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NONUNIVERSALITY FOR STRUCTURAL PHASE TRANSITIONS NEAR THE DISPLACIVE LIMIT

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I. INTRODUCTION

The structural phase transitions have been studied within the framework of the fluctuation theory of critical phenomena by means of the parquet approximation [1] as well as by the Wilson renormalization group approach [2,3] to first order of both the ϵ- and $1/n$-expansions [4]. The relevance of the Matsubara frequency for the quantum-to-classical crossover phenomena is clarified in the paper [5], where a variety of generalized Ginzburg-Landau models are considered to first order in $\epsilon = d_c - d$. Here d denotes the space dimensionality, whereas d_c is the borderline dimensionality.

In this paper we present the results, obtained for the exact recursion relations and the critical exponents to second order in ϵ for a model of a structural phase transition, considered in refs. [1,4]. We use the method, described in ref. [6] as "the large b limit". We have investigated the general recursion relations in two extreme cases: (i) The finite temperature case ($T_c \neq 0$), which turns out to be the classical one [6]. Here we have no deviation from universality. The borderline dimension is $d = 4 + O(\epsilon)$. (ii) The limit of utmost interest is $T_c \to 0$, which is in fact the quantum mechanical case. In this case the quantum fluctuations modify the dynamic behaviour so that we obtain a new ϵ-dependent fixed point (f.p.) and its corresponding critical exponents. Universality still holds place to first order in $\epsilon = 3 - d$ (here $d_c = 3 + O(\epsilon)$ in accordance with ref. [5]). In second order in ϵ, however, it breaks down. What we mean by this is that the ϵ-dependent critical exponents to first order in ϵ are the same as for a Wilson f.p. (with $\epsilon = 3 - d$ instead of $\epsilon = 4 - d$), but the analysis up to second order in ϵ proves that the dynamic exponent differs from those, predicted for a Wilson f.p.

II. MODEL

We consider the following generalized Ginzburg-Landau model [1,4] : $H = H_0 + H_I$,

$$H_0 = - \sum_{a, q} G_0^{-1}(q)\, \phi_a^*(q)\, \phi_a(q) \ , \tag{1}$$

$$H_I = -\frac{(uT)}{V}\sum_{\alpha\beta;\, q_1, q_2, q_3}\phi^*_\alpha(q_1)\phi^*_\beta(q_2)\phi_\alpha(q_3)\phi_\beta(q_1+q_2-q_3), \quad (2)$$

where H_0 and H_I are the free and the interaction parts of the Hamiltonian, respectively. In (1-2): $\phi(q) = \{\phi_\alpha(q), \alpha = 1, \ldots, n/2\}$ is a $n/2$ -dimensional complex vector function, depending on $q = (\underset{\sim}{k}, \omega_\ell)$, where $\underset{\sim}{k}$ is the wave vector and $\omega_\ell = 2\pi\ell T$ ($\ell = 0, \pm1, \pm2, \ldots$) is the Matsubara frequency. The Fourier transform $\Phi(x, \tau)$ of $\phi(q)$ is also $(n/2)$ -dimensional complex vector function, depending on the space vector $\underset{\sim}{x}$ and the imaginary time τ [1,4]. Thus formulated, the model is equivalent to the corresponding one with n -component classical real order parameter $\psi(x, \tau)$. We consider a d -dimensional system with a volume $V = L^d$; T stands for the temperature. The unperturbed correlation function (see (1)) is:

$$G_0^{-1}(q) = \{\omega_\ell^2 + c\underset{\sim}{k}^\sigma + r\}, \quad (3)$$

where σ is a number; c, r and the interaction constant u in H are parameters of the theory. The grand canonical partition function, corresponding to H, is $Z = \mathrm{Tr}(\exp(H))$, where the trace symbol denotes integration over the degrees of freedom $\phi_\alpha(q)$. The Feynman diagrams [8] for the Hamiltonian (1)-(2) are standard. The diagrammatic representation of H_I is shown on fig.1. Note that the model (1-2) is used for the investigation of the singlet-singlet model in the theory of itinerant magnetism [5].

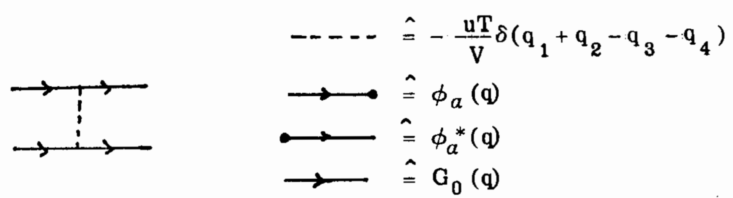

Fig.1

III. RECURSION RELATIONS TO ORDER ϵ^2

The general exact recursion relations up to ϵ^2 are:

$$\omega_\ell'^2 = e^{s(2-\eta)}\{\omega_\ell^2 - 2(n+2)(uT)^2\Delta K\omega\}, \quad (4)$$

$$c' = e^{s(2-\eta-\sigma)}\{c - 2(n+2)(uT)^2\left[\frac{\Delta K_k}{(ke^{-s})^\sigma}\right]\}, \quad (5)$$

$$r' = e^{s(2-\eta)}\{r + (n+2)(uT)I_1(r) - (n+2)^2 I_1(r)I_2(r)(uT)^2 - 2(n+2)K(r,0;0)(uT)^2\}, \quad (6)$$

$$(uT)' = e^{s(4-d-2\eta)}\{(uT) - (n+8)I_2(r)(uT)^2 + (uT)^3[(n^2+6n+20)I_2^2(r) + 2(n+2)(n+8)I_1(r)I_3(r) + 4(5n+22)J(r)]\}, \quad (7)$$

where e^s is the rescaling factor, η is the anomalous dimensionality [2-6] of the field $\phi_\alpha(q)$. The following expressions appear in (4-7):

$$I_m(r) = \sum_{\omega_\ell}\int^1 d\underset{\sim}{k}\, G_0^m(q), \quad (m = 1,2,3), \quad (8)$$

$$J(r) = \sum_{\omega_{\ell_1}\omega_{\ell_2}}\int^1 d\underset{\sim}{k}_1 d\underset{\sim}{k}_2\, G_0(q_1)G_0(q_2), \quad (9)$$

$$K(\underset{\sim}{k}e^{-s}, \omega_\ell, r) = \sum_{\omega_{\ell_1}\omega_{\ell_2}}\int^1 d\underset{\sim}{k}_1 d\underset{\sim}{k}_2\, G_0(q_1)G_0(q_2)G_0(q'+q_1-q_2), \quad [q' \equiv (\underset{\sim}{k}e^{-s}, \omega_\ell)], \quad (10)$$

and

$$\Delta K_\omega = K(r, \underset{\sim}{k}e^{-s}, \omega_\ell) - K(r, ke^{-s}, 0), \quad (11)$$

$$\Delta K_k = K(r, ke^{-s}, 0) - K(r, 0, 0). \quad (12)$$

The last two expressions (with $\int' d\underset{\sim}{k} \equiv \int_{e^{-s}\Lambda}^{\Lambda} d\underset{\sim}{k}$; Λ is the basic cutoff of the model) are constructed from (10) and they will be evaluated to order ϵ^0 (ΔK_ω for $r = 0$ and $d = d_c$ and ΔK_k for $\omega_\ell = 0$, $r = 0$ and $d = d_c$). Everywhere we have already replaced the summation in $\underset{\sim}{k}$ with integration. The diagrams, corresponding to the various analytic contributions, are presented on figs.2-5 (for the rest of the diagrams related to (7), refer to [10]).

The summation in equations (8)-(10) yields the following integrals:

$$I_1(r) = \frac{1}{2T}\int' d\underset{\sim}{k}\,\frac{\coth\left[\frac{a(k)}{2T}\right]}{a(k)}, \quad a(k) = \sqrt{c\underset{\sim}{k}^\sigma + r}, \quad (13)$$

$$I_2(r) = -\frac{d}{dr}I_1(r), \quad I_3(r) = \frac{1}{2}\frac{d^2}{dr^2}I_1(r), \quad (14)$$

$$K(\underset{\sim}{k}e^{-s}, \omega_\ell, r) = \int' d\underset{\sim}{k}_1 d\underset{\sim}{k}_2\, S_K(\underset{\sim}{k}e^{-s}, \omega_\ell, r), \quad (15)$$

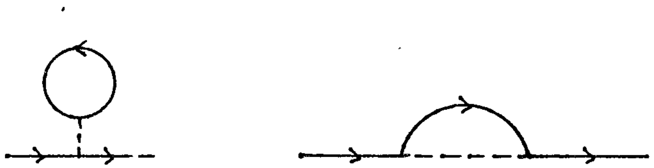

Fig.2

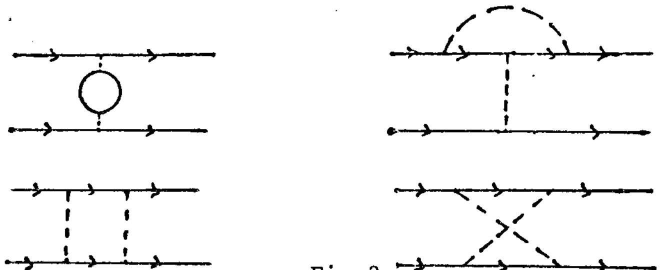

Fig.3

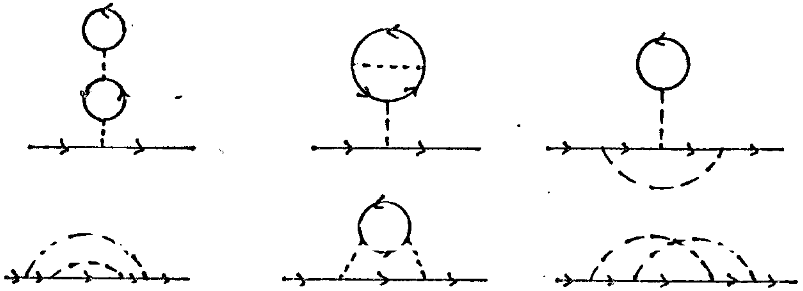

Fig.4

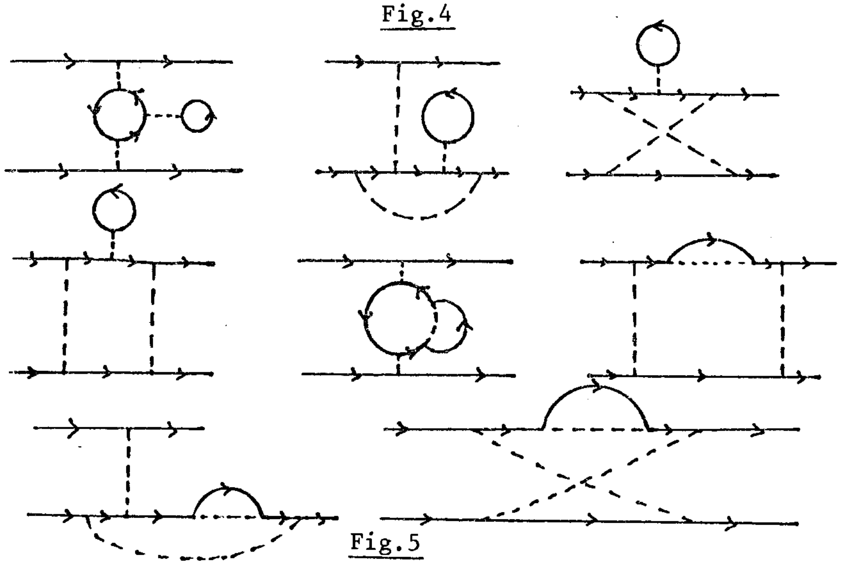

Fig.5

where

$$S_K(\underset{\sim}{k}e^{-s},\ \omega_\ell,\ r) = \frac{1}{16T^2 a_1 a_2 a_3} \times$$

$$\times\{[\coth(\frac{a_3}{2T}) - \coth(\frac{a_2}{2T})][\coth(\frac{a_3-a_2}{2T}) - \coth(\frac{a_1}{2T})]\cdot\frac{a_3-a_2-a_1}{\omega_\ell^2+(a_3-a_2-a_1)^2} +$$

$$\times[\coth(\frac{a_2}{2T}) - \coth(\frac{a_3}{2T})][\coth(\frac{a_1}{2T}) + \coth(\frac{a_3-a_2}{2T})]\cdot\frac{a_3-a_2+a_1}{\omega_\ell^2+(a_3-a_2+a_1)^2} +$$

$$+[\coth(\frac{a_2}{2T}) + \coth(\frac{a_3}{2T})][\coth(\frac{a_1}{2T}) - \coth(\frac{a_2+a_3}{2T})]\cdot\frac{a_3+a_2+a_1}{\omega_\ell^2+(a_3+a_2-a_1)^2} +$$

$$+[\coth(\frac{a_2}{2T}) + \coth(\frac{a_3}{2T})][\coth(\frac{a_2+a_3}{2T}) + \coth(\frac{a_1}{2T})]\cdot\frac{a_1+a_2+a_3}{\omega_\ell^2+(a_1+a_2+a_3)^2}\}, \qquad (16)$$

with

$$a_i = \sqrt{ck_i^\sigma + r},\quad (i = 1,2),\quad a_3 = [(\underset{\sim}{k}e^{-s} + \underset{\sim}{k}_1 - \underset{\sim}{k}_2)^\sigma + r]^{1/2}, \qquad (17)$$

and

$$I(r) = \frac{1}{2}\int d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 \frac{1}{a_1}[\frac{\partial}{\partial a_1} S_K(a_1, a_2, a_3)] \qquad (18)$$

The treatment of the general recursion relations (4)-(7) with the integrals, taken in the form (11)-(12) and (14)-(18), is highly complicated. Note that in these recursion relations both the critical dynamics and the critical statics are incorporated. The dynamics follows from the recursion relation (4) for ω_ℓ. We shall consider separately the two cases of physical interest: (1) $T_c \neq 0$ (classical case) and (2) the quantum limit $T_c \to 0$ (for a structural transition it is called the displacive limit [4]).

IV. FINITE TEMPERATURE CRITICAL BEHAVIOUR

In this case we consider $T_c \neq 0$. This means that (at $T \sim T_c, k \sim 0$) $a(k) \ll T_c$ and consequently $\coth(\frac{a}{T_c}) \approx \frac{T_c}{a}$. Such approximation leads to an immediate coincidence with the recursion relations of ref. [6] to order ϵ^2 with $\sigma = 2$ (see ref. [6] with $4u_0 = (uT)$). The borderline dimension is $d_c = 4 + 0(\epsilon)$. But here we have an additional recursion-recursion relation for the additional parameter ω_ℓ. From this relation one can obtain the dynamic critical exponent z to second order in $\epsilon = 4-d$.

V. ZERO-TEMPERATURE LIMIT

This section contains the main results of the present communication. The limit $T_c \to 0$ is achieved through the approximation $\coth[\frac{a(k)}{T}] \approx 1$ in the general expressions (4)-(18). Then we obtain for the recursion relations:

$$\omega_\ell'^{\,2} = e^{s(2-\eta)} \{ \omega_\ell^2 - (\frac{n+2}{2}) u^2 \Delta K^\circ_\omega \} , \tag{19}$$

$$c' = e^{s(2-\eta-\sigma)} \{ c - \frac{(n+2)}{2} u^2 [\frac{\Delta K^\circ_{\underset{\sim}{k}}}{(\underset{\sim}{k} e^{-s})^\sigma}] \} , \tag{20}$$

$$r' = e^{s(2-\eta)} \{ r + \frac{n+2}{2} u I^\circ_1 (r) - \frac{(n+2)^2}{8} u^2 I^\circ_1 (r) I^\circ_2 (r) - \frac{(n+2)}{2} u^2 K^\circ (r, 0, 0) \} , \tag{21}$$

$$(uT)' = e^{s(4-d-2\eta)} T \{ u - \frac{n+8}{4} u^2 I^\circ_2 (r) + u^3 [\frac{3(n+2)(n+8)}{16} I^\circ_1 (r) I^\circ_3 (r) + \frac{n^2+6n+20}{16} I^{\circ 2}_2 (r) + \frac{(5n+22)}{2} J^\circ (r) , \tag{22}$$

with the integrals:

$$I^\circ_1 (r) = \int' d\underset{\sim}{k}\; a^{-1} (\underset{\sim}{k}) , \tag{23}$$

$$I^\circ_2 (r) = \int' d\underset{\sim}{k}\; a^{-3/2} (\underset{\sim}{k}) , \tag{24}$$

$$K^\circ (r, 0, 0) = \int' d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 \frac{1}{a_1 a_2 a_3 (a_1 + a_2 + a_3)} , \tag{25}$$

$$I^\circ_3 (r) = \int' d\underset{\sim}{k}\; a^{-5/2} (\underset{\sim}{k}) , \tag{26}$$

$$J^\circ (k) = \int' d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 \frac{2a_1 + a_3 + a_2}{(a_1 + a_2 + a_3)^2 a_1^3 a_2 a_3} , \tag{27}$$

$$\Delta K^\circ_\omega = \int d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 \{ \frac{a_1 + a_2 + a_3}{a_1 a_2 a_3 [\omega_\ell^2 + (a_1 + a_2 + a_3)^2]} - \frac{1}{a_1 a_2 a_3 (a_1 + a_2 + a_3)} \} , \tag{28}$$

$$\Delta K_{\underset{\sim}{q}} = \int d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 \{ \frac{1}{a_1 a_2 a_3 (a_1 + a_2 + a_3)} - [\frac{1}{a_1 a_2 a_3 (a_1 + a_2 + a_3)}]_{\underset{\sim}{k}=0} \} . \tag{29}$$

The equation (19) is related [7] to the temperature T. Using (19) and (22), one can see that the borderline dimensionality is $d_c' = 3 + O(\epsilon)$. The evaluation of the integrals to the necessary order in $\epsilon \equiv \epsilon' = 3-d$ yields:

$$I^\circ_1 (r) = \frac{K_d}{2c^{1/2}} \{ \Lambda^2 (1 - e^{-2s})(1 + \frac{\epsilon}{2}) - \epsilon \Lambda^2 \ln\Lambda + \epsilon (\Lambda e^{-s})^2 \ln(\Lambda e^{-s}) - \frac{r}{c} s \} , \tag{30}$$

$$I^\circ_2 (r) = \frac{K_d}{c^{3/2}} \{ s + \frac{\epsilon}{2} s^2 - \epsilon s \ln\Lambda + \frac{3}{4} \frac{r}{c\Lambda^2} (1 - e^{2s}) \} , \tag{31}$$

$$I^\circ_3 (r) = \frac{K_3}{2c^{5/2} \Lambda^2} (e^{2s} - 1) , \tag{32}$$

$$\Delta K^\circ_\omega = - \frac{\omega^2}{c^3} \frac{K_2 K_3}{16\pi} s , \tag{33}$$

$$\Delta K_{\underset{\sim}{q}} = - \frac{q^2 e^{-2s}}{64 \pi^4 c^2} s , \tag{34}$$

$$K^\circ (r, 0, 0) \approx 0 , \tag{35}$$

$$J^\circ (r) = \frac{K_2 K_3}{4\pi c^3} (s^2 + s) , \tag{36}$$

where $K_d = 2^{1-d} \pi^{-d/2} / \Gamma(d/2)$, $\Gamma(x)$ is the gamma function. Note that to order ϵ^1:

$$K_{3-d} = \frac{1}{2\pi^2} \{ 1 + \epsilon \ln[\frac{2\sqrt{\pi}}{e^B}] \} , \tag{37}$$

where:

$$B = \frac{c_E}{2} - \sum_{p=2}^{\infty} \frac{(-1)^p \zeta(p)}{2^p} , \tag{38}$$

$\zeta(x)$ is the Riemann dzeta function, c_E is the Euler constant. Note that $K^\circ(r,0,0) \approx 0$ to order ϵ° in the large limit [6], but $(\frac{\partial}{\partial r} K^\circ)_{r=0}$ is not. The last integral appears in the analysis of the recursion relations. Performing the standard procedure [6], one finds two different f.p. The Gaussian f.p. ($T^* = r^* = u^* = 0$) is stable with respect to u-pertutbations for $d > d_c' = 3$; it is unstable for $d<d'_c$. The critical exponents for $d>d'_c$ are classical (without ϵ-corrections). For $d<d_c$ we have obtained a new f.p.:

$$T^* = 0 \Leftarrow \text{from Eq.(19)}, \tag{39}$$

$$r^* = -\frac{(n+2)\,c\Lambda^2}{(n+8)}\,\epsilon\{1+\epsilon[\frac{1}{2}+\frac{9n+42}{(n+8)^2}]\}, \tag{40}$$

$$u^* = \frac{8\pi^2}{n+8}\,c^{3/2}\,\epsilon\{1+\epsilon[\frac{9n+42}{(n+8)^2}+\ln(\frac{\Lambda e^B}{2\sqrt{\pi}})]\}. \tag{41}$$

One can see that to order ϵ^1, r^* and u^* have exactly the Wilson f.p. values with $\epsilon = 4-d \to \epsilon^1 = 3-d$, but they have essentially different values in order ϵ^2 (see ref.[6]).

The critical exponents, corresponding to the new f.p., are:

$$\eta = \frac{(n+2)}{2(n+8)^2}\,\epsilon^2, \tag{42}$$

$$z = 1 + O(\epsilon), \tag{43}$$

$$\nu = \frac{1}{2} + \frac{n+2}{2(n+8)^2}\,\epsilon + \frac{n+2}{4(n+8)^3}(n^2+22n+52)\,\epsilon^2, \tag{44}$$

$$J_u = -\epsilon + \frac{9n+42}{n+8}\,\epsilon^2. \tag{45}$$

The last exponent (defined by $u' = e^{sJ}\cdot u$) gives corrections to the scaling laws (see ref.[9]). Any critical exponent which might be of some interest could be found using the well-known scaling relations [2,3,9].

VI. FINAL REMARKS

We have presented the general exact recursion relations up to order ϵ^2 for a model describing second order structural phase transitions. This analysis can be used for further discussion on the scaling properties near such transition points.

Our analysis of the finite temperature case leads to universality, namely, for $d>4+O(\epsilon)$ the Gaussian critical behaviour (with classical values of the critical exponents) is stable and for dimensionality $d<4$ the stable f.p. is the one, discovered by Wilson and Fisher [2,9]. The critical exponents, corresponding to this f.p., are well-known functions of the dimensionality $d=4-\epsilon$ and the symmetry index n of the order parameter.

The influence of the quantum correlations in the zero-temperature limit $T_c \to 0$ is inevitable. In this limit the decrease of the borderline dimensionality from d_c to another value d'_c (depending on the structure of the unperturbed correlation function) is a well-known classical-to-quantum crossover phenomenon. So far in the literature it has been generally acknowledged [4,5] that up to first order in $\epsilon' = d'_c - d$ universality preserves its validity; i.e., for $d>d'_c$ one finds again a Gaussian stable behaviour, whereas for $d<d'_c$ a Wilson-type f.p. is the stable one. The values of the f.p. coordinates and the corresponding critical exponents are the same as in the case $T_c \neq 0$, but now with $\epsilon' = d'_c - d$ (and not $\epsilon = 4-d$).). Our results confirm that all this is true up to ϵ'^1.

However we prove that this classical-to-quantum crossover is not the only effect of the quantum correlations when second order (in $\epsilon' = 3-d$) contributions are taken into consideration. For the model under discussion we find nonuniversality (in the above-mentioned sense). It is exhibited in the new values of the stable f.p. (for $d<3$) and of the dynamic exponent. This conclusion is a new point in the understanding of the competition between the interacting classical fluctuations and the quantum correlations. Having in mind the results in ref.[7] one can see that the quantum effects account for a critical behaviour which is more nonuniversal than it was expected. Although the new effect appears in second order in ϵ', it is in our opinion interesting from theoretical point of view. Further steps in the discussed field would be investigations of other models to second order in ϵ'. The direct calculation of the critical exponents for the model, considered here, to higher than the second order is another problem to be solved. Investigations in this direction could be useful for the profound explanation of the classical-to-quantum crossover phenomena in various systems.

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Милев И.Т., Узунов Д.И. E17-82-22

Неуниверсальность критического поведения структурного перехода типа смещения

Рассмотрен обобщенный гамильтониан Гинзбурга-Ландау-Вильсона для описания структурной неустойчивости методом ренормгруппы. Получены рекуррентные соотношения до второго порядка по $\epsilon = d_c - d$ в случае $T_c \neq 0$ ($d_c = 4$) и $T_c = 0$ ($d'_c = 3$). Для $T_c \neq 0$ имеет место универсальное критическое поведение При $T_c \to 0$: 1/ в первом порядке по $\epsilon = 3 - d$ универсальность сохраняется, 2/ во втором порядке по $\epsilon = 3 - d$ обнаружена неуниверсальность критического поведения.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Millev Y.T., Uzunov D.I. E17-82-22

Nonuniversality for Structural Phase Transitions near the Displacive Limit

A quantum-mechanical treatment of a structural phase transition model Hamiltonian with a quartic anharmonicity is carried out to second order in $\epsilon = d_c - d$ by the Wilson renormalization group approach, where d is the space dimensionality and d_c is the borderline dimensionality. Two distinct cases are investigated: $T_c \neq 0$ and $T_c \to 0$. For $T_c \neq 0$ we obtain coincidence with the universal (in the sense of Wilson) critical exponents. The striking result is that for $T_c \to 0$ nonuniversality appears in second order in $\epsilon = 3 - d$ whereas to order ϵ^1 universality still holds place.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1982