Unification of the standard and gradient theories of phase transition

B. I. Lev and A. G. Zagorodny
Bogolyubov Institute for Theoretical Physics, NAS Ukraine, Metrolohichna 14-b, Kyiv 03680, Ukraine
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We show that the standard model of phase transition can be unified with the gradient model of phase transitions using the description in terms of the gradient of order parameter. The generalization of the gradient theory of phase transitions with regard to the fourth power of the order parameter and its gradient is proposed. Such generalization makes it possible to describe wide class of phase transitions within a unified approach. In particular it is consistent with the nonlinear models that can be used to describe a phase transition with the formation of spatially inhomogeneous distribution of the order parameter. Typical examples of such structures (with or without defects) are considered. We show that formation of spatially inhomogeneous distributions of the order parameter in the course of a phase transition is a characteristic feature of many nonlinear models of phase transitions.

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Withing the context of the general theory of phase transitions a system treated as a continuous medium is assumed to have a ground state which can always be described in terms of the order parameter. Such order parameter can have various geometrical presentations, for example, a scalar field in the case of condensed matter [1], a fundamental scalar field in the quantum field theory [2], a magnetization vector in the theory of magnetism [3], a second-rank tensor in the liquid crystal theory [4], etc.

To introduce the order parameter that determines a stable state of condensed matter, we have to consider possible deformations of the distribution of the field, in particular, the disordered configuration of the ground state.

The phase transition associated with the system with broken continuous symmetry can be described in terms of the relevant order parameter. In particular, according to the Landau theory the free energy density can be presented in terms of the order parameter as given by

\[ f = (\nabla \varphi(r))^2 + W(\varphi(r)) \]  

where \( \varphi(r) \) is the order parameter and \( W(\varphi(r)) \) describes the order parameter dependence of the free energy that is assumed to be known.

In the well-known standard model of phase transitions

\[ W(\varphi(r)) = \frac{1}{2} a \varphi^2(r) + \frac{1}{4} b \varphi^4(r). \]  

(2)

With the dimensionless variable \( \varphi^2(r) = \frac{b}{a} \varphi^2(r) \) being introduced the standard dimensionless free energy reduced to the form given by

\[ f = l^2 (\nabla \varphi(r))^2 + (|\varphi(r)|^2 - 1)^2 \]  

(3)

with the potential being written in the standard form and \( l^2 = \frac{2}{a} \) being the characteristic length. Making use of this expression for the free energy, we can find the spatial distribution of the order parameter and thus, describe the properties of the new states which can be formed after the phase transition.

It should be noted that in the case of system with the gradient of the order parameter, it looks reasonable to introduce into the free energy functional the term responsible for possible interaction between the order parameter and its gradient. This coupling can regularize possible perturbations of the order parameter and thus confine the spatially inhomogeneous state of the system.

On the other hand, singular perturbation models, involving higher order of the the spatial derivations have provided a new insight on the role of additional physical features of the system under consideration, on the details of phase transitions, in particular on the way how to describe the contribution of the surface energy. In this case restricting the accuracy of the free energy functional by the first order derivatives of the order parameter leads to the solution with the homogeneous distribution of the order parameter only.

The main idea of the present contribution is to generalize the phenomenological theory of phase transitions by introducing the second-order spatial derivatives into the order parameter dependence of the free energy. Such generalization is reasonable in view both mathematical and physical arguments. From the mathematical point of view, our argument is that the order parameter can be treated as a vector quantity and thus it is possible to rewrite the free energy (1) in the form

\[ f = l^2 (\nabla \varphi(r))^2 + (|\varphi(r)|^2 - 1)^2 \]  

(4)

where the order parameter is a vector function. Such problem arises if we assume that the order parameter \( \varphi(r) \) can be presented in term of a gradient of some other scalar function \( \nabla u(r) \). This assumption leads to the known presentation of the free energy in the Aviles-Giga form [5,6], i.e.

\[ f = l^2 (|\nabla u(r)|^2 + (|\nabla u(r)|^2 - 1)^2 \]  

(5)

As is known, this presentation has various physical applications, e.g. the description of smectic liquid crystals [5], thin film blisters [7,8] and convective pattern formation [9]. Physically, such model can be regarded as...
the Landau model applied to a system with vector order parameter. Some well-known Landau theories have similar features. For example, the energy of a smectic-A liquid crystal has been described within such model \( \mathbb{R} \) where \( \frac{\nabla u(r)}{|u(r)|} \) represents the director field of the liquid crystal. The observed focal-conic defect structures can also be described in terms of this functional \( \mathbb{R} \). The micro-magnetics give one more example of the application of the functional \( \mathbb{R} \). In particular, it can be used to describe magnitization constrained by \(|m|=1\) within and \(m=0\) outside the micro-magnetics \( \mathbb{R} \). The unknown \( u(r) \) is purely curl-free, while \(|m|\) just prefers to be divergence-free. Moreover, \(|m|\) is restricted to unit vectors, while \( u(r) \) prefers to have unit magnitude. But the similarity should be clear, particularly for an isotropic ferromagnet \( \mathbb{R} \).

Another motivation to use the functional \( \mathbb{R} \) arises from recent phenomenological modeling of blisters in compressed thin films \( \mathbb{R} \). Early it has been suggested that the fold patterns of such blisters could be described by minimizing the sum of membrane and bending energies \( \mathbb{R} \). With some simplification, this problem can be reduced to the free energy, given by \( \mathbb{R} \). The same free energy can also be obtained for an equilibrium state of a free surface. In this case \( u(r) \) represents the height profile of the sheet (relative to a flat reference state). This model describes a fluctuating fluid membrane.

The interpretation of the free energy appears also in the phase diffusion theory of pattern formation proposed by Cross and Newell \( \mathbb{R} \). Of course, the physical justification of the models discussed above can be criticized \( \mathbb{R} \). Nevertheless, they demonstrate the need to introduce new representations for the free energy functional in term of the order parameter. We have referred informally to the existence of an asymptotic variational problems. Now, let us consider the possibility to generalize the representation of the free energy to the case when it depends not only on the order parameter, and its gradient, but also on their combination. Such generalization looks quite reasonable if one bears in mind that, in the case of the functional with the first order spatial derivative, the order parameter describes a phase transition in a spatially homogeneous system, while the presence of the second-order derivative makes it possible to describe the formation of spatially inhomogeneous structures. Thus, we can expect that the combination of the gradient terms with the scalar order parameter can be responsible for the self-consistent influence of the order parameter on the spatial distribution and parameters of the ordered structures. In other words, the coupling between the order parameter and its derivatives can influence possible deformations and confine possible inhomogeneous stable structures of the system.

So, let us postulate, that the order-parameter dependence of the free energy is given by

\[
f = a l^2 (|\nabla \varphi(r)|)^2 + b (|\varphi(r)|)^2 - 1)^2 + 
+ m l^4 (|\nabla \nabla \varphi(r)|)^2 + n l^2 (|\nabla \varphi(r)|)^2 - 1)^2 + 
+ c \varphi^2(r) (l \nabla \varphi(r))^2
\]

where \( l \) is the length of the order-parameter changing, \( a, b, m, n, c \) and \( c \) are parameters describing the influence of the gradient order parameter and coupling between the order parameter and the appropriate derivative of this parameter. Having introduced the operator \( D = l \nabla \) we can rewrite the free energy density as

\[
f = a (D \varphi(r))^2 + b (|\varphi(r)|)^2 - 1)^2 + 
+ m (D^2 \varphi(r))^2 + n (l^2 (D \varphi(r))^2 - 1)^2 + 
+ c \varphi^2(r) (D \varphi(r))^2
\]

If all the coefficients except \( a \) and \( b \) are equal to zero, we come to the standard theory of phase transitions. If \( a, b, c \) vanish we come to the standard gradient theory. In the case of large values of \( m \) ( \( m \) is larger than other coefficients) we obtain the eikonal equation \( \nabla \varphi(r) = 1 \) which we supplement with the boundary conditions \( \varphi(r) = 0 \) at the boundary. This eikonal equation has no smooth solution, but it has immitely many Lipschitz solutions. We can suggest that the energy can be concentrated at the discontinuities of \( \varphi(r) \). Thus, the singular part of the order parameter can provide a selection mechanism for the perturbations of the eiconal equation solutions which minimize the free energy.

In the general case, the minimum of the free energy satisfies the Euler-Lagrange equation:

\[
\frac{\delta f}{\delta \varphi(r)} = \frac{\partial f}{\partial \varphi(r)} - D \frac{\partial f}{\partial D \varphi(r)} + D^2 \frac{\partial f}{\partial D^2 \varphi(r)}
\]

which is reduced in our case to:

\[
m D^4 \varphi(r) - (a - 2 n + 6 n (D \varphi(r))^2 + c \varphi^2(r)) D^2 \varphi(r) 
- c \varphi(r) (D \varphi(r))^2 - 2 b \varphi(r) (1 - \varphi^2(r)) = 0
\]

Let us consider in the one dimensional case some probable solutions of the Euler-Lagrange equation for various combinations of the coefficients introduced.

a) Linear solutions

i) We shall look for a solution similar to the solution of the equation \( D \varphi = - \varphi \) and \( D^2 \varphi = \varphi \). Substituting this solution in the Euler-Lagrange equation yields

\[
m \varphi - (a - 2 n + c \varphi^2 + 6 n \varphi^2) \varphi - c \varphi^3 - 2 b \varphi (1 - \varphi^2) = 0
\]

This equation leads us to the following relations between the coefficients, \( m - a = 2 (b - n) \) and \( b - c = 3 m \). In the standard model of phase transitions \( a = b = 1 \) and thus we have \( m + 2 n = 3 \) and \( c = 1 - 3 n \). If \( m = n = 1 \) the coupling constant \( c = -2 \). If \( a = 1 \) and \( b = -1 \) and \( m = 1 \) and \( n = -1 \) the coupling constant \( c = 2 \). In the case of the gradient presentation \( a = b = 0 \) the exponential solution can be realized only for \( n = 1, m = -2 \) and
c = 3. In the case of standard model with n = m = 0 the exponential solution exists for \( b = 1, a = -2 \) and \( c = 1 \). Thus, the exponential solution is realized for various combination of the introduced coefficients.

ii) Now let us look for another possible linear solution in the form of a periodical function, namely \( \varphi(r) = \varphi \exp(ikr) \). This solution satisfies the equation

\[
D^2 \varphi(r) = -k^2 \varphi(r) \]

Substituting of this solution into Euler-Lagrange relations into Euler-Lagrange equation one finds that thus solution satisfies an equation with the high-order derivatives. Such generalization can be employed for standard and gradient theories of the phase transitions by introducing the coupling between the order parameter and its gradient. Such generalization can be employed to describe the phase transitions from spatially homogeneous to inhomogeneous states. It is shown, that the solution of the standard and gradient models of phase transitions can be inconsistent with the Euler-Lagrange equation generated by the generalized functional of the free energy. In the general case the requirement of consistency of the known solutions with the generalized description can be archived by the appropriate choice of the coupling between the order parameter and its gradient.

Specific examples considered in the present contribution shows, that the structure formation observed experimentally can be described by various phenomenological free energy functional which correspond to various sets of coefficients, i.e. there is no unique functional representation of the free energy related to the chosen spatially inhomogeneous configuration of the order parameter. This uncertainty is generated by the phenomenological description and could be eliminated in the microscopic calculations.

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