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LOCALIZATION OF BENDING VIBRATIONS IN THE SINGLE-WALL CARBON NANOTUBES

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The main result of this work is that the small-amplitude long wavelength bending oscillations of carbon nanotubes (CNT) become localized ones if the intensity of initial excitation exceeds some threshold which depends on the CNT length. This localization results from the intensive resonant interaction of zone-boundary and nearest modes in the weakly nonlinear regime that leads to loss of stability of the zone-boundary mode as to the first step. The further development of resonant interaction leads to effective confinement of energy in the part of the system only. We study this process in the terms of Limiting Phase Trajectories and demonstrate the usefulness of transition from "modal" to "effective particles" representation for description of the system under consideration. We also show that the similar tendency to localization of oscillation is the common property of the systems, the eigenvalue spectra of which are non-equidistant ones near their edges.

Keywords: carbon nanotubes, bending, nonlinear energy localization.

1. Introduction

The carbon nanotubes (CNTs) are of great interest not only as the objects that can have large potential use in nanotechnology processes and devices, but also as ideal model systems to check the many physical principles. This work deals with the analysis of localization of bending vibrations of single-walled carbon nanotubes. Such an analysis has to demonstrate both a new phenomenon – localization of bending vibrations of CNTs – and the efficiency of the used approach for description of specific strongly nonlinear behavior which cannot be adequately understood in terms of nonlinear normal modes.

2. The model

To consider the nonlinear localization of CNTs vibrations we should to reduce the description of CNT to that of some effective one-dimensional system. Keeping in mind this objective we consider a single-wall carbon nanotube of a finite length and cut it ideally into the N rings by planes which are perpendicular to the tube axis (Fig. 1). The actual choice of the ring width has to reflect the real properties of the CNT (in particularly, its chirality). From the other side the width has not to be too large, because the deformation of the ring along the axis is regarded as a constant one.

It is known that the mechanical properties of single-wall carbon nanotubes are well described within the continuum approach, when the tube is replaced by a cylinder shell with an effective thickness δ. In this framework the potential energy of the CNT can be represented as the sum of deformation energy of the individual rings

$$U_n = \int_0^{2\pi} \left[\frac{1}{2} ESR\varepsilon^2 + \frac{1}{2} EJR\kappa^2 \right] d\theta \qquad (1)$$

and the interaction energy between neighbor rings, which should be described as

$$V_n = \int\limits_0^{2\pi} \left[\frac{1}{2}EJ'R\kappa_{||}^2 + \frac{1}{2}E\varepsilon_{||}^2\right] d\theta \tag{2}$$

Here ε is the deformation of the contour length, κ is the flexural deformation of the ring (curvature), $\kappa_{||}$ is the bending strain along the tube axis, $\varepsilon_{||}$ is the longitudinal strain (along the tube axis), E, J, J' is Young's modulus, moment of inertia of the ring and the moment of inertia in the plane passing through the axis of the tube, $S = R\delta$ is the effective square of the element of the section of the ring. Because we deal with the small-amplitude vibrations, the energy of the Van der Waals interactions is negligible. To obtain the total potential energy of the CNT we should sum the expressions $(1, 2)$ along the tube axis.

One of the main types of nanotube deformation is bending one. In particular, the action of concentrated external forces which are perpendicular to the axis of the CNT leads to a strain that can be represented as a pure bending in the plane perpendicular to the axis of CNTs in combination with a bend along the cylinder. In the first approximation we can ignore the deformation of the middle surface and consider only the bending deformation. (Accounting for the average tensile strain of the surface somewhat complicates the calculations but does not lead to qualitatively new results.) Thus, the observed deformation is a combination of two modes along the CNT axis (a homogeneous deformation with the wave vector $k_z = 0$ and the mode with $k_z = 2\pi/N$), the ring being changed its form into elliptical one (see Fig. 1).

Then we can characterize the deformation of carbon nanotubes by a single variable – the amplitude of the elliptical deformation. Indeed, assuming that the bending strain in each section of the CNT is presented as $X\cos 2\theta$, where θ – the azimuth angle, and X – the amplitude, after integration over the angle θ, we obtain the following expression for the strain energy:

$$U_{tot} = \pi \sum_{n=1}^{N} \left[\frac{1}{2}EJR\kappa_n^2 + \beta\kappa_n^4 + \frac{1}{2}EJ'\kappa_{||,n}^2\right], \tag{3}$$

$$\kappa_n = \frac{X_n}{R}, \quad \kappa_{||,n} = \frac{X_{n+1} - 2X_n + X_{n-1}}{R}, \tag{4}$$

where κ_n is the deformation of the n-th ring and $\kappa_{||,n}$ – corresponds to inter-ring interaction. The strain energy (3) contains also the anharmonic terms ($\sim \beta\kappa_n^4$), which must be taken into account when calculating the dynamics of carbon nanotubes. First of all, it concerns to the vibrations of the ring profile. From symmetry considerations it follows that the anharmonic contribution is the fourth-order strain. Its exact form can be derived directly from the atomic interaction potentials. When the flexural deformation of the ring contour occurs, the main part of the deformation energy corresponds to angular component of interatomic potentials, which is characterized by the nonlinearity of soft type. So the coefficient β should be negative.

It is easy to see that the potential energy in the form of (3) reduces the problem of small-amplitude oscillations of carbon nanotubes to a system of ordinary differential-difference equations for the variables X_n. The significant characteristic feature of the eigenvalue spectrum of such a system is the existence of a gap determined by the bending oscillations of the ring with a frequency $\omega_2 \sim EJR/a^2$, where a – "lattice constant", i.e. effective width of the ring, and the second one – the spectrum crowdling near its edges corresponding to the wave numbers $k_z = 0$ and $k_z = \pi$.

$$\omega^2 = \omega_0^2 + 16c^2 \sin^4 \frac{k_z}{2}, \quad \omega_0^2 = \frac{\pi EJR}{a^2}; \quad c^2 = \frac{\pi ERJ'}{a^2}$$

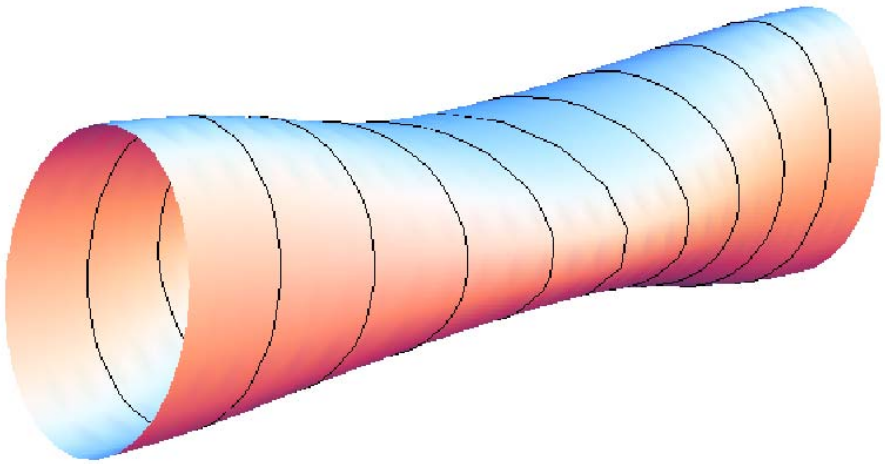


Fig. 1. CNT under external forces applied in the center of CNT in the direction which is perpendicular to the tube axis. Thin lines show the boundaries of the effective rings

Such peculiarities of the spectrum make it to be similar to that of the one-dimensional chain (involving longitudinal bonds), on an elastic support (i.e. the model of the Klein-Gordon or the Frenkel-Kontorova). A similar model with periodic boundary conditions was recently considered by us [1], where the asymptotic analysis of the equations of motion was discussed in detail. It was shown that while the amplitude of excitation increases the significant role of resonant interaction between closely spaced modes can be revealed (it relates especially the interaction between zone-boundary mode and the nearest to it). In the present case it corresponds to the modes with wave numbers $k_z = 0$ and $k_z = 2\pi/N$ along the CNT , which describe the deformation of carbon nanotubes as a result of the excitation (Fig. 1). The influence of resonant interaction of non-linear normal modes leads to a loss of stability of the boundary mode ($k_z = 0$), and eventually to the emergence of the energy localization in the system. Qualitatively, this process can be described as follows: a resonant interaction of two closely spaced modes with small amplitudes leads to periodic redistribution of energy with a characteristic time which is inversely proportional to the frequency difference. This process can be naturally regarded as the beats between the "effective" particles, each of which contains about half of the system's atoms. Such a behavior is specific for the harmonic system, where the period does not depend on the amplitude. The effect of nonlinearity leads to the nonlinear beats. At a certain critical level of excitation the zone-boundary mode becomes unstable in the systems with soft nonlinearity ($\beta < 0$). The loss of stability of the boundary mode leads to the emergence of new stationary solutions and a separatrix passing through the unstable stationary point. At the same time the behavior of the trajectories corresponding to the beats remaines without qualitatively changes. The fundamental change occurs when the excitation energy reaches the value, at which the energy of the beating becomes equal to that of the separatrix. In this case, the beats in the system are generally prohibited and the energy is "trapped" in the domain of initial excitation. Of course, such localization covers large areas corresponding approximately to a half of the chain (in the framework of two-mode approach, we have not the tools to describe a higher degree of localization, because it requires a participation of the shorter nonlinear modes). Therefore, we have a qualitative picture, so to say the manifestation of the nucleing of the localization, that clarifies the origin of the breathers formation. As the result of computer simulations, we can accurately estimate in this model the threshold of localization, and the profile of the localized

solutions. The energy contribution ot other modes to this process does not usually exceed 10-20% of the initial excitation energy.

The procedure for analysis of dynamic equations and the determination of thresholds in the asymptotic approach are discussed in detail in [1, 2]. In this case, we want to obtain an estimate of the localization threshold, without resorting to complex analytical calculations. We represent the variable X_n as a combination of the two modes (this representation adequately describes the deformation of CNTs, as it is shown in Fig. 1):

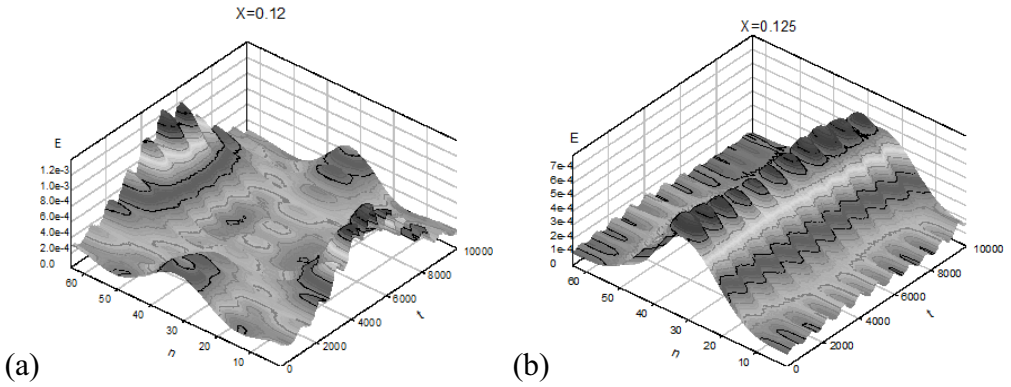
$$X_n(t) = \chi_0(t) + \chi_1(t)\cos\frac{2\pi n}{N} \tag{5}$$

where $\chi_0(t)$ and $\chi_1(t)$ are the amplitudes of the modes, which are the periodic functions with period $2\pi/\omega_0$ and $2\pi/\omega_1$ in the harmonic limit; ω_0 and ω_1 – the smallest eigenvalues (see (4)). However, the above-mentioned "effective particles" are described by a linear combination of normal modes:

$$\varphi_1 = \frac{\chi_0 + \chi_1}{\sqrt{2}}, \quad \varphi_2 = \frac{\chi_0 - \chi_1}{\sqrt{2}}, \tag{6}$$

and each of the "effective particles" corresponds to specific function φ. For these variables, the total "number of excitations" $Y = |\varphi_1|^2 + |\varphi_2|^2 = |\chi_0|^2 + |\chi_1|^2$ is preserved. As it becomes apparent from expression (6), the beats realizing the energy transfer from one "effective particle" to another correspond to transition from one "pure" state (in the terms of effective particles φ_j) to another "pure" state, while the zone-boundary normal mode corresponds to some "mixed" state. The "pure" states bound the attraction domains of χ_0 and they are the limiting phase trajectories (LPTs) [1]. The cessation of energy transfer from one "effective" particle to another one occurs when the energy of "effective" particles becomes equal to that of normal mode χ_0. At that the LPT coincides with the separatrix that leads to the prohibition of the transition from "particle" φ_1 to the "particle" φ_2. After substitution of expressions (5)–(6) into (3) and performation of some simple algebra we obtain the expression for threshold level of excitation:

$$|\chi_0|^2 + |\chi_1|^2 = \frac{4N(\omega_0^2 - \omega_1^2)}{3\beta} \sim -\frac{64N\sin^4\frac{\pi}{N}}{3\beta} \sim -\frac{1}{\beta N^3}, \quad (\beta < 0) \tag{7}$$



(a) (b)

Fig. 2. 3D surface of energy distribution in the CNT with $N = 64$: (a) before and (b) after localization threshold. The beating corresponds to energy transfer from the central part of CNT ("particle" φ_1) to the edge parts of it ("particle" φ_2) and inversely. When the localization occurs the energy is confined in the central part of the CNT. n is the ring number; the time t is measured in the periods of zone-boundary mode $T_0 = \dfrac{2\pi}{\omega_0}$

The above estimates (7) (with an accuracy about 10%) are in a good accordance with the threshold of localization observed in computer simulations (Fig. 2). In the following example, the numerical estimate of the threshold amplitude according to (5) gives a value of $\chi_0 = \chi_1 \sim 0.1258$ while the localization is observed even at $\chi_0 = \chi_1 \sim 0.1258$.

3. Conclusion

The brief qualitative analysis of the bending vibrations of CNT allows us to reveal the origin of non-linear behavior of the system under consideration. First of all, we observed the new nonlinear modes, which do not exist in the linear system and are created from the resonant interaction of the normal modes. The accurate asymptotic analysis which is similar to that made in [1, 2] leads to the clear manifestation of new normal modes. The transformation of the phase space originated from these new modes appearence leads to topological structure of phase space with some domains corresponding to the states with energy localization. We describe adequately the transition from intensive energy exchange between "pure" bending states to energy localization in terms of LPTs. And finally, the comparison with the previous papers [1, 2] allows us to conclude that such a behavior is a specific one for the system with unstable zone-boundary mode and the non-equidistant spectrum of linearized system. We suppose that the approach developed in the paper will be useful for investigations of the nonlinear systems of very different nature.

References

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