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The structure and collective oscillations of linear systems of particles with van der Waals interaction

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The simulation of a system of particles, located in the plane, with van der Waals interaction described by the Lennard-Jones potential is carried out. The possibility of the existence of a solitary chain of particles, as well as the formation of linear systems of two and three chains, has been established. The spectrum of vibrations of the systems was determined for various configurations and the characteristic frequencies of the vibrations were found. The dispersion law of collective modes is calculated theoretically by the method of equations of motion for small displacements of atoms from their equilibrium position when analyzing the compatibility condition for the arising system of equations. The obtained values of the characteristic frequencies are in rather good agreement with the results obtained in the Fourier analysis of the time dependence of the displacements of particles from their equilibrium positions along and across the system.

Keywords: simulating of low-dimensional systems, dispersion of collective oscillations, systems of particles with van der Waals interaction, Lennard-Jones potential, Fourier analysis of spectra.

1. Introduction

Last years the methods of numerical simulation of behavior and investigation of various properties of low-dimensional systems, especially charged ones, have become increasingly important. The computer simulation of the systems consisting of a small number of atoms gives the possibility to study in detail their properties under various conditions including those that are difficult or impossible to implement in a real physical experiment. The additional interest in the numerical modeling is also due to serious difficulties in using traditional experimental methods arising from the low density of the studied systems and the extremely low level of the corresponding measuring signals, the impossibility of using contact methods for measuring conductivity, etc. For example, in the case of widely studied quasi-two-dimensional and quasi-one-dimensional systems of charges (surface electrons, SEs) over liquid helium [1] by using a numerical experiment it was possible to establish interesting features of the phase transitions of SEs into the crystalline state, the effect of restricted geometry and external confining potential on the configuration of linear SE systems [2–5]. It was shown that the characteristic frequencies of plasma oscillations in such systems are in good agreement with the values that follow from the laws of dispersion of collective modes calculated theoretically in the quasi-crystalline approximation by the method of equations of motion for small displacements of particles from their equilibrium position [6–8]. It was demonstrated that the dispersion law of collective plasma oscillations strongly depends on the type of configuration of the system [3, 9, 10]. This makes experimental studies of the collective properties of SE a promising tool for identifying the types of SE systems that arise when the parameters of the system change.

The collective properties of low-dimensional SE systems are determined by the long-range Coulomb interaction, which intensity decreases with the distance between a pair of particles according to the law $\sim |\mathbf{r}-\mathbf{r}'|^{-1}$, so one should take into account the pair interactions of the entire ensemble of particles. At the same time, the similar studies of systems of particles with short-range interactions are of great interest. Such systems, first of all, should include quasi-one-dimensional structures formed by atoms of inert gases on the surface of bundles of carbon nanotubes [11–14]. The phonon spectra and densities of phonon states in such structures formed by inert gas atoms are studied as well as the contribution of such states to the vibrational heat capacity of linear chains of inert gases, including taking into account the inhomogeneity of the bundle structure (see [15] and literature references therein). The interaction of a pair of particles at a distance $|\mathbf{r}-\mathbf{r}'|$ in the studied systems is due to the van der Waals interaction, which can be described with good accuracy by the Lennard-Jones potential (potential "6–12")

$$U(\mathbf{r}-\mathbf{r}') = 4\varepsilon\left[\left(\frac{\sigma}{|\mathbf{r}-\mathbf{r}'|}\right)^{12} - \left(\frac{\sigma}{|\mathbf{r}-\mathbf{r}'|}\right)^{6}\right], \qquad (1)$$

where ε and σ are empirical interaction parameters depending on the nature of interacting particles. Potential energy (1) decreases very quickly with increasing distance between particles. That is why one can, describing the properties of the system, almost always to account only pair interactions with the nearest neighbors, neglecting the absolutely negligible contribution from particles located at larger distances.

The systems with van der Waals interaction (1) are fundamentally different from Coulomb systems. Since the Coulomb interaction between electrons is exclusively repulsive the formation of a stable two-dimensional structure on the surface of liquid helium requires an external electric field which most essentially affects the structure and properties of electronic systems. The properties of systems with van der Waals interaction can be determined exclusively by inter-atomic interaction itself except that in two-dimensional systems (or quasi-one-dimensional) systems on a plane the presence of a substrate is implied, which, under certain conditions, ensures the existence of these systems. These circumstances provide the relevancy of simulating the particle systems with van der Waals interactions. The aim of the present work is to establish the configurations that arise in systems of particles interacting according to the law (1), as well as to calculate the dispersion law of collective modes. We restrict ourselves to a plane system of particles, which greatly simplifies the calculations. In the future, it is planned to generalize the modeling and calculations to three-dimensional model systems corresponding to the arrangement of quasi-one-dimensional structures on the surface of nanobundles.

2. Simulation procedure

A characteristic parameter of van der Waals systems is the distance corresponding to the minimum of the pair interaction potential. When modeling it is advisable at least the initial distribution of atoms be selected in such a way that the average distance between atoms to be comparable to this characteristic distance. To implement such an arrangement of particles, one should introduce appropriate boundary conditions (periodic, reflections from boundaries, etc.). In this paper for the spatial localization of a system of atoms it is assumed that there is a substrate of monolayer of atoms, the interaction of which with each other is that of van der Waals and is characterized by the parameters ε_s и σ_s of potential "6–12". The number of substrate atoms is proportional to its area. The interaction of the studied system of adatoms with substrate atoms can be described by a potential (1) with parameters $\varepsilon_{as} = \sqrt{\varepsilon\varepsilon_s}$ and $\sigma_{as} = \frac{1}{2}(\sigma + \sigma_s)$. It is assumed that adatoms are at the same equilibrium distance from the substrate $d = 2^{1/6}\sigma_{as}$ corresponding to the minimum of the interaction potential of the adatom with the substrate atoms. This allows us to restrict ourselves to the interaction energy $U \sim 1/|\mathbf{r}-\mathbf{r}'|^6$ corresponding to attraction when considering the interaction of the selected adatom with the substrate atoms.

The substrate acts to the adatom by a force equal to the sum of the forces acting from the side of individual atoms of the substrate to this adatom. We are interested in the projection of this force onto the plane in which the adatoms are located. The magnitude of the force can be estimated in the continuum approximation neglecting the discreteness of the substrate structure which means that, at calculating the force, the summation can be replaced by integration. In this case, for a rectangular substrate with dimensions L and M we obtain the following expression for the components of the force acting on the adatom from the side of the substrate in the plane of the studied system:

$$f_x(x,y) = \frac{24\varepsilon_{as}\sigma_{as}^6 2^{1/3}\sigma_s^2}{ML} \times \int_{-M/2}^{M/2} d\beta \int_{-L/2}^{L/2} d\alpha \frac{(\alpha - x)}{\left[(\alpha-x)^2 + (\beta-y)^2 + d^2\right]^4}, \qquad (2)$$

$$f_y(x,y) = \frac{24\varepsilon_{as}\sigma_{as}^6 2^{1/3}\sigma_s^2}{ML} \times \int_{-L/2}^{L/2} d\alpha \int_{-M/2}^{M/2} d\beta \frac{(\beta - y)}{\left[(\alpha-x)^2 + (\beta-y)^2 + d^2\right]^4}. \qquad (3)$$

Calculating the integrals in (2) and (3) and introducing the function

$$g(l_1,\mu_1,l_2,\mu_2,d) = \frac{24\varepsilon_{as}\sigma_{as}^6 2^{1/3}\sigma_s^2}{ML} \times \left\{ \frac{l_1-\mu_1}{4\left[(l_2-\mu_2)^2+d^2\right]\left[(l_2-\mu_2)^2+(l_1-\mu_1)^2+d^2\right]} + \frac{3(l_1-\mu_2)}{8\left[(l_2-\mu_2)^2+d^2\right]\left[(l_2-\mu_2)^2+(l_1-\mu_1)^2+d^2\right]} + \frac{3}{8\left[(l_2-\mu_2)^2+d^2\right]^{5/2}} \arctan\frac{(l_1-\mu_1)}{\sqrt{(l_2-\mu_2)^2+d^2}} \right\} \qquad (4)$$

one obtains the following components of the force:

$$\begin{aligned} f_x(x,y) &= g(M/2,y,-L/2,x,d) - g(-M/2,y,-L/2,x,d) \\ &\quad - g(M/2,y,L/2,x,d) + g(-M/2,y,L/2,x,d); \\ f_y(x,y) &= g(L/2,x,-M/2,y,d) - g(-L/2,x,-M/2,y,d) \\ &\quad - g(L/2,x,M/2,y,d) + g(-L/2,x,M/2,y,d). \end{aligned} \qquad (5)$$

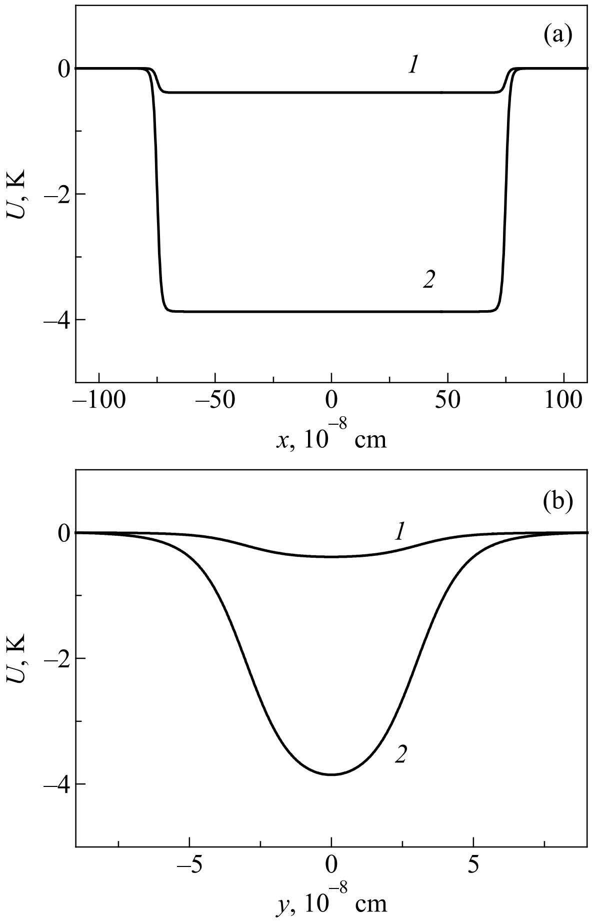

Fig. 1. The potential energy characterizing the localization of helium atoms above the substrate as a function of the distance from the center of the substrate along the axes x (a) and y (b) for two values $\varepsilon_{sa} = 0.1$ K (*1*) and 1 K (*2*).

Choosing the dimensions of the plane region and the parameters of the interaction potential of the substrate with the atoms under study, one can influence the boundary conditions determined by the field of van der Waals forces, which can be easily changed by changing the parameters of the potential. If $\varepsilon_{as} = 0$ the substrate does not affect the studied system.

In this paper, the helium atoms were taken as the system under study. The pair potential of interaction "6–12" between them is characterized by the following parameters: $\varepsilon = 10.22$ K, $\sigma = 2.576\cdot 10^{-8}$ cm. The value of parameter σ_s characterizing the interaction of the substrate atoms is chosen $\sigma_s = 2\cdot 10^{-8}$ cm, in this case, the distance of the two-dimensional system of helium atoms from the substrate is $d = 2^{1/6}(\sigma + \sigma_s)/2 = 2.57\cdot 10^{-8}$ cm.

At the first step of the calculation, the number of helium atoms and the dimensions of the spatial region were taken comparable with the expected dimensions of the modeled configuration. The initial velocities and coordinates of the atoms were chosen randomly within a given spatial region. The condition was imposed on the velocities that the total kinetic energy corresponds to the selected temperature of the system. In the calculations this temperature was in the range $10^{-2} - 10^{-4}$ K. Then the system of linearized equations of motion of atoms in the field of forces acting from all other atoms was solved step by step, taking into account the influence of the substrate. At the initial stage of calculations the energy of interaction of helium atoms with the substrate was chosen to be high ($\varepsilon_{sa} \sim 100$ K), but after the formation of a stable ordered system, it decreased to low values ($\varepsilon_{sa} = 1$ K or $\varepsilon_{sa} = 0.1$ K) at which the determination of the possible vibration frequencies was mainly carried out. In some cases, the vibrations in systems were also studied for $\varepsilon = 0$. It should be noted that the quantities $\varepsilon_{sa} = 1$ K and $\varepsilon_{sa} = 0.1$ K are much less than the corresponding value of the pair interaction potential He–He ($\varepsilon = 10.22$ K) so that the properties of the system under study were almost completely determined by the interaction of helium atoms with each other, and the effect of the substrate could be treated as negligible.

The helium atoms were held in a certain region of two-dimensional space due to their attraction to the substrate. The energy that characterizes this attraction $\left[U_x = \int dx \cdot f_x(x, y=0) \text{ and } U_y = \int dy \cdot f_y(x=0, y)\right]$, is shown in Fig. 1 for substrate dimensions $L = 1.5\cdot 10^{-6}$ cm and $M = 6\cdot 10^{-8}$ cm, i.e., $L \gg M$, depending on the distance of the atom on the substrate from the center of the substrate in two directions for the values $\varepsilon_{sa} = 0{,}1$ and 1 K (1 and 2, respectively). It is shown in Fig. 1 that there is an energy barrier that prevents the atom from leaving the considered region of space.

3. The dispersion of collective modes

The dispersion law of collective oscillations in systems with van der Waals interaction is determined by the short-range nature of the particle interaction, which we describe by the Lennard-Jones potential (1). The results are highly dependent on the system configuration.

3.1. The solitary chain

We start our consideration with a solitary linear chain of particles, the stability of which can be expected at zero temperature. Under the simulation, the temperature was taken low but still nonzero in order to provide a sufficient amplitude of oscillations necessary to determine the natural frequencies. Additionally if in the theoretical calculation of the dispersion law of oscillations the chain was assumed to be so long that the edge effects can be neglected, in the simulation process it is assumed that from the very beginning the chain has a finite length. The motion of atoms at the ends of the chain and in its center is different which affects the stability of the configuration. As a consequence if after the formation of the chain during the simulation we remove the external field from the side of the substrate the chain turns out to be unstable primarily at the ends and overtime forms a zigzag structure. Therefore the properties of a linear chain were determined in the presence of a substrate that ensures the stability of the system.

The presence of a substrate gives us grounds to disregard the condition of the fulfillment, for the chain itself, of the elastic moduli tensor symmetry condition, with respect to the permutation of pairs of indices, which is the condition for the correct transition of the equations of lattice dynamics to equations of the theory of elasticity (see, for example, [16]) and assume that this condition is satisfied the entire system as a whole, including the substrate.

We determined the structures and vibration frequencies of the chains consisting of different numbers of atoms $N = 10, 20$, and 50 and this fact provided the possibility of determining the vibration frequencies corresponding to different wave vectors. The finite length of the chain, even in the absence of a substrate, ensures the convergence of the rms amplitudes of atomic vibrations, that is, the dynamic stability of the system. In this case, the phonon spectrum of the chain, of course, will begin at a frequency other than zero. However, if we do not interested in studying the stability margin of the system and do not consider "compressed" chains with negative dispersion of transversely polarized modes [15], the chain can be considered infinite in calculations and its spectrum can be considered starting from zero.

The chains were placed on a substrate characterized by the parameter $\varepsilon_{sa} = 1$ K. This value, as noted above, is much less than the corresponding value of the "6–12" potential for the interaction between helium atoms. As a result, the average distance between particles along the chain with high accuracy turned out to be $a = 2^{1/6}\sigma$, corresponding to the minimum of potential (1) for a pair of helium atoms.

An example of a stable linear chain consisting of 20 atoms is shown in Fig. 2(a). The possibility of the stable existence of the chain provides the possibility of the theoretical determining the dispersion law of collective modes, assuming the chain to be unbounded in the direction x.

In equilibrium positions [see Fig. 2(a)], the particles of a free solitary chain are located at points with coordinates x_{0i} with distance a between neighbors. To find the dispersion law for the collective oscillations we introduce small displacements from the equilibrium positions: ξ_i along the chain of particles (axis x) and across the chain, η_i and λ_i along the axes y and z, respectively. Expanding the potential energy of interaction to quadratic terms, we obtain the following Lagrange function describing small oscillations of the system:

$$L_1 = \frac{m}{2}\sum_i \left(\dot{\xi}_i^2 + \dot{\eta}_i^2 + \dot{\lambda}_i^2\right) - \delta U_1,$$

$$\delta U_1 = \frac{6\varepsilon\sigma^6}{a^8}\left\{\left[\frac{26\beta^6}{|i-j|^{14}} - \frac{7}{|i-j|^8}\right]\left(\xi_i - \xi_j\right)^2 - \left[\frac{2\beta^6}{|i-j|^{14}} - \frac{1}{|i-j|^8}\right]\left[\left(\eta_i - \eta_j\right)^2 + \left(\lambda_i - \lambda_j\right)^2\right]\right\}, \quad (6)$$

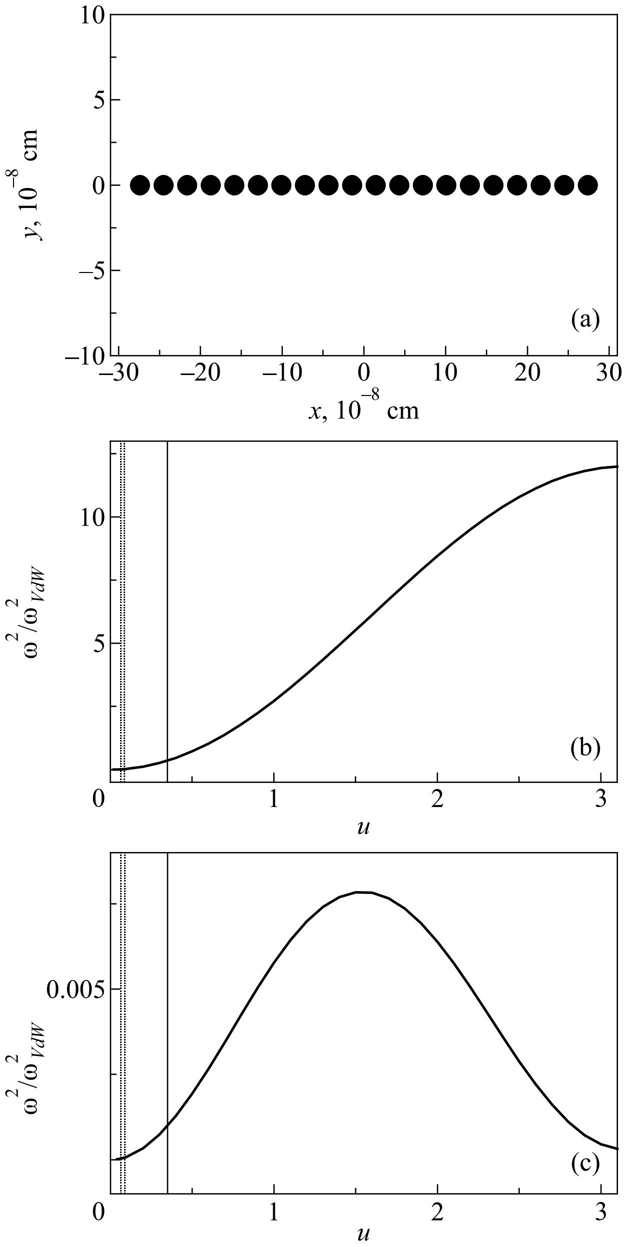

Fig. 2. The schematic representation of a solitary chain of particles with van der Waals interaction (a) and the functions determining the dispersion laws of the longitudinal (b) and transverse (c) branches of the collective oscillations of a solitary chain.

where $\beta = \sigma / a$ and m is particle mass. In L_1, we disregard, in view of $\varepsilon_{sa} \ll \varepsilon$, the contribution of the substrate potential.

Writing the equations of motion for the Fourier-transformed displacements $\xi_i = \sum_q \xi_q \exp\left(iqx_{0i} - i\omega t\right)$ by coordinates x_{0i} and time t (and similarly for η_i and λ_i) and taking into account the periodicity of the system along the x axis, we obtain three branches of the dispersion law of collective modes. One of these branches corresponds to longitudinal vibrations along the chain is

$$\omega_{\|}^2 = \omega_{vdW}^2 F_{\text{line}}^{(\|)}(qa),$$

$$F_{\text{line}}^{(\|)}(u) = \sum_{n\geq 1}\left(\frac{26\beta^6}{n^6}-7\right)\left(\frac{1-\cos un}{n^8}\right),\ \omega_{vdW}^2 = \frac{48\varepsilon\beta^6}{ma^2}. \quad (7)$$

The other two branches, corresponding to particle oscillations across the chain (along the axes y and z) possesses the dispersion law

$$\omega_{\perp}^2 = \omega_{vdW}^2 F_{\text{line}}^{(\perp)}(qa),\ F_{\text{line}}^{(\perp)}(u) = \sum_{n\geq 1}\left(1-\frac{2\beta^6}{n^6}\right)\left(\frac{1-\cos un}{n^8}\right). \quad (8)$$

Note that due to the absence of the requirement, for the chain itself, to satisfy the symmetry condition of the elastic moduli tensor with respect to the permutation of pairs of indices, the dispersion law of the transverse mode (8) in the long-wavelength limit is linear (sound-like), and not quadratic (flexural) [17].

From the structure of function $F_{\text{line}}^{(\perp)}(u)$ it follows that in the long-wavelength limit $|u| \ll 1$ this function is always positive if $\beta \leq 2^{-1/6}$ that is, the average distance between the equilibrium positions of particles in the chain satisfies the condition $a \geq 2^{1/6}\sigma$, and if this inequality is not satisfied $F_{\text{line}}^{(\perp)}(u)$ may become negative. This according to (8) leads to the negativeness of the square of the frequency of transverse vibrations of particles meaning the instability of the given configuration of the system, i.e., the solitary chain. Note that if $\beta = 2^{-1/6}$, $a = 2^{1/6}\sigma$, that is neighboring particles along the axis in equilibrium states are at the distance a from one another, corresponding to the minimum energy of pair interaction of neighbors according to the law (1). In this case $\omega_{vdW}^2 = 24\varepsilon/(ma^2)$. Recall that exactly at this distance, according to the simulation results, the particles are located along the chain.

Functions $F_{\text{line}}^{(\|)}(u)$ and $F_{\text{line}}^{(\perp)}(u)$ at $\beta = 2^{-1/6}$ are written in the form

$$F_{\text{line}(m)}^{(\|)}(u) = \sum_{n\geq 1}\left(\frac{13}{n^6}-7\right)\left(\frac{1-\cos un}{n^8}\right),$$

$$F_{\text{line}(m)}^{(\perp)}(u) = \sum_{n\geq 1}\left(1-\frac{1}{n^6}\right)\left(\frac{1-\cos un}{n^8}\right). \quad (9)$$

Their graphs are shown in Figs. 2(b) and 2(c) for the argument interval from zero to the boundary of the first Brillouin zone $u = \pi$.

The series in (9) converge so quickly that the results of their summation almost coincide with their values obtained undertaken into account only the first nonvanishing term in them, that is $n = 1$ in $F_{\text{line}(m)}^{(\|)}$ which corresponds to the approximation of the first nearest neighbors when we restrict ourselves to the interaction of a particle with neighbors located at a distance a from the given one. At the same time, this approximation turns out to be insufficient for $F_{\text{line}(m)}^{(\perp)}$ since, as follows from (9), the term of the series for $F_{\text{line}(m)}^{(\|)}$ with $n = 1$ equals to zero and the first nonvanishing term corresponds to $n = 2$ which corresponds to the interaction of the particle with the particles following the nearest neighbors (second nearest neighbors) located at a distance $2a$ from the given one. In the limit $u \ll 1$, we have the following asymptotic expressions for the functions $F_{\text{line}(m)}^{(\|)}$ and $F_{\text{line}(m)}^{(\perp)}$:

$$F_{\text{line}(m)}^{(\|)} \simeq \frac{1}{2}\left[13\zeta(12)-7\zeta(6)\right]u^2 \simeq 2.94u^2,$$

$$F_{\text{line}(m)}^{(\perp)} \simeq \frac{1}{2}\left[\zeta(6)-\zeta(12)\right]u^2 \simeq 8.55\cdot 10^{-3}u^2, \quad (10)$$

where $\zeta(x)$ is the Riemann zeta function. This means linear acoustic dispersion of modes (10) in the limit $|qa| \ll 1$, when $\omega_{\|(\perp)} \simeq c_{\|(\perp)}q$, $c_{\|} \simeq 1.71\omega_{vdW}a$, $c_{\perp} \simeq 9.25\cdot 10^{-2}\omega_{vdW}a$, that is the ratio of the velocities of the longitudinal and transverse modes is $c_{\|}/c_{\perp} \simeq 18.5$. Attention is drawn to the smallness of the velocity of the transverse mode in comparison with the longitudinal one. In the approximation of the first nearest neighbors, the frequency of the transverse mode vanishes and becomes finite only when the interparticle interaction at distances exceeding the average distance from the particle in the chain to the nearest neighbor is taken into account.

An interesting feature of the function $F_{\text{line}(m)}^{(\perp)}$ describing the dispersion of transverse modes is the nonmonotonic character. The function has a maximum at the point $u_{\max} \simeq 1.54$, where $u_{\max}$ is the root of the equation

$$\sum_{n\geq 1}\left(1-\frac{1}{n^6}\right)\frac{\sin nu}{n^7} = 0.$$

The value $u_{\max}$ slightly different from $u_{\max}^{(0)} = \pi/2 \simeq 1.57$ obtained in the approximation of the second nearest neighbors when in the series in (9) we leave only the first nonvanishing term with $n = 2$. The presence of a maximum means that the group velocity of the transverse modes turns out to be positive at $|q| < u_{\max}/a$, is zero at the point $|q| = u_{\max}/a$, and becomes negative at larger values of the wavenumber. In general, it can be noted that the function $F_{\text{line}(m)}^{(\perp)}$ almost symmetric with respect to $u \simeq \pi/2$.

The positivity of the squared frequency of the longitudinal and transverse modes at $\beta = 2^{-1/6}$ in the entire range of wavenumbers corresponding to the first Brillouin zone $0 < |q| < \pi/a$ means the stability of a solitary chain with respect to small vibrations both along and across it. Note that a chain of particles with a long-range Coulomb interaction, in contrast to the chain with a short-range van der Waals interaction considered here, is unstable with respect to small transverse vibrations (negative square of the transverse mode frequency) and is stabilized only in the presence of an external confining potential [10].

The characteristic values of the frequencies of the natural oscillations of the chain were also estimated from the vibration spectrum established by means of a Fourier analysis of the time dependence of small displacements of particles from the equilibrium position along x and y axes. Examples of such spectra are shown in Fig. 3 for the chains of different lengths consisting of $N = 10$, 20, and 50 atoms. The wave vectors $\pi / L = \pi / [(N-1)a]$ corresponding to chains of different lengths (different N) are shown by vertical lines in Figs. 2(b) and 2(c). The triangles in Fig. 3 show the vibration frequencies calculated theoretically. As one can see, the agreement between the result of the theoretical calculation of the dispersion law and the simulation results seems rather good. Note that the ratio of the velocities of the modes shown by triangles corresponds to the previously indicated relation $c_{\parallel} / c_{\perp} \simeq 18.5$ (10).

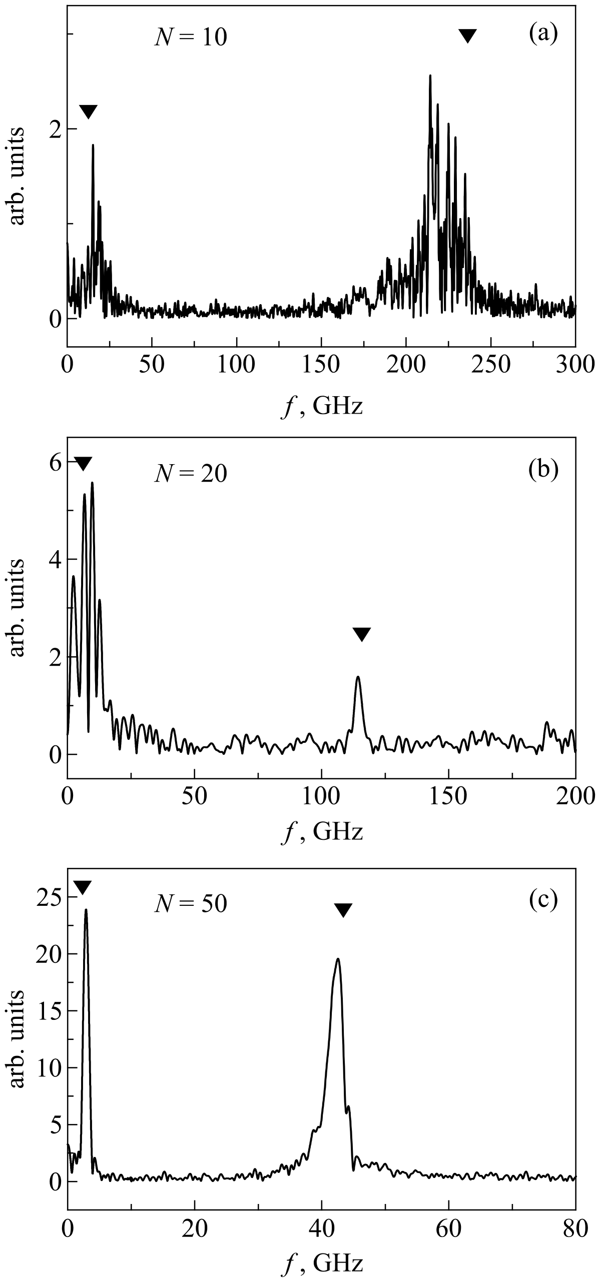

Fig. 3. The spectrum of vibrations of a solitary chain of atoms interacting according to the law (1) for chains with different numbers of particles $N = 10$ (a), 20 (b), and 50 (c). The triangles mark the vibration frequencies calculated using Eq. (9).

3.2. Two chains with van der Waals interaction

In this subsection, we will consider collective oscillations in a system of particles interacting according to the law (1) and consisting of two parallel chains separated by a distance D which are assumed to be located in the plane $\{xy\}$ [Fig. 4(a)]. As noted in the previous subsection such zigzag systems naturally arise from a solitary chain during simulation if there is no external potential of the substrate. In addition, a zigzag configuration is formed under specially specified external conditions from the initial random distribution of particles if the transverse size of the system is limited from the very beginning. To analyze the parameters of the system in Fig. 4(a) let us consider the potential energy of interaction of particles located in different chains (without taking into account their small displacements from the equilibrium position):

$$U_{21} = 4\varepsilon \sum_{ij} \left[\frac{\sigma^{12}}{\left(X_{ij}^2 + D^2\right)^6} - \frac{\sigma^6}{\left(X_{ij}^2 + D^2\right)^3} \right], \qquad (11)$$

where the notation is introduced $X_{ij} = x_{2i}^{(0)} - x_{1j}^{(0)}$ (or $x_{1i}^{(0)} - x_{2j}^{(0)}$), $x_{ki}^{(0)}$ are equilibrium positions of the particles in a chain $k = 1, 2$. Furthermore in each of the chains, the distance between neighboring particles is a. For simplicity in (11) we can restrict ourselves to the approximation of the nearest neighbors and consider the interaction of ith atom of the one of the chains with the nearest atoms j and $j+1$ of the another chain. If we denote $X = X_{ij}$ one obtains:

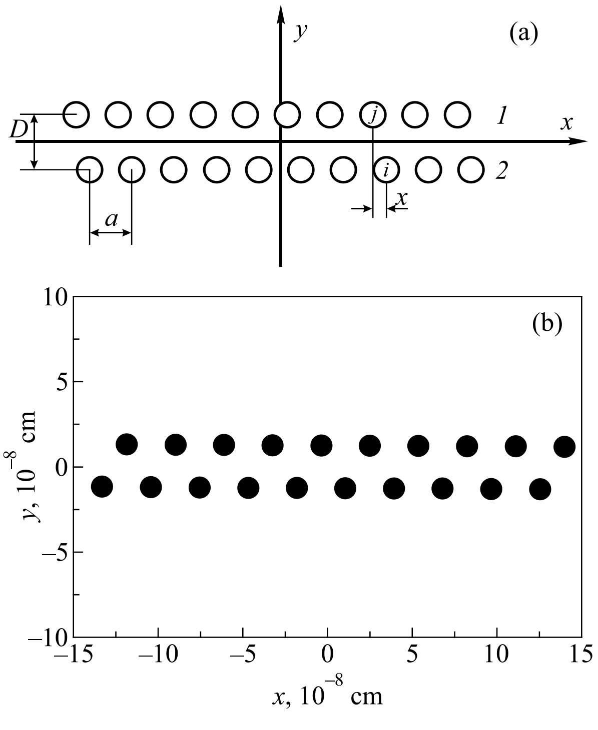

Fig. 4. Two-chain configuration of particles interacting according to the law (1): schematic diagram to explain the scheme for determining the parameters $X = X_{ij}$ and D (in the text) (a) and the result of numerical simulation (b).

$$U_{21}^{(i,j,j+1)} \simeq 4\varepsilon\left\{\frac{\sigma^{12}}{\left(X^2+D^2\right)^6}-\frac{\sigma^6}{\left(X^2+D^2\right)^3}+\frac{\sigma^{12}}{\left[\left(a-X\right)^2+D^2\right]^6}-\frac{\sigma^6}{\left[\left(a-X\right)^2+D^2\right]^3}\right\}. \qquad (12)$$

To calculate X and D we solve the equations $\partial U_{21}^{(i,j,j+1)}/\partial X=0$ and $\partial U_{21}^{(i,j,j+1)}/\partial D=0$. Their nontrivial solutions give $X=a/2$ and $D=\sqrt{3}a/2$, if we take $a=2^{1/6}\sigma$, that is to consider the particles located along the chain at a distance corresponding to the minimum of the pair interaction energy of neighboring atoms.

The system simulation results in Fig. 4(b) are in complete agreement with this result. As the simulation results show when a zigzag configuration is formed the particles are arranged in such a way that one chain is displaced relative to the other by a distance $a/2$ (the equilibrium distance between particles in each of the chains is still a). In this case, the unit cell is an equilateral triangle with $D=\sqrt{3}a/2$. As for the solitary chain, the simulation gives $a=2^{1/6}\sigma$.

Note once more that the zigzag configuration of two atomic lines [Fig. 4(b)] is very stable in the absence of an external field. At some simulation steps the double-chain system can be displaced as a whole in the plane, but the relative arrangement of the atoms in the zigzag stays the same. The formation of such a configuration at low temperature from an initial random distribution of atoms often leads to a structure with defects. In this case, annealing was carried out, that is a smooth increase in temperature followed by its decrease, which led to the formation of a defect-free structure.

The Lagrange function of the system, up to quadratic terms in small displacements from the equilibrium position, can be written as

$$L_2 = L_1^{(2)} + \delta U_{21}, \qquad (13)$$

where the function $L_1^{(n)}$ is the result of summing the functions L_1 from (6) written for each of the chains $k=1,\,2,\,\ldots,\,n$ (in the case considered here $n=2$), and the term δU_{12} corresponds to the interaction of particles located in chains 1 and 2:

$$\begin{aligned}\delta U_{21} ={}& \frac{12\varepsilon\sigma^6}{a^8}\sum_{i,j}\left\{\frac{2\beta^6\left[13\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^8}-\frac{\left[7\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^5}\right\}\left(\xi_{2i}-\xi_{1j}\right)^2\\ &+\frac{12\varepsilon\sigma^6}{a^8}\sum_{i,j}\left\{\frac{2\beta^6\left[13\alpha^2-\left(\nu_{2i}-\nu_{1j}\right)^2\right]}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^8}-\frac{\left[7\alpha^2-\left(\nu_{2i}-\nu_{1j}\right)^2\right]}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^5}\right\}\left(\eta_{2i}-\eta_{1j}\right)^2\\ &+\frac{12\varepsilon\sigma^6}{a^8}\sum_{i,j}\left\{\frac{1}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^4}-\frac{2\beta^6}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^7}\right\}\left(\lambda_{2i}-\lambda_{1j}\right)^2\\ &+\frac{96\varepsilon\sigma^6}{a^8}\alpha\sum_{i,j}\left(\nu_{2i}-\nu_{1j}\right)\left\{\frac{7\beta^6}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^8}-\frac{2}{\left[\left(\nu_{2i}-\nu_{1j}\right)^2-\alpha^2\right]^5}\right\}\left(\xi_{2i}-\xi_{1j}\right)\left(\eta_{2i}-\eta_{1j}\right),\end{aligned} \qquad (14)$$

where the notation are introduced $\nu_{ki}=x_{ki}^{(0)}/a$ and $\alpha=D/a$. The last term in Eq. (14) describes the coupling of particle displacements from the equilibrium position along the chains and across to them. With an increase in the distance between particles along the axis x, increase $\left|\nu_{2i}-\nu_{1j}\right|$ under conditions $(\nu_{2i}-\nu_{1j})^2 \gg \alpha^2$, this term decreases proportionally $(\nu_{2i}-\nu_{1j})^{-15}$ (in the first term in this term) and $(\nu_{2i}-\nu_{1j})^{-9}$ in the second term, that is one degree stronger than the corresponding terms in the first three terms of Eq. (14). Because of this during the summation in (14), the contribution of the last term will be less than the contribution from the remaining terms if the summation process is extended to a large number of terms, as it happens with long-wave oscillations. Similarly when considering oscillations of chains with long-range Coulomb interaction of particles in [10], a similar term corresponding to the coupling of oscillations along and across electron chains turned out to be negligible when considering long-wave oscillations, affecting however the dispersion of collective modes at $|qa|\geq 1$. For systems of particles with a short-range van der Waals interaction considered in this work, the first and in some cases second nearest neighbors make the overwhelming contribution to the summation of the series in (14). Under these conditions, the last term in (14), generally speaking, seems to be necessary to take into account along with the first three in the entire wavenumber interval within the first Brillouin zone.

To obtain the dispersion laws for collective oscillations, we write down the equations of motion for small oscillations based on the Lagrange function (13) and carry out the Fourier transform in these equations in the same way as it was done for the solitary chain in the previous subsection. As a result, we obtain the coupled equations for the displacements ξ_{nq} and η_{nq} in the plane $\{xy\}$ and separately equations for displacements λ_{ni} in the z direction, that is normally to the plane of arrangement of particle chains. The dispersion law for frequencies is calculated by solving the compatibility equations for systems of equations with respect to the corresponding displacements.

If we define $\kappa=\omega^2/\omega_{vdw}^2$ then the dispersion equation for collective modes in the plane $\{xy\}$ for $\beta=2^{-1/6}$ and $\alpha=\sqrt{3}/2$ can be written in the form

$$\left[(\kappa-F_{L1})^2-F_{L2}^2\right]\left[(\kappa-F_{T1})^2-F_{T2}^2\right]-2F_{LT}^2\left[(\kappa-F_{L1})(\kappa-F_{T1})-F_{L2}F_{T2}-\frac{F_{LT}^2}{2}\right]=0. \tag{15}$$

Here

$$F_{L1}(u)=F_{\text{line}(m)}^{(\|)}(u)+\sum_{n\ge1}\left[\frac{26n^2-26n+5}{2(n^2-n+1)^8}-\frac{7n^2-7n+1}{(n^2-n+1)^5}\right]\simeq F_{\text{line}(m)}^{(\|)}(u)+1.44,$$

$$F_{L2}(u)=\sum_{n\ge1}\left[\frac{26n^2-26n+5}{2(n^2-n+1)^8}-\frac{7n^2-7n+1}{(n^2-n+1)^5}\right]\cos\left[\left(n-\frac{1}{2}\right)u\right],$$

$$F_{T1}(u)=F_{\text{line}(m)}^{(\perp)}(u)+\sum_{n\ge1}\left[\frac{19-2n^2+2n}{2(n^2-n+1)^8}-\frac{5-n^2+n}{(n^2-n+1)^5}\right]\simeq F_{\text{line}(m)}^{(\perp)}(u)+4.49,$$

$$F_{T2}(u)=\sum_{n\ge1}\left[\frac{19-2n^2+2n}{2(n^2-n+1)^8}-\frac{5-n^2+n}{(n^2-n+1)^5}\right]\cos\left[\left(n-\frac{1}{2}\right)u\right],$$

$$F_{LT}(u)=\sqrt{3}\sum_{n\ge1}\left(n-\frac{1}{2}\right)\left[\frac{7}{(n^2-n+1)^8}-\frac{4}{(n^2-n+1)^5}\right]\sin\left[\left(n-\frac{1}{2}\right)u\right].$$

As in the case of the solitary chain, here $u=|qa|$. The presence of function $F_{LT}(u)$ in (15) is a consequence of the presence of the last term in (14).

Equation (15) is a fourth-degree equation with respect to κ. We solved it by numerical methods. The results are shown in Fig. 5.

As can be seen from the figure two branches of the spectrum of collective vibrations are Goldstone, starting from zero value at $u=|qa|=0$, and two are optical, which at $u=0$ have finite values. There is a point of maximum convergence of optical modes (anti-crossing) near the middle of the Brillouin zone at u close to $\pi/2$.

To test the influence $F_{LT}(u)$ on the mode dispersion law in the long-wavelength limit $u=|qa|\le1$ we depicted in Fig. 6 the dispersion laws obtained by solving Eq. (15) (solid lines) together with the results of solving this equation

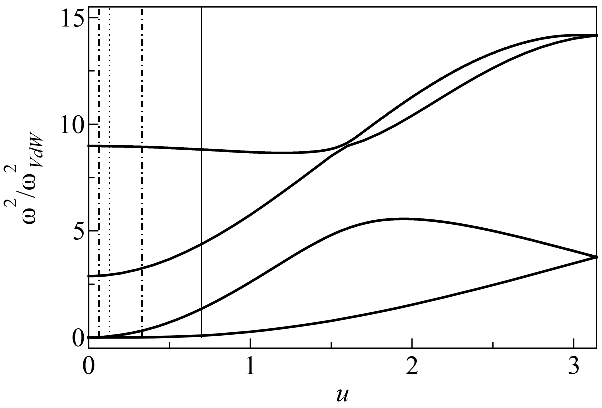

Fig. 5. The reduced squares of the frequencies of collective oscillations of two linear chains with van der Waals interaction for the motion of particles in the plane of the chains.

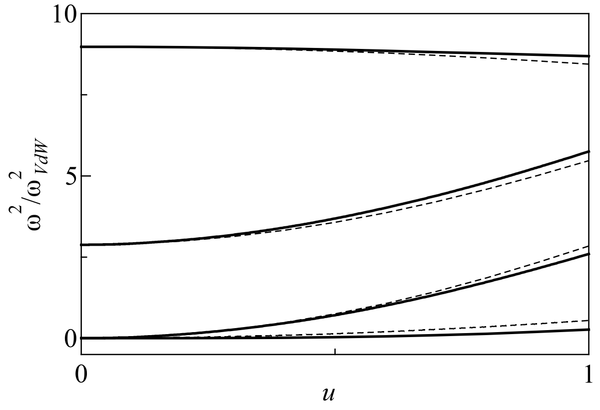

Fig. 6. Exact (solid lines) and approximate (16) — dashed lines are functions that determine the dispersion laws of collective modes in the long-wavelength limit.

in the limit $F_{LT}(u) = 0$ (dashed lines). It is easy to see from (15) that if $F_{LT}(u) = 0$ four solutions of Eq. (15) degenerate into two, which have the form

$$\kappa_{1,2} = F_{L1} \pm F_{L2}, \quad \kappa_{3,4} = F_{T1} \pm F_{T2}. \tag{16}$$

Dashed lines in Fig. 6 are described by Eq. (16). As can be seen from Fig. 6, the influence of the F_{LT} on the dispersion of coupled vibrations turns out to be rather weak in the long-wavelength limit. When $u > 1$ exact solutions of Eq. (15) differ markedly from those of Eq. (16). We do not present a comparison of exact solutions of Eqs. (15) and (16) in this interval $|qa|$ due to the low cognition of the corresponding drawing with a large number of intersecting solid and dotted lines.

It can be seen from Eq. (15) that Eq. (16) gives the roots of the exact Eq. (15) for $u = 0$ when $F_{LT}(0) = 0$. This makes it possible to evaluate analytically the starting values κ in optical modes in Fig. 5 as $F_{L1}(0) + F_{L2}(0) = 2F_{L1}(0) \simeq 2.88$ and $F_{T1}(0) + F_{T2}(0) = 2F_{T1}(0) \simeq 8.78$ in complete agreement with the results of the numerical solution of the dispersion Eq. (15). Another possibility of analytical analysis of solutions (15) is available for $u = \pi$ that is at the upper boundary of the first Brillouin zone. In this limit the functions $F_{L2}(\pi) = F_{T2}(\pi) = 0$ and Eq. (15) degenerates into a square, two roots of which are

$$\kappa_{(\pm)}(\pi) = \frac{F_{L1} + F_{T1}}{2} \pm \sqrt{\frac{\left(F_{L1} - F_{T1}\right)^2}{4} + F_{LT}^2}\,. \tag{17}$$

Substituting into (17) the values of F_{L1}, F_{T1}, and F_{LT} taken at $u = \pi$, we obtain $\kappa_{(+)} \simeq 14.16$ and $\kappa_{(-)} \simeq 3.77$ in excellent agreement with the results of the numerical solution (15) presented in Fig. 5.

When considering collective oscillations in the direction of the axis z, that is, perpendicular to the plane in which two chains of particles are located, one introduces the functions

$$F_{T3} = F^{(\perp)}_{\text{line}(m)}(u) + \sum_{n\ge1}\left[\frac{1}{\left(n^2 - n + 1\right)^4} - \frac{1}{\left(n^2 - n + 1\right)^7}\right]$$

$$\simeq F^{(\perp)}_{\text{line}(m)}(u) + 0.0124,$$

$$F_{T4}(u) = \sum_{n\ge1}\left[\frac{1}{\left(n^2 - n + 1\right)^4} - \frac{1}{\left(n^2 - n + 1\right)^7}\right]\cos\left[\left(n - \frac{1}{2}\right)u\right].$$

As a result the equations of motion for small displacements λ_{ni} $(n = 1, 2)$ lead to the following dispersion equation for collective oscillations along the z axis:

$$\left(\kappa - F_{T3}\right)^2 - F_{T4}^2 = 0 \tag{18}$$

with two obvious independent roots $\kappa_{5,6}(u) = F_{T3}(u) \pm F_{T4}(u)$ and with graphs shown in Fig. 7.

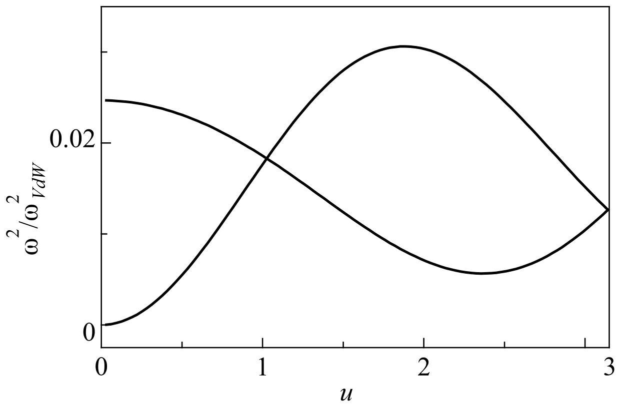

Fig. 7. Same as in Fig. 5, but for the oscillations of particles in the direction perpendicular to the plane of the two chains.

It should be emphasized that the κ_5 and κ_6 are small in comparison with the corresponding functions in Fig. 5 describing coupled vibrations in the $\{x, y\}$ plane. This is due to the fact that the functions F_{T3} and F_{T4} determining κ_5 and κ_6 in the nearest-neighbor approximation vanish if only the term with $n = 1$ is left in Eq. (18). Thus, the dispersion of vibrations in the direction z manifests itself only when the interaction of particles with the second nearest and next neighbors is taken into account [small terms of the series with $n \ge 2$ in (18)].

One of the branches of the spectrum in Fig. 7, namely κ_5, is optical, starting from $\kappa_5(0) = 2F_{T3}(0)$ with asymptotic $\kappa_5 \simeq 0.0248 - 6.420 \cdot 10^{-3}u^2$ at $u \ll 1$, and second one κ_6 is Goldstone, having asymptotic in the long-wavelength limit $\kappa_6 \simeq 0.0235u^2$ with linear dispersion of the corresponding mode. Curves $\kappa_5(u)$ and $\kappa_6(u)$ intersect at $u_{\text{cr}} \simeq 1.02$, where u_{cr} is the root of equation $F_{T4}(u) = 0$. The value u_{cr} is very close to $u^{(0)}_{\text{cr}} = \pi/3$ which is a root if at summing in F_{T4} we restrict ourselves to the first nonvanishing term with $n = 2$. We also note the nonmonotonic character of the curves in Fig. 7 that show the minimum on the curve $\kappa_5(u)$ at the point $u_{\min} \simeq 2.37$, $u^{(0)}_{\min} \simeq 2.38$, summing in (18) is restricted by $n = 2$, and maximum $\kappa_6(u)$ at the point $u_{\max} \simeq 1.88$ ($u^{(0)}_{\max} \simeq 1.91$). Both solutions of dispersion Eq. (18) coincide at the point $u = \pi$ and are equal $\kappa_5(\pi) = \kappa_6(\pi) = F_{T3}(\pi)$ because $F_{T4}(\pi) = 0$.

The intersection of the functions $\kappa_5(u)$ and $\kappa_6(u)$ is due to the fact that the solutions of Eq. (18) are independent, in contrast to coupled modes for oscillations in the plane $\{xy\}$ in Fig. 5, where the repulsion of the optical modes of the spectrum is observed at the point of their closest approach — the anti-crossing of the modes.

In conclusion of the subsection, we note that from the form of the Lagrange function (13) it is easy to see that in the limit $D \to \infty$ the function $L_2 = L_1^{(2)}$. This means that the collective modes of the zigzag system turn into modes of two solitary chains. In the opposite limit $D \to 0$, we obtain again the mode dispersion of a solitary chain but

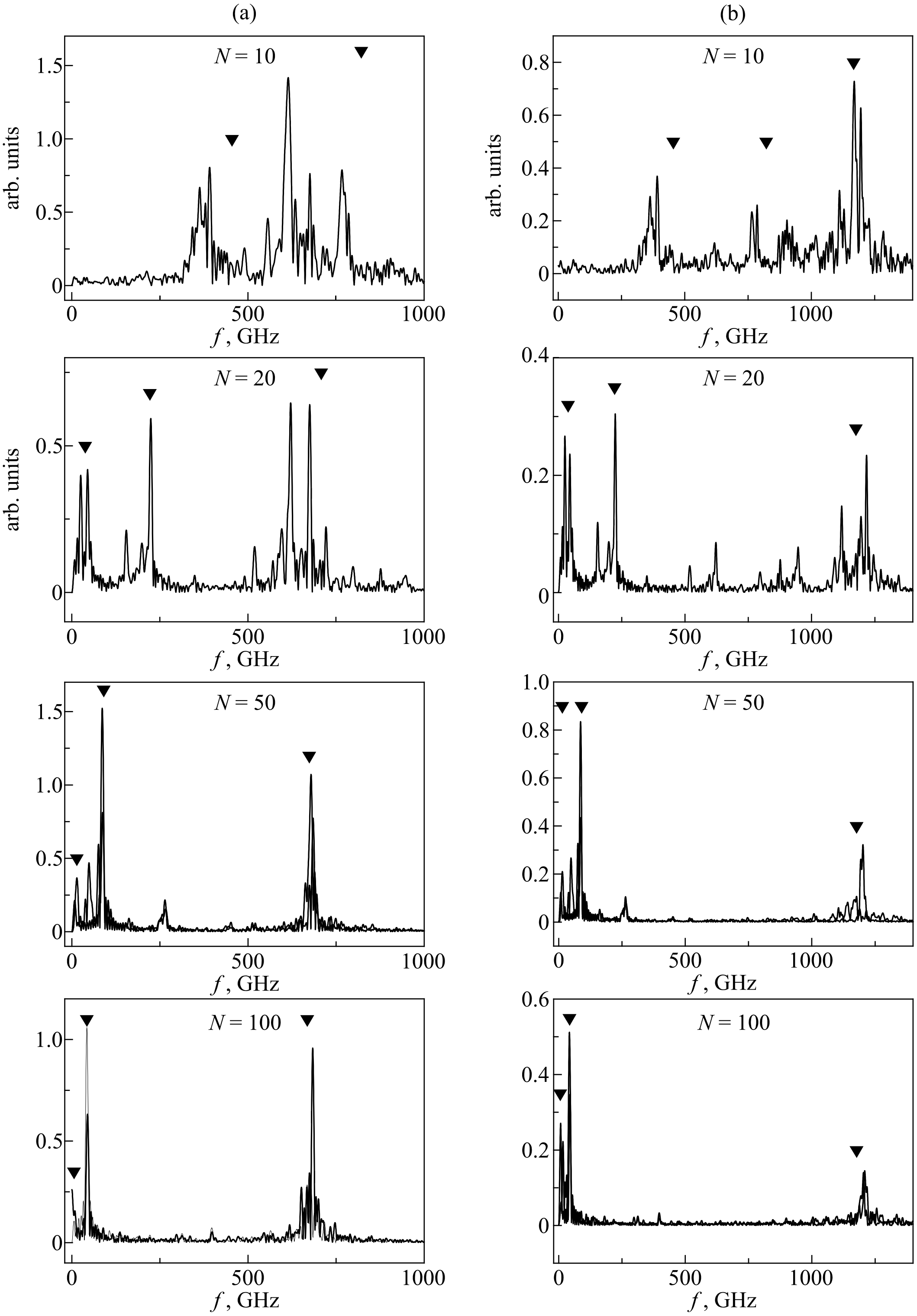

Fig. 8. Spectra of vibrations of a two-chain system of atoms interacting according to law (1) in the case of a different number of particles in the system. Spectra (a) are obtained for displacements of atoms along the x axis, whereas (b) along the y axis.

with an average distance between particles $a/2$. In this case, solutions of the dispersion equation for oscillations along x, y, and z transform into dispersion laws of two longitudinal and two transverse oscillation modes of a solitary chain with a step $a/2$ and with phase shift π between the corresponding dispersion laws (dispersion of the modes along z is the same as for vibrations along y).

As in the case of a solitary chain, considered in Subsec. 3.1, the characteristic values of the frequencies of the natural vibrations of the double-chain configuration were established in the Fourier analysis of the vibration spectrum. The study of vibration frequencies in the system was carried out at the value $\varepsilon_{sa} = 0.1$ K. Examples of the obtained spectra are shown in Fig. 8 for chains of different lengths consisting of $N = 10$, 20, 50, and 100 atoms. Wave numbers π / L, corresponding to chains of different lengths for different N, are shown by vertical lines in Fig. 5. The triangles in Fig. 8 show the vibration frequencies calculated theoretically and presented in Fig. 5. In Fig. 8, spectra (a) were obtained by analyzing x-coordinates of atoms, and spectra (b) — y-coordinates. The agreement between the results of the theoretical calculation of the dispersion law and the analysis of the vibration spectrum should be treated as quite satisfactory, and this agreement is especially manifested for longer chains. In spectrum (a) for a chain with $N = 10$, in addition to the frequencies following from the theory, a peak with a frequency of about 700 GHz, which is well reproduced in different series of calculations, is also observed. One can speculate that this is a combination frequency, the excitation of which is facilitated by the small size of this chain.

3.3. Collective oscillations in a system of three chains

In this Subsec., we will consider collective oscillations of a system of particles with van der Waals interaction, which consists of three chains (Fig. 9), in which the configuration is shown at different (a) and identical (b) scales along the coordinate axes. This configuration is formed from a random initial distribution of particles with a limitation of the spatial region of their location under conditions when the transverse size is approximately one and a half times greater than that for which the formation of a zigzag is characteristic. Configurations with a larger number of particle lines are not considered in this work.

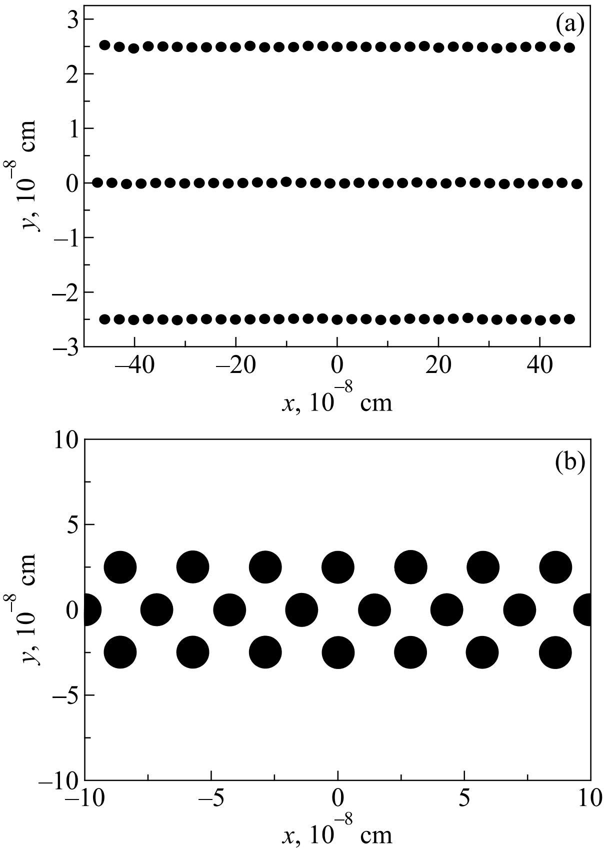

Fig. 9. Configuration of particles interacting according to the law (1), consisting of three lines of atoms in different (a) and the same (b) scales along the coordinate axes.

As before, we assume that the system is located in the plane $\{xy\}$ with axis x along the chains. The distance between the extreme chains 1 and 3 is considered equal D and correspondingly $D/2$ between the central chain 2 and the outer ones. Note that x — the coordinates of the equilibrium positions of particles in chains 1 and 3 coincide, and x — the coordinates of such positions for the particles of chain 2 are shifted by $a/2$ relative to the corresponding positions in chains 1 and 3. It is also important that now, when considering chains 2 and 1 or 2 and 3, we have, in contrast to the situation considered in the previous subsection, $D = \sqrt{3}a$.

The determination of the parameters of the system, similar to what was carried out at the beginning of Subsec. 3.2, the case of three chains is generalized in a trivial way if we take into account the interaction of only the nearest neighbors. In this case, the problem of the structure of three chains splits into separate problems of the pairwise interactions of two neighboring chains with a completely analogous result — the formation of a triangular structure of particles.

The procedure for determining the dispersion laws of collective oscillation modes in the case of three chains is straightforward. Lagrange function:

$$L_3 = L_1^{(3)} + \delta U_{21} + \delta U_{31} + \delta U_{32} \tag{19}$$

now includes contributions δU_{ij} from pairwise interactions of particles located in three different chains, $i, j = 1, 2, 3$. These expressions are similar to those that were written out in the previous subsection for the interaction of particles in two chains, but taking into account the geometry of the system, the mutual arrangement of particles, and the distance between the chains (see Fig. 9). From the structure of the Lagrange function and the equations of motion following from it, it results that for $D \to \infty$ the corresponding equations and the dispersion law of collective oscillations are obtained for an isolated chain of particles, and at $D \to 0$ — a solitary chain of particles with a half mean distance $a/2$ between particles.

The dispersion equation is obtained as the compatibility condition for the system of equations with respect to the Fourier-transformed displacements of particles from the equilibrium position ξ_{iq} and η_{iq} along and across the chains in the plane $\{xy\}$ and λ_{iq} normal to the plane of the chains ($i = 1, 2, 3$). As in the case of two chains, considered in the previous subsection, the equations for the squared frequencies ω^2 of the oscillations in the plane of the chains are coupled, and the condition of their compatibility (dispersion equation) is reduced to the equality of the determinant of the sixth order to zero. Equations for λ_{iq} are "splitted off" from the corresponding equations for oscillations in the plane of the chains, while the dispersion equation

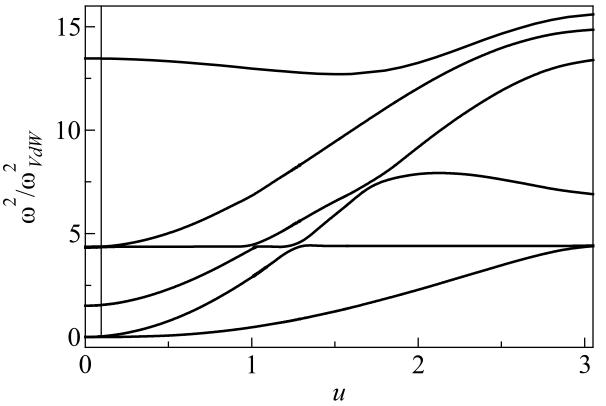

Fig. 10. Reduced squares of oscillation frequencies in the plane of a three-chain system of particles interacting according to the law (1).

for ω^2 here is determined by the vanishing of the third-order determinant. We solved both dispersion equations by numerical methods taking $\beta = 2^{-1/6}$. At Fig. 10 there are shown six branches of the dispersion law for vibrations in the $\{xy\}$ plane.

As can be seen from the figure, two branches of oscillations are Goldstone, and the other four are optical. There are three anti-crossing points.

Normalized squares of frequencies of three vibration modes in the direction of the axis z are shown in Fig. 11. One of the spectrum branches turns out to be Goldstone, the other two are optical and these modes demonstrate two anti-crossing points. As in the case of two chains of particles the values of the squares of the mode frequencies in the direction normal to the plane of the chains are much smaller in magnitude than the squares of the vibration frequencies in the plane of the chains at Fig. 10.

An example of a spectrum of collective vibrations obtained using a Fourier analysis of the time dependence of particle displacements from the equilibrium positions in the plane $\{xy\}$ is shown at Fig. 12 for wave number π / L marked with a vertical line in Fig. 10 for the number of atoms in the system $N = 100$. The spectra were obtained by analyzing the displacements of atoms in the directions x (a) and y (b). A good agreement is observed between the frequencies (triangles) theoretically calculated when determining the mode dispersion law with the frequencies obtained in the simulation. However, it should be noted that not all of the possible frequencies are sufficiently clearly manifested in the simulation in the case of a system of three chains.

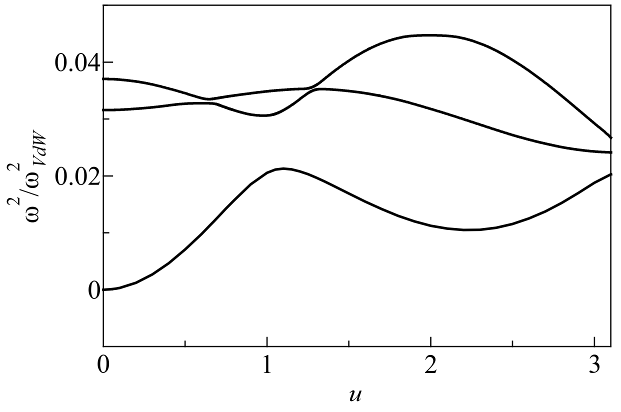

Fig. 11. Same as in Fig. 10, but for the oscillations along the z axis.

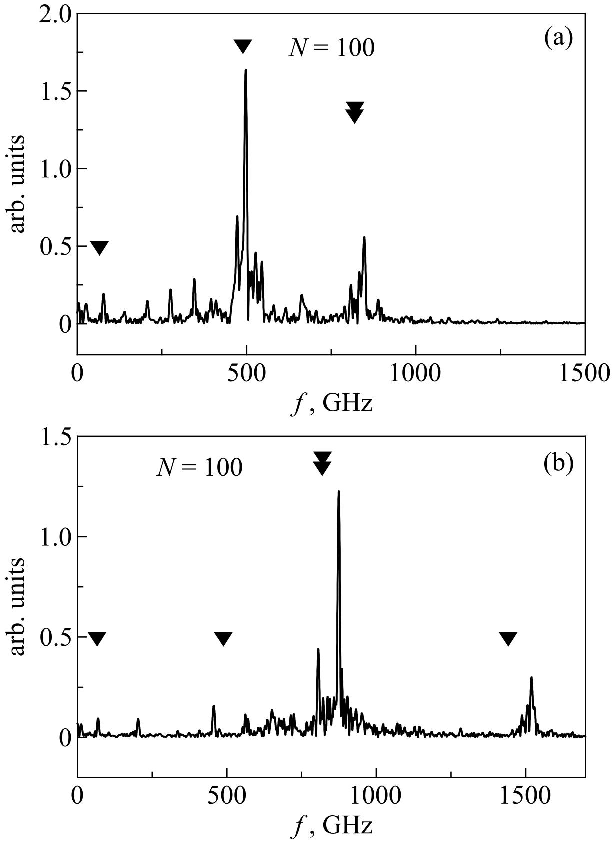

Fig. 12. Spectra of vibrations of a three-chain system of atoms interacting according to the law (1) for 100 particles. Spectra (a) and (b) are obtained for displacements of atoms along the x axis and y axis, respectively.

Conclusion

In this paper by means of computer simulation, we investigated the conditions for the appearance of linear systems of particles, located in a plane, with van der Waals interaction for the description of which the Lennard-Jones potential was used. It is shown that with a change in the temperature and the external holding potential of the substrate single-chain structures can form, and two- and three-chain configurations appear even in the absence of an external potential. For one-, two- and three-chain planar systems of atoms interacting according to the "6–12" law, the parameters of the arising particle configurations have been established. Using the Fourier analysis of the time dependence of the displacements of particles along and across the system, the values of the characteristic frequencies of collective oscillations are found. The obtained results are in good agreement with the theoretical calculation of the dispersion laws of collective modes due to the van der Waals interaction. The dispersion law is obtained as a result of equating to zero the determinant of the system of equations of motion for small displacements of particles from the equilibrium position both in the plane of the particle chains and in the direction normal to this plane. The results were obtained in the quasi-crystalline approximation for the wave number interval q inside the first Brillouin zone. It was found that among the collective modes there are both Goldstone modes starting from zero frequency at $q = 0$ and optical, starting from a finite value at zero wave number. The dispersion laws of collective oscillations turn out to be significantly different in systems with different numbers of particle chains.

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1. Y. P. Monarkha and K. Kono, *Two-dimensional Coulomb Liquids and Solids*, Springer-Verlag, Berlin (2003).
2. V. E. Syvokon and S. S. Sokolov, *Fiz. Nizk. Temp.* **41**, 1097 (2015) [*Low Temp. Phys.* **41**, 858 (2015)].
3. V. E. Syvokon and I. V. Sharapova, *Fiz. Nizk. Temp.* **45**, 1498 (2019) [*Low Temp. Phys.* **45**, 1267 (2019)].
4. G. Piacente, I. V. Schweigert, J. J. Betouras, and F. M. Peeters, *Phys. Rev. B* **69**, 045324 (2004).
5. V. E. Syvokon, S. S. Sokolov, and I. V. Sharapova, *Fiz. Nizk. Temp.* **45**, 58 (2019) [*Low Temp. Phys.* **45**, 49 (2019)].
6. A. V. Chaplik, *Pis'ma Zh. Eksp. Teor. Fiz.* **31**, 275 (1980) [*JETP Lett.* **31**, 252 (1980)].
7. S. S. Sokolov and O. I. Kirichek, *Fiz. Nizk. Temp.* **20**, 761 (1994) [*Low Temp. Phys.* **20**, 599 (1994)].
8. S. S. Sokolov, J.-P. Rino, and N. Studart, *Phys. Rev. B* **75**, 233405 (2007).
9. S. S. Sokolov and V. E. Syvokon, *J. Low Temp. Phys.* **187**, 427 (2017).
10. V. E. Syvokon, E. S. Sokolova, and S. S. Sokolov, *Fiz. Nizk. Temp.* **46**, 1171 (2020) [*Low Temp. Phys.* **46**, 991 (2020)].
11. M. I. Bagatskii, M. S. Barabashko, A. V. Dolbin, and V. V. Sumarokov, *Fiz. Nizk. Temp.* **38**, 667 (2012) [*Low Temp. Phys.* **38**, 523 (2012)].
12. M. I. Bagatskii, M. S. Barabashko, and V. V. Sumarokov, *Fiz. Nizk. Temp.* **39**, 568 (2013) [*Low Temp. Phys.* **39**, 441 (2013)].
13. M. I. Bagatskii, V. G. Manzhelii, V. V. Sumarokov, and M. S. Barabashko, *Fiz. Nizk. Temp.* **39**, 801 (2013) [*Low Temp. Phys.* **39**, 618 (2013)].
14. M. I. Bagatskii, M. S. Barabashko, and V. V. Sumarokov, *JETP Lett.* **99**, 461 (2014).
15. E. V. Manzhelii, S. B. Feodosyev, and S. A. Gospodarev, *Fiz. Nizk. Temp.* **45**, 404 (2019) [*Low Temp. Phys.* **45**, 355 (2019)].
16. A. M. Kossevich, *The Crystal Lattice* (*Phonons, Solitons, Dislocations*), WILEY-VCH Verlag Berlin GmBH, Berlin (1999).
17. E. V. Manzhelii, S. B. Feodosyev, I. A. Gospodarev, E. S. Syrkin, and K. A. Minakova, *Fiz. Nizk. Temp.* **41**, 718 (2015) [*Low Temp. Phys.* **41**, 557 (2015)].

Структура й колективні коливання лінійних систем частинок з ван-дер-ваальсовою взаємодією

V. E. Syvokon, E. S. Sokolova, S. S. Sokolov

Проведено моделювання розташованої в площині системи частинок з ван-дер-ваальсовою взаємодією, яка описана потенціалом Леннарда-Джонса. Установлено можливість існування одного ланцюжка частинок, а також формування лінійних систем із двох та трьох ланцюжків. Визначено спектр коливань системи при різних конфігураціях та встановлено характерні частоти коливань. Закон дисперсії колективних мод розраховано теоретично методом рівнянь руху для малих зсувів атомів з положення рівноваги при аналізі умови спільності системи рівнянь, яка виникає. Знайдені значення характерних частот перебувають у гарній згоді з результатами, які отримані при фур'є-аналізі часової залежності зсувів частинок з положень рівноваги уздовж та поперек системи.

Ключові слова: моделювання низьковимірних систем, дисперсія колективних коливань, системи частинок з ван-дер-ваальсовою взаємодією, потенціал Леннарда-Джонса, фур'є-аналіз спектрів.