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The 3D solitons and vortices in 3D discrete monatomic lattices with cubic and quartic nonlinearity*

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By virtue of the method of multiple-scale and the quasi-discreteness approach, we have discussed the nonlinear vibration equation of a 3D discrete monatomic lattice with its nearest-neighbours interaction. The 3D simple cubic lattices have the same localized modes as a 1D discrete monatomic chain with cubic and quartic nonlinearity. The nonlinear vibration in the 3D simple cubic lattice has 3D distorted solitons and 3D envelop solitons in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/6a_0$ in the Brillouin zone, as well as has 3D vortices in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/a_0$ in the Brillouin zone.

Keywords: 3D simple cubic lattice, Brillouin zone, envelop soliton, distorted soliton, vortices
PACC: 0320, 0430

1. Introduction

Nonlinear discrete systems are abundant in nature. In optics, a typical example is a closely spaced nonlinear waveguide array. When the waveguide array is embedded in a nonlinear medium, a balance between discrete diffraction and nonlinear self-focusing gives rise to the so-called discrete solitons.[1] Optical vibration modes and electron–phonon interactions[2] are also the examples of this kind. In nonlinear lattices, they are discrete modes with the vibration excited by a short wavelength wave. The examples of nonlinear discrete lattices include the interaction of a kink soliton with a breather in a Fermi–Pasta–Ulam chain,[3] discrete breathers and Anderson modes,[4] envelope-kink phonon localized modes in a homogeneous anharmonic chain,[5] the gap solitons in discrete diatomic lattice,[6−8] the breathers in a one-dimensional molecular chain[9] and the soliton of nonlinear lattice with damping interaction.[10] In this paper we discuss the nonlinear vibration equation of a 3D discrete monatomic lattice by virtue of the method of multiple-scale and the quasi-discreteness approach. Taking their nearest-neighbours interaction into account, the 3D simple cubic lattices have the same localized modes (distorted solitons and envelop solitons) as a 1D discrete monatomic chain with cubic and quartic nonlinearity. The nonlinear vibration in 3D simple cubic lattices has 3D distorted solitons and 3D envelop solitons in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/6a_0$ in the Brillouin zone, and has 3D vortices in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/a_0$ in the Brillouin zone.

2. The 3D distorted solitons of the nonlinear vibration in 3D discrete monatomic lattices with cubic nonlinearity

3D monatomic lattices are shown in Fig.1. By taking into account the interaction between the lattice and its nearest-neighbours, the Hamiltonian of the system with a cubic anharmonic potential is given by

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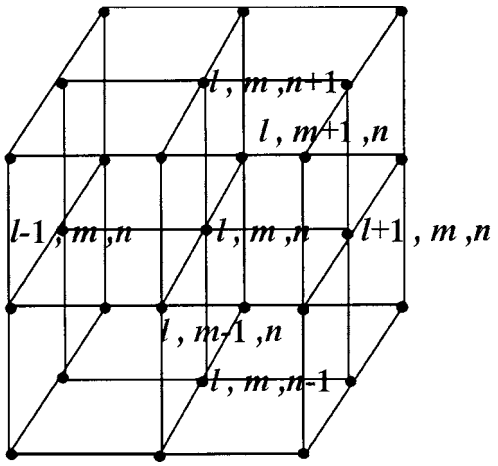


Fig.1. 3D simple cubic lattices.

$$
\begin{aligned}
H = \sum_{l,m,n} \Bigg[& \frac{p_{l,m}^2}{2M} + \frac{1}{2} K_x \left(u_{l+1,m,n} - u_{l,m,n}\right)^2 \\
& + \frac{1}{3} \alpha_x K_x \left(u_{l+1,m,n} - u_{l,m,n}\right)^3 \Bigg] \\
& + \sum_{l,m,n} \Bigg[\frac{1}{2} K_y \left(u_{l,m+1,n} - u_{l,m,n}\right)^2 \\
& + \frac{1}{3} \alpha_y K_y \left(u_{l,m+1,n} - u_{l,m,n}\right)^3 \Bigg] \\
& + \sum_{l,m,n} \Bigg[\frac{1}{2} K_z \left(u_{l,m,n+1} - u_{l,m,n}\right)^2 \\
& + \frac{1}{3} \alpha_z K_z \left(u_{l,m,n+1} - u_{l,m,n}\right)^3 \Bigg], \qquad (1)
\end{aligned}
$$

where $M, p_{l,m,n}, u_{l,m,n}$ are the mass, momentum and displacement of an atom; K_x, K_y and K_z are force constants in the x-direction, y-direction and z-direction, respectively. The nonlinear vibration equation for a 3D lattice is obtained by $\dot{p}_{l,m,n} = M\ddot{u}_{l,m,n} = -\partial H/\partial u_{l,m,n}$, where

$$
\begin{aligned}
M\ddot{u}_{l,m} = & K_x \left(u_{l+1,m,n} + u_{l-1,m,n} - 2u_{l,m,n}\right) \\
& + \alpha_x K_x [\left(u_{l+1,m,n} - u_{l,m,n}\right)^2 \\
& - \left(u_{l-1,m,n} - u_{l,m,n}\right)^2] \\
& + k_y \left(u_{l,m+1,n} + u_{l,m-1,n} - 2u_{l,m,n}\right) \\
& + \alpha_y K_y [\left(u_{l,m+1,n} - u_{l,m,n}\right)^2 \\
& - \left(u_{l,m-1,n} - u_{l,m,n}\right)^2] \\
& + k_z \left(u_{l,m,n+1} + u_{l,m,n-1} - 2u_{l,m}\right) \\
& + \alpha_z K_z [\left(u_{l,m,n+1} - u_{l,m,n}\right)^2 \\
& - \left(u_{l,m,n-1} - u_{l,m,n}\right)^2]. \qquad (2)
\end{aligned}
$$

According to the method of multiple-scale and the quasi-discreteness approach, we assume

$$
\begin{aligned}
u_{l,m,n}(t) = & \varepsilon u^{(1)} \left(\xi_l, \zeta_m, \varsigma_n, \tau, \phi_{l,m,n}\right) \\
& + \varepsilon^2 u^{(2)} \left(\xi_l, \zeta_m, \varsigma_n, \tau, \phi_{l,m,n}\right) \\
& + \varepsilon^3 u^{(3)} \left(\xi_l, \zeta_m, \varsigma_n, \tau, \phi_{l,m,n}\right) + \cdots \\
= & \sum_{\gamma=1}^{\infty} \varepsilon^\gamma u^{(\gamma)} \left(\xi_l, \zeta_m, \varsigma_n, \tau, \phi_{l,m,n}\right) \\
= & \sum_{\gamma=1}^{\infty} \varepsilon^\gamma u_{lmn,lmn}^{(\gamma)}, \qquad (3)
\end{aligned}
$$

where ε is a small ordering parameter denoting the relative amplitude of the excitation and $u_{lmn,lmn}^{(\gamma)} = u^{(\gamma)} \left(\xi_l, \zeta_m, \varsigma_n, \tau, \phi_{l,m,n}\right)$. $\xi_l = \varepsilon(la - \lambda t)$, $\zeta_m = \varepsilon(mb - \eta t)$, $\varsigma_n = \varepsilon(nc - \mu t)$ and $\tau = \varepsilon^2 t$ are multiple-scales slow variables. The fast variable, $\phi_{l,m,n} = lk_x a + mk_y b + nk_z c - \omega t$, represents the phase of the carrier wave. k_x, k_y, k_z, ω are the numbers and frequency of the carrier wave, respectively . Here a, b and c are lattice constants. λ, η, μ are the parameters to be determined later. We perform the Taylor expansion as follows:

$$
\begin{aligned}
u_{l\pm1,m,n}^{(\gamma)} = & u_{lmn,(l\pm1)mn}^{(\gamma)} \pm \varepsilon a \frac{\partial u_{lmn,(l\pm1)mn}^{(\gamma)}}{\partial \xi_l} + \frac{\varepsilon^2 a^2}{2!} \frac{\partial^2 u_{lmn,(l\pm1)mn}^{(\gamma)}}{\partial \xi_l^2} \pm \frac{\varepsilon^3 a^3}{3!} \frac{\partial^3 u_{lmn,(l\pm1)mn}^{(\gamma)}}{\partial \xi_l^3} + \cdots, \\
u_{l\pm1,m,n} = & \sum_{\gamma=1}^{\infty} \varepsilon^\gamma \left[\sum_{q=0}^{\infty} \frac{1}{q!} \left(\pm \varepsilon a \frac{\partial}{\partial \xi_l} \right)^q u_{lmn,(l\pm1)mn}^{(\gamma)} \right], \\
u_{l,m\pm1,n}^{(\gamma)} = & u_{lmn,l(m\pm1)n}^{(\gamma)} \pm \varepsilon b \frac{\partial u_{lmn,l(m\pm1)n}^{(\gamma)}}{\partial \zeta_m} + \frac{\varepsilon^2 b^2}{2!} \frac{\partial^2 u_{lmn,l(m\pm1)n}^{(\gamma)}}{\partial \zeta_m^2} \pm \frac{\varepsilon^3 b^3}{3!} \frac{\partial^3 u_{lmn,l(m\pm1)n}^{(\gamma)}}{\partial \zeta_m^3} + \cdots, \\
u_{l,m\pm1,n} = & \sum_{\gamma=1}^{\infty} \varepsilon^\gamma \left[\sum_{q=0}^{\infty} \frac{1}{q!} \left(\pm \varepsilon b \frac{\partial}{\partial \zeta_m} \right)^q u_{lmn,l(m\pm1)n}^{(\gamma)} \right],
\end{aligned}
$$

$$u_{l,m,n\pm1}^{(\gamma)} = u_{lmn,lm(n\pm1)}^{(\gamma)} \pm \varepsilon c \frac{\partial u_{lmn,lm(n\pm1)}^{(\gamma)}}{\partial \varsigma_n} + \frac{\varepsilon^2 c^2}{2!} \frac{\partial^2 u_{lmn,lm(n\pm1)}^{(\gamma)}}{\partial \varsigma_n^2} \pm \frac{\varepsilon^3 c^3}{3!} \frac{\partial^3 u_{lmn,lm(n\pm1)}^{(\gamma)}}{\partial \varsigma_n^2} + \cdots,$$

$$u_{l,m,n\pm1} = \sum_{\gamma=1}^{\infty} \varepsilon^{\gamma} \left[\sum_{q=0}^{\infty} \frac{1}{q!} \left(\pm \varepsilon c \frac{\partial}{\partial \varsigma_n} \right)^q u_{lmn,lm(n\pm1)}^{(\gamma)} \right]. \tag{4}$$

By virtue of the method of the chain, we make the transformation as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} - \lambda\varepsilon \frac{\partial}{\partial \xi_l} - \eta\varepsilon \frac{\partial}{\partial \zeta_m} - \mu\varepsilon \frac{\partial}{\partial \varsigma_n} + \varepsilon^2 \frac{\partial}{\partial \tau}, \tag{5a}$$

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}t^2} =& \frac{\partial^2}{\partial t^2} - 2\lambda\varepsilon \frac{\partial^2}{\partial t \partial \xi_l} - 2\eta\varepsilon \frac{\partial^2}{\partial t \partial \zeta_m} - 2\mu\varepsilon \frac{\partial^2}{\partial t \partial \varsigma_n} + 2\varepsilon^2 \frac{\partial^2}{\partial t \partial \tau} + \lambda^2\varepsilon^2 \frac{\partial^2}{\partial \xi_l^2} + 2\lambda\eta\varepsilon^2 \frac{\partial^2}{\partial \xi_l \partial \zeta_m} \\ &+ 2\lambda\mu\varepsilon^2 \frac{\partial^2}{\partial \xi_l \partial \varsigma_n} - 2\lambda\varepsilon^3 \frac{\partial^2}{\partial \xi_l \partial \tau} + \eta^2\varepsilon^2 \frac{\partial^2}{\partial \zeta_m^2} + 2\eta\mu\varepsilon^2 \frac{\partial^2}{\partial \zeta_m \partial \varsigma_n} - 2\eta\varepsilon^3 \frac{\partial^2}{\partial \zeta_m \partial \tau} \\ &+ \mu^2\varepsilon^2 \frac{\partial^2}{\partial \varsigma_n^2} - 2\mu\varepsilon^3 \frac{\partial^2}{\partial \varsigma_n \partial \tau} + \varepsilon^4 \frac{\partial^2}{\partial \tau^2}. \end{aligned} \tag{5b}$$

Substituting Eqs.(3), (4) and (5) into Eq.(2), we have

$$\begin{aligned} &\varepsilon \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial t^2} - 2\lambda\varepsilon^2 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial t \partial \xi_l} - 2\eta\varepsilon^2 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial t \partial \zeta_m} - 2\mu\varepsilon^2 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial t \partial \varsigma_n} \\ &+ 2\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial t \partial \tau} + \lambda^2\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \xi_l^2} + 2\lambda\eta\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \xi_l \partial \zeta_m} + 2\lambda\mu\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \xi_l \partial \varsigma_n} \\ &- 2\lambda\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \xi_l \partial \tau} + \eta^2\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \zeta_m^2} + 2\eta\mu\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \zeta_m \partial \varsigma_n} - 2\eta\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \zeta_m \partial \tau} \\ &+ \mu^2\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \varsigma_n^2} - 2\mu\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \varsigma_n \partial \tau} + \varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(1)}}{\partial \tau^2} \\ &+ \varepsilon^2 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial t^2} - 2\lambda\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial t \partial \xi_l} - 2\eta\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial t \partial \zeta_m} - 2\mu\varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial t \partial \varsigma_n} \\ &+ 2\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial t \partial \tau} + \lambda^2\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \xi_l^2} + 2\lambda\eta\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \xi_l \partial \zeta_m} + 2\lambda\mu\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \xi_l \partial \varsigma_n} \\ &- 2\lambda\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \xi_l \partial \tau} + \eta^2\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \zeta_m^2} + 2\eta\mu\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \zeta_m \partial \varsigma_n} - 2\eta\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \zeta_m \partial \tau} \\ &+ \mu^2\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \varsigma_n^2} - 2\mu\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \varsigma_n \partial \tau} + \varepsilon^6 \frac{\partial^2 u_{lmn,lmn}^{(2)}}{\partial \tau^2} \\ &+ \varepsilon^3 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial t^2} - 2\lambda\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial t \partial \xi_l} - 2\eta\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial t \partial \zeta_m} - 2\mu\varepsilon^4 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial t \partial \varsigma_n} \\ &+ 2\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial t \partial \tau} + \lambda^2\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \xi_l^2} + 2\lambda\eta\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \xi_l \partial \zeta_m} + 2\lambda\mu\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \xi_l \partial \varsigma_n} \\ &- 2\lambda\varepsilon^6 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \xi_l \partial \tau} + \eta^2\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \zeta_m^2} + 2\eta\mu\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \zeta_m \partial \varsigma_n} - 2\eta\varepsilon^6 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \zeta_m \partial \tau} \\ &+ \mu^2\varepsilon^5 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \varsigma_n^2} - 2\mu\varepsilon^6 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \varsigma_n \partial \tau} + \varepsilon^6 \frac{\partial^2 u_{lmn,lmn}^{(3)}}{\partial \tau^2} \end{aligned}$$

$$
\begin{aligned}
=&\frac{K_x}{M}\Bigg(\varepsilon u^{(1)}_{lmn,(l+1)mn}+\varepsilon u^{(1)}_{lmn,(l-1)mn}-2\varepsilon u^{(1)}_{lmn,lmn}\pm\varepsilon^2 a\frac{\partial u^{(1)}_{lmn,(l\pm1)mn}}{\partial\xi_l}+\frac{\varepsilon^3a^2}{2!}\frac{\partial^2u^{(1)}_{lmn,(l\pm1)mn}}{\partial\xi_l^2}+\cdots\\
&+\varepsilon^2u^{(2)}_{lmn,(l+1)mn}+\varepsilon^2u^{(2)}_{lmn,(l-1)mn}-2\varepsilon^2u^{(2)}_{lmn,lmn}\\
&\pm\varepsilon^3a\frac{\partial u^{(2)}_{lmn,(l\pm1)mn}}{\partial\xi_l}+\frac{\varepsilon^4a^2}{2!}\frac{\partial^2u^{(2)}_{lmn,(l\pm1)mn}}{\partial\xi_l^2}+\cdots+\varepsilon^3u^{(3)}_{lmn,(l+1)mn}+\varepsilon^3u^{(3)}_{lmn,(l-1)mn}\\
&-2\varepsilon^3u^{(3)}_{lmn,lmn}\pm\varepsilon^4a\frac{\partial u^{(3)}_{lmn,(l\pm1)mn}}{\partial\xi_l}+\frac{\varepsilon^5a^2}{2!}\frac{\partial^2u^{(3)}_{lmn,(l\pm1)mn}}{\partial\xi_l^2}+\cdots\Bigg)\\
&+\frac{K_x\alpha_x}{M}\left[\left(\varepsilon u^{(1)}_{lmn,(l+1)mn}-\varepsilon u^{(1)}_{lmn,lmn}\right)^2-\left(\varepsilon u^{(1)}_{lmn,(l-1)mn}-\varepsilon u^{(1)}_{lmn,lmn}\right)^2+\cdots\right]\\
&+\frac{K_y}{M}\Bigg(\varepsilon u^{(1)}_{lmn,l(m+1)n}+\varepsilon u^{(1)}_{lmn,l(m-1)n}-2\varepsilon u^{(1)}_{lmn,lmn}\pm\varepsilon^2b\frac{\partial u^{(1)}_{lmn,l(m\pm1)n}}{\partial\zeta_m}+\frac{\varepsilon^3b^2}{2!}\frac{\partial^2u^{(1)}_{lmn,l(m\pm1)n}}{\partial\zeta_m^2}+\cdots\\
&+\varepsilon^2u^{(2)}_{lmn,l(m+1)n}+\varepsilon^2u^{(2)}_{lmn,l(m-1)n}-2\varepsilon^2u^{(2)}_{lmn,lmn}\\
&\pm\varepsilon^3b\frac{\partial u^{(2)}_{lmn,l(m\pm1)n}}{\partial\zeta_m}+\frac{\varepsilon^4b^2}{2!}\frac{\partial^2u^{(2)}_{lmn,l(m\pm1)n}}{\partial\zeta_m^2}+\cdots+\varepsilon^3u^{(3)}_{lmn,l(m+1)n}+\varepsilon^3u^{(3)}_{lmn,l(m-1)n}\\
&-2\varepsilon^3u^{(3)}_{lmn,lmn}\pm\varepsilon^4b\frac{\partial u^{(3)}_{lmn,l(m\pm1)n}}{\partial\zeta_m}+\frac{\varepsilon^5b^2}{2!}\frac{\partial^2u^{(3)}_{lmn,l(m\pm1)n}}{\partial\zeta_m^2}+\cdots\Bigg)\\
&+\frac{K_y\alpha_y}{M}\left[\left(\varepsilon u^{(1)}_{lmn,l(m+1)n}-\varepsilon u^{(1)}_{lmn,lmn}\right)^2-\left(\varepsilon u^{(1)}_{lmn,l(m-1)n}-\varepsilon u^{(1)}_{lmn,lmn}\right)^2+\cdots\right]\\
&+\frac{K_z}{M}\Bigg(\varepsilon u^{(1)}_{lmn,lm(n+1)}+\varepsilon u^{(1)}_{lmn,lm(n-1)}-2\varepsilon u^{(1)}_{lmn,lmn}\pm\varepsilon^2c\frac{\partial u^{(1)}_{lmn,lm(n\pm1)}}{\partial\varsigma_n}+\frac{\varepsilon^3c^2}{2!}\frac{\partial^2u^{(1)}_{lmn,lm(n\pm1)}}{\partial\varsigma_n^2}+\cdots\\
&+\varepsilon^2u^{(2)}_{lmn,lm(n+1)}+\varepsilon^2u^{(2)}_{lmn,lm(n-1)}-2\varepsilon^2u^{(2)}_{lmn,lmn}\\
&\pm\varepsilon^3c\frac{\partial u^{(2)}_{lmn,lm(n\pm1)}}{\partial\varsigma_n}+\frac{\varepsilon^4c^2}{2!}\frac{\partial^2u^{(2)}_{lmn,lm(n\pm1)}}{\partial\varsigma_n^2}+\cdots+\varepsilon^3u^{(3)}_{lmn,lm(n+1)}+\varepsilon^3u^{(3)}_{lmn,lm(n-1)}\\
&-2\varepsilon^3u^{(3)}_{lmn,lmn}\pm\varepsilon^4c\frac{\partial u^{(3)}_{lmn,lm(n\pm1)}}{\partial\varsigma_n}+\frac{\varepsilon^5c^2}{2!}\frac{\partial^2u^{(3)}_{lmn,lm(n\pm1)}}{\partial\varsigma_n^2}+\cdots\Bigg)\\
&+\frac{K_z\alpha_z}{M}\left[\left(\varepsilon u^{(1)}_{lmn,lm(n+1)}-\varepsilon u^{(1)}_{lmn,lmn}\right)^2-\left(\varepsilon u^{(1)}_{lmn,lm(n-1)}-\varepsilon u^{(1)}_{lmn,lmn}\right)^2+\cdots\right].
\end{aligned}
\tag{6}
$$

Comparing the powers of ε in Eq.(6), we can obtain the following equations:

$$
\begin{aligned}
\varepsilon^1:&\frac{\partial^2u^{(1)}_{lmn,lmn}}{\partial t^2}-\frac{K_x}{M}\left(u^{(1)}_{lmn,(l+1)mn}+u^{(1)}_{lmn,(l-1)mn}-2u^{(1)}_{lmn,lmn}\right)\\
&-\frac{K_y}{M}\left(u^{(1)}_{lmn,l(m+1)n}+u^{(1)}_{lmn,l(m-1)n}-2u^{(1)}_{lmn,lmn}\right)\\
&-\frac{K_z}{M}\left(u^{(1)}_{lmn,lm(n+1)}+u^{(1)}_{lmn,lm(n-1)}-2u^{(1)}_{lmn,lmn}\right)=0,
\end{aligned}
\tag{7a}
$$

$$
\begin{aligned}
\varepsilon^2:&\frac{\partial^2u^{(2)}_{lmn,lmn}}{\partial t^2}-\frac{K_x}{M}\left(u^{(2)}_{lmn,(l+1)mn}+u^{(2)}_{lmn,(l-1)mn}-2u^{(2)}_{lmn,lmn}\right)\\
&-\frac{K_y}{M}\left(u^{(2)}_{lmn,l(m+1)n}+u^{(2)}_{lmn,l(m-1)n}-2u^{(2)}_{lmn,lmn}\right)\\
&-\frac{K_z}{M}\left(u^{(2)}_{lmn,lm(n+1)}+u^{(2)}_{lmn,lm(n-1)}-2u^{(2)}_{lmn,lmn}\right)
\end{aligned}
$$

$$
\begin{aligned}
=&2\lambda\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial t\partial\xi_l}+2\eta\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial t\partial\zeta_m}+2\mu\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial t\partial\varsigma_n}+\frac{K_x a}{M}\frac{\partial}{\partial\xi_l}\left(u^{(1)}_{lmn,(l+1)mn}-u^{(1)}_{lmn,(l-1)mn}\right)\\
&+\frac{K_y b}{M}\frac{\partial}{\partial\zeta_m}\left(u^{(1)}_{lmn,l(m+1)n}-u^{(1)}_{lmn,l(m-1)n}\right)+\frac{K_z c}{M}\frac{\partial}{\partial\varsigma_n}\left(u^{(1)}_{lmn,lm(n+1)}-u^{(1)}_{lmn,lm(n-1)}\right)\\
&+\frac{K\alpha_x}{M}\left[\left(u^{(1)}_{lmn,(l+1)mn}-u^{(1)}_{lmn,lmn}+\cdots\right)^2-\left(u^{(1)}_{lmn,(l-1)mn}-u^{(1)}_{lmn,lmn}+\cdots\right)^2\right]\\
&+\frac{K_y\alpha_y}{M}\left[\left(u^{(1)}_{lmn,l(m+1)n}-u^{(1)}_{lmn,lmn}\cdots\right)^2-\left(u^{(1)}_{lmn,l(m-1)n}-u^{(1)}_{lmn,lmn}+\cdots\right)^2\right]\\
&+\frac{K_z\alpha_z}{M}\left[\left(u^{(1)}_{lmn,lm(n+1)}-u^{(1)}_{lmn,lmn}\cdots\right)^2-\left(u^{(1)}_{lmn,lm(n-1)}-u^{(1)}_{lmn,lmn}+\cdots\right)^2\right],
\end{aligned}
\tag{7b}
$$

$$
\begin{aligned}
\varepsilon^3:&\frac{\partial^2 u^{(3)}_{lmn,lmn}}{\partial t^2}-\frac{K_x}{M}\left(u^{(3)}_{lmn,(l+1)mn}+u^{(3)}_{lmn,(l-1)mn}-2u^{(3)}_{lmn,lmn}\right)\\
&-\frac{K_y}{M}\left(u^{(3)}_{lmn,l(m+1)n}+u^{(3)}_{lmn,l(m-1)n}-2u^{(3)}_{lmn,lmn}\right)-\frac{K_z}{M}\left(u^{(3)}_{lmn,lm(n+1)}+u^{(3)}_{lmn,lm(n-1)}-2u^{(3)}_{lmn,lmn}\right)\\
=&2\lambda\frac{\partial^2 u^{(2)}_{lmn,lmn}}{\partial t\partial\xi_l}+2\eta\frac{\partial^2 u^{(2)}_{lmn,lmn}}{\partial t\partial\zeta_m}+2\mu\frac{\partial^2 u^{(2)}_{lmn,lmn}}{\partial t\partial\varsigma_n}-\left(\lambda^2\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial\xi_l^2}+\eta^2\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial\zeta_m^2}+\mu^2\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial\varsigma_n^2}\right)\\
&-\left(2\lambda\eta\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial\xi_l\partial\zeta_m}+2\lambda\mu\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial\xi_l\partial\varsigma_n}+2\eta\mu\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial\zeta_m\partial\varsigma_n}+2\frac{\partial^2 u^{(1)}_{lmn,lmn}}{\partial t\partial\tau}\right)\\
&+\frac{K_x}{M}\left[a\frac{\partial}{\partial\xi_l}\left(u^{(2)}_{lmn,(l+1)mn}-u^{(2)}_{lmn,(l-1)mn}\right)+\frac{a^2}{2}\frac{\partial^2}{\partial\xi_l^2}\left(u^{(1)}_{lmn,(l+1)mn}+u^{(1)}_{lmn,(l-1)mn}\right)\right]\\
&+\frac{K_y}{M}\left[b\frac{\partial}{\partial\zeta_m}\left(u^{(2)}_{lmn,l(m+1)n}-u^{(2)}_{lmn,l(m-1)n}\right)+\frac{b^2}{2}\frac{\partial^2}{\partial\zeta_m^2}\left(u^{(1)}_{lmn,l(m+1)n}+u^{(1)}_{lmn,l(m-1)n}\right)\right]\\
&+\frac{K_z}{M}\left[b\frac{\partial}{\partial\varsigma_n}\left(u^{(2)}_{lmn,lm(n+1)}-u^{(2)}_{lmn,lm(n-1)}\right)+\frac{b^2}{2}\frac{\partial^2}{\partial\varsigma_n^2}\left(u^{(1)}_{lmn,lm(n+1)}+u^{(1)}_{lmn,lm(n-1)}\right)\right]\\
&+\frac{K\alpha_x}{M}\left[\left(u^{(1)}_{lmn,(l+1)mn}-u^{(1)}_{lmn,lmn}+\cdots\right)^2-\left(u^{(1)}_{lmn,(l-1)mn}-u^{(1)}_{lmn,lmn}+\cdots\right)^2\right]\\
&+\frac{K_y\alpha_y}{M}\left[\left(u^{(1)}_{lmn,l(m+1)n}-u^{(1)}_{lmn,lmn}\cdots\right)^2-\left(u^{(1)}_{lmn,l(m-1)n}-u^{(1)}_{lmn,lmn}+\cdots\right)^2\right]\\
&+\frac{K_z\alpha_z}{M}\left[\left(u^{(1)}_{lmn,lm(n+1)}-u^{(1)}_{lmn,lmn}\cdots\right)^2-\left(u^{(1)}_{lmn,lm(n-1)}-u^{(1)}_{lmn,lmn}+\cdots\right)^2\right].
\end{aligned}
\tag{7c}
$$

Equation (7a) has the same form as that of the vibration equation of the 3D harmonic monatomic lattice, which has the solution

$$
u^{(1)}_{lmn,lmn}=A_0\left(\xi_l,\zeta_m,\varsigma_n,\tau\right)+A\left(\xi_l,\zeta_m,\varsigma_n,\tau\right)\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}+\text{c.c.} \tag{8}
$$

where c.c. denotes complex conjugate, which is also used hereinafter.

The dispersion relation is

$$
\begin{aligned}
\omega^2=&-\frac{K_x}{M}\left(\mathrm{e}^{\mathrm{i}k_x a}+\mathrm{e}^{-\mathrm{i}k_x a}-2\right)-\frac{K_y}{M}\left(\mathrm{e}^{\mathrm{i}k_y b}+\mathrm{e}^{-\mathrm{i}k_y b}-2\right)-\frac{K_z}{M}\left(\mathrm{e}^{\mathrm{i}k_z c}+\mathrm{e}^{-\mathrm{i}k_z c}-2\right)\\
=&\frac{2K_x}{M}\left(1-\cos k_x a\right)+\frac{2K_y}{M}\left(1-\cos k_y b\right)+\frac{2K_z}{M}\left(1-\cos k_z c\right).
\end{aligned}
\tag{9}
$$

Substituting Eq.(8) into Eq.(7b), we have

$$\begin{aligned}
&\frac{\partial^2 u^{(2)}_{lmn,lm^n}}{\partial t^2} - \frac{K_x}{M}\left(u^{(2)}_{lmn,(l+1)mn} + u^{(2)}_{lmn,(l-1)mn} - 2u^{(2)}_{lmn,lmn}\right)\\
&- \frac{K_y}{M}\left(u^{(2)}_{lmn,l(m+1)n} + u^{(2)}_{lmn,l(m-1)n} - 2u^{(2)}_{lmn,lmn}\right) - \frac{K_z}{M}\left(\left(u^{(2)}_{lmn,lm(n+1)} + u^{(2)}_{lmn,lm(n-1)} - 2u^{(2)}_{lmn,lmn}\right)\right)\\
=&-\mathrm{i}2\omega\left(\lambda\frac{\partial A}{\partial \xi_l}\cdot + \eta\frac{\partial A}{\partial \zeta_m} + \mu\frac{\partial A}{\partial \varsigma_n}\right)\cdot \mathrm{e}^{\mathrm{i}\phi_{l,m,n}}\\
&+\mathrm{i}\frac{2}{M}\left(K_x a\sin k_x a\frac{\partial A}{\partial \xi_l} + K_y b\sin k_y b\frac{\partial A}{\partial \zeta_m} + K_z c\sin k_z c\frac{\partial A}{\partial \varsigma_n}\right)\cdot \mathrm{e}^{\mathrm{i}\phi_{l,m,n}}\\
&-\mathrm{i}\frac{8}{M}\left(K_x\alpha_x\sin k_x a\sin^2\frac{k_x a}{2} + K_y\alpha_y\sin k_y b\sin^2\frac{k_y b}{2} + K_z\alpha_z\sin k_z c\sin^2\frac{k_z c}{2}\right)A^2\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}} + \text{c.c.} \qquad (10)
\end{aligned}$$

The terms proportional to $\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}$ on the right-hand side of Eq.(10) are secular terms which must be eliminated for the theory being valid. Thus we have

$$\begin{aligned}
&\frac{\partial^2 u^{(2)}_{lmn,lmn}}{\partial t^2} - \frac{K_x}{M}\left(u^{(2)}_{lmn,(l+1)mn} + u^{(2)}_{lmn,(l-1)mn} - 2u^{(2)}_{lmn,lmn}\right)\\
&- \frac{K_y}{M}\left(u^{(2)}_{lmn,l(m+1)n} + u^{(2)}_{lmn,l(m-1)n} - 2u^{(2)}_{lmn,lmn}\right) - \frac{K_z}{M}\left(\left(u^{(2)}_{lmn,lm(n+1)} + u^{(2)}_{lmn,lm(n-1)} - 2u^{(2)}_{lmn,lmn}\right)\right)\\
=&-\mathrm{i}\frac{8}{M}\left(K_x\alpha_x\sin k_x a\sin^2\frac{k_x a}{2} + K_y\alpha_y\sin k_y b\sin^2\frac{k_y b}{2} + K_z\alpha_z\sin k_z c\sin^2\frac{k_z c}{2}\right)A^2\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}}, \qquad (11a)
\end{aligned}$$

$$2\left(\lambda - \frac{K_x a}{M\omega}\sin k_x a\right)\frac{\partial A}{\partial \xi_l} + 2\left(\eta - \frac{K_y b}{M\omega}\sin k_y b\right)\frac{\partial A}{\partial \zeta_m} + 2\left(\mu - \frac{K_z c}{M\omega}\sin k_z c\right)\frac{\partial A}{\partial \varsigma_n} = 0. \qquad (11b)$$

According to Eq.(11b), we know $\lambda = \dfrac{K_x a}{M\omega}\sin k_x a$, $\eta = \dfrac{K_y b}{M\omega}\sin k_y b$ and $\mu = \dfrac{K_z c}{M\omega}\sin k_z c$, because $\dfrac{\partial A}{\partial \xi_l} \neq 0$, $\dfrac{\partial A}{\partial \zeta_m} \neq 0$ and $\dfrac{\partial A}{\partial \varsigma_n} \neq 0$ (If $\dfrac{\partial A}{\partial \xi_l} = 0$, $\dfrac{\partial A}{\partial \zeta_m} = 0$ and $\dfrac{\partial A}{\partial \varsigma_n} = 0$, A=constant, the solution (8) is the solution of vibration in the 3D harmonic lattice), and from Eq.(11a) we obtain

$$\begin{aligned}
u^{(2)}_{lmn,lmn} =& B_0\left(\xi_l,\zeta_m,\varsigma_n,\tau\right) + \left\{B\left(\xi_l,\zeta_m,\varsigma_n,\tau\right)\mathrm{e}^{\mathrm{i}\phi_{l,m,n}} + \mathrm{i}\left[\alpha_x\mathrm{ctg}\left(\frac{k_x a}{2}\right) + \alpha_y\mathrm{ctg}\left(\frac{k_y b}{2}\right)\right.\right.\\
&\left.\left. + \alpha_z\mathrm{ctg}\left(\frac{k_z c}{2}\right)\right]A^2\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}} + \text{c.c.}\right\}.
\end{aligned}$$

In fact we can let B =0, because it can be transformed into the lowest-order solution (8). Substituting $u^{(1)}_{lmn,lmn}$ into Eq.(7c) and taking the following relation into account:

$$\begin{aligned}
&\frac{K\alpha_x}{M}\left[\left(u^{(1)}_{lmn,(l+1)mn} - u^{(1)}_{lmn,lmn} + \cdots\right)^2 - \left(u^{(1)}_{lmn,(l-1)mn} - u^{(1)}_{lmn,lmn} + \cdots\right)^2\right]\\
&+ \frac{K_y\alpha_y}{M}\left[\left(u^{(1)}_{lmn,l(m+1)n} - u^{(1)}_{lmn,lmn}\cdots\right)^2 - \left(u^{(1)}_{lmn,l(m-1)n} - u^{(1)}_{lmn,lmn} + \cdots\right)^2\right]\\
&+ \frac{K_z\alpha_z}{M}\left[\left(u^{(1)}_{lmn,lm(n+1)} - u^{(1)}_{lmn,lmn}\cdots\right)^2 - \left(u^{(1)}_{lmn,lm(n-1)} - u^{(1)}_{lmn,lmn} + \cdots\right)^2\right]\\
=&\left\{2\varepsilon\left(\cos k_x a - 1\right)\left(A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}} + A^*\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right) + \mathrm{i}2\varepsilon^2\alpha_x\mathrm{ctg}\left(\frac{k_x a}{2}\right)\left(\cos 2k_x a - 1\right)\left(A^2\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}} + A^{*2}\mathrm{e}^{-2\mathrm{i}\phi_{l,m,n}}\right)\right.\\
&\left. + \mathrm{i}2\varepsilon^2 a\sin k_x a\left(\frac{\partial A}{\partial \xi_l}\mathrm{e}^{\mathrm{i}\phi_{l,m,n}} - \frac{\partial A^*}{\partial \xi_l}\mathrm{e}^{-i\phi_{l,m,n}}\right)\right\}\left\{\mathrm{i}2\varepsilon\sin k_x a\left(A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}} - A^*\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right.\\
&\left. + 2\varepsilon^2\alpha_x\mathrm{ctg}\left(\frac{k_x a}{2}\right)\sin 2k_x a\left(A^{*2}\mathrm{e}^{-2\mathrm{i}\phi_{l,m,n}} - A^2\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}}\right) + 2\varepsilon^2 a\cos k_x a\left(\frac{\partial A}{\partial \xi_l}\mathrm{e}^{\mathrm{i}\phi_{l,m,n}} + \frac{\partial A^*}{\partial \xi_l}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right\}\frac{K_x\alpha_x}{M}
\end{aligned}$$

$$
\begin{aligned}
&+\left\{2\varepsilon\left(\cos k_y b-1\right)\left(A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}+A^{*}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)+\mathrm{i}2\varepsilon^{2}\alpha_y\mathrm{ctg}\left(\frac{k_y b}{2}\right)\left(\cos 2k_y b-1\right)\left(A^{2}\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}}+A^{*2}\mathrm{e}^{-2\mathrm{i}\phi_{l,m,n}}\right)\right.\\
&\left.+\mathrm{i}2\varepsilon^{2}b\sin k_y b\left(\frac{\partial A}{\partial\zeta_m}\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}-\frac{\partial A^{*}}{\partial\zeta_m}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right\}\left\{\mathrm{i}2\varepsilon\sin k_y b\left(A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}-A^{*}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right.\\
&\left.+2\varepsilon^{2}\alpha_y\mathrm{ctg}\left(\frac{k_y b}{2}\right)\sin 2k_y b\left(A^{*2}\mathrm{e}^{-2\mathrm{i}\phi_{l,m,n}}-A^{2}\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}}\right)+2\varepsilon^{2}b\cos k_y b\left(\frac{\partial A}{\partial\zeta_m}\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}+\frac{\partial A^{*}}{\partial\zeta_m}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right\}\frac{K_y\alpha_y}{M}\\
&+\left\{2\varepsilon\left(\cos k_z c-1\right)\left(A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}+A^{*}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)+\mathrm{i}2\varepsilon^{2}\alpha_z\mathrm{ctg}\left(\frac{k_z c}{2}\right)\left(\cos 2k_z c-1\right)\left(A^{2}\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}}+A^{*2}\mathrm{e}^{-2\mathrm{i}\phi_{l,m,n}}\right)\right.\\
&\left.+\mathrm{i}2\varepsilon^{2}c\sin k_z c\left(\frac{\partial A}{\partial\varsigma_n}\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}-\frac{\partial A^{*}}{\partial\varsigma_n}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right\}\left\{\mathrm{i}2\varepsilon\sin k_z c\left(A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}-A^{*}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right.\\
&\left.+2\varepsilon^{2}\alpha_z\mathrm{ctg}\left(\frac{k_z c}{2}\right)\sin 2k_z c\left(A^{*2}\mathrm{e}^{-2\mathrm{i}\phi_{l,m,n}}-A^{2}\mathrm{e}^{2\mathrm{i}\phi_{l,m,n}}\right)+2\varepsilon^{2}c\cos k_z c\left(\frac{\partial A}{\partial\varsigma_n}\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}+\frac{\partial A^{*}}{\partial\varsigma_n}\mathrm{e}^{-\mathrm{i}\phi_{l,m,n}}\right)\right\}\frac{K_z\alpha_z}{M},
\end{aligned}
$$

we obtain

$$
\begin{aligned}
&\frac{\partial^{2}u^{(3)}_{lmn,lmn}}{\partial t^{2}}-\frac{K_x}{M}\left(u^{(3)}_{lmn,(l+1)mn}+u^{(3)}_{lmn,(l-1)mn}-2u^{(3)}_{lmn,lmn}\right)\\
&-\frac{K_y}{M}\left(u^{(3)}_{lmn,l(m+1)n}+u^{(3)}_{lmn,l(m-1)n}-2u^{(3)}_{lmn,lmn}\right)-\frac{K_y}{M}\left(u^{(3)}_{lmn,lm(n+1)}+u^{(3)}_{lmn,lm(n-1)}-2u^{(3)}_{lmn,lmn}\right)\\
=&\left(\frac{K_x a}{M}\cos k_x a-\lambda^{2}\right)\frac{\partial^{2}A_0}{\partial\xi_l^{2}}+2\lambda\eta\frac{\partial^{2}A_0}{\partial\xi_l\partial\zeta_m}+\left(\frac{K_y b}{M}\cos k_y b-\eta^{2}\right)\frac{\partial^{2}A_0}{\partial\zeta_m^{2}}+2\lambda\mu\frac{\partial^{2}A_0}{\partial\xi_l\partial\varsigma_n}+2\eta\mu\frac{\partial^{2}A_0}{\partial\zeta_m\partial\varsigma_n}\\
&+\left(\frac{K_z c}{M}\cos k_z c-\mu^{2}\right)+\frac{8K_x\alpha_x a}{M}\sin^{2}k_x a\frac{\partial\left|A\right|^{2}}{\partial\xi_l}+\frac{8K_y\alpha_y b}{M}\sin^{2}k_y b\frac{\partial\left|A\right|^{2}}{\partial\zeta_m}+\frac{8K_z\alpha_z c}{M}\sin^{2}k_z c\frac{\partial\left|A\right|^{2}}{\partial\varsigma_n}\\
&+\frac{8K_x\alpha_x a}{M}\left(\cos k_x a-1\right)\cos k_x a\frac{\partial\left|A\right|^{2}}{\partial\xi_l}+\frac{8K_y\alpha_y b}{M}\left(\cos k_y b-1\right)\cos k_y b\frac{\partial\left|A\right|^{2}}{\partial\zeta_m}\\
&+\frac{8K_z\alpha_z c}{M}\left(\cos k_z c-1\right)\cos k_z c\frac{\partial\left|A\right|^{2}}{\partial\varsigma_n}\\
&+\frac{4K_x\alpha_x}{M}\mathrm{ctg}\left(\frac{k_x a}{2}\right)\left(\cos 2k_x a-1\right)\sin k_x a\left|A\right|^{2}A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}\\
&-\frac{4K_x\alpha_x}{M}\mathrm{ctg}\left(\frac{k_x a}{2}\right)\left(\cos k_x a-1\right)\sin 2k_x a\left|A\right|^{2}A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}\\
&+\frac{4K_y\alpha_y}{M}\mathrm{ctg}\left(\frac{k_y b}{2}\right)\left(\cos 2k_y b-1\right)\sin k_y b\left|A\right|^{2}A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}-\frac{4K_y\alpha_y}{M}\mathrm{ctg}\left(\frac{k_y b}{2}\right)\left(\cos k_y b-1\right)\sin 2k_y b\left|A\right|^{2}A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}\\
&+\frac{4K_z\alpha_z}{M}\mathrm{ctg}\left(\frac{k_z c}{2}\right)\left(\cos 2k_z c-1\right)\sin k_z c\left|A\right|^{2}A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}-\frac{4K_z\alpha_z}{M}\mathrm{ctg}\left(\frac{k_z c}{2}\right)\left(\cos k_z c-1\right)\sin 2k_z c\left|A\right|^{2}A\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}\\
&+\left[\mathrm{i}2\omega\frac{\partial A}{\partial\tau}+\left(\frac{K_x a}{M}\cos k_x a-\lambda^{2}\right)\frac{\partial^{2}A}{\partial\xi_l^{2}}+2\lambda\eta\frac{\partial^{2}A}{\partial\xi_l\partial\zeta_m}+\left(\frac{K_y b}{M}\cos k_y b-\eta^{2}\right)\frac{\partial^{2}A}{\partial\zeta_m^{2}}+2\lambda\mu\frac{\partial^{2}A}{\partial\xi_l\partial\varsigma_n}+2\eta\mu\frac{\partial^{2}A}{\partial\zeta_m\partial\varsigma_n}\right.\\
&\left.+\left(\frac{K_z c}{M}\cos k_z c-\mu^{2}\right)\frac{\partial^{2}A}{\partial\varsigma_n^{2}}\right]\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}. \qquad (12)
\end{aligned}
$$

There are two types of secular terms in Eq.(12). One type is functions of the slow variables only which will gives rise to terms explicitly in t in $u^{(3)}_{n,n}$. Removal of these and the secular terms $\mathrm{e}^{\mathrm{i}\phi_{l,m,n}}$ on the right-hand side of Eq.(12) gives

$$
\begin{aligned}
&2\omega\left(\alpha\frac{\partial^{2}A_0}{\partial\xi_l^{2}}+\frac{\lambda\eta}{\omega}\frac{\partial^{2}A_0}{\partial\xi_l\partial\zeta_m}+\beta\frac{\partial^{2}A_0}{\partial\zeta_m^{2}}+\frac{\lambda\mu}{\omega}\frac{\partial^{2}A_0}{\partial\xi_l\partial\varsigma_n}+\frac{\eta\mu}{\omega}\frac{\partial^{2}A_0}{\partial\zeta_m\partial\varsigma_n}+\gamma\frac{\partial^{2}A_0}{\partial\varsigma_n^{2}}\right)\\
&-\frac{8K_x\alpha_x a}{M}\cos k_x a\frac{\partial\left|A\right|^{2}}{\partial\xi_l}-\frac{8K_y\alpha_y b}{M}\cos k_y b\frac{\partial\left|A\right|^{2}}{\partial\zeta_m}-\frac{8K_z\alpha_z c}{M}\cos k_z c=0, \qquad (13a)
\end{aligned}
$$

$$
\mathrm{i}\frac{\partial A}{\partial\tau}+\alpha\frac{\partial^{2}A}{\partial\xi_l^{2}}+\frac{\lambda\eta}{\omega}\frac{\partial^{2}A}{\partial\xi_l\partial\zeta_m}+\frac{\lambda\mu}{\omega}\frac{\partial^{2}A}{\partial\xi_l\partial\varsigma_n}+\frac{\eta\mu}{\omega}\frac{\partial^{2}A}{\partial\zeta_m\partial\varsigma_n}+\gamma\frac{\partial^{2}A}{\partial\varsigma_n^{2}}+\beta\frac{\partial^{2}A}{\partial\zeta_m^{2}}+\chi\left|A\right|^{2}A=0, \qquad (13b)
$$

where

$$\chi = \frac{4K_x\alpha_x}{\omega M}\mathrm{ctg}\left(\frac{k_x a}{2}\right)(\cos k_x a - 1)\sin k_x a + \frac{4K_y\alpha_y}{\omega M}\mathrm{ctg}\left(\frac{k_y b}{2}\right)(\cos k_y b - 1)\sin k_y b + \frac{4K_z\alpha_z}{\omega M}\mathrm{ctg}\left(\frac{k_z c}{2}\right)(\cos k_z c - 1)\sin k_z c$$

and

$$\alpha = \frac{1}{2\omega}\left(\frac{K_x a^2}{M}\cos k_x a - \lambda^2\right), \quad \beta = \frac{1}{2\omega}\left(\frac{K_y b^2}{M}\cos k_y b - \eta^2\right), \quad \gamma = \frac{1}{2\omega}\left(\frac{K_z c^2}{M}\cos k_z c - \mu^2\right).$$

Taking Eqs.(3) and (8) and the method of multiple-scale into account, we have $A = u/\varepsilon$, $\xi_l = \varepsilon(la - \lambda t) = \varepsilon X_l$, $\zeta_m = \varepsilon(mb - \eta t) = \varepsilon Y_m$, $\varsigma_n = \varepsilon(nc - \mu t) = \varepsilon Z_n$ and $\tau = \varepsilon^2 t$. Equation (13) can be written as

$$2\omega\left(\alpha\frac{\partial^2 u_0}{\partial X_l^2} + \frac{\lambda\eta}{\omega}\frac{\partial^2 u_0}{\partial X_l \partial Y_m} + \beta\frac{\partial^2 u_0}{\partial Y_m^2} + \frac{\lambda\mu}{\omega}\frac{\partial^2 u_0}{\partial X_l \partial Z_n} + \frac{\eta\mu}{\omega}\frac{\partial^2 u_0}{\partial Y_m \partial Z_n} + \gamma\frac{\partial^2 u_0}{\partial Z_n^2}\right) - \frac{8K_x\alpha_x a}{M}\cos k_x a\frac{\partial |u|^2}{\partial X_l} - \frac{8K_y\alpha_y b}{M}\cos k_y b\frac{\partial |u|^2}{\partial Y_m} - \frac{8K_z\alpha_z c}{M}\cos k_z c\frac{\partial |u|^2}{\partial Z_n} = 0, \tag{14a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} + \alpha\frac{\partial^2 u}{\partial X_l^2} + \frac{\lambda\eta}{\omega}\frac{\partial^2 u}{\partial X_l \partial Y_m} + \beta\frac{\partial^2 u}{\partial Y_m^2} + \frac{\lambda\mu}{\omega}\frac{\partial^2 u}{\partial X_l \partial Z_n} + \frac{\eta\mu}{\omega}\frac{\partial^2 u}{\partial Y_m \partial Z_n} + \gamma\frac{\partial^2 u}{\partial Z_n^2} + \chi |u|^2 u = 0. \tag{14b}$$

Here we discuss several types of particular conditions. When the lattice has the same structure as the simple cubic lattice we have $a = b = c = a_0$, $K_x = K_y = K_z = K$, $\alpha_x = \alpha_y = \alpha_z = \alpha_0$, and $\alpha = \beta = \gamma = \frac{Ka_0^2}{8M\omega}(3\cos ka_0 - 1)$, $\frac{\lambda\eta}{\omega} = \frac{\lambda\mu}{\omega} = \frac{\eta\mu}{\omega} = \frac{Ka_0^2}{6M\omega}(\cos ka_0 + 1)$ in the direction of $k_x = k_y = k_z = k$ in the Brillouin zone. Equation (14) can be transformed into the following forms:

$$\frac{Ka_0^2}{4M}(3\cos ka_0 - 1)\left(\frac{\partial^2}{\partial X_l^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Y_m} + \frac{\partial^2}{\partial Y_m^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Z_n} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial Y_m \partial Z_n} + \frac{\partial^2}{\partial Z_n^2}\right)u_0 - \frac{8K\alpha_0 a_0}{M}\cos ka_0\left(\frac{\partial}{\partial X_l} + \frac{\partial}{\partial Y_m} + \frac{\partial}{\partial Z_n}\right)|u|^2 = 0, \tag{15a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} + \frac{Ka_0^2}{8M\omega}(3\cos ka_0 - 1)\left(\frac{\partial^2}{\partial X_l^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Y_m} + \frac{\partial^2}{\partial Y_m^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Z_n} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial Y_m \partial Z_n} + \frac{\partial^2}{\partial Z_n^2}\right)u + \chi |u|^2 u = 0. \tag{15b}$$

When $k = \pm\frac{\pi}{6a_0}$, Eq.(15) are transformed as follows:

$$\left(\frac{\partial}{\partial X_l} + \frac{\partial}{\partial Y_m} + \frac{\partial}{\partial Z_n}\right)^2 u_0 = \frac{32\alpha_0}{a_0}\left(\frac{\partial}{\partial X_l} + \frac{\partial}{\partial Y_m} + \frac{\partial}{\partial Z_n}\right)|u|^2, \tag{16a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} - \frac{Ka_0^2}{16M\omega}\left(\frac{\partial}{\partial X_l} + \frac{\partial}{\partial Y_m} + \frac{\partial}{\partial Z_n}\right)^2 u + \chi |u|^2 u = 0, \tag{16b}$$

where $\chi = -3\alpha_0\sqrt{\frac{3K}{M}} < 0$. With the transformation $X_l = X(r,s,g) = r + s + g$, $Y_m = Y(r,s,g) = r - s + g$, $Z_n = Z(r,s,g) = r + s - g$, we have

$$\frac{\partial}{\partial r} = \frac{\partial}{\partial X_l}\frac{\partial X_l}{\partial r} + \frac{\partial}{\partial Y_m}\frac{\partial Y_m}{\partial r} + \frac{\partial}{\partial Z_n}\frac{\partial Z_n}{\partial r} = \left(\frac{\partial}{\partial X_l} + \frac{\partial}{\partial Y_m} + \frac{\partial}{\partial Z_n}\right),$$

$$\frac{\partial}{\partial s} = \frac{\partial}{\partial X_l}\frac{\partial X_l}{\partial s} + \frac{\partial}{\partial Y_m}\frac{\partial Y_m}{\partial s} + \frac{\partial}{\partial Z_n}\frac{\partial Z_n}{\partial s} = \left(\frac{\partial}{\partial X_l} - \frac{\partial}{\partial Y_m} + \frac{\partial}{\partial Z_n}\right),$$

$$\frac{\partial}{\partial g} = \frac{\partial}{\partial X_l}\frac{\partial X_l}{\partial g} + \frac{\partial}{\partial Y_m}\frac{\partial Y_m}{\partial g} + \frac{\partial}{\partial Z_n}\frac{\partial Z_n}{\partial g} = \left(\frac{\partial}{\partial X_l} + \frac{\partial}{\partial Y_m} - \frac{\partial}{\partial Z_n}\right).$$

Equation (16) can be written as

$$\frac{\partial u_0}{\partial r} = \frac{32\alpha_0}{a_0}|u|^2, \tag{17a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} = \frac{Ka_0^2}{16M\omega}\frac{\partial^2 u}{\partial r^2} + 3\alpha_0\sqrt{\frac{3K}{M}}|u|^2 u. \tag{17b}$$

If the initial state of lattice is static, we can obtain $u_0 = 0$ from Eq.(17a); and for Eq.(17b), we can assume that its solution has the form of $u = u(r)\,\mathrm{e}^{-\mathrm{i}(s+g)}$. Thus the solution is

$$u(r,s,g,t) = \sqrt{c}\,\mathrm{sech}\left[\frac{6}{a_0}\sqrt{2\alpha_0 c}\,(r-vt)\right] \times \mathrm{e}^{-\mathrm{i}\frac{8M\omega v}{Ka_0^2}(r-vt)+\mathrm{i}\omega_0 t-\mathrm{i}(s+g)}. \tag{18}$$

Substituting the transformation $r = \dfrac{Y_m + Z_n}{2}$, $s = \dfrac{X_l - Y_m}{2}$, and $g = \dfrac{X_l - Z_n}{2}$ into the solution (18), we have

$$u(l,m,n,t) = \sqrt{c}\,\mathrm{sech}\left\{\delta_0\left[(m+n)a_0 - (\eta+\mu+2v)t\right]\right\} \times \mathrm{e}^{-\mathrm{i}(la_0+\delta_1 ma_0+\delta_2 na_0-\delta_3 t)}, \tag{19}$$

where c, v and ω_0 are integration parameters and $\delta_0 = \dfrac{3}{a_0}\sqrt{2\alpha_0 c}$, $\delta_1 = \delta_2 = \dfrac{1}{2} + \dfrac{4M\omega v}{Ka_0^2}$, $\delta_3 = \omega_0 + \dfrac{4M\omega v}{Ka_0^2}(\eta+\mu+2v)$.

According to Eq.(17a), we obtain

$$u_0 = \frac{8a_0}{9}\delta_0 \mathrm{th}\left\{\delta_0\left[(m+n)a_0 - (\eta+\mu+2v)t\right]\right\}. \tag{20}$$

So the solution of Eq.(2) has the following form:

$$u = \frac{8a_0}{9}\delta_0 \mathrm{th}\left\{\delta_0\left[(m+n)a_0 - (\eta+\mu+2v)t\right]\right\} + \sqrt{c}\,\mathrm{sech}\left\{\delta_0\left[(m+n)a_0 - (\eta+\mu+2v)t\right]\right\} \times \mathrm{e}^{-\mathrm{i}(la_0+\delta_1 ma_0+\delta_2 na_0-\delta_3 t)}. \tag{21}$$

From the solution (21) we know that the solution of the nonlinear vibration of the 3D simple cubic lattice has the same form as that of a 1D discrete monatomic chain with cubic nonlinearity.[11]

The solution (21) has the forms shown in Figs.2(a) and (b). The nonlinear vibration of a 3D simple cubic lattice with the cubic nonlinearity has the 3D distorted solitons, in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/6a_0$ in the Brillouin zone.

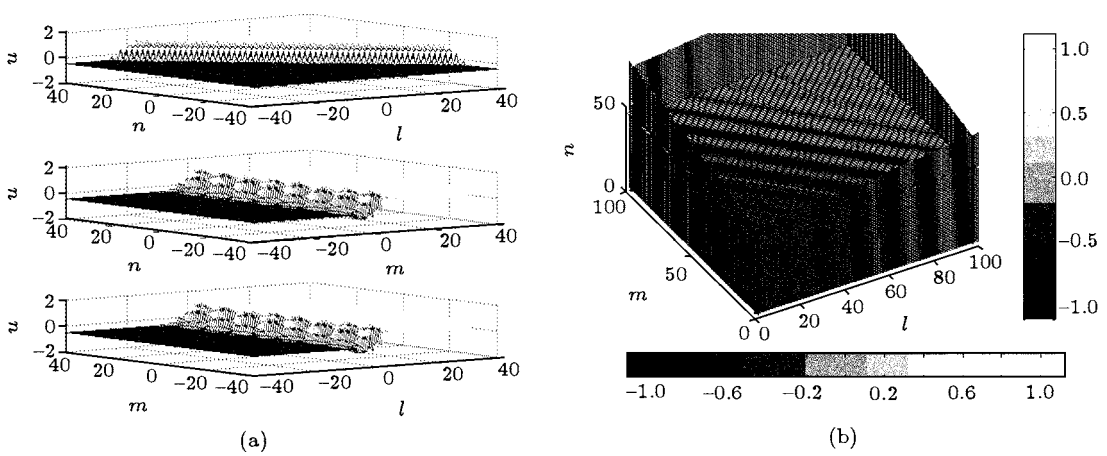


Fig.2. (a) The 3D distorted solitons of a 3D simple cubic lattice; (b) The 3D distorted solitons of a 3D simple cubic lattice.

3. The 3D envelop solitons and the 3D vortices of the nonlinear vibration in 3D discrete monatomic lattices with quartic nonlinearity

The 3D monatomic lattices are shown in Fig.1. Taking the interaction between the lattice and its nearest-neighbours into account, the Hamiltonian of the system with quartic anharmonic potential is given by

$$
\begin{aligned}
H = & \sum_{l,m,n} \left[\frac{p_{l,m}^2}{2M} + \frac{1}{2} K_x \left(u_{l+1,m,n} - u_{l,m,n} \right)^2 \right. \\
& \left. + \frac{1}{4} \beta_x K_x \left(u_{l+1,m,n} - u_{l,m,n} \right)^4 \right] \\
& + \sum_{l,m,n} \left[\frac{1}{2} K_y \left(u_{l,m+1,n} - u_{l,m,n} \right)^2 \right. \\
& \left. + \frac{1}{4} \beta_y K_y \left(u_{l,m+1,n} - u_{l,m,n} \right)^4 \right] \\
& + \sum_{l,m,n} \left[\frac{1}{2} K_z \left(u_{l,m,n+1} - u_{l,m,n} \right)^2 \right. \\
& \left. + \frac{1}{4} \beta_z K_z \left(u_{l,m,n+1} - u_{l,m,n} \right)^4 \right]. \qquad (22)
\end{aligned}
$$

By taking the same procedure as the above, we obtain

$$
\begin{aligned}
& 2\omega \left(\alpha \frac{\partial^2 u_0}{\partial X_l^2} + \frac{\lambda\eta}{\omega} \frac{\partial^2 u_0}{\partial X_l \partial Y_m} + \beta \frac{\partial^2 u_0}{\partial Y_m^2} + \frac{\lambda\mu}{\omega} \frac{\partial^2 u_0}{\partial X_l \partial Z_n} \right. \\
& \left. + \frac{\eta\mu}{\omega} \frac{\partial^2 u_0}{\partial Y_m \partial Z_n} + \gamma \frac{\partial^2 u_0}{\partial Z_n^2} \right) = 0, \qquad (23a)
\end{aligned}
$$

$$
\begin{aligned}
& \mathrm{i} \frac{\partial u}{\partial t} + \alpha \frac{\partial^2 u}{\partial X_l^2} + \frac{\lambda\eta}{\omega} \frac{\partial^2 u}{\partial X_l \partial Y_m} \\
& + \beta \frac{\partial^2 u}{\partial Y_m^2} + \frac{\lambda\mu}{\omega} \frac{\partial^2 u}{\partial X_l \partial Z_n} + \frac{\eta\mu}{\omega} \frac{\partial^2 u}{\partial Y_m \partial Z_n} \\
& + \gamma \frac{\partial^2 u}{\partial Z_n^2} + \chi |u|^2 u = 0. \qquad (23b)
\end{aligned}
$$

When

$$
\begin{aligned}
\chi = & \frac{4K_x\beta_x}{M\omega} [\sin^2 k_x a \left(\cos k_x a - 1 \right) \\
& + 2 \left(\cos k_x a - 1 \right)^2 \left(2 \cos k_x a - 1 \right)] \\
& + \frac{4K_y\beta_y}{M\omega} [\sin^2 k_y b \left(\cos k_y b - 1 \right) \\
& + 2 \left(\cos k_y b - 1 \right)^2 \left(2 \cos k_y b - 1 \right)] \\
& + \frac{4K_z\beta_z}{M\omega} [\sin^2 k_z c \left(\cos k_z c - 1 \right) \\
& + 2 \left(\cos k_z c - 1 \right)^2 \left(2 \cos k_z c - 1 \right)],
\end{aligned}
$$

$\beta_x = \beta_y = \beta_z = \beta_0$, and $k = \pm \dfrac{\pi}{6a_0}$, by the same transformation we have

$$
\frac{\partial^2 u_0}{\partial r^2} = 0, \qquad (24a)
$$

$$
\mathrm{i} \frac{\partial u}{\partial t} = \frac{K a_0^2}{16 M \omega} \frac{\partial^2 u}{\partial r^2} + 3\beta_0 \sqrt{\frac{3K}{M}} |u|^2 u. \qquad (24b)
$$

If the initial state of lattice is static, we can obtain $u_0 = 0$ from Eq.(24a), and for Eq.(24b) we can assume that its solution has the form of $u = u(r) \mathrm{e}^{-\mathrm{i}(s+g)}$. Thus the solution is

$$
\begin{aligned}
u(r, s, g, t) = & \sqrt{c} \operatorname{sech} \left[\frac{6}{a_0} \sqrt{2\beta_0 c} \left(r - vt \right) \right] \\
& \times \mathrm{e}^{-\mathrm{i} \frac{8 M \omega v}{K a_0^2} (r - vt) + \mathrm{i}\omega_0 t - \mathrm{i}(s+g)}. \qquad (25)
\end{aligned}
$$

Substituting the transformation $r = \dfrac{Y_m + Z_n}{2}$, $s = \dfrac{X_l - Y_m}{2}$, $g = \dfrac{X_l - Z_n}{2}$ into the solution (25), we have

$$
\begin{aligned}
u(l, m, n, t) = & \sqrt{c} \operatorname{sech} \{ \delta_0 [(m + n) a_0 \\
& - (\eta + \mu + 2v) t] \} \\
& \times \mathrm{e}^{-\mathrm{i}(l a_0 + \delta_1 m a_0 + \delta_2 n a_0 - \delta_3 t)}, \qquad (26)
\end{aligned}
$$

where c and v are integration parameters and

$$
\begin{aligned}
\delta_0 &= \frac{3}{a_0} \sqrt{2\beta_0 c}, \\
\delta_1 &= \delta_2 = \frac{1}{2} + \frac{4 M \omega v}{K a_0^2}, \\
\delta_3 &= \omega_0 + \frac{4 M \omega v}{K a_0^2} \left(\eta + \mu + 2v \right).
\end{aligned}
$$

From the solution (26) we know that the solution of the nonlinear vibration of the 3D simple cubic lattice has the same form as that of a 1D discrete monatomic chain with quartic nonlinearity.[11]

The solution (26) has the form shown in Figs.3(a) and (b). The nonlinear vibration of the 3D simple cubic lattice with the quartic nonlinearity has the 3D envelop solitons, in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/6a_0$ in the Brillouin zone.

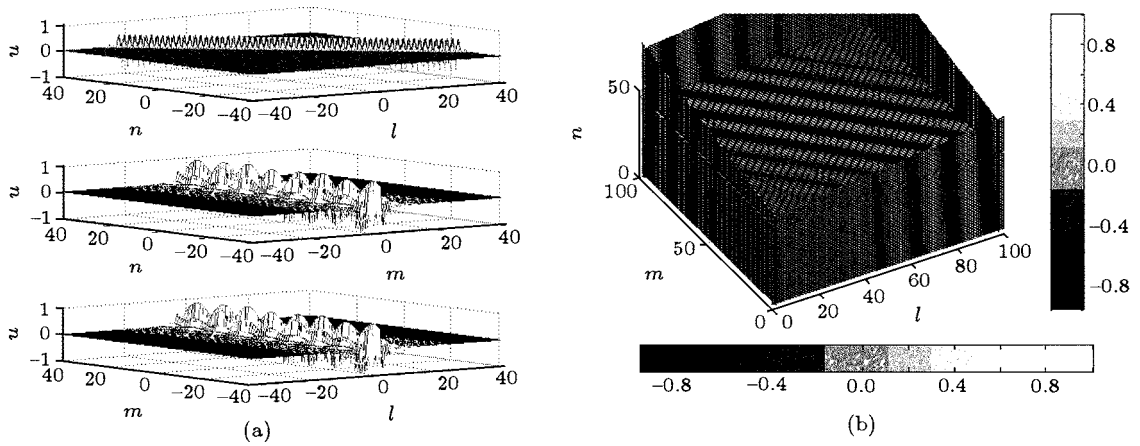


Fig.3. (a) The 3D envelop solitons of a 3D simple cubic lattice; (b) The 3D envelop solitons of a 3D simple cubic lattice.

When $\beta_x = \beta_y = \beta_z = \beta_0$, $\alpha = \beta = \gamma = \dfrac{Ka_0^2}{8M\omega}(3\cos ka_0 - 1)$, and $\dfrac{\lambda\eta}{\omega} = \dfrac{\lambda\mu}{\omega} = \dfrac{\eta\mu}{\omega} = \dfrac{Ka_0^2}{6M\omega}(\cos ka_0 + 1)$, Equations (23a) and (23b) can be transformed into the following forms:

$$\frac{Ka_0^2}{4M}(3\cos ka_0 - 1)\left(\frac{\partial^2}{\partial X_l^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Y_m} + \frac{\partial^2}{\partial Y_m^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Z_n} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial Y_m \partial Z_n} + \frac{\partial^2}{\partial Z_n^2}\right)u_0 = 0, \tag{27a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} + \frac{Ka_0^2}{8M\omega}(3\cos ka_0 - 1)\left(\frac{\partial^2}{\partial X_l^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Y_m} + \frac{\partial^2}{\partial Y_m^2} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial X_l \partial Z_n} + 2\frac{\cos ka_0 + 1}{3(3\cos ka_0 - 1)}\frac{\partial^2}{\partial Y_m \partial Z_n} + \frac{\partial^2}{\partial Z_n^2}\right)u + \chi|u|^2 u = 0. \tag{27b}$$

When $k = \pm\dfrac{\pi}{a_0}$, we have

$$\frac{Ka_0^2}{M}\left(\frac{\partial^2}{\partial X_l^2} + \frac{\partial^2}{\partial Y_m^2} + \frac{\partial^2}{\partial Z_n^2}\right)u_0 = 0, \tag{28a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} - \frac{Ka_0^2}{2M\omega}\left(\frac{\partial^2}{\partial X_l^2} + \frac{\partial^2}{\partial Y_m^2} + \frac{\partial^2}{\partial Z_n^2}\right)u + \chi|u|^2 u = 0. \tag{28b}$$

Let $r^2 = X_l^2 + Y_m^2 + Z_n^2$, Eqs.(23a) and (23b) can be transformed into the following forms:

$$\frac{Ka_0^2}{M}\frac{\partial^2 u_0}{\partial r^2} = 0, \tag{29a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} - \frac{a_0^2}{4}\sqrt{\frac{K}{3M}}\frac{\partial^2 u}{\partial r^2} - 144\beta_0\sqrt{\frac{K}{3M}}|u|^2 u = 0. \tag{29b}$$

If the initial state of lattice is static, from Eq.(29a) we can obtain $u_0 = 0$, Thus the solution is

$$u(r,t) = \sqrt{c}\,\mathrm{sech}\left[\frac{12}{a_0}\sqrt{2\beta_0 c}(r - vt)\right] \times \mathrm{e}^{\mathrm{i}\left(-\frac{2v}{a_0^2}\sqrt{\frac{3M}{K}}\right)(r - vt) + \mathrm{i}\omega_0 t}, \tag{30}$$

where c, v and ω_0 are integration parameters.

From the solution (30) we know that the solution of the nonlinear vibration of the 3D simple cubic lattice has the same form as that of the 1D discrete monatomic chain with quartic nonlinearity.[11]

The solution (30) has the form shown in Figs.4(a) and (b). The nonlinear vibration of the 3D simple cubic lattice with the quartic nonlinearity has the 3D vortices in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/a_0$ in the Brillouin zone.

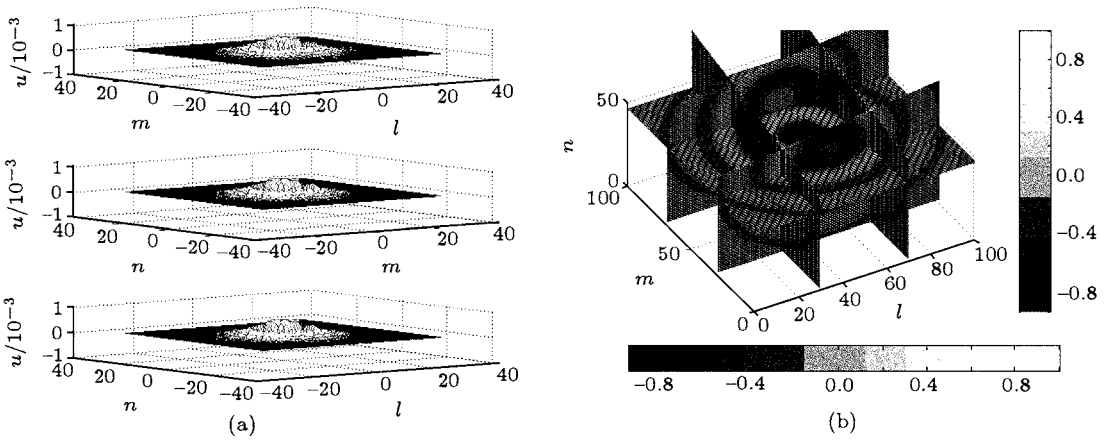


Fig.4. (a) The 3D vortices of a 3D simple cubic lattice; (b) The 3D vortices of a 3D simple cubic lattice.

4. The 3D distorted solitons of the nonlinear vibration in 3D discrete monatomic lattices with cubic and quartic nonlinearity

The 3D monatomic lattices are shown in Fig.1. Taking the interaction between the lattice and its nearest-neighbours into account, the Hamiltonian of the system with a cubic and quartic anharmonic potential is given by

$$H=\sum_{l,m,n}\left[\frac{p_{l,m}^2}{2M}+\frac{1}{2}K_x\left(u_{l+1,m,n}-u_{l,m,n}\right)^2+\frac{1}{3}\alpha_xK_x\left(u_{l+1,m,n}-u_{l,m,n}\right)^3+\frac{1}{4}\beta_xK_x\left(u_{l+1,m,n}-u_{l,m,n}\right)^4\right]$$
$$+\sum_{l,m,n}\left[\frac{1}{2}K_y\left(u_{l,m+1,n}-u_{l,m,n}\right)^2+\frac{1}{3}\alpha_yK_y\left(u_{l,m+1,n}-u_{l,m,n}\right)^3\frac{1}{4}\beta_xK_x\left(u_{l+1,m,n}-u_{l,m,n}\right)^4\right]$$
$$+\sum_{l,m,n}\left[\frac{1}{2}K_z\left(u_{l,m,n+1}-u_{l,m,n}\right)^2+\frac{1}{3}\alpha_zK_z\left(u_{l,m,n+1}-u_{l,m,n}\right)^3\frac{1}{4}\beta_xK_x\left(u_{l+1,m,n}-u_{l,m,n}\right)^4\right]. \tag{31}$$

By taking the same procedure as the above, we obtain

$$2\omega\left(\alpha\frac{\partial^2u_0}{\partial X_l^2}+\frac{\lambda\eta}{\omega}\frac{\partial^2u_0}{\partial X_l\partial Y_m}+\beta\frac{\partial^2u_0}{\partial Y_m^2}+\frac{\lambda\mu}{\omega}\frac{\partial^2u_0}{\partial X_l\partial Z_n}+\frac{\eta\mu}{\omega}\frac{\partial^2u_0}{\partial Y_m\partial Z_n}+\gamma\frac{\partial^2u_0}{\partial Z_n^2}\right)$$
$$-\frac{8K_x\alpha_xa}{M}\cos k_xa\frac{\partial\left|u\right|^2}{\partial X_l}-\frac{8K_y\alpha_yb}{M}\cos k_yb\frac{\partial\left|u\right|^2}{\partial Y_m}-\frac{8K_z\alpha_zc}{M}\cos k_zc\frac{\partial\left|u\right|^2}{\partial Z_n}=0, \tag{32a}$$

$$\mathrm{i}\frac{\partial u}{\partial t}+\alpha\frac{\partial^2u}{\partial X_l^2}+\frac{\lambda\eta}{\omega}\frac{\partial^2u}{\partial X_l\partial Y_m}+\beta\frac{\partial^2u}{\partial Y_m^2}+\frac{\lambda\mu}{\omega}\frac{\partial^2u}{\partial X_l\partial Z_n}+\frac{\eta\mu}{\omega}\frac{\partial^2u}{\partial Y_m\partial Z_n}+\gamma\frac{\partial^2u}{\partial Z_n^2}+\chi\left|u\right|^2u=0, \tag{32b}$$

where

$$\chi=\frac{4K_x\alpha_x}{\omega M}\mathrm{ctg}\left(\frac{k_xa}{2}\right)\left(\cos k_xa-1\right)\sin k_xa$$
$$+\frac{4K_y\alpha_y}{\omega M}\mathrm{ctg}\left(\frac{k_yb}{2}\right)\left(\cos k_yb-1\right)\sin k_yb+\frac{4K_z\alpha_z}{\omega M}\mathrm{ctg}\left(\frac{k_zc}{2}\right)\left(\cos k_zc-1\right)\sin k_zc$$
$$+\frac{4K_x\beta_x}{M\omega}\left[\sin^2k_xa\left(\cos k_xa-1\right)+2\left(\cos k_xa-1\right)^2\left(2\cos k_xa-1\right)\right]$$
$$+\frac{4K_y\beta_y}{M\omega}\left[\sin^2k_yb\left(\cos k_yb-1\right)+2\left(\cos k_yb-1\right)^2\left(2\cos k_yb-1\right)\right]$$
$$+\frac{4K_z\beta_z}{M\omega}\left[\sin^2k_zc\left(\cos k_zc-1\right)+2\left(\cos k_zc-1\right)^2\left(2\cos k_zc-1\right)\right],$$

$k=\pm\dfrac{\pi}{6a_0}$. By the same transformation, we have

$$\frac{\partial u_0}{\partial r} = \frac{32\alpha_0}{a_0}|u|^2, \tag{33a}$$

$$\mathrm{i}\frac{\partial u}{\partial t} = \frac{Ka_0^2}{16M\omega}\frac{\partial^2 u}{\partial r^2} + \frac{3K}{2M\omega}(\alpha_0 + 3\beta_0)|u|^2 u. \tag{33b}$$

So the solution of Eq.(32) has the following form:

$$\begin{aligned} u =& \frac{8a_0}{9}\delta_0 \mathrm{th}\{\delta_0[(m+n)a_0 - (\eta+\mu+2v)t]\} \\ &+ \sqrt{c}\,\mathrm{sech}\{\delta_0[(m+n)a_0 - (\eta+\mu+2v)t]\} \\ &\times \mathrm{e}^{-\mathrm{i}(la_0+\delta_1 ma_0+\delta_2 na_0-\delta_3 t)}, \end{aligned} \tag{34}$$

where c and v are integration parameters and $\delta_0 = \frac{2}{a_0}\sqrt{3(\alpha_0+3\beta_0)c}$, $\delta_1 = \delta_2 = \frac{1}{2} + \frac{4M\omega v}{Ka_0^2}$, $\delta_3 = \omega + \frac{4M\omega v}{Ka_0^2}(\eta+\mu+2v)$.

From the solution (34) we know that the solution of the nonlinear vibration of the 3D simple cubic lattice has the same form as that of a 1D discrete monatomic chain with cubic and quartic nonlinearity.[11] The solution (34) has also the form shown in Fig.2(a) and (b). The nonlinear vibration of the 3D simple cubic lattice with the cubic and quartic nonlinearity has the 3D distorted solitons in the direction of $k_x = k_y = k_z = k$ and $k = \pm\pi/6a_0$ in the Brillouin zone.

5. Conclusion

The above results show that the nonlinear vibration of a 3D simple cubic lattice has the same behaviours as the nonlinear vibration of a 1D discrete monatomic chain, and they are different from results of 2D compared with the results in Ref.[11]. There are following two main reasons. On the one hand, in the aspect of structural symmetry, a 3D simple cubic lattice is the same as a 1D monatomic chain, but different from 2D simple lattice . For example, when taking the interaction between the lattice and its nearest-neighbours into account, we assume that lattice vibration is transported along the crystal direction that is the same as the z-direction. In the x-direction and y-direction, the 3D simple cubic lattice and 1D monatomic chain have the same symmetry, but for the 2D simple lattice it is another story. On the other hand, in the aspect of symmetric interaction, the assumption is the same as the previous. In the x-direction and y-direction, the 3D simple cubic lattice and 1D monatomic chain have the same symmetric interaction. In the case of the 2D simple lattice the situation is different. The nonlinear vibration of lattice correlates closely to the above two factors, so there is 3D simple cubic lattice and 1D discrete monatomic chain have the same behaviour, but for the 2D simple lattice the situation is different.

From Figs.2(a) and (b) we know that the nonlinear vibrations of the 3D simple cubic lattice with only the cubic nonlinearity and with both the cubic nonlinearity and quartic nonlinearity have the same localized model—3D distorted solitons. From Figs.3(a), 3(b), 4(a) and 4(b) we know that the nonlinear vibration of 3D simple cubic lattice with only the quartic nonlinearity has the 3D envelop solitons and the 3D vortices which are different from the previous forms. The main reason is that the quartic nonlinear potential is a symmetric potential. Its action is what a symmetric localized model produces. The behaviour in any place, but for the position of localized model is the same as that without the potential action. The cubic nonlinear potential is a distorted potential. Its action is what a distorted model produces, and the positions of the localized model coincide with those with the quartic potential. So the localized states with a cubic and quartic potential are similar to those with only the cubic potential. The difference only lies in amplitude and frequency of the localized model.

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