MODULATED STRUCTURES IN MATERIALS UNDER IRRADIATION

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The models describing phase transitions in systems with a few control parameters are considered. Such models are necessary for studying phase transitions in materials under irradiation. Describing of the phase transitions in the systems with a few control parameters demands taking into account higher gradients and nonlinearities of order parameters. One of the features of such systems is a possibility of modulated phases existence. By analogy with the theory of the phase transitions near tricritical Lifshits points the generalization of existed models was proposed. The role of mixed terms in the thermodynamic potential which are necessary for modulated structures stability is explained.

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INTRODUCTION

One of the important problems of both radiation physics and physics of phase transitions (PT) is studying of critical phenomena in materials under irradiation [1]. The importance of such problems is determined by different reasons. On the one hand irradiation influence on materials properties, so it is necessary to take into account these effects while description of phase transitions. On the other hand some radiation effects might be reasons of phase transitions. Another important reason of necessity of studying of PT under irradiation is that one of the best methods of experimental studying of PT (particularly of the incommensurate phases) is method based on elastic neutron scattering [2]. Elastic neutron scattering is the application of neutron scattering to the determination of the magnetic structure of a material. A sample to be examined is placed in a beam of thermal or cold neutrons to obtain a diffraction pattern that provides information of the structure of the material. Studying of the possible effects of the neutron irradiation on PT is very important to correct using of such techniques.

In order to describe PT in materials under irradiation one need to use models with a few control parameters. Let's consider the thermodynamic potential of the following form [3], [4]:

$$\Phi = \Phi_0 + a_2 \cdot \varphi^2 + a_4 \cdot \varphi^4 + a_6 \cdot \varphi^6 + \ldots + c_1 \cdot \left(\nabla \varphi\right)^2 + c_2 \cdot \left(\nabla^2 \varphi\right)^2 + \ldots, \qquad (1)$$

here Φ – is the t thermodynamic potential; φ – is an order parameters; a_i and b_i – are some material parameters that depend on control parameters. If there is no irradiation than the most common control are temperature, pressure and concentration. To describe PT in the simplest case of system with one control parameter (usually T – temperature) one need to take into account the first three terms in Eq. (1). If there are more than one control parameters in the system than it is necessary to take into account some terms with higher powers and gradients of order parameters. Systems with the higher powers of the order parameters are known as systems with multicritical points, systems with the higher gradients of the order parameters are known as systems with Lifshitz points. In some cases it is necessary to consider systems with critical points of mixed types. An example of a phase transition in the simplest system with a critical point with properties of the both Lifshitz and multicritical points (known as tricritical Lifshitz point) is the phase transition in ferroelectrics of type $Sn_2P_2(Se_xS_{1-x})_6$. A lot of theoretical and experimental results of investigation of the PTs of those types have been obtained recently. One of the main features of such systems is an existence of modulated phases. The thermodynamic potential of such system looks as follows [5]:

$$\Phi = \Phi_0 + \int dx \left\{ c_2 (\varphi'')^2 - g(\varphi\varphi')^2 - c_1 (\varphi')^2 + a_2\varphi^2 + a_4\varphi^4 + a_6\varphi^6 \right\}. \qquad (2)$$

The control parameters of this PT are temperature, pressure and concentration, so 3 of the terms in corresponding thermodynamic potential must change sign at the critical point ($a_2=a_4=c_1=0$), but there is an additional term $g(\varphi\varphi')^2$ in (2). The reason of necessity of taking it into account is discussed below.

If the number of the control parameters is larger than 3, then it is necessary to consider terms with the both higher nonlinearities and gradients of OP in thermodynamic potential. One of the features of the systems with Lifshitz points of high order is a necessity to take into account a possibility of appearance of anisotropic phases. Below a model that makes possible description of such systems is discussed.

APPLICABILITY OF MEAN FIELD APPROXIMATION FOR STUDYING OF CRITICAL PHENOMENA IN SYSTEMS WITH CRITICAL POINTS OF MIXED TYPE

The model that allows one to describe the systems with joint multicritical and Lifshitz behavior was introduced and studied in papers [5]. The Hamiltonian of such model in a vicinity of a critical point may be written as follows:

$$H = \int d^m x_i d^{d-m} x_c \left\{ \frac{r}{2}\varphi^2 + \frac{\gamma}{2}\left(\Delta^{\frac{1}{2}}{}_i \varphi\right)^2 + \frac{\delta}{2}\left(\Delta^{\frac{1}{2}}{}_c \varphi\right)^2 + \right.$$

$$\left.\frac{\beta}{2}\left(\Delta^{\frac{p}{2}}{}_i\varphi\right)^2 + u\varphi^{N+1}\right\}. \quad (3)$$

In order to study as general case as possible such model parameters as *d* (dimension of the physical space), *p* (an order of the order parameters gradients) and *(N+1)* (a power of the model nonlinearity) are considered as arbitrary real numbers. Derivatives of a fractional order in such case might be determined via an opposite Fourier transform. There only the leading terms are taken into account in Eq. (3), because other terms are not necessary for our purposes. Of course it is necessary to take them in to account in order to study a behavior of the systems far from the critical point. Here $r, \gamma, \delta, \beta, u$ are some material parameters. Physical space with a dimension *d* is divided into 2 subspaces with dimensions *m* and *d-m*. There is modulation in the first one and no in the second one. The critical point under considerations determines by the equation: $r = \gamma = 0$. Here and below in this paper the notion of Hamiltonian is used instead of the notion of thermodynamic potential, as it is accepted in modern theory of critical phenomena. The connection between these notions is explained in [6].

In the papers [7] both critical dimensions (lower and upper) were found. The lower critical dimension (d_l) determines a range of an existence of ordering states: there are no PTs at nonzero temperature if the space dimension is less than the lower critical dimension, in other words at the lower critical dimension Goldstone bosons start interacting strongly. I.e. appearing of ordering states is possible only if $d > d_l$. The upper critical dimension (d_u) determines a range of applicability of a mean field approximation in the theory of critical phenomena. For the model under consideration the critical dimensions:

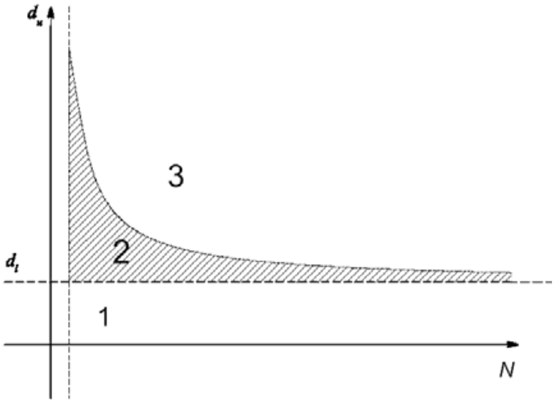
$$d_l = m\left(1 - \frac{1}{p}\right) + 2, \quad (4)$$

$$d_u = m\left(1 - \frac{1}{p}\right) + 2\frac{N+1}{N-1}. \quad (5)$$

The critical dimensions are the borders that determine a fluctuation region. In the fluctuation region PTs are possible, but in order to find the critical exponents it is necessary to use methods based on renormalization group. The width of the fluctuation region:

$$\Delta = d_u - d_l = \frac{4}{N-1}. \quad (6)$$

It is clear that $\lim\limits_{N\to\infty} \Delta = 0$, so the fluctuation region decreases as a function of power of nonlinearity (Figure). This fact is physically reasonable, because strong coupling suppresses the fluctuations. As it is expected, the lower critical dimension of any systems is not less then 2.



Dependence of the upper critical dimension on the power of nonlinearity of the model. The region labeled 2 is the fluctuation region

The critical dimensions are important not only as “borders”. They are the necessary elements of the methods based on renormalization group. Moreover, systems in spaces with dimensions that coincide with the critical one have a number of interesting properties. Corresponding models are renormalizable, they allow variational scale invariance. Moreover, in isotropic cases they are invariant under conformal transformations. These properties are very important while solving corresponding variational equations [8].

As was mentioned above the system of type Eq. (2) is the most thoroughly studied system with joint multicritical and Lifshitz behavior. Let’s write the corresponding Hamiltonian with *N=5* and *p=2* in isotropic case at the critical point:

$$H = \int d^d x \left\{\frac{\beta}{2}(\Delta\varphi)^2 + u\varphi^6\right\}. \quad (7)$$

As was mentioned above there is an additional term $g(\varphi\varphi')^2$ in (2). This term is necessary to explain experimental data. There is impossible to describe incommensurate states without introducing it [9]. Let’s see if it is possible to get this term in different way. In the space with a dimension coinciding with the upper one our system allow the variational scale invariance. Let’s add a “mixed” term of form:

$$\left(\Delta^{\frac{k}{2}}\varphi\right)^2 \varphi^m, \quad (8)$$

and check on what condition it is not break scale invariance. The upper critical dimension d_u*=6* in this case. One should transform the expression:

$$d^6 x \left(\Delta^{\frac{k}{2}}\varphi\right)^2 \varphi^m, \quad (9)$$

with following transformation: $\varphi = e^a\varphi^*, x = e^{-a}x^*$:

$$d^6 x^* \left(\Delta^{\frac{k}{2}}\varphi^*\right)^2 \varphi^{*m}\, e^{6a-2a-2ka+am}. \quad (10)$$

It leads to the condition on k and m:

$$2k + m = 4. \quad (11)$$

Taking into account that k and m have to be integer it easy to see that there is only one option: *k=1, m=2*. Therefore the only one term that keep scale invariance is $\left(\Delta^{\frac{1}{2}}\varphi\right)^2\varphi^2$. Therefore, demanding of keeping of the variational scale invariance leads to the right expression for "g-term".

One can use the same procedure for arbitrary integer values of N and p in order to construct analogs of "g-term" for the models with the higher order parameters gradients and nonlinearities. Let's write the Hamiltonian of the isotropic system in space with dimension d_u at the critical point:

$$H=\int d^{d_u}x\left\{\frac{\beta}{2}\left(\Delta^{\frac{p}{2}}\varphi\right)^2+u\varphi^{N+1}\right\}, \tag{12}$$

here

$$d_u=2p\frac{N+1}{N-1}. \tag{13}$$

This Hamiltonian is invariant under the scale transformation with the generator:

$$\widehat{X}=\frac{\partial}{\partial\varphi}-\frac{N-1}{2p}\frac{\partial}{\partial x}, \tag{14}$$

the corresponding transformation might be written as follows:

$$\varphi=e^a\varphi^*, x=e^{-\frac{N-1}{2p}a}x^*. \tag{15}$$

We want to find what terms of the type:

$$\left(\Delta^{\frac{k}{2}}\varphi\right)^2\varphi^m, \tag{16}$$

don't break the symmetry Eq. (15). Let's transform the expression Eq. (16) with the transformation Eq. (15) taking into account that:

$$d_u=2p\frac{N+1}{N-1}, \tag{17}$$

after the transformation Eq.(15) takes the form:

$$d^{d_u}x^*\left(\Delta^{\frac{k}{2}}\varphi^*\right)^2\varphi^{*m}\,e^{-(N+1)a}e^{-ma}e^{2a}e^{\frac{(N-1)}{p}ka}. \tag{18}$$

The Hamiltonian Eq. (12) with additional terms of type Eq. (16) will keep the invariance if:

$$2p+(N-1)k+mp-(N+1)p=0. \tag{19}$$

It leads to Diophantine equation for *k* and *m*:

$$(N-1)k+pm=(N-1)p, \tag{20}$$

with boundary conditions:

$$0\le k\le p, 0\le m\le N-1.$$

Let's analyze Eq. (20). There are always at least 2 "boundary" solutions for any integer *N* and *p*: $(k=0,m=N-1)\,and\,(k=p,m=0)$. They correspond to "unmixed" terms φ^{N+1} and $\left(\Delta^{\frac{p}{2}}\varphi\right)^2$. If *n* is the greatest common divisor of *N-1* and *p* then the Hamiltonin looks as follows:

$$H=\int d^{d_u}x\left\{\frac{\beta}{2}\left(\Delta^{\frac{p}{2}}\varphi\right)^2+\sum_{i=0}^{n}g_i\varphi^{m_i}\left(\Delta^{\frac{k_i}{2}}\varphi\right)^2+u\varphi^{N+1}\right\}. \tag{21}$$

Finally: if *N-1* and *p* are coprimes then there one no "mixed" terms in the Hamiltonian.

CONCLUSIONS

Conditions of existence of "mixed" terms in the model (3) were found. Next step is to determine a parametric evolution of a spatial distribution of an order parameter field. It is determined by solving of variational equations for corresponding functionals of the thermodynamic potentials. These equations even in the simplest case (2) are nonlinear differential equations of high order. There is no general way of solving such equations. Therefore any steps in solving or just simplification of this problem are very important. An important role in solving this problem plays finding of exact partial solutions of corresponding equations. They don't always describe real physical distributions, but they are necessary elements of different methods of finding physical solutions. For example, they might be used like seeds for expansions or for some numerical methods. One of the promising numerical methods is a method based on using genetic algorithms [10]. One of the ways of finding exact partial solutions of differential equations is the group analysis. We showed that if the dimension of the space coincides with the upper critical one than Hamiltonian allow Eq. (21) is invariant under scale variational transformations. This fact on the one hand allows reducing of the order of corresponding variational equations by 2 and on the other hand allows searching of exact solutions by methods of group analysis.

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МОДУЛИРОВАННЫЕ СТРУКТУРЫ В МАТЕРИАЛАХ ПОД ОБЛУЧЕНИЕМ

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Рассмотрены модели фазовых переходов в системах с несколькими управляющими параметрами. Модели такого типа необходимы для описания фазовых переходов в материалах под воздействием облучения. Описание фазовых переходов в системах с несколькими управляющими параметрами требует учета высших градиентов и нелинейностей параметров порядка. Одной из особенностей таких систем является возможность существования фаз с несоизмеримыми структурами параметров порядка. По аналогии с теорией фазовых переходов вблизи трикритических точек Лифшица предложено обобщение ранее существовавших моделей. Обоснована роль смешанных слагаемых в термодинамическом потенциале, необходимых для устойчивости модулированных структур параметров порядка.

МОДУЛЬОВАНІ СТРУКТУРИ В МАТЕРІАЛАХ ПІД ОПРОМІНЕННЯМ

А.В. Бабіч, О.М. Кіценко, В.Ф. Клепіков

Розглянуто моделі фазових перетворень у системах з декількома управляючими параметрами. Моделі такого типу є необхідними для опису фазових переходів у матеріалах під впливом опромінення. Опис фазових переходів у системах з декількома управляючими параметрами потребує обліку вищих нелінійностей і градієнтів параметрів порядку. Однією із особливостей таких систем є можливість існування фаз з модульованими станами параметрів порядку. По аналогії з теорією фазових перетворень поблизу трикритичних точок Ліфшиця запропоновано узагальнення раніш існуючих моделей. Обґрунтовано роль змішаних доданків у термодинамічному потенціалі, які є необхідними для існування модульованих структур параметрів порядку.