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RESEARCH ARTICLE

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Dispersion relation for two-dimensional simple cubic lattices

Abstract The linear wave equation for the simple cubic lattice is given in this paper. The dispersion relations of both longitudinal and transverse waves are given analytically for the acoustic mode and the optical mode, respectively.

Keywords dispersion relation, simple cubic lattice, two-dimensional (2-D) lattice

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1 Introduction

Recently, many researchers have become interested in nonlinear waves in many fields of physics [1–3], such as in the soft condensed matter, Bose-Einstein condensate, lattice, etc. Lattices with a reduced dimensionality are an interesting topic. These lattices consist of particles that arrange themselves in a crystalline structure in the presence of external and interparticle forces. Typical examples of two-dimensional systems are colloidal suspensions [4], electrons on liquid helium [5], and Langmuir monolayers [6]. A number of interesting physical processes have been studied in these lattices, e.g., solid-liquid phase transitions, phonon propagation, and sublimation. We can find typical one-dimensional (1-D) systems [7, 8]: 1-D surface states such as chains of H atoms on Ni (110) [9], O on Cu (110) [10], ion chains trapped in a storage ring [11], nonlinear dynamics of sliding chain in a periodical potential [12], and optically bound chains of microspheres in a colloid [13]. Another way of preparing a lattice with reduced dimensionality is to use a plasma crystal, in which micron-size charged particles interact with each other via a Yukawa or screened-Coulomb potential. Most commonly, particles are levitated in a 2-D lattice in the plasma sheath of a lower electrode, where an upward electric force balances gravity in the downward direction [14–17]. When the crystal anneals, a triangular lattice with hexagonal symmetry is formed. Experiments by Konopka *et al*. [18] and simulations by Schweigert *et al*. [19] have verified that in the plane of the 2-D lattice, the interaction potential is modelled by a Yukawa potential. Hence, a 2-D plasma crystal belongs to the general class of 2-D Yukawa lattices. Similarly, 1-D chains can be formed by shaping the particle suspension with a fence or a groove in an electrode [20].

In a 2-D plasma crystal, two eigenwave modes can propagate; a longitudinal and a transverse wave. The longitudinal wave is a wave of compression propagating parallel to the particle motion. The transverse wave, sometimes called the shear wave, is a wave propagating perpendicular to the particle motion. In the linear wave regime, i.e., regime where wave amplitude is much smaller than the mean interparticle spacing, both longitudinal and transverse modes have already been observed in several experiments and the measured dispersion relations agreed with theoretical predictions [21–23]. Here,

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we summarize the characteristics of wave dispersion relations of longitudinal and transverse modes in 2-D plasma crystals, which have been verified in the above mentioned experiments and theories. Both modes have acoustic behavior. The sound speeds of these two modes are different; the longitudinal mode propagates faster than the transverse mode. Dispersion relations exhibit anisotropy, which is more pronounced in large values of k. In addition to the longitudinal and transverse waves, which are elastic deformations of the lattice, there are several other modes of particle motion. If the lattice has a finite size, and is confined by an external potential, it will have eigenmodes including the sloshing mode, which is a rigid-body oscillation of the entire lattice in the confining potential. An indirect observation of the presence of the sloshing mode at the same time as a longitudinal wave was reported previously [24, 25]. In addition, a lattice can be deformed with a plastic deformation, i.e., with a breaking of interparticle bonds. When bonds are broken, energy is consumed in an irreversible process, unlike an elastic deformation which involves no breaking of bonds and is reversible in the absence of any friction. A shear in the particle velocity profile is particularly effective in breaking bonds. After bonds have been broken in a plastic deformation process, it is possible for particles to circulate in a vortex, driven by any shear force that might be present. This vortex can be thought of as yet another kind of mode for particle motion. For all these modes, gas friction can lead to a damping.

In this paper, we study both longitudinal and transverse waves for two-dimensional simple cubic lattice. The dispersion relations are obtained in this paper.

2 Equation of motion

In this section, we derive general differential equations for the propagation of a linear 2-D form. Figure 1 shows the monolayer simple cubic lattice in two dimensions. We now want to find the equation of motion for arbitrary particle (n, m)th. We only consider the forces exerted on the particle (n, m)th produced only by the eight nearest particles. At equilibrium, the distances from the particle (n, m)th to the eight nearest particles are a or $\sqrt{2}a$. These eight nearest particles are expressed by No.1, 2, 3, 4, 5, 6, 7 and 8 respectively, see Fig. 1. We now set up the two-dimensional (x, y) plane. Let the (n, m)th particle be in the origin of this plane, then the positions of particles 1, 2, 3, 4, 5, 6, 7 and 8 at equilibrium are $(-a, a)$, $(0, a)$, (a, a), $(-a, 0)$, $(a, 0)$, $(-a, -a)$, $(0, -a)$, and $(a, -a)$, respectively. However, if the particles are not at their equilibrium positions, we define the eight variables of length l_1, l_2, l_3, l_4, l_5, l_6, l_7 and l_8 to represent the distances from particle $(n, m)th$ to the particles 1, 2, 3, 4, 5, 6, 7 and 8 respectively.

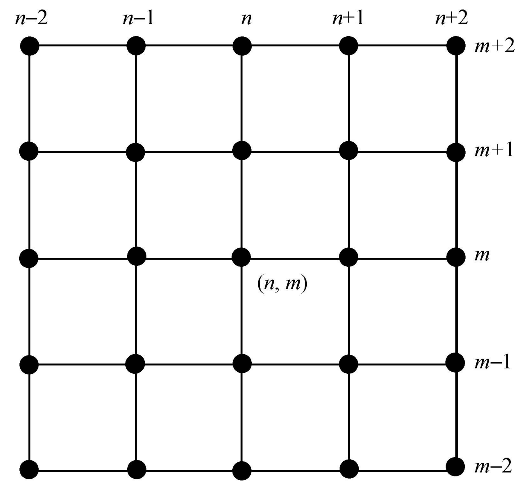

Fig. 1 Two-dimensional (2-D) simple cubic lattice.

$$l_p = \sqrt{(x_p + \Delta u_p)^2 + (y_p + \Delta v_p)^2} \tag{1}$$

where $p = 1, 2, 3, 4, 5, 6, 7, 8$, and

$$\begin{pmatrix} x_1 & y_1 & \Delta u_1 & \Delta v_1 \\ x_2 & y_2 & \Delta u_2 & \Delta v_2 \\ x_3 & y_3 & \Delta u_3 & \Delta v_3 \\ x_4 & y_4 & \Delta u_4 & \Delta v_4 \\ x_5 & y_5 & \Delta u_5 & \Delta v_5 \\ x_6 & y_6 & \Delta u_6 & \Delta v_6 \\ x_7 & y_7 & \Delta u_7 & \Delta v_7 \\ x_8 & y_8 & \Delta u_8 & \Delta v_8 \end{pmatrix}$$
$$= \begin{pmatrix} -a & a & u_{n-1,m+1} - u_{n,m} & v_{n-1,m+1} - v_{n,m} \\ 0 & a & u_{n,m+1} - u_{n,m} & v_{n,m+1} - v_{n,m} \\ a & a & u_{n+1,m+1} - u_{n,m} & v_{n+1,m+1} - v_{n,m} \\ -a & 0 & u_{n-1,m} - u_{n,m} & v_{n-1,m} - v_{n,m} \\ a & 0 & u_{n+1,m} - u_{n,m} & v_{n+1,m} - v_{n,m} \\ -a & -a & u_{n-1,m-1} - u_{n,m} & v_{n-1,m-1} - v_{n,m} \\ 0 & -a & u_{n,m-1} - u_{n,m} & v_{n,m-1} - v_{n,m} \\ a & -a & u_{n+1,m-1} - u_{n,m} & v_{n+1,m-1} - v_{n,m} \end{pmatrix} \tag{2}$$

where $u_{i,j}$ and $v_{i,j}$ are the displacements of the particles (i, j)th from their equilibrium positions in the x and y directions, respectively. We assume that all the particles (atoms or ions) are the same. The mass of each particle is M. The potential between the two nearest particles is $U(r)$. We also assume that at equilibrium the distance between the two nearest particles is a_0, the potential between them is, therefore, $U(a_0)$. If there is a displacement from the equilibrium position between two particles, then the distance between them becomes $r = a_0+\delta$, the potential becomes $U(r)$. We only consider the case of $\delta \ll a_0$, then we expand $U(r)$ as follows:

$$U(r) = U(a_0) + \left(\frac{\mathrm{d}U}{\mathrm{d}r}\right)_{a_0} \delta + \frac{1}{2}\left(\frac{\mathrm{d}^2U}{\mathrm{d}r^2}\right)_{a_0} \delta^2 + \cdots$$

Then, the force between two particles can be written as

$$F = -\beta\delta$$

where $\beta = \left(\frac{\mathrm{d}^2U}{\mathrm{d}r^2}\right)_{a_0}$.

The two components of the forces in the x and y directions exerted to the particle $(n, m)th$ by the nearest particles $1, 2, 3, 4, 5, 6, 7$ and 8 are given by

$$F_x = \sum_{i=1}^{8} F_i \frac{x_i + \Delta u_i}{l_i}$$

and

$$F_y = \sum_{i=1}^{8} F_i \frac{y_i + \Delta v_i}{l_i}$$

where $F_i = -\beta\delta_i$, $i = 1, 2, 3, 4, 5, 6, 7, 8$, $\delta_i = l_i - l_0$, $l_0 = a_0$ for the particles of $2, 4, 5, 7$, and $l_0 = \sqrt{2}a_0$ for the particles of $1, 3, 6, 8$. Now, we only consider the case of small amplitude vibration, i.e., $\Delta u_i \ll l_0$ and $\Delta v_i \ll l_0$, where $i = 1, 2, 3, 4, 5, 6, 7, 8$. By using the Taylor expansion, we then obtain the equation of motion for the arbitrary particle $(n, m)th$ as follows:

$$\begin{aligned}\frac{\partial^2 u_{n,m}}{\partial t^2} = &\frac{1}{M}[\beta_1(u_{n+1,m} + u_{n-1,m} - 2u_{n,m}) \\ &+\frac{\beta_2}{2}(u_{n+1,m+1} + u_{n+1,m-1} + u_{n-1,m+1} \\ &+u_{n-1,m-1} - 4u_{n,m} + v_{n+1,m+1} \\ &+v_{n-1,m-1} - v_{n+1,m-1} - v_{n-1,m+1})]\end{aligned} \quad (3)$$

and

$$\begin{aligned}\frac{\partial^2 v_{n,m}}{\partial t^2} = &\frac{1}{M}[\beta_1(v_{n,m+1} + v_{n,m-1} - 2v_{n,m}) \\ &+\frac{\beta_2}{2}(v_{n+1,m+1} + v_{n+1,m-1} + v_{n-1,m+1} \\ &+v_{n-1,m-1} - 4v_{n,m} + u_{n+1,m+1} \\ &+u_{n-1,m-1} - u_{n+1,m-1} - u_{n-1,m+1})]\end{aligned} \quad (4)$$

where $\beta_1 = \left(\frac{\mathrm{d}^2U}{\mathrm{d}r^2}\right)_a$, and $\beta_2 = \left(\frac{\mathrm{d}^2U}{\mathrm{d}r^2}\right)_{\sqrt{2}a}$.

3 Dispersion relations

It is well noted that there are two kinds of waves in the lattice, i.e., longitudinal and transverse waves in the different propagation directions. First, we study the dispersion relation of longitudinal waves which propagate in the direction of n. Assume that $u = u_0\mathrm{e}^{\mathrm{i}(kna-\omega t)}$, and then we obtain the dispersion relation as follows:

$$\omega_{\mathrm{L}}^2 = \frac{4}{M}(\beta_1 + \beta_2)\sin^2\frac{ka}{2}$$

Similarly, we study the dispersion relation of transverse waves propagating in the direction of m. Assume that $u = u_0\mathrm{e}^{\mathrm{i}(kma-\omega t)}$, we obtain

$$\omega_{\mathrm{T}}^2 = \frac{4}{M}\beta_2\sin^2\frac{ka}{2}$$

The dispersion relation propagating in the m direction is the same as that in the n direction because of the symmetry of the lattice. Therefore, it is enough that we only study the dispersion relation in the n direction for both longitudinal and transverse waves. Figure 2 shows the dispersion relation for both longitudinal and transverse waves, where ω_{L} denotes the frequency of the longitudinal waves and the ω_{T} stands for the frequency of the transverse waves. It indicates that the frequency of the longitudinal waves are larger than that of the transverse waves. Here, we only study the waves propagating in either the n or the m directions. However, they are only two particular directions. The dispersion relations may be much more complex for any other directions since the lattices are anisotropic. For generality, we assume that the waves propagate in the direction of $(1, \alpha)$. For this case, $v = \alpha u$. Letting

$$u = u_0\mathrm{e}^{\mathrm{i}(kna+k\alpha ma-\omega t)}$$

$$v = \alpha u_0\mathrm{e}^{\mathrm{i}(kna+k\alpha ma-\omega t)}$$

Substituting these equations into Eqs. (3) and (4), we find that there are real solutions only when $\alpha = 1$. More-

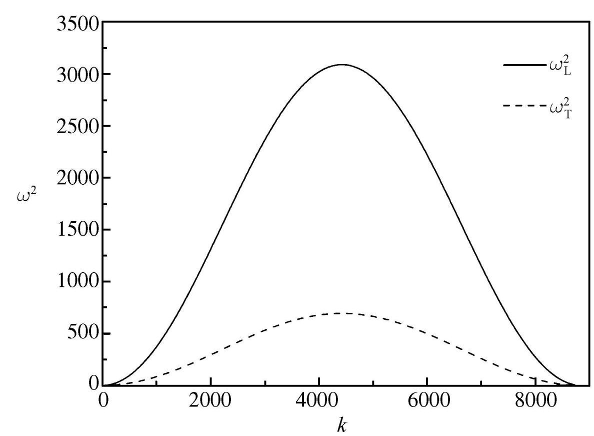

Fig. 2 Dispersion relations for both longitudinal and transverse waves in the direction of (1,0) or (0,1).

over, the dispersion relations of the longitudinal and the transverse waves propagating in the direction of (1,1) are obtained, respectively, as follows:

$$\omega_l^2 = \frac{4\beta_1}{M}\sin^2\frac{ka}{2} + \frac{4\beta_2}{M}\sin^2(ka) \tag{5}$$

$$\omega_T^2 = \frac{4\beta_1}{M}\sin^2\frac{ka}{2} \tag{6}$$

It is found that the linear waves can only propagate in the direction of (1,1), (1,0) and (0,1). The dispersion relations for both longitudinal and the transverse waves propagating in the direction of (1,1) are shown in Fig. 3, where ω_{L} denotes the frequency of the longitudinal waves and ω_{T} stands for the frequency of the transverse waves. It seems that the frequency of the longitudinal waves is a little bit larger than that of transverse waves. However, it is different from that propagating in the directions of (1,0) or (0,1). The anisotropic character of the lattice are given from these results.

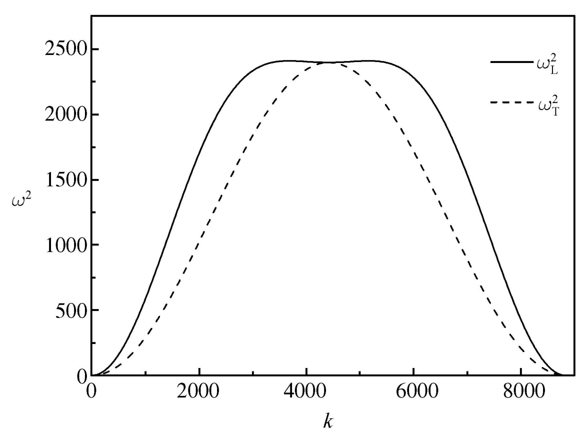

Fig. 3 Dispersion relations for both longitudinal and transverse waves in the direction of (1,1).

For bi-atomic lattice, as shown in Fig. 4, we assume that there are two kinds of different particles. Their masses are also different. Let M_1 and M_2 represent the masses of two different kinds of particles. Suppose that if $m + n = 2l$, the mass of the particle is M_1, while if $m + n = 2l + 1$, the mass of the particle is M_2, where $l = 0, \pm 1, \pm 2, \pm 3, \cdots$. Similarly, the equation of motion for this system can be obtained as follows for particle M_1

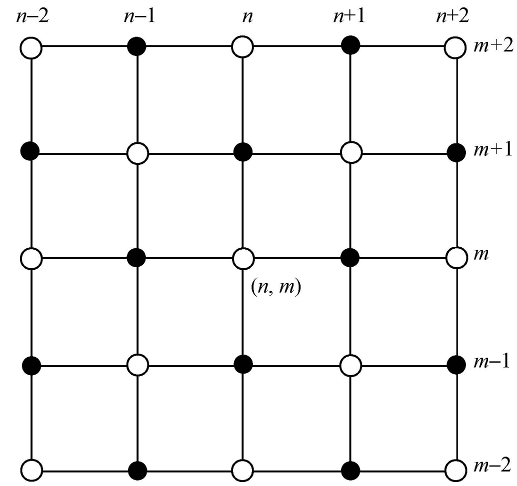

Fig. 4 Two-dimensional (2-D) simple cubic bi-atomic lattice.

$$\begin{aligned}\frac{\partial^2 u_{n,2l-n}}{\partial t^2} = \frac{1}{M_1}[&\beta_1(u_{n+1,2l-n} + u_{n-1,2l-n} \\ &-2u_{n,2l-n}) + \frac{\beta_2}{2}(u_{n+1,2l-n+1} \\ &+u_{n+1,2l-n-1} + u_{n-1,2l-n+1} \\ &+u_{n-1,2l-n-1} - 4u_{n,2l-n} \\ &+v_{n+1,2l-n+1} + v_{n-1,2l-n-1} \\ &-v_{n+1,2l-n-1} - v_{n-1,2l-n+1})]\end{aligned} \tag{7}$$

and for particle M_2

$$\begin{aligned}\frac{\partial^2 u_{n,2l-n+1}}{\partial t^2} = \frac{1}{M_2}[&\beta_1(u_{n+1,2l-n+1} + u_{n-1,2l-n+1} \\ &-2u_{n,2l-n+1}) + \frac{\beta_2}{2}(u_{n+1,2l-n+2} \\ &+u_{n+1,2l-n} + u_{n-1,2l-n+2} \\ &+u_{n-1,2l-n} - 4u_{n,2l-n+1} \\ &+v_{n+1,2l-n+2} + v_{n-1,2l-n} \\ &- v_{n+1,2l-n} - v_{n-1,2l-n+2})]\end{aligned} \tag{8}$$

The similar equation can be given for the displacements of $v_{i,j}$. First, we consider the compressional waves and assume that $u_{n,2l-n} = A\mathrm{e}^{\mathrm{i}(nka-\omega t)}$ for particles with mass M_1, $u_{n,2l-n+1} = B\mathrm{e}^{\mathrm{i}(nka-\omega t)}$ for particles with mass M_2. Then, we find that the dispersion relation is given by

$$\begin{pmatrix}\omega_{1L}^2 \\ \omega_{2L}^2\end{pmatrix} = \frac{1}{M_1M_2}\begin{pmatrix}(M_1+M_2)(\beta_1+\beta_2-\beta_2\cos(ka)) \\ (M_1+M_2)(\beta_1+\beta_2-\beta_2\cos(ka))\end{pmatrix} + \frac{1}{M_1M_2}\begin{pmatrix}-[(M_2-M_1)^2(\beta_1+\beta_2-\beta_2\cos(ka))^2+4M_1M_2\beta_1^2\cos(ka)^2)]^{1/2} \\ +[(M_2-M_1)^2(\beta_1+\beta_2-\beta_2\cos(ka))^2+4M_1M_2\beta_1^2\cos(ka)^2)]^{1/2}\end{pmatrix} \tag{9}$$

It is easy to find from Eq. (9) that there are two frequencies for longitudinal waves propagating in the n direction of (1,0). As usual, we define the two waves as acoustic mode and the optic mode. $\omega_{1\mathrm{L}}$ is defined as the frequency of the acoustic mode, $\omega_{2\mathrm{L}}$ as that of the optic mode. Figure 5 shows the dispersion relation given by Eq. (9), where we select the parameters of $M_1 = 6.8\times10^{-13}$kg, $M_2 = 9.0\times10^{-13}$kg [23]. The maximum value of ω_{1L} is given by $\omega_{1L_{\max}} = \left[\dfrac{2(\beta_1+\beta_2)}{M_2}\right]^{1/2}$. However, the minimum value of ω_{2L} is given by $\omega_{2L_{\min}} = \left[\dfrac{2(\beta_1+\beta_2)}{M_1}\right]^{1/2}$. It is noted that the maximum value of ω_{1L} is less than the minimum value of ω_{2L}. Therefore, we find that the frequency of the optical mode is always larger than that of the acoustic mode.

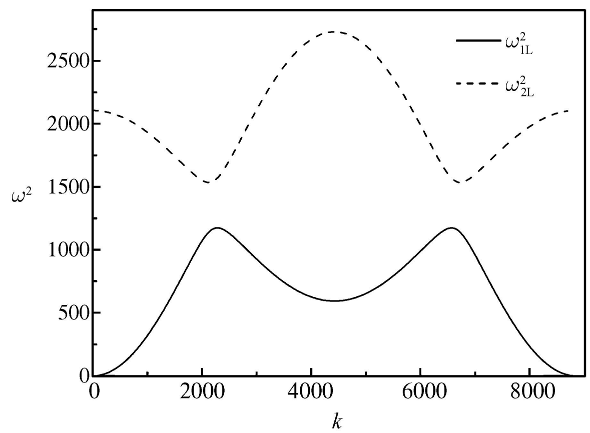

Fig. 5 Dispersion relation of the longitudinal waves of both acoustic and optic modes for bi-atomic lattice.

Second, we study the transverse waves in this system and assume that $u_{n,2l-n} = A\mathrm{e}^{\mathrm{i}[(2l-n)ka-\omega t]}$ for particles M_1, and $u_{n,2l-n+1} = B\mathrm{e}^{\mathrm{i}[(2l-n+1)ka-\omega t]}$ for particles M_2. Then, we find the dispersion relation for the transverse wave

$$\begin{pmatrix}\omega_{1T}^2\\ \omega_{2T}^2\end{pmatrix} = \frac{\beta_2}{M_1M_2} \cdot\begin{pmatrix}M_1+M_2-[M_1^2+M_2^2+2M_1M_2\cos(2ka)]^{1/2}\\ M_1+M_2+[M_1^2+M_2^2+2M_1M_2\cos(2ka)]^{1/2}\end{pmatrix} \qquad (10)$$

We also find that there are two frequencies for transverse waves propagating in the n direction of (1,0). Similar results can be obtained in the (0,1) direction. We also define two waves as acoustic mode and the optic mode. ω_{1T} is the frequency of the acoustic mode, ω_{2T} the optic mode. Figure 6 shows the dispersion relation given by Eq. (6), where we also select the parameters of $M_1 = 6.8\times10^{-13}$kg, $M_2 = 9.0\times10^{-13}$kg [23]. We also find that the frequency of the optic mode is larger than that of the acoustic mode which is similar with that of longitudinal waves.

To find the dependence of the frequencies on the different mass ratio of $\gamma = M_2/M_1$, we have calculated the dispersion relations of ω_{1L}, ω_{2L}, ω_{1T} and ω_{2T} with different mass ratio of $\gamma = 0.5, 0.7, 1.0, 1.5, 2.0$ respectively, which are shown in Figs.7, 8, 9, and 10, respectively, where the M_1 is a constant. $M_1 = 6.8\times10^{-13}$kg. We find that all the four frequencies decrease as γ increases.

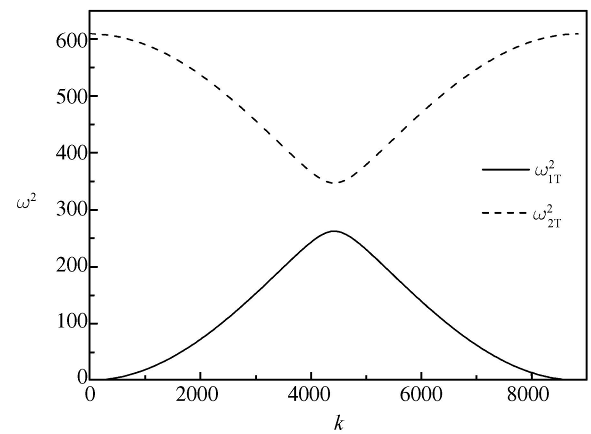

Fig. 6 Dispersion relation of the transverse waves of both acoustic and optic modes for bi-atomic lattice.

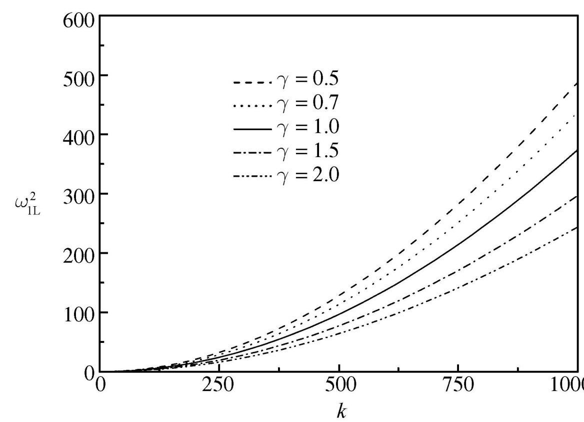

Fig. 7 Dispersion relation of acoustic mode for longitudinal wave for different mass ratios.

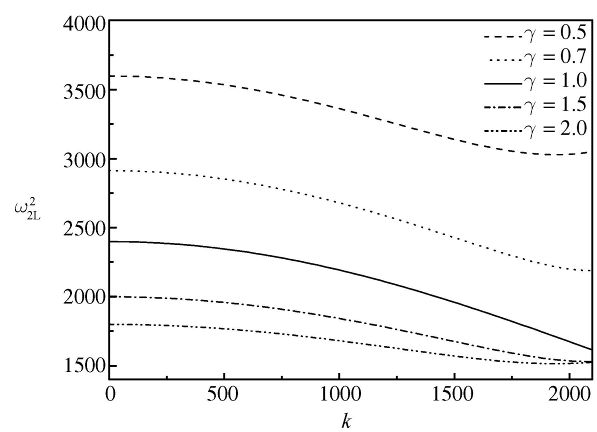

Fig. 8 Dispersion relation of optic mode for longitudinal wave for different mass ratios.

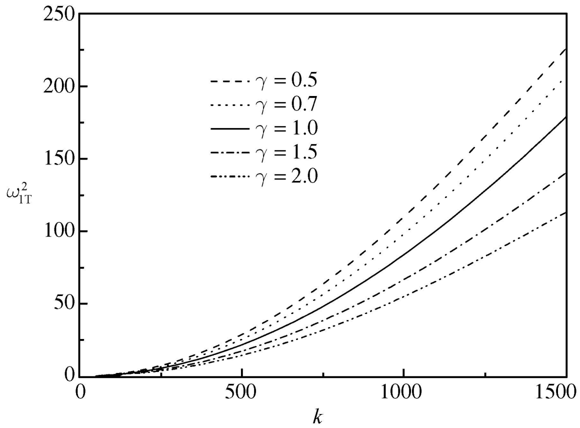

Fig. 9 Dispersion relation of acoustic mode for transverse wave for different mass ratios.

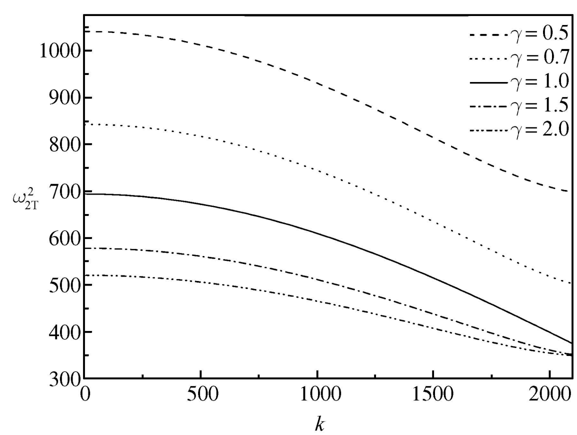

Fig. 10 Dispersion relation of optic mode for transverse wave for different mass ratios.

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