2015 International Symposium on Nonlinear Theory and its Applications
NOLTA2015, Kowloon, Hong Kong, China, December 1-4, 2015

Dynamics of Discrete Breathers in Carbon Nanotube

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Abstract—In this talk, we propose numerical method for investigating dynamics of discrete breathers (DBs) in carbon nanotube (CNT) by molecular dynamics (MD) based simulations. Method for Numerical precise periodic solutions of DBs are derived in various geometrical configurations of CNTs such as zig-zag CNTs and armchair CNTs. Linear stability of DB is also investigated numerically.

1. Introduction

Recently, discrete breathers (DBs) or intrinsic localized modes (ILMs)[1] have attracted great interests in the field of nonlinear physics, material science and mechanical engineering[2, 3]. DB is a time-periodic solution which has localized structure. Discreteness of the system and nonlinearity between elements in the system support such a structure, since nonlinearity supports the vibration out of dispersion band which is limited in finite ranges of frequency due to the discreteness of the system. It has been known that DB can be exited in a wide range of theoretical lattice model such as Fermi-Pasta-Ulam (FPU) β lattice, discrete nonlinear Klein-Gordon (NKG) lattice and discrete nonlinear Schrödinger system. In these systems, existence, structure and stability of DB have been investigated. It should be noted that existence of DB is not require special property except nonlinearity and discreteness. Therefore DB can be excited whether considering system is integralable or not. This means that DB can be excited in a wide range of physical systems. Recently it has been reported that DB can be excited in various physical systems such as micro-[4] and macro-[5] mechanical systems, magnet-mechanical systems[6] and optical systems[7].

One of the promising physical systems in which excitation of DB is expected is crystal structure. In a microscopic view, crystal structure is just a discrete structure of atoms. Usually, interaction between atoms is considered as linear interaction. However, in the case of large deformation of materials and dynamics of atoms in large amplitude, interaction between atoms can be described as nonlinear function. Therefore in these situation, nonlinearity and discreteness become dominant in dynamics of the system. Discreteness of crystals appears in dispersion bands in phonon dispersion relation. Nonlinearity of crystal leads to excitation of vibration of higher or lower frequency of dispersion band. Therefore DB can be excited as atomic vibration in a region of a few atomic length.

There have been a lot of reports on DB in crystals. In early stage, one-dimensional lattice with a realistic model potential is considered. Kiselev has been investigated DB in a one-dimensional lattice with Born-Mayer-Coulomb potentials[8]. Cuevas has been reported interaction of DB with defects in a one-dimensional lattice with Morse potentials[9]. DBs in more complex crystals, such as two dimensional hexagonal systems with Lennard-Jones potential[10], and three dimensional bcc metals with EAM potential[11] has been also investigated by using molecular dynamic (MD) method.

Carbon structure such as carbon nanowire, graphene and carbon nanotube (CNT) has been attracted significant interests since they have special characteristics in mechanics, electrics and vibrations other than previous carbon compounds such as diamonds and graphite. It is also expected that DB can be excited in these carbon structures. Yamayose has been reported that DB can be excited in graphene from modulational instability[12]. DB is excited in three directions which can be corresponds to direction of bond of hexagonal lattice. Kinoshita has been reported that DB can be excited in CNT by the same way of graphene[**?**]. Lifetime of DB in CNTs depends on its chirality, since curvature along to circumference affect on stability of DBs. Linear stability of DB in graphene has been investigated numerically by Doi[14]. In there report, stability depends on strain enforced in graphene and unstable perturbation mode sometimes forms shear motion against the motion of DB. This result imply that DB in graphene becomes trigger of the deformation or rearrangement of structure of atoms. Shimada have performed direct simulation of dynamics of DB in strained CNT[15]. In their simulations, DB in the strained CNT becomes a trigger of Stone-Wales transformation, which transforms four hexagons into two pentagons and two heptagons.

In this study, we investigate the dynamics of DB in CNT from the view point of linear stability and direct simulation by MD method. MD method is a powerful tools for investigating deformation of materials. MD is performed by direct integration of equation of motion which is estimated by the heuristic model potential describing the interaction between atoms. We couple the MD method with linear stability analysis based on nonlinear dynamics. At first, we search localized solution in CNT by a iteration method coupled with MD method. Then we investigate linear stability

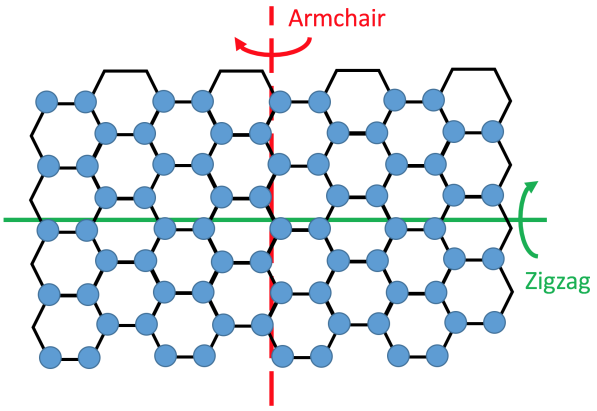

Figure 1: Schematic description of formation of CNT from graphene.

of DB in CNT. Detailed procedure is described in the following sections.

2. Models

We consider two types of CNT with different structure: armchair CNT and zigzag CNT. Fig. 1 shows schematic description of structure of armchair CNT and zigzag CNT. CNT can be formed by rolling the graphene. Difference of structure between armchair CNT and zigzag CNT is due to difference of direction of rolling. As a result of difference of direction of rolling, armchair CNT has bonds which is parallel to circumference of CNT. Zigzag CNT, on the other hand, has bonds which is parallel to the rolling axis.

CNT consists of carbon atoms. We use the heuristic interaction potential for hydrocarbon atoms proposed by Brenner. Brenner potential is described as follows:

$$H = \sum_{i}^{N} \sum_{\alpha} \frac{(p_i^\alpha)^2}{2M} + \frac{1}{2} \sum_{i}^{N} \sum_{j \neq i}^{N} \sum_{k \neq i,j}^{N} \Phi_{ijk}(r_{ij}, r_{jk}, \theta_{ijk}), \quad (1)$$

where N is the number of atoms in the system, α is the coordinates x, y and z, i, j and k are the indices of the atoms, M is the mass of carbon atom, p_i^α is the momentum of i-th atom in α coordinate, Φ_{ijk} is interaction potential, $r_{ij} = \sqrt{\sum_\alpha (q_j^\alpha - q_i^\alpha)^2}$ is bond length of between i-th and j-th atoms, θ_{ijk} is the angle between bond $i-j$ and bond $i-k$, q_i^α is the position of i-th atom in α coordinate. The function Φ_{ijk} is determined from the mechanical properties of hydrocarbon crystal.

CNT is placed in the simulation region such that rolling axis of CNT is parallel to the z-axis. Periodic boundary conditions for x-, y- and z-axis is considered. Length of simulation cell in x- and y-axis is wide enough to effect from mirroring simulation cell is negligible. In z-axis, CNT is connected at boundary.

We consider the condition for very low temperature. Atoms except for DB is excited are at rest. Energy conservation in the system is also considered. Therefore, any heat bath is not connected to the system.

3. Simulation

We investigate the dynamics of atoms in CNT by MD method. Equations of motions for i-th atom is given as follows:

$$\dot{q}_i^\alpha = \frac{\partial H}{\partial p_i^\alpha} \quad (2)$$

$$\dot{p}_i^\alpha = -\frac{\partial H}{\partial q_i^\alpha}. \quad (3)$$

We integrate these equations of motion numerically. The integration method is 4-th order symplectic integration method. As discussed in the above section, we do not consider any heat bath to the system since we consider energy conservation dynamics. MD method also used in the calculation of temporal evolution in iteration method and linear stability analysis.

We also investigate numerically exact solution of DB in graphene. Consider a state in the phase space $\mathbf{X}_0 = \{q_1^x, q_1^y, q_1^z, q_2^x, \ldots, q_N^z, p_1^x, p_1^y, p_1^z, p_2^x, \ldots, p_N^z\}^T$. Temporal evolution from $\mathbf{X}_0$ is described by the equation of motion (2)-(3). Let $\mathbf{V}(\mathbf{X})$ be a vector field defined as follows:

$$\mathbf{V}(\mathbf{X}) = \mathcal{A}_T(\mathbf{X}) - \mathbf{X}, \quad (4)$$

where $\mathcal{A}_{t'}$ is a map defined as follows:

$$\mathcal{A}_{t'}\mathbf{X} = \mathbf{X}(t + t'). \quad (5)$$

If $\mathbf{X}_0$ is on the periodic orbit in period T in the phase space. The following relation holds,

$$\mathbf{V}(\mathbf{X}_0) = \mathcal{A}_T(\mathbf{X}_0) - \mathbf{X}_0 = \mathbf{0}. \quad (6)$$

When we consider a small error $\delta\mathbf{X}$ around $\mathbf{X}_0$, we obtain the difference δX for the Newton-Raphson method by using Taylor expansion for vector filed,

$$\delta\mathbf{X} = -(\partial\mathcal{A}(\mathbf{X}_0) - \mathbf{I})^{-1}\mathbf{V}(\mathbf{X}_0), \quad (7)$$

where $\partial\mathcal{A}(\mathbf{X}_0)$ is a tangent map. The tangent map $\partial\mathcal{A}(\mathbf{X}_0)$ can be calculated numerically by solving the linearized equation of (2)-(3) with initial conditions which have only nonzero component. Main periodic orbit which appears in coefficient in the linearized equation can be estimated from the numerical results for MD method. Therefore, Newton-Raphson method for the DB in CNT is constructed by the following procedure:

1. Calculate the temporal evolution of the orbit in the phase space from a initial guess X by numerical integration of equation of motion (2)-(3) by MD method.

2. Evaluate the vector field (4). If $\mathbf{V}(\mathbf{X})$ is small enough. The initial guess is numerically exact solution of DB.

3. If $\mathbf{V}(\mathbf{X})$ is not small enough, we construct a tangent map $\partial\mathcal{A}(\mathbf{X})$ by integrating the linearized equation of motion on the periodic orbit calculated in procedure 1.

4. Calculate the correct vector (7) and update the initial guess from $\mathbf{X}$ to $\mathbf{X} + \delta\mathbf{X}$.

We also investigate linear stability of the obtained numerically exact solution of DB in CNT. Once numerically exact solution is obtained, linearized equation of motion around the solution is obtained,

$$\dot{\xi}_i^\alpha = \sum_{(j,\beta)\neq(i,\alpha)} \left.\frac{\partial^2 H}{\partial p_i^\alpha \partial q_j^\beta}\right|_{\mathbf{X}_{DB}} \xi_j^\beta + \sum_{j,\beta} \left.\frac{\partial^2 H}{\partial p_i^\alpha \partial p_j^\beta}\right|_{\mathbf{X}_{DB}} \eta_j^\beta \tag{8}$$

$$\dot{\eta}_i^\alpha = -\sum_{(j,\beta)\neq(i,\alpha)} \left.\frac{\partial^2 H}{\partial q_i^\alpha \partial q_j^\beta}\right|_{\mathbf{X}_{DB}} \xi_j^\beta - \sum_{j,\beta} \left.\frac{\partial^2 H}{\partial q_i^\alpha \partial p_j^\beta}\right|_{\mathbf{X}_{DB}} \eta_j^\beta, \tag{9}$$

where ξ_i^α and η_i^α are perturbations around q_i^α and p_i^α, respectively.

Consider that the numerically exact solution of DB has period T. Coefficient of Eq.(8)-(9) is T-periodic. Therefore, Eq.(8)-(9) is rewritten as follows:

$$\dot{\mathbf{Y}} = \mathbf{C}\mathbf{Y}, \tag{10}$$

$$\mathbf{C}(t) = \mathbf{C}(t+T), \tag{11}$$

where $\mathbf{Y} = \{\xi_1^x, \xi_1^y, \xi_1^z, xi_2^x, \ldots, \eta_N^z, \eta_1^x, \eta_1^y, \eta_1^z, \eta_2^x, \ldots, \eta_N^z\}^T$. It is known that equation of motion (10) with T-periodic coefficient matrix (11) has temporal evolution with following linear relation:

$$\mathbf{Y}(t+T) = \mathbf{M}(T)\mathbf{Y}(t). \tag{12}$$

The matrix $\mathbf{M}(T)$ is known as the monodromy matrix. The monodromy matrix gives information of linear stability of the periodic solution. By solving eigenvalue problem of $\mathbf{M}(T)$

$$\mathbf{M}(T)\mathbf{Y}_n = \sigma_n \mathbf{Y}_n, \tag{13}$$

we obtain the growth rate of the perturbation and the pattern of corresponding perturbation mode $\mathbf{Y}_n$. Using the result of eigenvalue problem, an arbitrary perturbation $\mathbf{Y}(t)$ is decomposed into

$$\mathbf{Y}(t) = \sum_n a_n(t)\mathbf{Y}_n, \tag{14}$$

where $a_n(t)$ is amplitude of n-th component of the perturbation. Using (12)-(14), temporal evolution of perturbation after one period of DB vibration is given as follows:

$$\mathbf{Y}(t+T) = \sum_n a_n(t)\sigma_n \mathbf{Y}_n. \tag{15}$$

Eq.(15) indicates that if $|\sigma_n| > 1$, corresponding perturbation mode grows during vibration. Therefore DB is unstable if there exists eigenvalues of the monodromy matrix with $|\sigma_n| > 1$. The system under consideration is Hamilton system. In this case, if σ_n is an eigenvalue, $1/\sigma_n$ is also eigenvalue. Therefore, the obtained DB is stable only if all eigenvalues $|\sigma_n| = 1$.

Monodromy matrix can be constructed numerically. Consider $3N$-vectors $\mathbf{d}_n$ as

$$\begin{aligned} \mathbf{d}_1 &= \{1,0,0,\ldots,0\}^T \\ \mathbf{d}_2 &= \{0,1,0,\ldots,0\}^T \\ &\vdots \\ \mathbf{d}_{3N} &= \{0,0,0,\ldots,1\}^T. \end{aligned} \tag{16}$$

Then we calculate temporal evolution during T of Eq.(8)-(9) from initial conditions (16). The monodromy matrix is obtained by arranging obtained vectors which describe the solution of $t = T$ of Eq.(8)-(9).

4. Conclusion

Using the proposed method, we can investigate numerical precise solution of DB in CNT. Adding to this, linear stability is also investigated using the method which is coupling method MD and stability theory. Some numerical results will be discussed in the presentation.

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