ON THE TYPE OF THE TEMPERATURE PHASE TRANSITION IN O(N) MODELS

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The temperature induced phase transition is investigated in the $O(N)$ models by using graphics processing units (GPU) for Monte Carlo simulations on a lattice. General purpose computing on GPU (GPGPU) technology allows to collect a huge amount of data that gives a possibility to investigate the type of the phase transition for a wide interval of coupling values. It is found that for the small values of λ a weak-first-order phase transition happens. It converts into a second order phase transition with the increase of λ. A comparison with analytic calculations in continuum field theory and lattice simulations obtained by other authors is given.

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1. INTRODUCTION

Scalar field models with orthogonal symmetry $O(N)$ are applied in various fields of physics, like quantum field theory, collective phenomena, quantum dots, high-temperature superconductivity, etc. In three spatial dimensions no analytic solutions exist, so different type approximations are used to estimate their physical relevance [1, 2]. In the literature various calculation schemes — daisy and super-daisy resummations, the optimized perturbation theory [3], the two-particle-irreducible (2PI) formalism [4], $1/N$ expansion [5] and renormalization group flow [2] — have been applied to investigate the thermodynamic behavior of models.

The temperature induced phase transition in the $O(N)$ models with a spontaneous symmetry breaking (SSB) was studied either by analytic methods or in lattice simulations (see Refs. [1, 2, 6] and references therein). It was observed in the daisy, super-daisy and some type beyond resummations [7] that the first order phase transition could occur in the $O(1)$-model. However, the lack of the expansion parameter happens near the phase transition temperature $T \sim T_c$ for various kind resummations. So, it is impossible to draw a reliable conclusion about the transition type even for small values of the coupling constant λ. In Ref. [8] some extended kind of resummations was used for the $O(N)$ model, and the phase transition of the second order was determined independently of the coupling value. The same result was also derived by applying the renormalization group approach [9]. Analogous observations have been obtained in Monte Carlo (MC) simulations on a lattice. On the contrary, in recent paper [10] within the 2PI formalism in the double-bubble approximation the first order phase transition was determined. As a result, nowadays the general believe is that the phase transition is of the second order and the perturbation theory fails in this problem. However, in the $O(N)$-models, the results of perturbation theory calculations coincide with the lattice MC ones in the limit of $N \to \infty$, only [7].

Recently, a new powerful computational platform — General Purpose computing on Graphics Processing Units (GPGPU) technology — has been put in force [11, 12] that gives a possibility to generate extremely large amount of MC data. Therefore the accuracy of calculations can be essentially increased and it becomes possible to shed light upon hidden peculiarities and details of different processes of interest studied by MC simulations. One of such unsolved problems is the kind of the temperature phase transition in the $O(N)$-models for small values of coupling constant λ and the reliability of the perturbation theory results.

In the present paper we investigate the temperature induced phase transition in the $O(N)$-models in a wide interval of the coupling constant λ using the GPGPU technology. We test our approach on $O(1)$-model as a simplest member of $O(N)$-models class. In order to determine the type of the phase transition, we apply a procedure known in the lattice quantum chromodynamics and compare the MC simulations obtained with the hot and cold starts. For small λ, $\lambda \leq \lambda_1 \simeq 10^{-3}$, an order parameter shows a hysteresis behavior near the phase transition temperature. Such kind behavior means the phase transition of the first order. With further increasing of λ the hysteresis behavior becomes less pronounced and disappears at all, reflecting the phase transition of the second order. Thus, the type of the phase transition is dependent

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on the value of coupling λ.

The paper is organized as follows. In Sec. 2 we describe the model and its realization on a lattice. In Sec. 3 a necessary information on the MC simulations is given. Sec. 4 summarizes the results obtained.

2. THE MODEL

In order to construct a self-consistent lattice version of the $O(N)$ ϕ^4-model we start with quantum field theory in the continuous space. The thermodynamical properties of the model are described by the generating functional

$$Z = \int D\varphi \; e^{-S[\varphi]}, \tag{1}$$

where φ is a real N-component scalar field, and the action is

$$S[\varphi] = \int dx \Big(\frac{1}{2} \partial_\mu \varphi_i \partial_\mu \varphi_i - \frac{1}{2} m^2 \varphi^2 + \frac{\lambda}{4} (\varphi^2)^2 \Big), \tag{2}$$

where

$$\varphi^2(x) = \sum_i \varphi_i(x) \varphi_i(x). \tag{3}$$

The standard realization of generating functional in MC simulations on a lattice assumes a space-time discretization and the probing random values of fields in order to construct the Boltzmann ensemble of field configurations. Then any macroscopic observable can be measured by averaging the corresponding microscopic quantity over this ensemble.

A direct lattice implementation of (1) encounters an evident problem: the fields $\varphi_i(x)$ are distributed uniformly in the infinite interval $(-\infty; \infty)$. However, a random number generator suitable in this case does not exist. Usually, one cuts the interval off, since the tails $\varphi \to \pm$ appear to be exponentially suppressed in actual simulations in any Metropolis algorithm. The cut scale is chosen in a way separating the unessential tails from the interval of physically important values of φ. But such kind scale cannot be predetermined being the result of an interplay between all the parameters entering the action. As a result, one has to adjust the cut scale manually for every set of the parameter values.

Since we are going to investigate the phase transition in a wide interval of couplings and temperatures, we prefer to rewrite the initial ϕ^4 model in the continuum space-time in the form allowing a further self-consistent lattice realization without manually adjusted cuts.

First we separate the absolute value from the direction of the vector φ_i:

$$\varphi_i(x) = R(x) n_i(x), \tag{4}$$

where $R(x) \in [0; \infty)$, and the vector $n_i(x)$ runs over the surface of the unit sphere:

$$n^2(x) = \sum_i n_i(x) n_i(x) = 1. \tag{5}$$

In the spherical coordinates:

$$\begin{aligned} n_1 &= \sin\theta_1 ... \sin\theta_{N-1}, \\ n_i &= \sin\theta_1 ... \sin\theta_{N-i}, \cos\theta_{N-i+1}, \\ &\quad (i = 2, ..., N-1) \\ n_N &= \cos\theta_1 \end{aligned} \tag{6}$$

with angles $\theta_{1,...,N-2}(x) \in [0; \pi]$ and $\theta_{N-1}(x) \in [0; 2\pi]$. These measure in the integral in (1) can be written in terms of new variables as

$$\begin{aligned} D\varphi &= \prod_x \prod_{i=1}^{N} d\varphi_i(x) \\ &= \prod_x R^{N-1} dR(x) \prod_{i=1}^{N-1} \sin\theta_i^{N-1-i} d\theta_i(x). \end{aligned} \tag{7}$$

The second step is to introduce one-to-one transformation $R(U)$ to a new field variable $U(x)$ defined in the finite interval $[0; 1)$. In what follows we assume that $U = 0$ corresponds to $R = 0$ ($\varphi = 0$). The measure in the integral in (1) becomes

$$\begin{aligned} D\varphi = \prod_x & R(U)^{N-1} R'(U) dU(x) \\ & \times \prod_{i=1}^{N-1} \sin\theta_i^{N-1-i} d\theta_i(x), \end{aligned} \tag{8}$$

where prime denotes the derivative, $R'(U) = dR/dU$.

Now the generating functional can be expressed in terms of field variables defined in finite intervals:

$$Z = \int \prod_x dU(x) \prod_{i=1}^{N-1} d\theta_i(x) \exp(-\tilde{S}[U, \theta]), \tag{9}$$

with the action

$$\begin{aligned} \tilde{S}[U, \theta] &= S[\varphi(U, \theta)] \\ &- \sum_x \log \left[R(U)^{N-1} R'(U) \prod_{i=1}^{N-1} \sin\theta_i^{N-1-i} \right]. \end{aligned} \tag{10}$$

The first term in the action is just the initial action with φ substituted by new field variables, whereas the second term arises from the measure transformation. For MC simulations we introduce a hypercubic lattice with hypertorous geometry. We use an anisotropic lattice with a spatial and a temporal lattice spacing a_s and $a_t = a_s/\zeta$ with $\zeta > 1$, respectively. The scalar field is defined in the lattice sites.

In the case of pure condensate field in some fixed direction in φ-space the action is determined by the potential

$$\begin{aligned} \tilde{V}[U] = & \frac{a_s^4}{\zeta} \left(-\frac{m^2}{2} R(U)^2 + \frac{\lambda}{4} R(U)^4 \right) \\ & - \log \left[R(U)^{N-1} R'(U) \right]. \end{aligned} \tag{11}$$

In order to get finite value of the potential at zero field ($U = 0$), we assume

$$R \sim U^{1/N}, \quad U \to 0. \tag{12}$$

Then, the potential has one local maximum at $U = 0$ and one global minimum at U_0. The spread between the values of the potential at the local maximum and the global minimum is

$$\Delta_V = \tilde{V}[0] - \tilde{V}[U_0]. \tag{13}$$

The quantities U_0 and Δ_V play a crucial role in MC simulations. Being equivalent in theory, different choices of these parameters can produce drastically different results in actual simulations. The reason is the finite number of simulations in an actual computer experiment. If rare but important events could be missed, then the MC algorithm will not converge to the Boltzmann ensemble of configurations. In case of $\sim 10^3$ iterations all the important probabilities have to be greater than 10^3.

Considering the phase transition, one must guarantee that the MC algorithm meets the field values compatible with both the phases to choose. If $U_0 \to 0$, then the broken phase can be missed since the corresponding field values are extremely rare events. On the other hand, $U_0 \to 1$ washes the unbroken phase out. It is also important to ensure finite probability of transition between those field values. The acceptance of non-zero condensate values of the field is ruled approximately by $\exp(\Delta_V)$ at each lattice site. If $\Delta_V \gg 1$, then the unbroken phase never occurs in actual simulations. If $\Delta_V \to 0$, then there is no broken phase. To study the phase transition in the model, we choose the following conditions:

$$U_0 = 0.25, \quad \Delta_V = 1. \tag{14}$$

Thus, the valuable part of generated field values realizes the global minimum of the 'effective' potential, and no phase will be accidentally missed. The probability to prefer condensate or non-condensate values will be of order $\sim 10^{-1}$ ensuring the fast convergence of MC algorithm. Of course, the choice (14) is not optimal for temperatures far away from the critical temperature.

To satisfy two conditions (14) we use a convenient two-parameter function

$$R[U] = m\xi K[U], \tag{15}$$
$$K[U] = \Big[N\Big(-\log(1-U) + \frac{\eta}{2}\log^2(1-U)\Big)\Big]^{1/N}$$

with $\xi > 0$ and $\eta > 0$. $R[U]$ ensures the limit (12).

Finally the lattice action $\tilde{S}[U,\theta]$ is

$$\begin{aligned}\tilde{S}[U,\theta] = {} & \sum_x \sum_\mu \Big[Y\sqrt{\frac{z}{\zeta\lambda}}\left(\mathcal{K}'[U(x)]\right)^2 \times \left(\frac{U(x+a_\mu\hat{\mu}) - U(x)}{a_\mu/a_s}\right)^2\Big] + \sum_x \sum_\mu \frac{2Y}{(a_\mu/a_s)^2}\sqrt{\frac{z}{\zeta\lambda}} \\ & \times \left(1 - \sum_{i=1}^{N} n_i(x+a_\mu\hat{\mu})n_i(x)\right)\mathcal{K}[U(x)]\Big(\mathcal{K}[U(x)] - \mathcal{K}'[U(x)]\Big(U(x+a_\mu\hat{\mu}) - U(x)\Big)\Big) \\ & + \sum_x \Big[-\frac{1}{4}\mathcal{G}[U(x)] - Y\mathcal{K}^2[U(x)] + Y^2 z\mathcal{K}^4[U(x)] + V_0\Big],\end{aligned} \tag{16}$$

where

$$Y = \frac{\mathcal{F}(U_0) - \mathcal{G}(U_0)}{2\mathcal{K}^2[U_0]}, \tag{17}$$
$$V_0 = -\Delta_V - \log(m\xi)^N - \log\pi,$$
$$\mathcal{F}[U] = N - 1 + \frac{\mathcal{K}''[U]\mathcal{K}[U]}{(\mathcal{K}'[U])^2},$$
$$\mathcal{G}[U] = 4[\log\left(\mathcal{K}'[U]\mathcal{K}^{N-1}[U]\right) - \Delta_V];$$

here the values of ξ and η have to be found as the solution of equations $\tilde{V}_0'[U_0] = 0$ and (13).

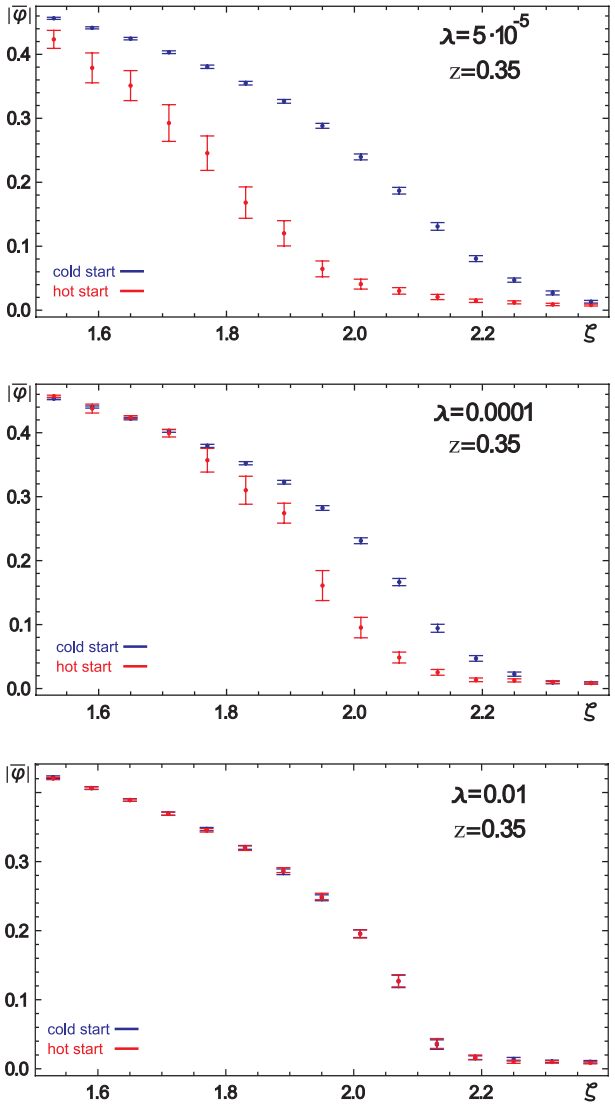
3. MONTE-CARLO SIMULATIONS

In this section we consider the results of MC simulations of $O(1)$ model. To determine the type of the phase transition we use the field condensate as an order parameter. It is non-zero in the broken phase and vanishing in the high-temperature phase. In case of the first-order transition, the overheated and supercooled states are possible. So, the MC simulations with the hot and cold starts have to lead to different phases near the critical temperature. Combining the MC simulations for the hot and cold starts we will see an exfoliation of data like a hysteresis plot. Such type procedure was successfully applied to determine the type of the phase transition in the lattice QCD.

The exfoliation of the simulated data in the vicinity of the critical temperature is a tiny effect. A large amount of simulation data must be prepared to observe it. In this regard, achieving the highest performance of computational hardware is a problem of great importance. To speed up essentially the simulation process we apply a GPU cluster of AMD/ATI Radeon GPUs: HD6970, HD5870, HD5850, HD4870 and HD4850 [13]. The peak performance of the cluster is up to 11 Tflops. The low-level AMD Intermediate Language (AMD IL) is used in order to obtain the maximal performance of the hardware. Some technical details of MC simulations on the ATI GPUs and the review of the AMD Stream SDK are given in Ref. [11] and references therein.

The MC simulations are realized at hypercubic lattices up to 64^4. Most of the obtained statistics come from the lattice 16^4. The lattice data are stored with the single precision. Updating the MC

configurations are also performed with the single precision, whereas all the averaging measurements are carried out with the double precision to avoid the accumulation of errors. The system is thermalized by passing 5000 MC iterations for every run. For measuring we use 1024 MC configurations separated by 10 bulk updates.



Temperature dependence of the absolute value of the averaged field $|\bar{\varphi}|$ *in* $O(1)$ *model for the lattice* 16^4 *at* $z = 0.35$ *for* $\zeta = [1.5; 2.4]$ *and different* $\lambda = 5{\cdot}10^{-5}$ *(top),* 10^{-4} *(center),* 10^{-2} *(bottom)*

We collect the data for the absolute value of the averaged field $|\bar{\varphi}|$ representing the field condensate. The temperature dependence of $|\bar{\varphi}|$ for the lattice 16^4 at $z = 0.35$ for $\zeta = [1.5; 2.5]$ is shown in the figure. The whole data set for every plot is divided into 15 bins. Different initial conditions are marked with different colors: the hot start is depicted in red (lower bins) and the cold start is represented in blue (upper bins). The mean values and the 95% confidence intervals are shown for each bin. Every bin contains 150 simulated points. As it is seen from the figure, for $\lambda = 0.01$ the temperature dependence of the field condensate is insensitive to the start configuration chosen. Both the cold and hot starts lead to the same behavior of the field condensate for various ζ. This means the phase transition to be of the second order, and this result is in agreement with the common opinion on the type of the phase transition stated in Refs. [1, 2, 8, 9]. However, therein this value of the coupling is considered as a small one.

Then, for smaller values of λ the overheated configurations occur in the broken phase for the hot start, and the supercooled states can be found for the cold start. That is, the exfoliation of the simulated data in the vicinity of the critical temperature is observed for different start configurations. Such a hysteresis behavior corresponds to the phase transition of the first order. With further decreasing of λ to the values of order $\lambda_0 \sim 10^{-5}$ the behavior of hot- and cold-started simulations becomes completely separated and independent of the temperature. Such type property means that the SSB does not happen even at zero temperature.

4. CONCLUSIONS

As it was discovered in the MC simulations, the temperature phase transition in the $O(1)$ ϕ^4 model is strongly dependent on a coupling value λ. There is the low bound $\lambda_0 \sim 10^{-5}$ determining the range where the SSB is not realized. Close to this value in the interval $10^{-5} \leq \lambda \leq 10^{-3}$ the phase transition is of the first order. For larger values of λ a second order phase transition happens. These types of the behavior have been determined on the lattices of different sizes. Our calculation procedure was developed to accelerate the MC procedure in the domain of parameters close to the phase transition for a wide range of coupling. For usually considered values of $\lambda \sim 0.01 ... 0.1$ it gives the results coinciding with the existing literature and signaling the second order phase transition.

Our observations, in particular, may serve as a guide for applicability of different kind resummations in perturbation theory. In fact, we see that the daisy and super daisy resummations give qualitatively correct results for small values of λ. For larger values they become non-adequate to the second-order nature of the phase transition. In this case other more complicated resummation schemes should be used.

The change of the phase transition type following due to the change of the coupling value is not a new phenomenon. For example, in the standard model of elementary particles it is well known that the electroweak phase transition is of the first order for small λ and it converts into the cross-over or the second order one for sufficiently large values of λ. Our investigation has shown that this takes also place even in the simple model with one coupling.

The research of order of the temperature phase transition depending on λ values for $O(N)$-models with $N > 1$ is in progress.

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О ТИПЕ ТЕМПЕРАТУРНОГО ФАЗОВОГО ПЕРЕХОДА В O(N)-МОДЕЛЯХ

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Исследован температурный фазовый переход в $O(N)$-моделях с помощью использования графических видеокарт (GPU) для Монте-Карло симуляций на решетке. Технология расчетов общего назначения на видеокартах (GPGPU) сделала возможным собрать огромное количество данных, позволивших исследовать тип фазового перехода в широком интервале значений константы связи. Найдено, что для малых значений величин λ наблюдается фазовый переход первого рода. С ростом константы связи λ фазовый переход становится фазовым переходом второго рода. Представлено сравнение результатов с результатами, полученными другими авторами с помощью аналитических вычислений в континуальной теории и решеточных симуляций.

ПРО ТИП ТЕМПЕРАТУРНОГО ФАЗОВОГО ПЕРЕХОДУ В O(N)-МОДЕЛЯХ

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Досліджено температурний фазовий перехід в $O(N)$-моделях за допомогою використання графічних відеокарт (GPU) у Монте-Карло симуляціях на решітці. Технологія розрахунків загального призначення на відеокартах (GPGPU) зробила можливим зібрати величезну кількість даних, які дозволили дослідити тип фазового переходу в широкому інтервалі значень константи зв'язку. Знайдено, що для малих значень величин λ спостерігається фазовий перехід першого роду. З ростом константи зв'язку λ фазовий перехід стає фазовим переходом другого роду. Представлено порівняння результатів з результатами, отриманими іншими авторами за допомогою аналітичних обчислень у континуальній теорії та симуляцій на решітках.