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RESEARCH ARTICLE

Structural transitions in systems with a triple-well potential

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Abstract
Objectives. Recently studied phenomena in condensed matter physics have prompted new insights into the dynamic theory of crystals. The results of numerous experimental data demonstrate the impossibility of their explanation within the framework of linear models of the dynamics of many-particle systems, resulting in the necessity to account for nonlinear effects. Analyzing the dynamics of systems in condensed matter physics containing a sufficiently large number of particles shows that modes of motion can undergo changes depending on the potential of interparticle interaction. This is also reflected in the presence of domains with essentially chaotic phase space having a number of degrees of freedom $N \geqslant 1.5$ and a certain set of interparticle interaction parameters. However, it is not only the dynamic model that appears to be strongly nonlinear. A similar nature of motion can be also observed in a static nonlinear many-particle system. The paper aims to study the influence of the external field specified by the interatomic triple-well potential on the equilibrium structure of a chain of interacting atoms.
Methods. Methods of Hamiltonian mechanics are used.
Results. Analytical expressions are obtained and analyzed for determining the phase portrait of the equilibrium structure of a chain of interacting atoms for various values of the parameter characterizing the local potential of the field in which each atom of the chain moves. Phase portraits of the equilibrium structure of the system are constructed in continuous and discrete representations of the equilibrium equations for various values of the parameter characterizing the local potential of the field in which each atom of the chain moves.
Conclusions. It is shown that both periodic and random chaotic arrangements of atoms are implemented depending on the magnitude of the external field.

Keywords: triple-well potential, chain, interaction, atom, phase portrait, chaos, structure

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НАУЧНАЯ СТАТЬЯ

Структурные переходы в системах с трехминимумным потенциалом

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Резюме
Цели. Явления, которые в последнее время изучаются физикой конденсированного состояния, привели к новым взглядам на проблемы динамической теории кристаллов. Результаты многочисленных экспериментальных данных показывают, что их невозможно объяснить, оставаясь в рамках линейных моделей динамики многочастичных систем. Необходимо учитывать существенно нелинейные эффекты. Анализ динамики систем в физике конденсированного состояния, содержащих достаточно большое число частиц, показывает, что они могут, в зависимости от потенциала межчастичного взаимодействия, испытывать смену режимов движения. Это проявляется и в том, что в фазовом пространстве такой системы с числом степеней свободы $N \geqslant 1.5$ при определенном наборе параметров межчастичного взаимодействия имеются области, в которых движение является по существу хаотическим. Однако не только динамическая модель оказывается сильно нелинейной. Подобный характер движения может проявляться и в статической нелинейной многочастичной системе. Цель работы – исследовать влияние внешнего поля, задаваемого межатомным трехъямным потенциалом, на равновесную структуру цепочки взаимодействующих атомов.
Методы. Использованы методы гамильтоновой механики.
Результаты. Получены и проанализированы аналитические выражения, определяющие фазовый портрет равновесной структуры цепочки взаимодействующих атомов при различных значениях параметра потенциала межчастичного взаимодействия, в котором движется каждый атом цепочки. Построены фазовые портреты равновесной структуры системы в континуальном и дискретном представлениях уравнений равновесия при различных значениях параметра, характеризующего межчастичный потенциал, в котором движется каждый атом цепочки.
Выводы. Показано, что в зависимости от величины внешнего поля реализуется как периодическое, так и случайное, хаотическое расположение атомов цепочки.

Ключевые слова: трехъямный потенциал, цепочка, взаимодействие, атом, фазовый портрет, хаос, структура

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INTRODUCTION

Recently studied phenomena in condensed state physics have prompted new approaches to problems in the dynamical theory of crystals [1, 2]. In order to explain numerous experimental data [3, 4], it has become necessary to allow for essentially nonlinear effects. However, it is not only the dynamical model that is strongly nonlinear. For example, it has been revealed [4, 5] that the type of crystal lattice depends on nonlinear properties of the interaction potential between crystal atoms even at absolute temperature $T = 0$ K.

From analyzing the dynamics of systems consisting of a sufficiently large number of particles shows [1–5] that a system can undergo a number of bifurcations occurring in the change of different types of motion depending on the nature and magnitude of interactions between particles. This is also reflected in the existence of regions in the phase space of such system having a number of degrees of freedom $N \geq 1.5$ at a certain set of parameters of the interparticle interaction potential, where motion is essentially chaotic [6–12].

This implies that the character of the system motion in such regions determinized by dynamic equations is such that it can be hardly distinguished from a random process. In addition, the presence of such regions implies that either deterministic or stochastic trajectories of motion can be realized in the system when the parameters of the interparticle interaction potential or initial conditions are changed. Such effects are best understood as a manifestation of the interparticle interaction potential nonlinearity.

The bifurcation phenomenon may also occur in a static system where the potential of interparticle interaction is nonlinear. In this case, such bifurcations imply the presence of structural transitions of different degrees of regularity up to chaotic.

In [3, 5], possible types of one-dimensional structures and transitions between them are studied. Distinguishing one-dimensional systems from their non-dimensional counterparts significantly simplifies the solution to the problem of atomic chain equilibrium due to the arrangement of atoms along one coordinate giving the meaning of "time" to this coordinate. The model of atomic one-dimensional chain in the periodic field and U(4) model are discussed in [13, 14] and [13], respectively. In the present work, the U(6) model is considered.

MATHEMATICAL MODEL

Following [4], we consider a one-dimensional chain of atoms interacting with their nearest neighbors in external field $V(u_n)$ determined by the atom number n in the chain interacting with the lattice atoms surrounding it. The Hamilton function (Hamiltonian) for this chain (system) has the following form (the atomic mass is assumed equal to 1):

$$H = \sum_{n=1}^{N} \left[\frac{1}{2} p_n^2 + \frac{1}{2} \chi a^2 \left(u_n - u_{n-1} - 1 \right)^2 + V\left(u_n\right) \right]. \quad (1)$$

Here u_n is displacement of the nth atom in units of interatomic distance a in the unperturbed chain, since at $V = 0$, the condition of minimum potential energy gives $u_{n+1} - u_n = 1$ for all numbers n; $p_n = a\dot{u}_n$, χ is the force interaction constant of chain atoms; $V(u_n)$ is the external potential field in which the nth atom moves. We define potential field $V(u_n)$ as the following function (the U(6) model):

$$V(u) = \varepsilon_0 u^2 (u^2 - 1)^2, \quad (2)$$

where $|\varepsilon_0|$ is the potential barrier value. The function has three minima and two maxima at $\varepsilon_0 > 0$ (Fig. 1), while two minima and three maxima occur at $\varepsilon_0 < 0$ (Fig. 2).

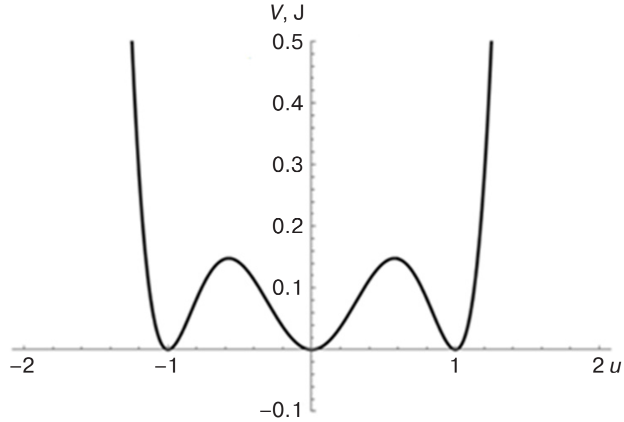

Fig. 1. Potential $V(u)$ at $\varepsilon_0 > 0$

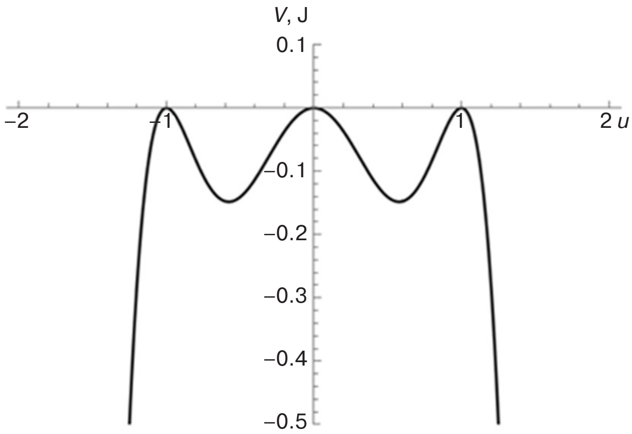

Fig. 2. Potential $V(u)$ at $\varepsilon_0 < 0$

ANALYZING THE MATHEMATICAL MODEL: CONTINUUM APPROXIMATION

1. Special points on a phase plane. The relative value of potential barrier $|\varepsilon_0|$ and energy of interatomic coupling $\approx \chi a^2$ between atoms in neighboring nodes of the chain are essential parameters affecting the properties of the chain having Hamiltonian (1) with external potential (2). If inequality $\chi a^2 \gg |\varepsilon_0|$ is satisfied, the equilibrium position of chain atoms would take the form of a spatial periodic wave. For $\chi a^2 \ll |\varepsilon_0|$, bonds between particles become insignificant so that the chain forms a "gas" of particles that are chaotically scattered over potential wells of the external field.

All possible configurations of the chain are solutions to equation

$$\chi a^2 \left(u_{n+1} - 2u_n + u_{n-1}\right) = \frac{dV}{du_n}. \tag{3}$$

Expression (3) is a difference equation. In the continuum approximation, where displacement values of atoms u_n slightly depend on index n, we have

$$u_{n+1} = u_n + \frac{du}{dx} + \frac{1}{2!} \cdot \frac{d^2u}{dx^2} + \ldots,$$
$$u_{n-1} = u_n - \frac{du}{dx} + \frac{1}{2!} \cdot \frac{d^2u}{dx^2} + \ldots,$$

while the equation describing the equilibrium form of the chain has the following form:

$$\chi a^2 \frac{d^2u}{dx^2} = \frac{dV}{du}. \tag{4}$$

For function $W = -V$, formula (4) is the equation of motion of a nonlinear oscillator provided that variable x is understood as time. This is equivalent to a system of two first-order equations:

$$\begin{cases} \chi a^2 \dfrac{du}{dx} = v, \\ \dfrac{dv}{dx} = \varepsilon_0 \left(6u^5 - 8u^3 + 2u\right). \end{cases}$$

Special points on phase plane (u, du/dx) are defined by conditions ($v = 0$, $dv/dx = 0$), i.e., by the following system of equations:

$$\begin{cases} v = 0, \\ 6u^5 - 8u^3 + 2u = 0. \end{cases}$$

This system defines five special points: $u = 0$, $u = \pm 1/\sqrt{3}$, $u = \pm 1$. At $\varepsilon_0 > 0$, points $u = 0, \pm 1$ are saddle points, while points $u = \pm 1/\sqrt{3}$ are centers. Conversely, points $u = 0, \pm 1$ are centers and points $u = \pm 1/\sqrt{3}$ are saddles at $\varepsilon_0 < 0$.

2. Phase trajectories of motion. Integrating Eq. (4) for once, the equation defining phase trajectories on plane (u, du/dx) is obtained:

$$\sqrt{\frac{\chi a^2}{2}} \cdot \frac{du}{dx} = \pm \sqrt{\varepsilon_0 \left(u^6 - 2u^4 + u^2\right) + E}, \tag{5}$$

where E – integration constant. The trajectories of the system motion (phase portrait) significantly depend on the sign of parameter ε_0. Therefore, we consider two cases.

2.1. Parameter $\varepsilon_0 > 0$. As follows from (5), at $\varepsilon_0 > 0$ in the finite depth potential well, periodic oscillations of atoms (periodic structures) exist only under condition $-4\varepsilon_0/27 \le E \le 0$.

Periodic oscillations and their corresponding periodic (ordered) chain structures are impossible within interval $E > 0$.

For $\varepsilon_0 > 0$, phase trajectories of the system motion on phase plane, based on Eq. (5), have the form shown in Fig. 3. It can be seen from the figure that the system phase portrait contains five main elements: special points of the "center" type at $u = \pm 1/\sqrt{3}$ and three special saddle points $u = 0, \pm 1$. The selected motion trajectory leaving one saddle and entering another is a separatrix. This curve separates the regions of phase plane with substantially different nature of motion: the separatrix separates periodic motions of the chain from aperiodic motions, i.e., ordered structures from disordered ones.

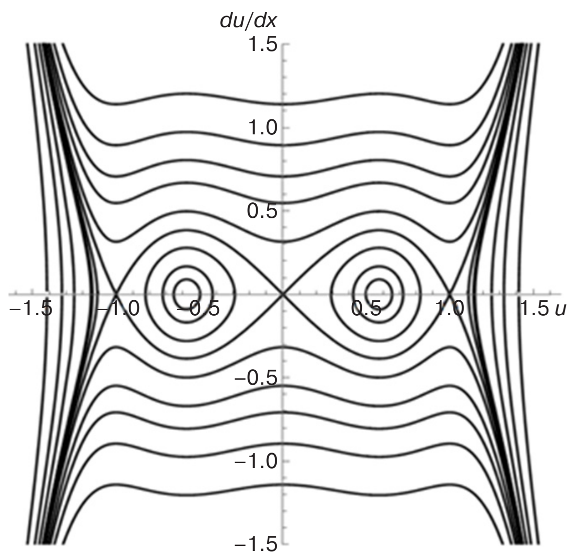

Fig. 3. Phase portrait of the system at $\varepsilon_0 > 0$

2.2. Parameter $\varepsilon_0 < 0$. Phase trajectories of the system motion on phase plane at $\varepsilon_0 < 0$ are shown in Fig. 4. It is evident from the figure that all phase trajectories in this case are closed, thus responding to the oscillatory motion of atoms in the chain and corresponding to the existence of its periodic structures. Here, separatrices have the form of loops beginning and ending in the same saddle to distinguish trajectories that correspond to oscillations of the chain with different nature; small-amplitude oscillations near minima $u = 0, \pm 1$ are separated by the separatrix from large-amplitude oscillations near the origin.

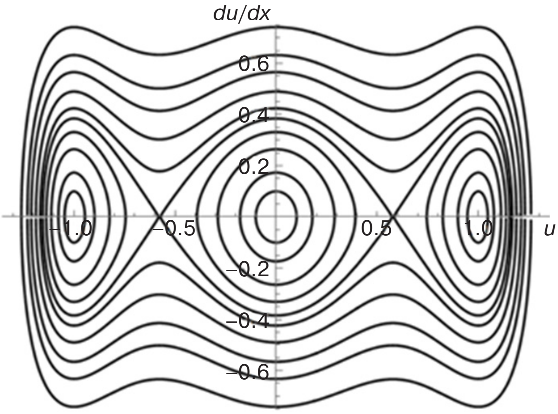

Fig. 4. Phase portrait of the system at $\varepsilon_0 < 0$

3. Analyzing solutions to Eq. (5). Next we consider solutions to Eq. (5) separately depending on the sign of parameter ε_0 in Eq. (2).

3.1. Parameter $\varepsilon_0 > 0$. After integrating Eq. (5) in this case, we denote $E_0 = E/\varepsilon_0$ and obtain the following

$$\int_{u_1}^{u_2} \frac{du}{\sqrt{u^6 - 2u^4 + u^2 + E_0}} = \int_{u_1}^{u_2} \frac{du}{\sqrt{P_6(u, E_0)}} = \pm \int_{x_0}^{x} \sqrt{\frac{2\varepsilon_0}{\chi a^2}} dx. \quad (6)$$

Here, value $P_6(u, E_0) = u^6 - 2u^4 + u^2 + E_0$. Limits of integration u_1, u_2 should satisfy condition $P_6(u, E_0) > 0$. We introduce a new integration variable using relation $u^2 = y$ and then transform expression (6) to the following form:

$$\int_{y_1}^{y_2} \frac{dy}{\sqrt{P_4(y, E_0)}} = \pm 2\sqrt{\frac{2\varepsilon_0}{\chi a^2}}\left(x - x_0\right). \quad (7)$$

Here, $P_4(y, E_0) = y^4 - 2y^3 + y^2 + E_0 y$. The graphs of function $P_4(y, E_0)$ for two different values of E_0 are shown in Fig. 5.

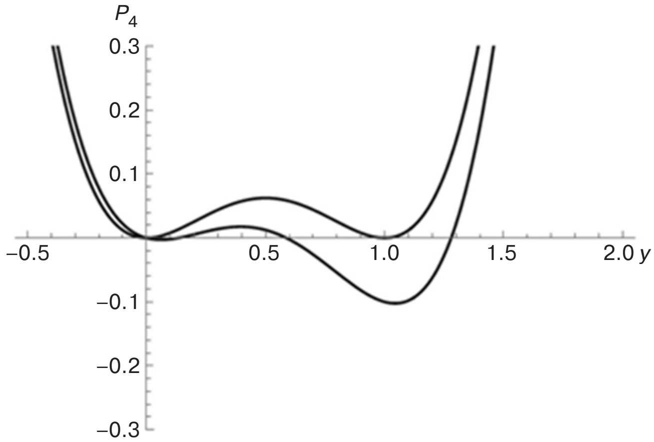

Fig. 5. Graphs of function $P_4(y, E_0)$ at $\varepsilon_0 > 0$

We study all possible cases of representing polynomial $P_4(y, E_0)$ in the form of a product of cofactors. At $E < -4\varepsilon_0/27$, polynomial $P_4(y, E_0)$ has two real and two complex conjugate roots. Given this, Eq. (7) takes the following form:

$$\int_{C_1}^{y} \frac{dy}{\sqrt{y\left(y - C_1\right)\left[\left(y - \alpha\right)^2 + \beta^2\right]}} = \pm 2\sqrt{\frac{2\varepsilon_0}{\chi a^2}}\left(x - x_0\right). \quad (8)$$

Here, C_1 is the real root of polynomial $P_4(y, E_0)$, the second real root $y = 0$, and complex roots $\alpha \pm i\beta$. The integral in the left part of Eq. (8) is expressed through elliptic Jacobi functions [15, 16], as follows:

$$\int_{C_1}^{y} \frac{dy}{\sqrt{y\left(y - C_1\right)\left[\left(y - \alpha\right)^2 + \beta^2\right]}} = \frac{1}{\sqrt{pq}} F\left(2\mathrm{arctg}\sqrt{\frac{q\left(y - C_1\right)}{py}};\ \frac{1}{2}\sqrt{\frac{\left(p + q\right)^2 + C_1^2}{pq}}\right). \quad (9)$$

Here, $p^2 = (C_1 - \alpha)^2 + \beta^2$, $q^2 = (2C_1 - \alpha)^2 + \beta^2$.

Introducing new variable $z = 2\sqrt{\frac{2\varepsilon_0 pq}{\chi a^2}}\left(x - x_0\right)$, the following is obtained from Eqs. (8) and (9):

$$z = \pm F\left(\gamma, k\right). \quad (10)$$

Here, $\gamma = 2\mathrm{arctg}\sqrt{\frac{q\left(y - C_1\right)}{py}}$, $k = \frac{1}{2}\sqrt{\frac{\left(p + q\right)^2 + C_1^2}{pq}}$, while $F(\gamma, k)$ is an elliptic integral of the first kind.

It follows from Eq. (10) that

$$\operatorname{sn}(z,k)=\sin(\gamma)=\sin\left(2\operatorname{arctg}\sqrt{\frac{q(y-C_1)}{py}}\right)= \\ =2\sqrt{\frac{q(y-C_1)}{py}}\left[1+\frac{q(y-C_1)}{py}\right]^{-1}. \quad (11)$$

Then

$$y=\frac{C_1 q\operatorname{sn}^2(z,k)}{q\operatorname{sn}^2(z,k)-p\left(1\pm\operatorname{cn}(z,k)\right)^2}. \quad (12)$$

Here, sn(z, k) and cn(z, k) are elliptic sine and cosine, respectively.

Function y defined by Eq. (12) is an even function with period T = 4K(k)/δ, where K(k) is the complete elliptic integral of the first kind, $\delta = 8|\varepsilon_0|pq/(\chi a^2)$. Hence,

$$u=\pm\frac{\operatorname{sn}(z,k)\sqrt{\alpha q}}{\sqrt{q\operatorname{sn}^2(z,k)-p\left(1\pm\operatorname{cn}(z,k)\right)^2}}. \quad (13)$$

In domain $-4/27\le E_0\le 0$, polynomial $P_4(y,\ E_0)$ has four real roots, $C_1 > C_2 > C_3 > C_4 = 0$. Roots C_1, C_2, C_3, and C_4 should satisfy the following conditions:

$$\begin{cases} C_1+C_2+C_3+C_4=-2, \\ C_1C_2+C_3C_4+(C_1+C_2)(C_3+C_4)=-1, \\ C_1C_2(C_3+C_4)+C_3C_4(C_1+C_2)=E_0, \\ -C_1C_2C_3C_4=0. \end{cases}$$

With allowance for the location of roots C_1, C_2, C_3, and C_4 on the real axis, polynomial $P_4(y, E_0) > 0$ in intervals $y\in(C_3,C_2)$ and

On interval $y\in(C_3,C_2)$, the integral on the left side of Eq. (7) has the following form:

$$\int\limits_{C_3}^{y}\frac{dy}{\sqrt{(C_1-y)(C_2-y)(y-C_3)y}}= \\ =\frac{2F(\gamma,q)}{\sqrt{(C_1-C_3)C_2}}. \quad (14)$$

Here, $\gamma=\arcsin\sqrt{\frac{C_2(y-C_3)}{(C_2-C_3)y}}$, $q=\sqrt{\frac{(C_2-C_3)C_1}{(C_1-C_3)C_2}}$.

We denote

$$z=\sqrt{\frac{2\varepsilon_0(C_1-C_3)C_2}{\chi a^2}}(x-x_0). \quad (15)$$

Then from (14), (15), we obtain that $z=\pm F(\gamma,q)$, so

$$\operatorname{sn}(z,q)=\sin\gamma=\sqrt{\frac{C_2(y-C_3)}{(C_2-C_3)y}}.$$

Hence,

$$u=\pm\left[\frac{C_2C_3}{C_2-(C_2-C_3)\operatorname{sn}^2(z,q)}\right]^{1/2}. \quad (16)$$

As above, function u is an even function with period T = 4K(k)/δ, where

$$\delta=\sqrt{\frac{2\varepsilon_0(C_1-C_3)C_2}{\chi a^2}}.$$

If we assume $C_1 = C_2$ in (16), then parameter q = 1 and solution (16) is a soliton solution having the following form:

$$u=\pm\sqrt{\frac{C_2C_3}{C_2-(C_2-C_3)\operatorname{th}^2 z}}. \quad (17)$$

Within the interval of values $y > C_1$, polynomial $P_4(y,\ E_0) > 0$. Substituting the necessary limits of integration into (8), periodic solutions at $E_0 > 0$ are obtained. Thus, we have the following:

$$\int\limits_{C_1}^{y}\frac{dy}{\sqrt{(y-C_1)(y-C_2)(y-C_3)y}}= \\ =\frac{2}{\sqrt{(C_1-C_3)C_2}}F(\varphi,k)=\pm2\sqrt{\frac{2\varepsilon_0}{\chi a^2}}(x-x_0), \quad (18)$$

where $\varphi=\arcsin\sqrt{\frac{C_2(y-C_1)}{C_1(y-C_2)}}$, $k=\sqrt{\frac{(C_2-C_3)C_1}{(C_1-C_3)C_2}}$.

Let $z=\sqrt{\frac{2\varepsilon_0(C_1-C_3)C_2}{\chi a^2}}(x-x_0)$.

Then $z=\pm F(\varphi,k)$ and hence,

$$\operatorname{sn}(z,k)=\sin\varphi=\sqrt{\frac{C_2(y-C_1)}{C_1(y-C_2)}}. \quad (19)$$

Given that $u=\pm y^{1/2}$, we obtain the following:

$$u=\pm\left[\frac{C_1C_2\left(1-\operatorname{sn}^2(z,k)\right)}{C_2-C_1\operatorname{sn}^2(z,k)}\right]^{1/2}. \quad (20)$$

For $C_1 = C_2$ ($k = 1$) from (20), the solution is bell-shaped:

$$u = \pm\left[\frac{C_1C_2\left(1-\text{th}^2(z)\right)}{C_2 - C_1\,\text{th}^2(z)}\right]^{1/2}.$$

At $z = 0$, u has the form of $u = \pm C_1^{1/2}$, while $u = 0$ at $z \to \pm\infty$.

3.2 Parameter $\varepsilon_0 < 0$. For $\varepsilon_0 < 0$, Eq. (5) has the following form:

$$\sqrt{\frac{\chi a^2}{2|\varepsilon_0|}}\frac{du}{dx} = \pm\sqrt{-u^6 + 2u^4 - u^2 + E_0}, \qquad (21)$$

where $E_0 = E/|\varepsilon_0|$.

Three points of stable equilibrium positions $u = 0, \pm 1$ and two points $u = \pm 1/\sqrt{3}$ corresponding to unstable positions are observed on the oscillator phase plane (u, du/dx).

We integrate Eq. (21):

$$\int_{u_1}^{u_2}\frac{du}{\sqrt{-u^6+2u^4-u^2+E_0}} = \int_{u_1}^{u_2}\frac{du}{\sqrt{P_6(u,E_0)}} = \pm\sqrt{\frac{2|\varepsilon_0|}{\chi a^2}}\int_{x_0}^{x}dx, \qquad (22)$$

where $P_6(u, E_0) = -u^6 + 2u^4 - u^2 + E_0$.

We introduce a new integration variable, $u^2 = y$, $du = dy/2\sqrt{y}$. Then (22) takes the following form:

$$\int_{u_3}^{u_4}\frac{dy}{\sqrt{P_4(y,E_0)}} = \pm 2\sqrt{\frac{2|\varepsilon_0|}{\chi a^2}}\left(x - x_0\right). \qquad (23)$$

Here, $P_4(y,E_0) = -y^4 + 2y^3 - y^2 + E_0 y$. The graphs of function $P_4(y, E_0)$ at two different values of E_0 are shown in Fig. 6.

As before, different cases of decomposing polynomial $P_4(y, E_0)$ into multipliers are also studied here. When polynomial $P_4(y, E_0)$ has two real $y = 0$, $y = C_1$ and two complex conjugate roots $y = \alpha \pm i\beta$, expression (23) is transformed to:

$$\int_0^y\frac{dy}{\sqrt{y\left(C_1-y\right)\left[\left(y-\alpha\right)^2+\beta^2\right]}} = \pm 2\sqrt{\frac{2|\varepsilon_0|}{\chi a^2}}\left(x-x_0\right),\ 0 < y < C_1. \qquad (24)$$

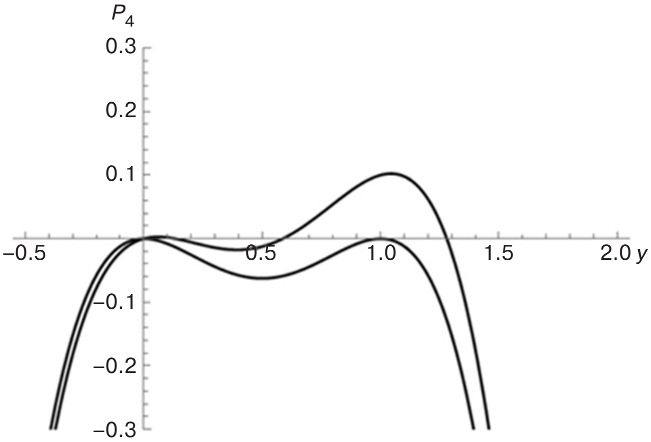

Fig. 6. Graphs of function $P_4(y, E_0)$ at $\varepsilon_0 < 0$

Since the integral in the left part of Eq. (24) is an elliptic Jacobi function, this equation can be represented as follows:

$$z = \pm F(\gamma, k), \qquad (25)$$

where $z = 2\sqrt{\frac{2|\varepsilon_0|}{\chi a^2}pq}\left(x - x_0\right)$, $\gamma = 2\,\text{arcctg}\sqrt{\frac{q\left(C_1 - y\right)}{py}}$,

$k = \frac{1}{2}\sqrt{\frac{-(p-q)^2 + C_1^2}{pq}}$, $q^2 = \alpha^2 + \beta^2$, $p^2 = \left(\alpha - C_1\right)^2 + \beta^2$,

$F(\gamma, k)$ is the Jacobi elliptic function.

It follows from Eq. (25) that

$$\text{sn}(z,k) = \sin\gamma = \sin\left(2\,\text{arcctg}\sqrt{\frac{q\left(C_1-y\right)}{py}}\right) = \frac{\sqrt{qpy\left(C_1-y\right)}}{py + q\left(C_1-y\right)}.$$

Hence, we obtain that $y = u^2$ and

$$y = \frac{qC_1\,\text{sn}^2(z,k)}{p\left(1 \pm \text{cn}(z,k)\right)^2 + q\,\text{sn}^2(z,k)}. \qquad (26)$$

Function y is an even periodic function with period $T = 4K(k)/\delta$. At $x = x_0$, the function becomes zero. Thus,

$$u = \pm\frac{\text{sn}(z,k)\sqrt{qC_1}}{\sqrt{p\left(1\pm\text{cn}(z,k)\right)^2 + q\,\text{sn}^2(z,k)}}. \qquad (27)$$

It follows from (27) that function u can be either even with period $T = 4K(k)/\delta$ or odd with period $T = 8K(k)/\delta$, $\delta = 8|\varepsilon_0|pq/(\chi a^2)$.

We consider the case when all roots C_1, C_2, C_3, and C_4 of polynomial $P_4(y, E_0)$ are real, where

$C_1 > C_2 > C_3 > C_4 = 0$. Then the integral in the left-hand part of (23) is transformed to the form under condition $0 < y < C_3$, as follows:

$$\int_0^y \frac{dy}{\sqrt{(C_1 - y)(C_2 - y)(C_3 - y)y}} = \frac{2}{\sqrt{(C_1 - C_3)C_2}} F(\beta, r) = \pm 2\sqrt{\frac{2|\varepsilon_0|}{\chi a^2}}(x - x_0). \tag{28}$$

Here, $\beta = \arcsin\sqrt{\frac{(C_1 - C_3)y}{(C_1 - y)C_3}}$, $r = \sqrt{\frac{C_3(C_1 - C_2)}{C_2(C_1 - C_3)}}$, $0 < y < C_3$.

It follows from expression (28) that

$$u = \pm\frac{\sqrt{C_1C_3}\,\mathrm{sn}(z, r)}{\sqrt{(C_1 - C_3) + C_3\,\mathrm{sn}^2(z, r)}}. \tag{29}$$

Here, $z = \sqrt{\frac{2|\varepsilon_0|}{\chi a^2}(C_1 - C_3)C_2}\,(x - x_0)$.

Equation (29) has a soliton solution in case of $C_2 = C_3$, with parameter $r = 1$. This solution has the following form:

$$u = \pm\frac{\sqrt{C_1C_3}\,\mathrm{th}\,z}{\sqrt{C_1 - C_3 + C_3\,\mathrm{th}^2 z}}. \tag{30}$$

Note that $u = 0$ at $z = 0$ while $u = \pm\sqrt{C_3}$ at $z \to \pm\infty$.

The polynomial $P_4(y, E_0)$ is also positive within interval $C_2 < y < C_1$.

Substituting the desired limits of integration from (23), we obtain:

$$\int_{C_2}^y \frac{dy}{\sqrt{y(C_1 - y)(y - C_2)(y - C_3)}} = \frac{2}{\sqrt{(C_1 - C_3)C_2}} F(\lambda, r) = \pm\sqrt{\frac{2|\varepsilon_0|}{\chi a^2}}(x - x_0), \tag{31}$$

where $\lambda = \arcsin\sqrt{\frac{(C_1 - C_3)(y - C_2)}{(C_1 - C_2)(y - C_3)}}$, $r = \sqrt{\frac{C_3(C_1 - C_2)}{C_2(C_1 - C_3)}}$.

With allowance for (31), we obtain the following:

$$u = \pm\sqrt{\frac{C_3(C_1 - C_2)\mathrm{sn}^2(z, r) - C_2(C_1 - C_3)}{(C_1 - C_2)\mathrm{sn}^2(z, r) - (C_1 - C_3)}}, \tag{32}$$

where $z = \sqrt{\frac{2|\varepsilon_0|}{\chi a^2}(C_1 - C_3)C_2}\,(x - x_0)$.

Thus, the results obtained in the continuum approximation (under conditions of weak external field) indicate that phase curves are closed and have the form of slightly deformed ellipses in the neighborhood of stable position points regardless of the ε_0 sign. Each curve corresponds to the equilibrium position of the chain in the form of a spatial periodic wave. Separatrices connecting the points of unstable position and limiting the domain of closed curves correspond to the equilibrium in the form of a bell-shaped solitary wave.

ANALYSING THE MATHEMATICAL MODEL: DISCRETE APPROXIMATION

When the external field potential is sufficiently large, function u_n cannot be considered to be weakly dependent on n, so it is necessary to return to difference equations.

Equation (3) can be visualized as a representation given the introduction of variable $I_n = (u_n - u_{n-1})$. Then Eq. (3) transforms into the universal representation [3]:

$$\begin{cases} I_{n+1} = I_n + \dfrac{dV_0}{du_n}, \\ u_{n+1} = u_n + I_{n+1}, \end{cases} \tag{33}$$

where $V_0 = V/(\chi a^2)$.

Representation (33) has periodic and chaotic solutions that determine the corresponding arrangements of atoms in the chain, i.e., its structure. Thus, studying equilibrium forms of the chain is reduced to studying sequences of points $\{u_n, I_n\}$ plotted on a plane. Depending on initial values (u_0, I_0), this sequence either regularly fits into closed lines or appears chaotically scattered in some domain on the coordinate plane.

Numerical solutions to the system of equations (33) with function V in form (2) are shown in Figs. 7 and 8 as phase portraits of the system at different values of parameter $\varepsilon_0' = \varepsilon_0/(\chi a^2)$.

The solution to system (33) in coordinates (u, I) at any initial values (u_0, I_0) is a straight line parallel to the u axis. At sufficiently small ε_0' (Fig. 7), the most of phase space is occupied by the sequence of points fitting into closed curves.

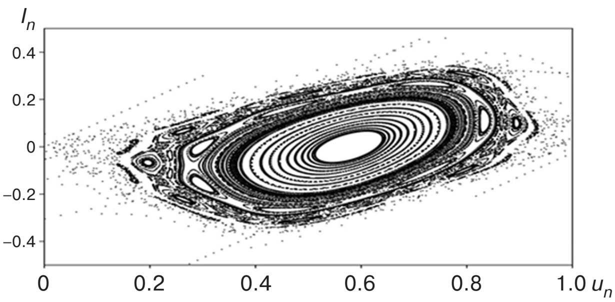

Fig. 7. Phase portrait of the system at $\varepsilon_0' = 0.4$

However, a disorderly distribution of sequential pairs (u_n, I_n) on the plane occurs in a minor part of the phase space, thus demonstrating the chaotic phenomenon for model (33). In the phase space, these pairs occupy narrow stochastic layers separated from each other by invariant curves. Separate domains on the phase plane are not occupied by stochastic trajectory points. Since these domains contain a finite measure of periodic trajectories, the conditions of KAM-theory (Kolmogorov–Arnold–Moser theory) are fulfilled in central parts of the domains [13]. This means that in case of ε_0' smallness, the stochastic layers are not connected to each other. This is the direct consequence of the KAM-theory [13] for the number of degrees of freedom $N \le 2$.

According to [3], the stochastic layer width δh can be estimated for $\varepsilon_0' \ll 1$:

$$\delta h \approx 2(2\pi)^4 e^{-\frac{\pi}{\sqrt{\varepsilon_0'}}}. \quad (34)$$

It follows from (34) that at arbitrarily small perturbations, an exponentially small stochastic layer appears that can be interpreted as a germ of structural chaos in the arrangement of chain atoms.

An increase in values of parameter ε_0' results in the growth of the stochastic layer width, thus leading, in turn, to the destruction of KAM curves and merging of stochastic layers and the subsequent formation of a stochastic sea containing islands of stability.

The system phase portrait at $\varepsilon_0' = 0.7$ is shown in Fig. 8.

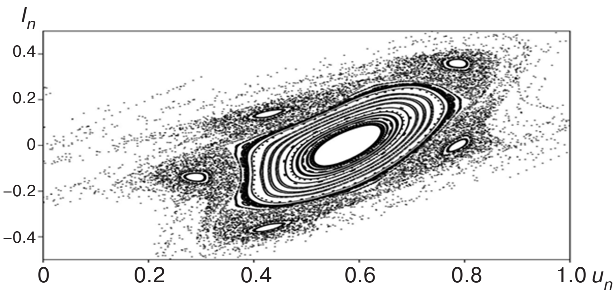

Fig. 8. Phase portrait of the system at $\varepsilon_0' = 0.7$

It is evident from Fig. 8 that the largest object of the phase portrait is the separatrix cell with saddle $u = \pm 1/\sqrt{3}$, which is destroyed to allow a stochastic structural layer to be formed in its place. The domain limited by this main layer contains a family of nested invariant curves that span point $I = 0$. Outside the domain limited by the main stochastic layer, a group of separatrix cells containing narrower stochastic layers is located. Invariant curves are beyond the cells. Thus, the system phase portrait consists of an infinite number of alternating invariant curves and stochastic layers. At $\varepsilon_0' \sim 1$, the merging of stochastic layers and formation of a common stochastic sea is observed indicating a transition to the formation of the chain chaotic structure.

At $|\varepsilon_0'| \gg 1$, almost the entire domain of phase space becomes the domain of stochastic motion. The exceptions are islands of stability, whose size is of $1/|\varepsilon_0'|$ order at $|\varepsilon_0'| \gg 1$. These islands are located in the neighborhood of elliptic points (points of stable equilibrium position) of the representation.

CONCLUSIONS

In the present paper, it is shown that closed phase curves in the continuum approximation under the conditions of a small external field have the form of slightly deformed ellipses in the neighborhood of stable position points regardless of the ε_0 sign. Each curve corresponds to the equilibrium position of the chain having the form of a spatial periodic wave. Separatrices connecting the points of unstable position and limiting the area of closed curves correspond to the chain equilibrium in the form of a bell-shaped solitary wave.

The numerical solutions to the system of equilibrium equations also demonstrate the implementation of that both periodic and random chaotic arrangements of chain atoms depending on the external field strength.

Authors' contribution. All authors equally contributed to the research work.

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