s^L \mu = \mu^* + \sum_{i \geqslant 1} t_i s^{y_i} e_i , \tag{10}$$

where e_i and s^{y_i} are eigenfunctions and eigenvalues of the RG-transformation operator $\hat{R}_s^L$ linearized in the vicinity of the fixed point, and t_i is the coefficient of the linear expansion of the quantity $\delta\mu = \mu - \mu^*$ into a series in eigenfunctions e_i's.

Let us note that the power laws of scaling theory (scaling laws) are determined by the greatest positive eigenvalue y_1 of the operator $\hat{R}_s^L$, given that $y_1 = 1/\nu$, where ν is the critical index of temperature dependence of the radius of the density fluctuation correlation, namely:

$$\xi = \xi_0 \tau^{-\nu}. \tag{11}$$

Here ξ_0 is the correlation radius amplitude which coincides in the order of magnitude with the intermolecular interaction radius, $\tau = (T - T_C)/T_C$ — is deviation of temperature T from its value T_C in the critical point, and ν is the critical index which equals 0.63 for $d = 3$ in the systems with a scalar (one-component) order parameter. Other eigenvalues $y_i (i \geqslant 2)$ specify different scaling corrections (see review [25]), making it possible to extend considerably the applicability limits of the phase transition theory with respect to the thermodynamic variables (temperature, density, pressure, etc.).

From all the aforementioned it definitely follows that the methods and mathematical tools employed in the modern fluctuation theory of phase transitions, on the one hand, and in quantum mechanics, on the other hand, are very similar. Indeed, both the problem of finding critical indices like the index ν and that of finding the quantum numbers are in essence Sturm-Liouville's problems. Moreover, this analogy (see Table) seems to be even closer in view of not only the common mathematical tools but also the basic symmetry reasons. The very fact of the existence of quantum numbers and stationary states has appeared as a manifestation of the fundamental properties of space and time symmetry as well as the processes in the microcosm. The existence of critical indices and universal commonality of properties pertaining to the systems of completely different nature displays a new class of symmetry, namely that defined by the renormalization group transformations. This new type of symmetry turns out to be inherent in all, not only micro- but also macroscopic, systems in the vicinity of their critical (bifurcation) points. A new phase, new ordered structures included, emerges in such systems due to fluctuation interaction which can be taken into account with use of the RG-method only.

Table

Correspondence between quantum mechanics and physics of phase transitions (synergetics)

Quantum Mechanics	*Phase Transitions (Synergetics)*
Hamiltonian $\hat{H}$	Linearized RG-operator $\hat{R}_s^L$
Eigenfunctions Ψ_n	Eigenfunctions of operator $\hat{R}_s^L$ – e_i
Eigenvalues E_n	Eigenvalues of operator $\hat{R}$ – s^{y_i}
Quantum numbers	Critical indices
Principal quantum number n	Critical index of correlation radius ν

Thus, based upon the concepts of scaling and renormalization group, the contemporary development of the phase transition theory makes it possible

i) to evaluate in a new fashion the validity and profundity of the known principle "via fluctuation to ordering";

ii) to give a new interpretation of the steps of the "Weisskopf quantum ladder".

СИНЕРГЕТИКА ТА ФАЗОВІ ПЕРЕХОДИ — ПІДЙОМ ПО "КВАНТОВИХ СХОДАХ"

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Аналізується проблема співвідношень двох підходів до живих систем — синергетики та квантової механіки. Особливу увагу приділено загальним методологічним аспектам у цих підходах, що грунтуються на фундаментальних ідеях сучасної теорії фазових переходів.

СИНЕРГЕТИКА И ФАЗОВЫЕ ПЕРЕХОДЫ — ВОСХОЖДЕНИЕ ПО "КВАНТОВОЙ ЛЕСТНИЦЕ"

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Обсуждена проблема соотношений между двумя подходами к живым системам — синергетикой и квантовой механикой. Особое внимание уделено общим методологическим аспектам в этих подходах, основанных на фундаментальных идеях современной теории фазовых переходов.

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