Nonlinear torsional dynamics of weakly coupled oscillatory chains

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Abstract

We present analysis of the torsion oscillations in the quasi-one-dimensional lattices with the periodic potentials of the nearest neighbor interaction. A one-dimensional chain of the point dipoles (spins) under external field as well as without the latter is a simplest realization of such a system. The normal oscillations of the crystal lattice are usually considered in the small-amplitude approximations because any collective motions of the atoms with the amplitudes, which exceed several per cents of the interatomic distances, lead to the melting or the destruction of the crystal lattice. However, some molecular crystals admit the torsion oscillations with the large amplitudes (up to the full rotation) without any violation of the crystal order. We obtained the dispersion relations for the nonlinear normal modes for the wide range of the oscillations amplitudes and wave numbers.

1 Introduction

The torsional movement is a wide spread type of motion which appears at the different scales from the rotation of the galaxies up to oscillations of the quantum magnets (spins). Many parts of the machines and devices undergo the torsional oscillations at the macroscale while the molecules and spins demonstrate the analogous mobility at the micro- and nanoscale. The most famous example of the torsional movement is the oscillatory dynamics of the rigid pendulum [1,2], for which thelaws of motion are well studied. Therefore, the latter is the often used model of the various phenomena both at the macro- and at the microscales [3,4].

In the majority of the systems where the torsional mobility occurs physically sensible are the torsional angles in the range $[0,2\pi]$, that is the effect of the periodicity of the interaction potentials. For example, the energy of the system of the interacting point-like dipoles (spins) is described as follows:

$$E = \sum \overrightarrow{d_j}\overrightarrow{d_{j+1}} \sim \sum \cos\left(\theta_{j+1} - \theta_j\right) \qquad (1)$$

where θ_j is the turning angle of j-th dipole $(\vec{d_j})$ with respect to some given axis.

The periodicity of the interaction potential has two important consequences. The first consists in fact that the torsion oscillations can be realized with the large amplitudes (up to the rotation) without a damage of the system integrity. In particular, such motion is possible for some molecular crystals, for example, for the crystals of the normal alkanes (paraffins), where the rotation of the flexible polymer chain with respect to its long axis is observed in the so called rotational phase without violation of the crystal order [5,6].

The second consequence is the essential nonlinearity of the equations of motion describing the systems under consideration. Therefore, each new problem in the area appears as a challenge for the researchers in spite of the significant progress in the nonlinear dynamics obtained in the last decades. Some simplification can be achieved in the framework of the quasi-one-dimensional approximation for the systems like the polymer crystals or the spin lattices. The well-known Frenkel-Kontorova model [3] is widely used for the description of various phenomena at the nano-scale (dislocations in solids, incommensurate phase on crystal surface, point-like defects in the polymer crystals, arrays of the Josephson junctionsetc.) and can be realized by the array of the coupled pendula [7]. The more complicate one-dimensional model (sine-lattice)with the nonlinear periodic interactionbetween nearest neighbours, similarly to eq. (1),assigned to the description of the planar ferromagnetic chain in a magnetic field, the rotational motion of CH_2 units in crystalline polyethylene and the plane-rotator model of bases in DNA macromolecule, was introduced by Takeno and Homma [8].The long wavelength limit of thementioned modelsleads to the integrable sine-Gordon equation in the systems of the infinite length [9-11]. This equation isone of the most popularnonlinear wave models, which is applicable tovarious physical systems.

The present study deals with essentially nonlinear dynamics of the discrete finite lattice with the interaction between nearest neighbours as well as the on-site potential in the form of periodic function of the torsional angle. The main goals of the study are the description of the nonlinear normal modes and the asymptotic analysis of the oscillation localization near the spectrum edges.

2 The model of torsional lattice

The ground state of the one-dimensional system with the energydescribed by eq. (1) corresponds to the “anti-ferromagnetic” configuration, when the neighbor spins are antiparallel, i.e. difference $\theta_{j+1} - \theta_j = \pi$. It is convenient to introduce new modulated variable $\varphi_j = (-1)^j \theta_j$. In such a case the ground state corresponds to $\varphi_j = 0$. If the system is under action of the external field (the magnetic one for the spin lattice or the field of the crystalline environment for the polymer crystal) energy (1)should be supplemented by the on-site potential, which depends on the local torsion angle φ_j. Let us write the Hamilton function as follows:

$$H = \sum_{j=1}^{N} \left(\frac{I}{2}\left(\frac{d\varphi_j}{dt}\right)^2 + \beta\left(1 - \cos\left(\varphi_{j+1} - \varphi_j\right)\right) + \sigma\left(1 - cos\varphi_j\right)\right), \tag{2}$$

where I is the moment of inertia, β is the coupling constant and σ is specified the action of the external field.N is the “length” of the system. It is obvious that the renormalization $t \to \sqrt{\beta/_I}\, t$ reduces the problem to the single parametric one. Therefore, in further we suppose $I = \beta = 1$.

The equations of motion corresponding to Hamilton function (2) are well known:

$$\frac{d^2\varphi_j}{dt^2} - \sin\left(\varphi_{j+1} - \varphi_j\right) + \sin\left(\varphi_j - \varphi_{j-1}\right) + \sigma \sin\varphi_j = 0. \tag{3}$$

Nonlinear normal modes In order to study the nonlinear normal modes, equations (3) should be completed the periodic boundary conditions: $\varphi_{N+1} = \varphi_1$. As it was shown [9] the adequate procedure to analyze equations (3) consists in the definition of the new complex variables:

$$\Psi_j = \frac{1}{\sqrt{2}}\left(\frac{i}{\sqrt{\omega}}\frac{d\varphi_j}{dt} + \sqrt{\omega}\varphi_j\right). \tag{4}$$

$$\varphi_j = \frac{1}{\sqrt{2\omega}}\left(\Psi_j + \Psi_j^*\right);\ \frac{d\varphi_j}{dt} = -i\sqrt{\frac{\omega}{2}}\left(\Psi_j - \Psi_j^*\right), \tag{5}$$

where ω is a unknown (yet) frequency and the asterisk marks the complex conjugated function.

Expanding the trigonometric functions into the Taylor series and taking into account expressions (5), one can rewrite equations (3) as follows:

$$i\frac{d}{dt}\Psi_j-\frac{\omega}{2}(\Psi_j-\Psi_j^{\,*})-\frac{1}{\sqrt{2\omega}}\sum_{k=0}\frac{(-1)^k}{(2k+1)!}\left(\frac{1}{\sqrt{2\omega}}\right)^{2k+1}((\Psi_{j+1}-\Psi_j+cc)^{k+1}-(\Psi_j-\Psi_{j-1}+cc)^{k+1}+$$

$$\sigma(\Psi_j+\Psi_j^*)^{k+1})=0, \qquad (6)$$

where "cc" replaces the complex conjugated terms.

We consider the stationary solution of equations (6) in the form

$$\Psi_j=\psi_j e^{-i\omega t} \qquad (7)$$

where $\psi_j=const(j)$.

Substituting expression (7) into equations (6) and multiplying the equations by factor $e^{i\omega t}$ one should integrate over the period $T={}^{2\pi}/_{\omega}$. Excluding the secular terms, we get the system of the transcendental equations:

$$\frac{\omega}{2}\psi_j-\frac{1}{\sqrt{2\omega}}\left(J_1\left(\sqrt{\frac{2}{\omega}}\left|\psi_{j+1}-\psi_j\right|\right)\frac{\psi_{j+1}-\psi_j}{|\psi_{j+1}-\psi_j|}-J_1\left(\sqrt{\frac{2}{\omega}}\left|\psi_j-\psi_{j-1}\right|\right)\frac{\psi_j-\psi_{j-1}}{|\psi_j-\psi_{j-1}|}+\sigma J_1\left(\sqrt{\frac{2}{\omega}}|\psi_j|\right)\frac{\psi_j}{|\psi_j|}\right)=0 \qquad (8)$$

where J_1 is the Bessel function of the first order.

One can be shown that functions

$$\psi_j=\sqrt{X}e^{i\kappa j};\quad \kappa=\frac{2\pi k}{N};\quad k=0,1,..N \qquad (9)$$

are the solutions of equations (8) if the frequency ω satisfies the relation

$$\frac{\omega}{2}\sqrt{X}-\frac{1}{\sqrt{2\omega}}\left(2J_1\left(\sqrt{\frac{2}{\omega}}\sqrt{X}\,sin\frac{\kappa}{2}\right)sin\frac{\kappa}{2}+\sigma J_1(\sqrt{\frac{2}{\omega}}\sqrt{X}))\right)=0. \qquad (10)$$

The dependence of the modulus of complex functions $\sqrt{X}$ on the amplitude of the oscillations Q can be determined from expression (4):

$$X=\frac{\omega}{2}Q^2. \qquad (11)$$

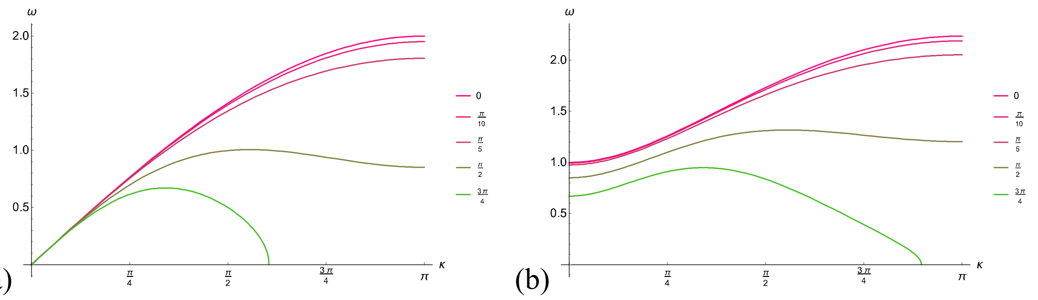
Thus, we can get the frequency ω corresponding to the wave number κ:

$$\omega^2=\frac{2}{Q}(\sigma J_1(Q)+2J_1\left(2Q sin\frac{\kappa}{2}\right)sin\frac{\kappa}{2}) \qquad (12)$$

Expression (12) shows the dispersion relation for nonlinear normal modes at the oscillations with the amplitude $Q\in[0,\pi]$. The low amplitude limit coincides with the dispersion relation for the linear system:

$$\omega^2=\sigma+4sin^2\frac{\kappa}{2} \qquad (13)$$

Fig. 1 represents the dispersion relations for the oscillations with various amplitudes.



(a) (b)

Figure 1. (a) Dispersion relations for the torsion lattice without external field ($\sigma=0$); (b) the same in the presence of the external field ($\sigma=1$). The legends show the oscillation amplitudes.

The analysis of Fig.1 shows that the oscillations with the large amplitudes are forbidden in the range of the short wavelength. It is the natural consequence of the periodicity of the intersite interactions. Really, if the difference $(\varphi_{j+1} - \varphi_j)$ exceeds the magnitude π, the interaction between neighboring spins turns out to be repulsive. Therefore, such oscillationscannot exist.

3 Long wavelength nonstationary dynamics

Equations (8) describe the nonlinear normal modes, i.e. the stationary oscillations, which are characterized by the wave number κ and the frequency ω. However, it is insufficient to describe the behavior of the essentially nonlinear system (3) because the normal modes can effectively interact under certain conditions in the contrast to the linear counterparts. It was shown that the resonant interaction of the nonlinear normal modes near the long wavelength edge of the spectrum leads to the modulation instability and the subsequent localization of the oscillations [12,13]. In order to study the non-stationary dynamics one should note that the energy of the system, corresponding to equations (8) is written as follows:

$$H = \sum_{j=1}^{N}(\frac{\omega}{2}|\psi_j|^2 + J_0\left(\sqrt{\frac{2}{\omega}}|\psi_{j+1} - \psi_j|\right) + \sigma J_0\left(\sqrt{\frac{2}{\omega}}|\psi_j|\right)), \quad (14)$$

where J_0 is the Bessel function of zero order.

One should notice that energy (14) does not depend on the time “t”, which determines the normal oscillation with frequency (13). (We will refer time “t” as the “fast time”.) However, one can assume that there is a slowly changed solutions, the non-stationarity of which is caused by the interactions between normal modes with the close frequencies. In such a case, the slowness of the amplitude variation is determined by difference of the modal frequencies. (One should notice, that the slowness of the changes does not mean their smallness.) In order to study the non-stationary dynamics, let us consider energy (14) as the Hamilton function for some system, the specific time scale of which is governed by the value of frequency detuning $\tau \sim 1/\Delta\omega$. We will refer this time as the “slow”. The equations of motion can be obtained from expression (14) as follows:

$$\frac{\partial \psi_j}{\partial \tau} = -\frac{\partial H}{\partial \psi_j^*}$$

The result is given by the equations:

$$i\frac{\partial \psi_j}{\partial \tau} + \frac{\omega}{2}\psi_j - \frac{1}{\sqrt{2\omega}}\left(J_1\left(\sqrt{\frac{2}{\omega}}|\psi_{j+1} - \psi_j|\right)\frac{\psi_{j+1}-\psi_j}{|\psi_{j+1}-\psi_j|} - J_1\left(\sqrt{\frac{2}{\omega}}|\psi_j - \psi_{j-1}|\right)\frac{\psi_j-\psi_{j-1}}{|\psi_j-\psi_{j-1}|} + \right.$$
$$\sigma J12\omega\psi j\psi j\psi j=0 \quad (15)$$

So, equations (15) describe the slow evolution of the system oscillations caused by the nonlinear normal modes’ interaction. For the large system $(N \gg 1)$ the long wavelength approximation leads to the linear equations at the absence of the external field $(\sigma = 0)$. Actually, in the framework of the long wavelength approximation we can write:

$$\psi_j = \psi\,;\psi_{j\pm1} \approx \psi \pm h\frac{\partial \psi}{\partial x} + \frac{h^2}{2}\frac{\partial^2 \psi}{\partial x^2} \quad (16)$$

where h is the lattice constant and $x = h\,j$.

Substituting expressions (16) into equations (15) and expanding the Bessel function into series, we get

$$i\frac{\partial \psi}{\partial \tau} + \frac{\omega}{2}\psi - \frac{h^2}{2\omega}\frac{\partial^2 \psi}{\partial x^2} = 0 \quad (17)$$

One can see that the stationary version of equation (17) $(\psi = const)$ leads to the linear normal mode with the dispersion relation $\omega \sim \kappa = \frac{2\pi\, k}{Nh}$ and the non-stationary solution $\psi = \sqrt{X}e^{i(\omega\tau - \kappa x)}$ shows the corrections to the mode with wave number κ, caused by a small frequency detuning$\Delta\omega$ ($\omega\tau = \omega\frac{\Delta\omega}{\omega}t = \Delta\omega\, t$). Such oscillations can be realized in the linear system under the respective initial conditions.

If the external field cannot be neglected ($\sigma \neq 0$), equations (15) keep the nonlinearity anywhere outside the small-amplitude approximation. It was shown [9, 12] that in the discrete systems, the resonant interaction of the nonlinear normal modes near long wavelength edge of the spectrum lead to the modulation instability of the uniform mode ($\kappa = 0$) and subsequent localization of the oscillations. The analysis has been restricted by two-mode approximation, in the framework of which we can describe a weak localization – the capture of the oscillation in one half of the chain ("coherent domain" [9]).On the other hand, the localized solutions for the discrete nonlinear systems (3) is not known. Therefore, it is difficult to compare the predictions of the asymptotic analysis.

As it was mentioned above, the long wavelength approximation for equations (3) leads to the sine-Gordon equation, the exact breather solutions of which have been obtained by the inverse scattering method [14,15]. Therefore, it is important the results of the asymptotic procedure discussed with the exact breather solution.

The long wavelength approximation of equations (15) for the large system leads to theequation in the form

$$i\frac{\partial\psi}{\partial\tau} + \frac{\omega}{2}\psi - \frac{h^2}{\sqrt{2\omega}}\frac{\partial^2\psi}{\partial x^2} - \sigma J_1\left(\sqrt{\frac{2}{\omega}}|\psi|\right)\frac{\psi}{|\psi|} = 0 \qquad (18)$$

In order to analyze this equation, we introduce the polar representation of complex function ψ:

$$\psi(x,\tau) = a(x,\tau)e^{i\theta(x,\tau)} \qquad (19)$$

Substituting expression (19) into equation (18) and separate the real and imaginary parts, we get the equations:

$$-a\frac{\partial\theta}{\partial\tau} - \frac{h^2}{2\omega}\left(\frac{\partial\theta}{\partial x}\right)^2 a + \frac{h^2}{2\omega}\frac{\partial^2 a}{\partial x^2} + \frac{1}{2}\omega\, a - \sigma\frac{1}{\sqrt{2\omega}}\mathrm{J}_1\left(\sqrt{\frac{2}{\omega}}a\right) = 0 \qquad (20.1)$$

$$\frac{\partial a}{\partial\tau} + \frac{h^2}{\omega}\frac{\partial a}{\partial x}\frac{\partial\theta}{\partial x} + \frac{h^2}{2\omega}a\frac{\partial^2\theta}{\partial x^2} = 0 \qquad (20.2)$$

Let us introduce the traveling-wave coordinate $\zeta = x - V\tau$. Multiplying equation (20.2) by 2a and integrating it once, we get:

$$-Va^2 + \frac{h^2}{\omega}a^2\theta' = C \qquad (21)$$

where C is the integration constant and the prime denotes the derivative with respect to ζ.

If C=0 next relation is valid

$$\theta' = \omega V = const.$$

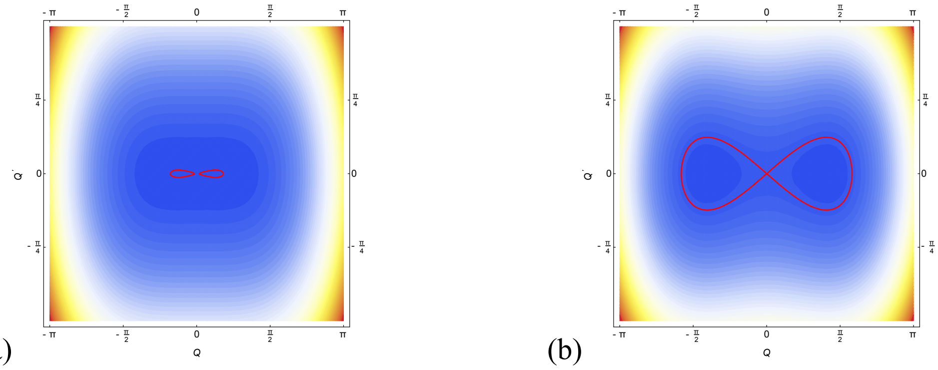
Taking into account this relation, one can rewrite equation (20.1) as follows:

$$\frac{h^2}{2\omega}\frac{\partial^2 a}{\partial x^2} + \frac{1}{2}\omega(1+V^2)\, a - \sigma\frac{1}{\sqrt{2\omega}}\mathrm{J}_1\left(\sqrt{\frac{2}{\omega}}a\right) = 0 \qquad (22)$$

The latter admits the first integral as follows:

$$\frac{1}{2}Q'^2 + \frac{1}{2}\omega^2(1+V^2)Q^2 + 4\sigma\mathrm{J}_0(Q) = E \qquad (23)$$

where $E = const$ and the modulus of complex function a is replaced by the oscillation amplitude $Q = \sqrt{\frac{2}{\omega}}a$. Equation (23) allows us to analyze the phase portrait of the system at various values of parameters ω and V. Some particular cases for the V=0 are shows in Fig.2.



(a) (b)

Figure 2. Phase portraits of system (23) at two values of the oscillation frequency: (a) $\omega = 0.99$, (b) $\omega = 0.95$. $\sigma = 1, V = 0$. The red homolinic separatrix corresponds to the breather.

In Fig. 2 the red curves correspond to the envelope solitons (breathers) at the constant $E = 0$. One can see that the amplitude of the breather is diminished essentially when the carrier frequency ω approaches to the unity. The breather amplitude becomes equal to zero, when the frequency reaches the gap value ($\omega_g = \sqrt{\sigma}$). The latter corresponds to the well-known fact that the breather are the gap solutions.

The exact breather solutions for the sine-Gordon equation can be written as follows:

$$\varphi = 4 \arctan \left[\tan \mu \frac{\sin (t\, cos\mu)}{\cosh (x\, sin\mu)}\right] \tag{24}$$

where 4μ is the breather's amplitude, $cos\mu = \omega$ – internal (carrier) breather's frequency and $sin\mu$ determines the breather's width (we assume $\sigma = 1$ and V=0).

In spite of that we have not analytical solution for equation (23), the breather's amplitude can be estimated numerically. Fig. 3 shows the comparison of the amplitudes of exact solutions (24) (blue solid curve) and numerically estimated by equation (23) (red dashed curve). One can see the accordance between exact and asymptotic data is well enough ($\leq 3\%$) in a wide range of frequency ω.

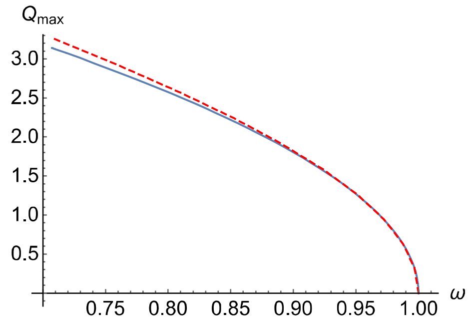


Figure 3. Comparison of the breather's amplitude (Q_{max})calculatedwith the exact solution (24) and asymptotic equation (23) (blue solid and red dashed curves, respectively).

4 Conclusions

The analysis of the torsion lattices performed above allows us to reveal the essential peculiarities of the torsion dynamics of the discrete systems at the large amplitudes of the oscillations. The analytical representation for the nonlinear normal modes and the frequencies of the normal oscillations have been obtained for the lattices under effect of the external field as well as without it. The decreasing the oscillation frequencies with a growth of the oscillation amplitude leads to the formation of the forbidden band, where the normal modes cannot exist. The analytical results are in a good accordance with the data of the numerical simulation of the torsion lattices of the various lengths.

We studied the nonlinear interaction of the normal modes near the edges of the spectrum of the discrete systems. In the long wavelength limit this interaction leads to the localization of the oscillation energy in some domain of the chain, if the oscillation amplitude exceeds some threshold value. In the chain of the infinite length such capture of the oscillations leads to the creation of breathers. The nonlinear Schrodinger equation for the chain of the infinite length have been obtained as the continuum limit of the discrete system equations. It can be considered as the complex representation of the sine-Gordon equation.
One should mention that the analysis performed above allows us to reveal the peculiarities of the torsion dynamics, which can be significant from the viewpoint of the understanding physical processes taking place in the dipole (spin) lattices, single molecules and crystals of the flexible polymers and biopolymers. The modern nanotechnologies are based on the fundamental properties of the single molecules and nanostructures. Therefore, the results obtained above can give very useful information for the development of the nano electro-mechanical resonators and other devices.

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