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Structure and Stability of Nonlinear Vibration Mode in Graphene Sheet

Yusuke Doi*, Akihiro Nakatani

*Department of Adaptive Machine Systems, Graduate School of Engineering, Osaka University
2-1 Yamadaoka, 565-0871 Suita, Japan

Abstract

Energy localization due to nonlinearity of atomic interactions in a graphene sheet is investigated. In nonlinear lattices, localized vibrational modes called discrete breather (DB) or intrinsic localized mode (ILM) exist. We search the DB in a graphene sheet as a periodic solution with larger frequency than phonon modes by a procedure combining the Newton-Raphson method and molecular dynamics (MD) method. We obtain long-alive vibrational modes. Some characteristics of the localized mode such as spatial structure, amplitude and vibrational frequency are discussed. Adding to this, we investigate the linear stability of the DB solutions by numerical analysis based on Floquet theory of periodic solutions. Dynamical instability of the vibrational mode is observed by MD simulations, which may lead to change of the structure of DB.

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1. Introduction

When we consider dynamics of large amplitude motion of systems, we find that nonlinearity of the system plays an important role in this dynamics. Nonlinearity can produce various phenomena in various systems, i.e., solitons in fluids, fluttering in structures and pattern formation in chemical reactions. Discrete breather (DB) or intrinsic localized mode (ILM) has attracted extensively interests in various fields[1] as nonlinear dynamics of discrete systems. DB is a time-periodic and space-localized structure in the nonlinear discrete systems. DB can be excited due to discreteness of the systems and nonlinearity of interaction between particles of the system. Frequency of vibration of particles in which DB is excited is usually larger than that of the linear eigenmode. DB can be excited in not only theoretical system such
as Fermi-Pasta-Ulam (FPU) β lattice, but also various realistic systems such as optical lattices, microcantilever arrays, and Bose-Einstein condensations (BEC)[2].

When we consider the vibration of atoms in crystal, the atomic systems can be regarded as a discrete system. In the case of vibration of small amplitude, linear approximation is valid. Vibration phenomena can be described as a combination of the linear modes within the phonon band in this approximation. However, in the case of the vibration with large displacement, nonlinearity of the interaction between atoms becomes dominant. In this case, atomic lattice can be regarded as nonlinear lattice. Therefore DB can be excited as vibration with large amplitude in crystal.

Molecular dynamics (MD) method is powerful method for investigating dynamics of solids in atomic scales, in which motion of all atoms is tracked by solving newton’s equations of motion. Interaction force acting on atoms is modeled heuristically. Some studies about DB in crystal have been done by molecular dynamics (MD) simulations. Marin et.al. has been studied mobile DBs in two dimensional Lenard-Jones lattices[3]. Excitation in static DB in two-dimensional graphene sheet[4], and carbon nanotubes[5] has been also studied. In these studies, energy localizations are excited after relaxation from particular phonon mode. The energy localizations survive in a finite lifetime.

DBs obtained by MD can become unstable during temporal evolution as due to thermal fluctuations from surrounding atoms. Numerical solution of DB in crystals is useful for studying structure and stability of DB in detail. In this study, we propose the numerical method combining MD and iteration method for obtaining numerical solutions of DB in the graphene sheet. Then we present structure and linear stability of the static DB excited in the graphene sheet.

2. Model

We consider a two-dimensional graphene sheet. Graphene sheets have honeycomb structure of carbon atoms (Fig. 1). Each atom has three nearest-neighbor atoms at equilibrium state. In order to describe the interaction of carbon atoms, we use a model potential proposed by Brenner[7]. Brenner potential describes interaction between two atoms and angle of two bonds. Motion of atoms is tracked by solving the equations of motion based on this potential considering a cutoff distance.

Fig. 1. Model of graphene sheet

We search the numerical solutions of DB by a numerical iteration method. Consider a graphene sheet which consists of N atoms, dynamics of N atoms correspond to an orbit in 4N dimensional phase space \( \{q_i, p_i\} \). The parameters \( q_i \) and \( p_i \) represent position and momentum in \( x \) and \( y \) directions of atoms. DB
which has internal frequency $\omega_{DB}$ corresponds to a periodic orbit in the phase space. Let $x(t_0) = \{q(t_0), p(t_0)\}$ as a point of the phase space at $t=t_0$. Temporal evolution of $x(t_0)$ is described by the equations of motion

$$\dot{x} = f(x),$$

(1)

where

$$f(x) = \{\frac{p}{m}, -\frac{\partial V(q)}{\partial q}\}.$$  

(2)

The function $V$ represents interaction potential. The point $x(t_0)$ moves to $x(t_0+\Delta t)$ by temporal evolution during $\Delta t$. Let $f_{\Delta t}$ as a map from a point $x(t_0)$ to a point $x(t_0+\Delta t)$ by temporal evolution of MD.

$$x(t_0+\Delta t) = f_{\Delta t}(x(t_0))$$

(3)

Consider $x(t_0)$ is on the periodic orbit which corresponds to DB of internal frequency $\omega_{DB}$, we obtain relation as follows:

$$x(t_0+2\pi/\omega_{DB}) = f_{2\pi/\omega_{DB}}(x(t_0)) = x(t_0)$$

(4)

Therefore it is found that searching numerical DB solution is equivalent to solving the equation

$$f_{2\pi/\omega_{DB}}(x) = x$$

(5)

for $x$. In numerical calculation, we search $x$ satisfying

$$|f_{2\pi/\omega_{DB}}(x) - x| = 0$$

(6)
by conjugate gradient method instead of solving (5). The map $f_{z\in DB}(x)$ is given as a result of the
temporal evolution of the point $x$ by the equations of motion.

In the iteration method, initial guess of the solution is important to find the suitable solutions. Adding
to this, obtaining the map $f_{z\in DB}(x)$ for large number of atoms requires large calculation. Therefore we
firstly start finding the DB solution of a system which has small number of degrees of freedom. Once we
have found the DB solution in that system. We construct a new system to find a solution, making some
surrounding atoms of the previous system to move. The previous numerical solution is used as initial
guess of the new system to find solutions. We repeat this procedure by effect of boundary on the DB
solution becomes sufficiently small.

3. Stability Analysis

Linear stability of the numerical DB solution can be discussed by Floquet theory. Consider equation
(1) has a periodic solution

$$x(t) = \Phi(t), \Phi(t+T) = \Phi(t)$$

(7)

Instituting $x = \Phi(t) + \xi(t)$ into equation (1) and linearizing the equation, we obtain the variational equation
as follows,

$$\dot{\xi} = \frac{\partial f(x)}{\partial x}_{x=\Phi(t)} \xi$$

(8)

It is found that coefficients of (8) is a periodic function with period $T$ since $f(t)$ is periodic. In this case,
monodromy matrix $M(T)$ is defined as a map from $\xi(t)$ to $\xi(t+T)$

$$\xi(t+T) = M(T)\xi(t)$$

(9)

If an eigenvalue of the monodromy matrix is greater than unity, perturbation grows duration one period $T$.
Corresponding eigenvector is an unstable perturbation mode. It is known that the monodromy matrix has
pair of eigenvalues $(\rho, \rho^{-1})$, since the perturbation equations are equations of motion of Hamilton system.
Therefore the periodic solution is unstable when there is eigenvalue which is not on the unit circle in
complex plane.

It is difficult to obtain explicit form of the monodromy matrix. However it is known that a
monodromy matrix can be obtained numerically. We perform temporal evolution of variational equations
(8) at the initial condition as following 4N orthonormal vectors

$$\xi_{(1)}(0) = \{1, 0, \cdots, 0\}^T, \xi_{(2)}(0) = \{0, 1, \cdots, 0\}^T, \ldots, \xi_{(4N)}(0) = \{0, 0, \cdots, 1\}^T.$$  \hspace{1cm} (10)

An monodromy matrix $M(T)$ can be constructed by vectors which are result of temporal evolution
duration $T$.

$$M(T) = [\xi_{(1)}(T), \xi_{(2)}(T), \cdots, \xi_{(4N)}(T)].$$  \hspace{1cm} (11)
4. Results

Fig. 2 shows a numerical result of DB in the graphene sheet. Fig. 2(a) shows the displacement pattern of DB excited in the center of the system. Two neighboring carbon atoms vibrate large amplitude. Direction of vibration is parallel to the bond of the vibrating atoms. Atoms surrounding the two atoms also vibrate but relatively small. Displacement of atoms goes to zero as distance from the DB become large. Fig. 2(b) shows temporal evolution of vibrating two atoms. Two atoms vibrate opposite direction. Internal frequency is $3.26 \times 10^{14}$ [rad/s]. This frequency is larger than $3.19 \times 10^{14}$ [rad/s] which is the maximum frequency of phonon band of graphene sheet modeled by Brenner potential.

![Fig. 2](image1)

Fig. 2. (a) displacement pattern of DB calculated by numerical simulation; (b) temporal evolution of displacement atoms on DB

Fig. 3 shows the relation between the maximum and minimum displacement form equilibrium position of carbon atoms and internal frequency of DB. It is found that DB’s amplitudes increase as the internal frequency increases. Adding to this, maximum and minimum amplitude is not equal. This is because DB’s amplitude depends on asymmetry of the interaction potential for a sign of deformation.

![Fig. 3](image2)

Fig. 3. Relation between internal frequency of DB and the maximum and minimum displacement
Fig. 4 shows the distribution of the eigenvalues of monodromy matrix in the complex plane with (a) T=18.9/fs; (b) T=19.1/fs and (c) T=19.3/fs. In each case, eigenvalue which is not on the unit circle exist. This means that DB have unstable perturbation mode in this case. Distribution of eigenvalue varies with DB’s period, which correspond the amplitude of localization. Therefore displacement pattern of perturbation modes varies with the amplitude of localization.

Fig. 4. Distribution of eigenvalues of DB with (a) T=18.9/fs; (b) T=19.1/fs; (c) T=19.3/fs

5. Conclusion

In this study, we search numerical solution of DB in graphene sheet by a method combining MD and iteration method. Structure and stability of DB which is obtained by numerical calculation are investigated in detail.

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