

Type of the ground magnetic state of the studied system was established from the calculation of the total energy of the magnetic configuration: it's the G-type antiferromagnetic state (G-AFM). Taking its total energy as zero, the energy for other magnetic configurations per formula unit is: 0.09 eV for C-AFM; 0.18 eV for A-AFM; 0.23 eV for FM. Thus, antiferromagnetic configurations lie under the ferromagnetic state and are separated by approximately the same energy value 90 meV. Considering that different directions of unit cell deformation correspond to different magnetic configurations, the use of the multiferroic YFeO_3 is promising in the composition of straintronic structures.

Acknowledgment

The authors thank the Belarusian Republican Foundation for Fundamental Research and the Ministry of education of the Republic of Belarus for partial financial support of the research by the grant M20MV-022.

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Geometrodynamics of the first-order phase transition in the generalized cosmological models and interface layers

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Abstract

The geometrodynamical model of the first-order phase transition in the generalized cosmological models and interface layers has been studied. The Euler-Lagrange equation system for the phase transition in the configuration space has been solved numerically. It has been shown that the production of the “true vacuum” phase nuclei with sizes much more than a critical one occurs at supersaturation of the system under the condition of rapid compression/expansion and is accompanied by appearing of the additional local minimum in the potential. It has been found that the “true vacuum” state and the metastable state is characterized by the Jacobi stability.

Keywords: first-order phase transition, cosmological model, geometrodynamics, pseudo-Finsler configuration space, Jacobi stability

Introduction

According to the representation of the actual cosmology, the phase transition occurred within the time range of the electroweak symmetry breaking $t \sim 10^{-11}$ s [1], as consequence of the spontaneous break in the symmetry of this scalar field. The theory of cosmological phase transition allows the existence of a large number of instanton configurations for the scalar field with a non-deep potential, in such a way that the energy density of the vacuum in domains does not exceed the general universe energy. The metric of cosmological transitions of first order should describe the

evolving domain of the true vacuum which is surrounded by domains of false vacuum. To describe the universe which is filled with barotropic fluid (dark energy or some scalar field) in Weil canonic coordinates and for negative cosmological constant Λ , can be used statistical solutions for the axially symmetric metric, which describes the dark hole in the vacuum [2]. The axially-symmetric metrics of Newman-Unti-Tamburino type are promising, as well, for describing cosmological phase transitions.

Thermodynamical models of cosmological phase transition of the first order is characterized by the stepwise change of the zero average value of the scalar field $\langle\phi\rangle$, which plays a role of the order parameter. The phase transition of the first order with a metastable state occurs in the models with strongly pronounced local minimum of the scalar potential at the zero temperature. The description of such transitions can be performed in the framework of the nucleation theory [3-5] but it should takes into account a nonlinear dependence of a nucleation rate on the level of supersaturation of the system. Kinetic nucleation models allow to describe the relaxation processes that are missing in the Van-der-Waals-Maxwell type models of the phase transitions. In such a way, the development of the geometric-thermodynamic approaches in cosmology needs to elaborate realistic models of the phase transitions of first order.

The modeling of the phase transition of first order by using Finsler geometry was earlier developed for 2-dimensional interphase systems without borders [6–10], such as Langmuir monolayers, and the proposed approach allows to consider the distribution of relaxation times and the interaction between the phase domains in a metastable dynamical system.

The model

We will consider the cosmological first-order phase transition as an evolution of the system from «false vacuum» state to the «true vacuum» state during nucleation process and following nuclei growth. The nucleation rate is considered to be a function of the time. The statistical distribution function of such system should accounts the times of the nuclei production t_i and relaxation times (life-times) τ_i of the nuclei:

$$p(\vec{r}_1, \vec{r}_1, t_1, \tau_1; \vec{r}_2, \vec{r}_2, t_2, \tau_2; \dots; \vec{r}_N, \vec{r}_N, t_N, \tau_N). \quad (1)$$

Let introduce an evolution parameter s in such a way that the following relationship fulfilled: $\tau_i = \Delta t_i / \Delta s$. In the macroscopic system, when the number of producing nuclei N is large enough ($N \rightarrow \infty$), one can pass to a limit:

$$\xi \equiv \tau_i = \frac{dt}{ds}. \quad (2)$$

Then the distribution function (1) can be rewritten in the form: $p(r(s), r(s), t(s), \xi(s))$. This means that in the continuum limit a point in phase space $\{r, r, t, \xi, s\}$ determines a configuration space \mathcal{M}_C of a contact statistical manifold. Here r is 2D radius-vector, $t \equiv \xi$ is a time coordinate, the derivatives over the evolution parameter s are denoted by the dots.

The dynamics of the system in the configuration space \mathcal{M}_C is determined by the axially-symmetric pseudo-Finsler metric [6-10]:

$$L = -dl_F^2 = -\left(A \frac{\xi^2}{r} + B\xi - \frac{C}{2} \frac{(r^2 + r^2 \phi^2)}{\xi} \right)^2, \quad (3)$$

and on the mass surface $\xi = 1$ by the metric function F [6-10]:

$$F^2 = A \frac{\xi^3}{r} + B \xi^2 - C \frac{(r^2 + r^2 \varphi^2)}{2}, \quad (4)$$

where $A(t, r)$ and $B(t, r)$ are functions defined by an effective potential U :

$$U(r, r, t; V) = -k \left[P_1 e^{\frac{2Vt}{r}} - \frac{2}{3} (Vt)^5 \left(6 - \frac{Vt}{r} \right) Ei \left[\frac{2Vt}{r} \right] - \frac{V}{r} \left(P_2 e^{\frac{2Vt}{r}} - \frac{4}{3} (Vt)^5 Ei \left[\frac{2Vt}{r} \right] \right) \right], \quad (5)$$

where

$$P_1 = -\frac{3}{4} r^5 + (Vt)r^4 + \frac{3}{4} (Vt)^2 r^3 + \frac{5}{6} (Vt)^3 r^2 + \frac{11}{6} (Vt)^4 r - \frac{1}{3} (Vt)^5,$$

$$P_2 = r^5 + \frac{1}{2} (Vt)r^4 + \frac{1}{3} (Vt)^2 r^3 + \frac{1}{3} (Vt)^3 r^2 + \frac{2}{3} (Vt)^4 r,$$

The metric parameters A and B have the following explicit form:

$$A = \tilde{p} V \left(P_2 e^{\frac{2Vt}{r}} - \frac{4}{3} (Vt)^5 Ei \left[\frac{2Vt}{r} \right] \right), \quad B = \lambda^2 - \tilde{p} \left(P_1 e^{\frac{2Vt}{r}} - \frac{2}{3} (Vt)^5 \left(6 - \frac{Vt}{r} \right) Ei \left[\frac{2Vt}{r} \right] \right), \quad (6)$$

Here k, p, λ are the phenomenological constants, V is a compression/expansion rate.

Results and discussion

Let us introduce the following denotes: $(x^j) = (t(s_w), r(s_w), \varphi(s_w))$ и $(y^j) = (\xi = \frac{dt}{ds_w}, r(s_w), \varphi(s_w)), j=1,2,3$. The dynamic is given by the Euler-Lagrange equations:

$$\frac{dy^i}{dt} + 2G^i = 0, \quad (7)$$

where

$$G^i = \frac{1}{4} g^{il} \left(\frac{\partial^2 L}{\partial x^k \partial y^l} y^k - \frac{\partial L}{\partial x^l} + \frac{\partial^2 L}{\partial y^l \partial r} \right), \quad g_{ij} = \frac{1}{2} \frac{\partial^2 L}{\partial y^i \partial y^j}.$$

The equations (7) has been solved numerically. The obtained result are shown in Figures 1 and 2.

As one can see in Figure 1b,d, at small compression/expansion rates V the nucleation rate is approximately constant and the sizes of the producing nuclei are close to critical one $\xi = 1$. At large values of V the system is destabilized with the energy and rate being enough to surmount the energy barrier and transfer the system in the supersaturated state. This process is revealed as appearing of the well-defined plateau in the isotherm (see Figure 1a, c) and as the producing of nuclei with the sized much more than critical one ($\xi > 40$ in configuration space with metric (3) (Figure 1b) and $\xi = 7$ for the phase transition on the mass surface (4)).

The potential U is defined the free energy of the nuclei. The dependence of U on the evolution parameter s has been calculated along the geodesics and is shown in Figure 2. At small values of V the potential is a single-well potential. The local minimum in the potential corresponds to the “false vacuum” state. The increase of the parameter V leads to appearing the additional local minimum (see Figure 2b, d) in the potential that is typical for a metastable state.

The Jacobi stability of the dynamical system solutions has been studied utilizing the Kosambi-Cartan-Chern (KCC) geometrical approach. We numerically calculated the eigenvalues of the second KCC-invariant

$$P_j^i = 2 \frac{\partial G^i}{\partial x^j} + 2G^s \frac{\partial N_j^i}{\partial y^s} - \frac{\partial N_j^i}{\partial x^s} y^s - N_s^i N_j^s - \frac{\partial N_j^i}{\partial t}, \quad N_j^i = \frac{\partial G^i}{\partial y^j} \quad (8)$$

that is called a curvature deviation tensor and defines the Jacobi field along the geodesic. The system is called the Jacobi stable one if the real parts of the eigenvalues of P_j^i are strongly negative, and the trajectories of the dynamical system converge in the vicinity of a critical point.

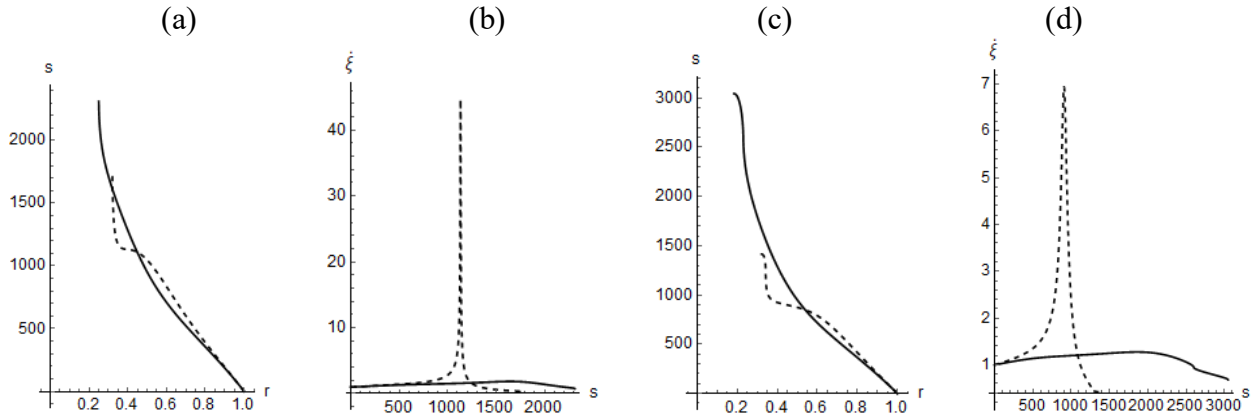


Figure 1. Isotherms $s(r)$ (a, c) and relaxation times distributions $\xi(s)$ (b, d) calculated along the geodesics in the configuration space with axially symmetric metric (3) (a,b) and on the mass surface with metric (4) (c,d). The parameters utilized are $V = 2 \cdot 10^{-4}$ (solid curves), $V = 2,6 \cdot 10^{-4}$ and $4 \cdot 10^{-4}$ (dashed curves)

As one can see in Figure 2, at the negative values of parameter s (for the “false vacuum” state) the eigenvalues Λ_1, Λ_2 have different signs in all studied cases. Λ_1, Λ_2 are smooth regular functions at small values of V . However at increase of rates V the singular behavior of Λ_1, Λ_2 is observed during the phase transition into the “true vacuum” state. The “true vacuum” state (the potential minimum at large values of s) is characterized with Jacobi stability as $\Lambda_1 < 0$ and $\Lambda_2 < 0$. The producing of the large nuclei (nuclei size is much more than critical one, $\xi \gg 1$) at high values of V is accompanied by the Jacobi unstable area ($\Lambda_1, \Lambda_2 > 0$) at $s \approx (900; 1000)$. In the model on the mass surface with metric (4) the metastable state is stable in the Jacobi sense.

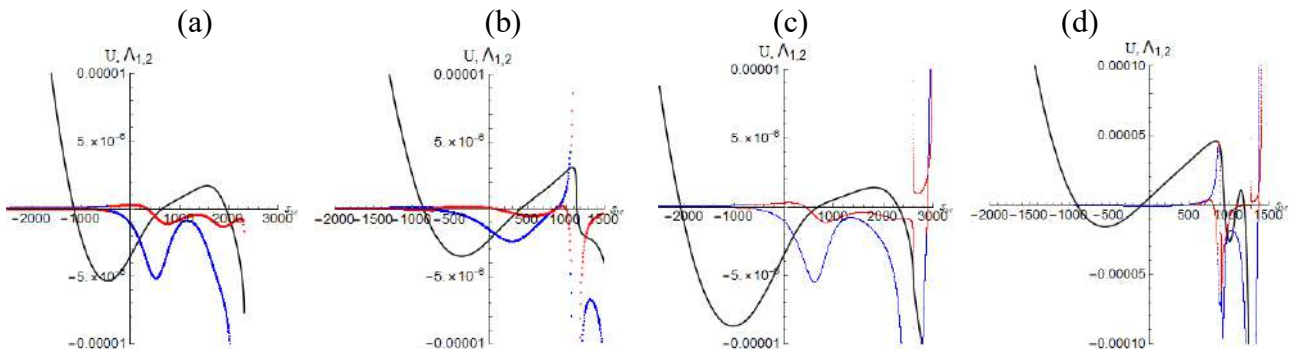


Figure 2. Effective potential U (black curves) and eigenvalues of the second KCC-invariant $\Lambda_{1,2}$ (blue and red points) calculated along the geodesics in the configuration space with axially symmetric metric (3) (a,b) and on the mass surface with metric (4) (c,d). The parameters utilized are $V = 2 \cdot 10^{-4}$ (a, c), $V = 2,6 \cdot 10^{-4}$ (b) and $4 \cdot 10^{-4}$ (d)

Conclusion

The studied geometrodynamical model of the first-order phase transition in the generalized cosmological models and interface layers in the configuration space demonstrates the nonlinear dependence of a nucleation rate on the level of supersaturation of the system that leads to production of the phase nuclei with sizes much more critical at high compression/expansion rate due to appearing the additional local minimum in the potential being typical to the metastable state.

Acknowledgment

The present work was developed under the auspices of the Project BRFFR No. F20RA-007, within the cooperation framework between Romanian Academy and Belarusian Republican Foundation for Fundamental Research.

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Jump diffusion of the lattice fluid on the two-level lattice

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Abstract

The diffusion properties of a lattice fluid with the interaction of nearest neighbors on the two-level non-rectangular lattice are considered. An analytical expression for estimating the jump diffusion coefficient is investigated. The results of the analytical calculations are compared with the MC simulation data. It is shown that the proposed analytical expression makes it possible to adequately assess the transport characteristics of the model from the qualitative point of view. The features of the behavior of the jump diffusion coefficient of the lattice fluid with the repulsive interaction of the nearest neighbors on two-level lattice are considered.

Keywords: lattice fluid, two-level lattice, jump diffusion coefficient, diagram approximation, Monte Carlo simulation.

Introduction

Mass transfer, and the associated charge transfer, through diffusion plays an important role in many physical, chemical and biological processes [1]. The lattice gas or lattice fluid model is one of the simplest models suitable for describing this process.

Within the framework of this model, particles can occupy the set of positions in space which forms the regular two- or three-dimensional lattice. These positions are called lattice sites. The