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PARAMETRIC REPRESENTATION AND BIFURCATION ANALYSIS OF THE CUBIC EQUATION SOLUTIONS WITH APPLICATION TO THE PHASE TRANSITIONS

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Real solutions representation for the cubic equation with real coefficients in a parametric form is given. The dependence of the solutions on the equation coefficients and the bifurcation conditions for these solutions are studied. In the parametric space regions with one and three real solutions are considered. Using parametric representations of the cubic equation solutions, the stability and bifurcation conditions of the equilibrium states for the thermodynamic systems described by the Landau-type kinetic potential are analyzed.

Keywords: *phase transitions, metastable state, bifurcation analysis.*

REPREZENTAREA PARAMETRICĂ ȘI ANALIZA BIFURCAȚIONALĂ A SOLUȚIILOR ECUAȚIEI CUBICE CU APLICARE LA TRANZIȚIILE DE FAZĂ

Este expusă reprezentarea soluțiilor reale pentru ecuația cubică cu coeficienți reali într-o formă parametrică. Sunt studiate dependența soluțiilor de coeficienții ecuației și condițiile de bifurcație pentru aceste soluții. În spațiul parametric sunt considerate regiuni cu una și trei soluții reale. Folosind reprezentările parametrice ale soluțiilor ecuației cubice, sunt analizate condițiile de stabilitate și de bifurcație ale stărilor de echilibru pentru sistemele termodinamice descrise de potențialul cinetic de tip Landau.

Cuvinte-cheie: *tranziții de fază, stare metastabilă, analiză bifurcațională.*

Introduction

Analysis of a large number of nonlinear processes from various fields of natural science leads to the study of the dependence of the cubic equation solutions on its coefficients. Despite the existence of the classical representations of the cubic equation solutions in the form of Cardano, their practical application, even with the use of powerful modern computer programs of symbolic calculations, is encountered, as experience shows, by significant difficulties connected with the multivaluedness of solutions and the determination of individual solutions.

In this study, we present the real solutions representation of the cubic equation with real coefficients in parametric form, which is extremely convenient for the solutions analysis, investigating their dependence on the equation coefficients, i.e. parameters of the thermodynamic systems under investigation, and realizing direct calculations with the use of modern computers.

1. Representation of the cubic equation solutions in parametric form. Analysis of solution bifurcations

Detailed solutions analysis of the cubic equations with real coefficients, constructing real solutions of these equations and regions of the parameter values, for which there are one or three real solutions, is presented. Some aspects of this issue were discussed in [1]. Let us consider the cubic equation

$$f(x;p,q,r) \equiv x^3 + px^2 + qx + r = 0, \tag{1}$$

where p, q and r are real parameters. For a fixed set of these parameters, Eq. (1) has one or three real solutions. In the parameter space p, q and r, the region for the parameter values of Eq. (1), for which there is only one real solution is denoted by D_1, and that with three real solutions by D_3. The values of parameters $p = p_*$, $q = q_*$, $r = r_*$ for which the change in the number of real solutions of Eq. (1) takes place, and the solutions $x_* = x(p_*, q_*, r_*)$ corresponding to these values are named bifurcation ones. The bifurcation values of parameters p_*, q_*, r_*, and the corresponding to them solutions $x_* = x(p_*, q_*, r_*)$, in accordance with the implicit function theorem [2], satisfy the relations

$$f(x;p,q,r) \equiv x^3 + px^2 + qx + r = 0, \ \ \partial f(x;p,q,r)/\partial x = 3x^2 + 2px + q = 0. \tag{2}$$

From relations (2) we arrive at an expression for bifurcation values $x = x_*$, that is

$$x_* = \frac{9r - pq}{2(p^2 - 3q)}\,. \tag{3}$$

Let us analyze separately the case when the condition $p^2 - 3q = 0$, so the denominator in Eq. (3) vanishes. Due to the finiteness of the bifurcation value of the parameter x_*, in the case under consideration, along with the condition $p^2 - 3q = 0$, at the same time the condition $9r - pq = 0$ must be met, so we arrive at the relations $q = \frac{p^2}{3}, r = \frac{p^3}{27}, f(x; p, q, r) = \left(x + \frac{p}{3}\right)^3$, and, as a result, the bifurcation value of parameter $x_* = -\frac{p}{3}$. Assuming further that $p^2 \neq 3q$, and substituting the value of $x = x_*$ from Eq. (3) into one of the Eqs. (2), we arrive at the expression in the form $\Phi(p, q, r) = 0$. In the parameter space p, q and r, a surface defined by this equation divides this parameter space into regions in each of which the Eq. (1) has either one (region D_1) or three real solutions (region D_3). For the values of parameters belonging to this surface the cubic equation (1) has three real solutions, two of which are identical. We note that the cubic equation in (2) is satisfied in the regions D_1 and D_3, while the second equation is replaced by an inequality, preserving certain signs in each of the regions. In order to identify the sign of inequality, it is sufficient to establish its value in any one point from each area by choosing such parameter sets, which are most convenient for this analysis. For the convenience of graphical representation of these regions let us introduce in Eq. (1) a new variable $\tilde{x} = x/\sqrt[3]{r}$ and two new parameters $\tilde{p} = p/\sqrt[3]{r}$, $\tilde{q} = q/\sqrt[3]{r^2}$, so that Eqs. (2), (3) and the equation $\Phi(p, q, r) = 0$ can be further represented as

$$\tilde{x}^3 + \tilde{p}\tilde{x}^2 + \tilde{q}\tilde{x} + 1 = 0,\ 3\tilde{x}^2 + 2\tilde{p}\tilde{x} + \tilde{q} = 0,\ \tilde{x}_* = \frac{9 - \tilde{p}\tilde{q}}{2(\tilde{p}^2 - 3\tilde{q})}, \tag{4}$$

$$\tilde{\Phi}(\tilde{p}, \tilde{q}) \equiv 27\left(\frac{2\tilde{p}^3}{27} - \frac{\tilde{p}\tilde{q}}{3} + 1\right)^2 - 4\left(\frac{\tilde{p}^2}{3} - \tilde{q}\right)^3 = 0. \tag{5}$$

In the plane of parameters $\tilde{p}$ and $\tilde{q}$ Eq. (5) describes a set of contours dividing this plane in regions with the values of parameters for which there is only one real solution of the cubic equations (1) or (4) in the region D_1 or three real solutions in the region D_1. The dependencies defined by Eq. (5) are shown in [3].

Let us analyze again the cubic equation in general form (1), and one can show that this equation, which depends on three parameters p, q, and r, can be transformed into its equivalent cubic form (canonical form) which depends on only one parameter

$$v^3 + \gamma v + 1 = 0,\ \gamma = \frac{P}{\sqrt[3]{Q^2}},\ P = -\frac{p^2}{3} + q,\ Q = \frac{2p^3}{27} - \frac{pq}{3} + r. \tag{6}$$

Conditions (2) for bifurcation of solutions and determination of the bifurcation values of parameters can be rewritten for canonical form of the cubic equation as

$$v^3 + \gamma v + 1 = 0,\ 3v^2 + \gamma = 0, \tag{7}$$

whence one can obtain the bifurcation values $v_* = \frac{1}{\sqrt[3]{2}}$ and $\gamma_* = -\frac{3}{\sqrt[3]{4}}$.

First, we note that this cubic equation has only one real solution $v_1 = v(\gamma_1) = -1$ for the value of parameter $\gamma_1 = 0$, and therefore, the equation has one real solution for the range of values $\gamma \in (\gamma_*, \infty)$, and there are three real solutions of the equation for $\gamma \in (-\infty, \gamma_*)$. We note also that the value $v = 0$ does not satisfy the cubic Eq. (7), which implies that the physically acceptable dependences $v(\gamma)$ defined by this equation take values of the same sign and, thus, the graphs for these dependencies are located entirely in one of the half-planes $v > 0$ or $v < 0$. Taking into account the bifurcation value $v_* = 1/\sqrt[3]{2} > 0$ from expressions (7), one can see that there are two real positive solutions in the upper half-plane region of the parameter values $\gamma \in (-\infty, \gamma_*)$ denoted hereafter by $v_2(\gamma)$ and $v_3(\gamma)$, and considering further that the value $v(0) = -1 < 0$ we conclude that there is only one real solution of the cubic Eq. (6) in the lower half-plane, which is denoted by $v_1(\gamma)$ and it is defined for all values of the parameter $\gamma \in (-\infty, \infty)$. Let us further consider the parametric representation of the real solutions of the cubic Eq. (6). For this purpose we solve this cubic equation with respect to the parameter $\gamma = -\frac{1+v^3}{v}$ and denote $v_1 = -\tau$, where $\tau > 0$ for the negative solution $v_1(\gamma) < 0$. As a result, the final parametric representation of $v_1(\gamma)$ can be written as follows:

$$v_1(\tau) = -\tau,\ \gamma(\tau) = \frac{1 - \tau^3}{\tau},\ \tau > 0. \tag{8}$$

We note that $\gamma(\tau)$ is a unique monotonic dependence of the parameter τ, that is, a unique relationship $v_1(\gamma)$ is determined by Eqs. (8), and $v_1(\gamma)$ is a monotonically increasing function of the parameter γ. Parametric relations of positive solutions can be written as

$$v(\tau) = \tau,\ \gamma(\tau) = -\frac{1+\tau^3}{\tau},\ \tau > 0, \tag{9}$$

where $v_1(\tau)$ is replaced here by $v(\tau)$.

In this case the relation for derivative $\gamma(\tau)$ becomes zero at $\tau_* = 1/\sqrt[3]{2}$, which corresponds to the bifurcation values $v_* = \tau_* = 1/\sqrt[3]{2}$ and $\gamma_* = -3/\sqrt[3]{4}$. There are two dependencies determined by relations (9). One of these dependencies, denoted here by $v_2(\gamma)$, has the parametric representation

$$v_2(\tau) = \tau,\ \gamma(\tau) = -\frac{1+\tau^3}{\tau},\ 0 < \tau \le \tau_*. \tag{10}$$

The last expression $v_3(\tau)$ is defined by parametric relations

$$v_3(\tau) = \tau,\ \gamma(\tau) = -\frac{1+\tau^3}{\tau},\ \tau_* \le \tau < \infty. \tag{11}$$

We note that the parametric representations of the real solutions for the cubic equation (6), i.e. Eq. (8) for $v_1(\gamma)$, Eq. (10) for $v_2(\gamma)$, and Eq. (11) for $v_3(\gamma)$ are significantly more convenient in the implementation of practical calculations than the well-known traditional Cardano's representation, and, in such a way, the given parametric representations along with Cardano's formula can be used as analytical expressions for the solutions of the cubic equation with real coefficients.

2. Stability and bifurcation analyses of the steady states for thermodynamic systems

Nowadays, the theory of supercooled liquids and glasses, proteins and molten polymers, and other complex nanomaterials is under intensive developing by means of computer simulations, as well as by parametric macroscopic modeling based on the Landau-type kinetic potential. In the present framework, we examine the generalized parametric model based on Landau-type kinetic potential by bifurcation and stability analysis for the first order phase transition in the presence of an intermediate metastable state. In particular, anomalous generation and extinction phenomenon of crystal nuclei at very low temperatures in non-equilibrium supercooled liquids containing hydroxyl group, namely *o*-benzylphenol, salol, and 2,2'-dihydroxybenzophenone [5-7]. Comprehensive presentation of these issues is done in [3, 8-12]. The main relations, which lead to the study of the cubic equation solutions dependence on the parameters, are given below. Let us consider the kinetic potential $U(x, y;\ \lambda, \mu, \gamma, \eta)$ in the form of a potential of fourth degree involving four control parameters and two order parameters *x* and *y* [3, 4], i.e.

$$U = \eta x + \frac{\lambda}{2}(x^2 + y^2) + \frac{\mu}{3}x^3 - \gamma x y^2 + \frac{1}{4}(x^4 + y^4), \tag{12}$$

which contains two control parameters λ and μ, namely diffusion and viscosity coefficients, coefficient γ is taken to weight the coupling term between *x* and *y*, as well as there is a coupling coefficient η with a constant external field in the linear term on the order parameter. Here λ, μ and γ are control parameters related to the intrinsic transition dynamics.

Following the methods described in [3, 10], the equilibrium states of the system given by Eq. (12) are solutions of the expressions $\frac{dx}{dt} = -\frac{\partial U}{\partial x} = 0$, $\frac{dy}{dt} = -\frac{\partial U}{\partial y} = 0$, so the steady states x_s and y_s satisfy accordingly the following system of equations regarding the parameters *x* and *y*:

$$-\eta - \lambda x - \mu x^2 + \gamma y^2 - x^3 = 0,\ -\lambda y + 2\gamma x y - y^3 = 0, \tag{13}$$

and the bifurcation conditions of the steady states (13) – by relations (see also Ref. [3])

$$(\lambda + 2\mu x + 3x^2)(\lambda - 2\gamma x + 3y^2) - 4\gamma^2 y^2 = 0. \tag{14}$$

Note that the analysis of equilibrium conditions (13) and bifurcations of the equilibrium states (14), taking into account the structure of the second equation in (13), is noticeably simplified when dividing the equilibrium states into two classes: (*x*, *y*=0) and (*x*, *y*≠0). In particular, for states (*x*, *y*=0), conditions (13) and (14) can be written in the form

$$x^3 + \mu x^2 + \lambda x + \eta = 0,\ (\lambda + 2\mu x + 3x^2)(\lambda - 2\gamma x) = 0,$$

and for states $(x, y \neq 0)$, conditions (13) take the form

$$-\eta - \lambda x - \mu x^2 + \gamma y^2 - x^3 = 0,\ y^2 = -\lambda + 2\gamma x. \tag{15}$$

Thus, using the second equation in (15), the order parameter *y* can be excluded from the equilibrium equations (15) and the bifurcation conditions (14), and, as a result, in both cases under consideration the analysis of equilibrium states reduces to the analysis of cubic equation solutions. A detailed analysis of the solutions with the effective use of their parametric representations is given in the Ref. [3].

Conclusions

In conclusion we note that the parametric representations of the real solutions for the cubic equation are essential more convenient in the framework of the present study with application to the phase transitions. One can also mention that the parametric representations of the real solutions for the cubic equation are significantly more convenient in the implementation of practical calculations than the well-known traditional Cardano's representation, and, in such a way, the given parametric representations along with Cardano's formula can be used as analytical expressions for the solutions of the cubic equation with real coefficients [3].

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