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Lattice Vibrations in the Frenkel-Kontorova Model. Ⅰ. Phonon Dispersion, Number Density, and Energy

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We studied the lattice vibrations of two inter-penetrating atomic sublattices via the Frenkel-Kontorova (FK) model of a linear chain of harmonically interacting atoms subjected to an on-site potential, using the technique of thermodynamic Green's functions based on quantum field-theoretical methods. General expressions were deduced for the phonon frequency-wave-vector dispersion relations, number density, and energy of the FK model system. As the application of the theory, we investigated in detail cases of linear chains with various periods of the on-site potential of the FK model. Some unusual but interesting features for different amplitudes of the on-site potential of the FK model are discussed. In the commensurate structure, the phonon spectrum always starts at a finite frequency, and the gaps of the spectrum are true ones with a zero density of modes. In the incommensurate structure, the phonon spectrum starts from zero frequency but at a non-zero wave vector; there are some modes inside these gap regions, but their density is very low. In our approximation, the energy of a higher-order commensurate state of the one-dimensional system at finite temperature may become indefinitely close to the energy of an incommensurate state. This finding implies that the higher-order incommensurate-commensurate transitions are continuous ones, and that the phase transition may exhibit a "devil's staircase" behavior at a finite temperature.

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I. Introduction

Recent investigations revealed that materials consisting of two interpenetrating incommensurate sub-lattices, such as Na_xCoO_2 [1], $Ca_3Co_4O_9$ [2, 3], and $Bi_{2-x}Pb_xSr_2Co_2O_y$ [2, 4], have very good thermoelectric properties. One reason for this is that these materials have very low lattice thermal conductivity [3]. To understand their lattice thermal conductivity, we need to know the lattice vibrational properties of two inter-penetrating sublattices. Some insights into this problem might be obtained from a studing the Frenkel-Knotorova (FK) model.

The FK model describes a chain of classical particles coupled to their neighbors, and subjected to a periodic on-site potential. This model has received much attention because of its relevance to a wide variety of physical problems. The FK model originally was proposed to model dislocations in epitaxial monolayers [5, 6], but its surprising ability to describe many physically important phenomena, such as the dynamics of absorbed layers of atoms on crystal surfaces [7, 8], charge-density waves [9, 10], ferro- or antiferro-magnetics [11], and superionic conductors [12], has attracted much attention from physicists working in solid-state physics.

Some simple classical models have been analyzed that describe an atomic chain with nearest-neighbor interactions and subjected to a periodic on-site potential [13~19]. For them, phonon dispersion, the dynamic structural factors of crystals with incommensurate lattices, were studied at the long-wavelength limit. If the effects of lattice discreteness are neglected, the long-wavelength limit transitions to the continuum-limit approximation, and the nonlinear differential equations of motion are obtained for these classical models. For the FK model, this approximation leads to the exactly integrable sine-Gordon equation that possesses many interesting properties and allows exact solutions describing different types of nonlinear excitations [20]. However, the FK model inherently is discrete and not exactly integrable [20].

Therefore, this simple approximation will engender some deviations. For example, Sutherland [21, 22] found that the phonon spectrum separates simply into two branches in the continuum-limit approximation. The lower branch represents the collective modes of lattice dislocations, while the upper one corresponds to renormalized phonons [13, 23]. Following standard procedures in the theory of lattice dynamics, the phonon spectrum may include multiple branches [7, 23]. Thus, the FK model at the simplest continuum limit intrinsically may be too simple, and misleading in some cases.

Typically, the FK model utilizes an on-site potential to describe the interaction between two interpenetrating sub-lattices. Classical theories have revealed some of the static- and dynamic-characteristics of lattice vibrations in such systems [13~23]. However, classical theories mainly give the results using a long-wavelength approximation, and temperature effects are not considered in any of the classical theories; indeed, and the discussion of lattice vibrations at low temperature is beyond the scope of the classical theory.

The present work was motivated by our desire to understand the thermodynamic properties of materials with two interpenetrating sub-lattices. The formulation of thermodynamic Green's functions leads naturally to the evaluation of the energy of a system via correlation functions; we have not identified any previous publication wherein the description of the energy of an FK model system has been evaluated quantum mechanically. In section Ⅱ, we deduce an expression for the correlation function resulting from the FK model, using thermodynamic Green's functions. From this correlation function, we obtained the phonon dispersion, the phonon number density, and the energy of the system. In section Ⅲ, we first use the general formulae deduced in section Ⅱ to calculate the properties of some low-order commensurate states, and then, from these results, we extend the calculation to commensurate states of any order, and to the incommensurate state. A detailed discussion of these findings is given; Section Ⅳ contains our summary and conclusions.

Ⅱ. General Formalism

A. The Hamiltonian

We consider a system consisting of a lattice of atoms with harmonic vibrations that interact with an external perturbing potential, i.e., the FK model. The total crystal Hamiltonian can be written as

$$H = H_0 + H_1 \tag{2.1}$$

where H_0 is the harmonic Hamiltonian of the unperturbed lattice given by

$$H_0 = \sum_{kj} \hbar\omega_{kj}\left(a_{kj}^{+}a_{kj} + \frac{1}{2}\right) = \frac{1}{4}\sum_{kj}\hbar\omega_{kj}\left(A_{kj}^{+}A_{kj} + B_{kj}^{+}B_{kj}\right) \tag{2.2}$$

H_1 is the perturbation Hamiltonian arising from the external on-site potentials of the FK model, and ω_{kj} is the frequency of a phonon with wave vector k and polarization index j. Hereafter, we use k to represent the pair of variables k and j. A_k and B_k are phonon operators that we define in terms of the usual phonon creation- and destruction-operators, a_k^{+} and a_k: $A_k = a_k + a_{-k}^{+} = A_{-k}^{+}$ and $B_k = a_k - a_{-k}^{+} = -B_{-k}^{+}$.

We can write the external on-site potential of the FK model as

$$H_1 = \sum_{l} V_0\left[1 - \cos(\mathbf{g}\cdot\mathbf{x}_1)\right] \tag{2.3}$$

where $\mathbf{g}$ is the wave vector of the periodic external potential, and $\mathbf{x}_1$ is the position of an atom, l, of the linear chain. For one dimension, $g = \frac{2\pi}{b}$, where b is the period of the on-site potential;

$x_l = al + u_l$, a is the lattice constant of the linear chain; l is an integer; and u_l describes a deviation from the lattice's original equilibrium position. V_0 is the amplitude of the on-site potential of the FK model. Assuming that u_l is small and only considering the one-dimensional case, H_1 can be written to the fourth-order in the deviations from the original equilibrium positions as follows:

$$H_1 = \sum_l V_0 \left\{ 1 - \cos(gla)\left[1 - \frac{1}{2!}(gu_l)^2 + \frac{1}{4!}(gu_l)^4\right] + \sin(gla)\left[gu_l - \frac{1}{3!}(gu_l)^3\right]\right\} \tag{2.4}$$

Using

$$u_l = \left(\frac{\hbar}{2Nm}\right)^{\frac{1}{2}} \sum_k \frac{1}{\omega_k^{\frac{1}{2}}} \exp(ikla) A_k \tag{2.5}$$

and ignoring the constant term in H_1, H_1 is

$$\begin{aligned} H_1 = {} & \sum_{k_1} C_1(k_1) A_{k_1} + \sum_{k_1,k_2} C_2(k_1,k_2) A_{k_1} A_{k_2} + \sum_{k_1,k_2,k_3} C_3(k_1,k_2,k_3) A_{k_1} A_{k_2} A_{k_3} \\ & + \sum_{k_1,k_2,k_3,k_4} C_4(k_1,k_2,k_3,k_4,) A_{k_1} A_{k_2} A_{k_3} A_{k_4} \end{aligned} \tag{2.6}$$

where, for a one-dimensional Bravais crystal of N atoms, each of mass m,

$$C_1(k_1) = -\frac{i\pi V_0}{b}\left(\frac{\hbar N}{2m}\right)^{\frac{1}{2}} \omega_{k_1}^{-\frac{1}{2}} \left[\Delta(k_1 + g) - \Delta(k_1 - g)\right] \tag{2.7a}$$

$$C_2(k_1,k_2) = \frac{\pi^2 \hbar V_0}{2mb^2} \left(\omega_{k_1}\omega_{k_2}\right)^{-\frac{1}{2}} \left[\Delta(k_1 + k_2 + g) + \Delta(k_1 + k_2 - g)\right] \tag{2.7b}$$

$$C_3(k_1,k_2,k_3) = \frac{i2\pi^3 V_0}{3b^3 N^{\frac{1}{2}}} \left(\frac{\hbar}{2m}\right)^{\frac{3}{2}} \left(\omega_{k_1}\omega_{k_2}\omega_{k_3}\right)^{-\frac{1}{2}} \left[\Delta(k_1 + k_2 + k_3 + g) - \Delta(k_1 + k_2 + k_3 - g)\right] \tag{2.7c}$$

$$C_4(k_1,k_2,k_3,k_4) = -\frac{\pi^4\hbar^2 V_0}{12m^2b^4N}\left(\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}\right)^{-\frac{1}{2}} \times\left[\Delta(k_1+k_2+k_3+k_4+g)+\Delta(k_1+k_2+k_3+k_4-g)\right] \tag{2.7d}$$

with $\Delta(k)=1$ for $k=0$; otherwise $\Delta(k)=0$.

B. Thermodynamic Green's function and time-correlation functions

To evaluate some necessary correlation functions, we need to know the thermodynamic Green's function for this model:

$$G_{qk}(t-t') = \left\langle\left\langle A_q(t), A_k^+(t')\right\rangle\right\rangle = -i\theta(t-t')\left\langle\left[A_q(t), A_k^+(t')\right]\right\rangle \tag{2.8}$$

$\theta(t)$ is the step function. The time correlation function is

$$Q_{kq}(t-t') = \left\langle A_k^+(t')A_q(t)\right\rangle \tag{2.9}$$

The brackets $\langle\cdots\rangle$ represent the thermodynamic average over a canonical ensemble. Namely, for any operator O

$$\langle O\rangle = \frac{Tre^{-\beta H}O}{Tre^{-\beta H}}$$

where $\beta = \frac{1}{k_BT}$, k_B is the Boltzmann constant, and T is the absolute temperature.

We define the Fourier transforms $\widetilde{G}_{qk}(\omega)$ and $J_{kq}(\omega)$ of the Green's function and the time correlation function as follows:

$$G_{qk}(t-t') = \int_{-\infty}^{\infty}\widetilde{G}_{qk}(\omega)e^{-i\omega(t-t')}d\omega \tag{2.10}$$

and,

$$Q_{kq}(t-t') = \int_{-\infty}^{\infty}J_{kq}(\omega)e^{-i\omega(t-t')}d\omega \tag{2.11}$$

$J_{kq}(\omega)$ is the spectral-density function and is related to the Green's function by

$$J_{kq}(\omega) = -\frac{2}{\exp(\beta\hbar\omega)-1}\operatorname{Im}\widetilde{G}_{qk}(\omega + i\varepsilon) \tag{2.12}$$

where $\varepsilon \to 0$ is implied.

Following Pathak's method [24], and the detailed presentation in Supplemental Material [25], the correlation functions can be obtained

$$Q_{kq}^{(1)}(t) = \left\langle a_k^+(0)a_q(t)\right\rangle = \frac{1}{4}\int_{-\infty}^{\infty}\left(1 + \frac{\omega}{\omega_k} + \frac{\omega}{\omega_q} + \frac{\omega^2}{\omega_k\omega_q}\right)J_{kq}(\omega)e^{-i\omega t}d\omega \tag{2.13a}$$

$$Q_{kq}^{(2)}(t) = \left\langle a_k(0)a_q^+(t)\right\rangle = \frac{1}{4}\int_{-\infty}^{\infty}\left(1 + \frac{\omega}{\omega_k} + \frac{\omega}{\omega_q} + \frac{\omega^2}{\omega_k\omega_q}\right)J_{qk}(\omega)e^{\beta\hbar\omega}e^{i\omega t}d\omega \tag{2.13b}$$

C. Calculation of the thermodynamic Green's function

As discussed above, Green's function must be known to calculate the correlation functions. We used Zubarev's method [26] for obtaining them in this paper. From the equation of motion for an operator $O(t)$

$$i\hbar\frac{\partial O(t)}{\partial t} = [O(t), H],$$

the equation of motion for the Green's function $G_{q,k}(t-t')$ is

$$i\frac{\partial G_{qk}}{\partial t} = \omega_q G_{qk}^{(1)} \tag{2.14a}$$

and,

$$\begin{aligned} i\hbar\frac{\partial G_{qk}^{(1)}}{\partial t} &= 2\hbar\delta(t-t')\delta_{qk} + \hbar\omega_q G_{qk} + 4\sum_{k_1}C_2(k_1,-q)G_{k_1k} \\ &+ 6\sum_{k_1k_2}C_3(k_1,k_2,-q)\left\langle\left\langle A_{k_1}A_{k_2}, A_k^+\right\rangle\right\rangle + 8\sum_{k_1k_2k_3}C_4(k_1,k_2,k_3,-q)\left\langle\left\langle A_{k_1}A_{k_2}A_{k_3}, A_k^+\right\rangle\right\rangle \end{aligned} \tag{2.14b}$$

where $G_{qk}^{(1)}(t-t') = \left\langle\left\langle B_q(t), A_k^+(t')\right\rangle\right\rangle = -i\theta(t-t')\left\langle\left[B_q(t), A_k^+(t')\right]\right\rangle$.

To obtain G_{qk}, we employed some approximations. For example, the last term of right side in Eq. (2.14b) was decoupled according to relation [24, 26]

$$\langle abcd \rangle = \langle ab \rangle \langle cd \rangle + \langle ac \rangle \langle bd \rangle + \langle ad \rangle \langle bc \rangle . \tag{2.15}$$

To discover the Green's function, $\Gamma^{(1)}_{k_1 k_2 k} = \langle\langle A_{k_1} A_{k_2}, A_k^+(t') \rangle\rangle$, contained in the third term of the right-hand side in Eq. (2.14b), we need other new Green's functions $\Gamma^{(2)}_{k_1 k_2 k} = \langle\langle B_{k_1} A_{k_2}, A_k^+(t') \rangle\rangle$, $\Gamma^{(3)}_{k_1 k_2 k} = \langle\langle A_{k_1} B_{k_2}, A_k^+(t') \rangle\rangle$, $\Gamma^{(4)}_{k_1 k_2 k} = \langle\langle B_{k_1} B_{k_2}, A_k^+(t') \rangle\rangle$, as is apparent from the following equations of motion

$$i \frac{\partial \Gamma^{(1)}_{k_1 k_2 k}}{\partial t} = \omega_{k_1} \Gamma^{(2)}_{k_1 k_2 k} + \omega_{k_2} \Gamma^{(3)}_{k_1 k_2 k} \tag{2.16a}$$

$$\begin{aligned} i\hbar \frac{\partial \Gamma^{(2)}_{k_1 k_2 k}}{\partial t} = {} & \hbar\omega_{k_2} \Gamma^{(4)}_{k_1 k_2 k} + \hbar\omega_{k_1} \Gamma^{(1)}_{k_1 k_2 k} + 2C_1(-k_1) G_{k_2 k} + 4\sum_{k_1^{'}} C_2\left(k_1^{'}, -k_1\right) \Gamma^{(1)}_{k_1^{'} k_2 k} \\ & + 6\sum_{k_1^{'} k_2^{'}} C_3\left(k_1^{'}, k_2^{'}, -k_1\right) \langle\langle A_{k_1^{'}} A_{k_2^{'}} A_{k_2}, A_k^+ \rangle\rangle \\ & + 8\sum_{k_1^{'} k_2^{'} k_3^{'}} C_4\left(k_1^{'}, k_2^{'}, k_3^{'}, -k_1\right) \langle\langle A_{k_1^{'}} A_{k_2^{'}} A_{k_3^{'}} A_{k_2}, A_k^+ \rangle\rangle \end{aligned} \tag{2.16b}$$

$$\begin{aligned} i\hbar \frac{\partial \Gamma^{(3)}_{k_1 k_2 k}}{\partial t} = {} & \hbar\omega_{k_1} \Gamma^{(4)}_{k_1 k_2 k} + \hbar\omega_{k_2} \Gamma^{(1)}_{k_1 k_2 k} + 2C_1(-k_2) G_{k_1 k} + 4\sum_{k_1^{'}} C_2\left(k_1^{'}, -k_2\right) \Gamma^{(1)}_{k_1 k_1^{'} k} \\ & + 6\sum_{k_1^{'} k_2^{'}} C_3\left(k_1^{'}, k_2^{'}, -k_2\right) \langle\langle A_{k_1} A_{k_1^{'}} A_{k_2^{'}}, A_k^+ \rangle\rangle \\ & + 8\sum_{k_1^{'} k_2^{'} k_3^{'}} C_4\left(k_1^{'}, k_2^{'}, k_3^{'}, -k_2\right) \langle\langle A_{k_1} A_{k_1^{'}} A_{k_2^{'}} A_{k_3^{'}}, A_k^+ \rangle\rangle \end{aligned} \tag{2.16c}$$

$$
\begin{aligned}
i\hbar\frac{\partial\Gamma^{(4)}_{k_1k_2k}}{\partial t} &= \hbar\omega_{k_1}\Gamma^{(3)}_{k_1k_2k} + \hbar\omega_{k_2}\Gamma^{(2)}_{k_1k_2k} + 2C_1(-k_1)G^{(1)}_{k_2k} + 2C_1(-k_2)G^{(1)}_{k_1k} \\
&+ 4\sum_{k_1'} C_2(k_1',-k_1)\Gamma^{(3)}_{k_1'k_2k} + 4\sum_{k_1'} C_2(k_1',-k_2)\Gamma^{(2)}_{k_1k_1'k} \\
&+ 6\sum_{k_1'k_2'} C_3(k_1',k_2',-k_2)\left\langle\left\langle B_{k_1}A_{k_1'}A_{k_2'}, A_k^+\right\rangle\right\rangle + 6\sum_{k_1'k_2'} C_3(k_1',k_2',-k_1)\left\langle\left\langle A_{k_1'}A_{k_2'}B_{k_2}, A_k^+\right\rangle\right\rangle \\
&+ 8\sum_{k_1'k_2'k_3'} C_4(k_1',k_2',k_3',-k_2)\left\langle\left\langle B_{k_1}A_{k_1'}A_{k_2'}A_{k_3'}, A_k^+\right\rangle\right\rangle \\
&+ 8\sum_{k_1'k_2'k_3'} C_4(k_1',k_2',k_3',-k_1)\left\langle\left\langle A_{k_1'}A_{k_2'}A_{k_3'}B_{k_2}, A_k^+\right\rangle\right\rangle
\end{aligned}
\tag{2.16d}
$$

To solve Eq. (2.16) to obtain these Green's functions, we neglected the five-operator Green's functions; and the four-operator Green functions can be decoupled as sums of the products of the two-operator correlation functions, and the two-operator Green's functions. Using Fourier transforms, and $N_k = \left\langle A_k^+ A_k \right\rangle$, Eqs. (2.15) and (2.16) become

$$
\omega\widetilde{G}_{q,k} = \omega_q\widetilde{G}^{(1)}_{q,k}
\tag{2.17a}
$$

$$
\begin{aligned}
\hbar\omega\widetilde{G}^{(1)}_{q,k} &= \frac{\hbar\delta_{qk}}{\pi} + \hbar\omega_q\widetilde{G}_{q,k} + 4\sum_{k_1} C_2(k_1,-q)\widetilde{G}_{k_1,k} + 6\sum_{k_1k_2} C_3(k_1,k_2,-q)\widetilde{\Gamma}^{(1)}_{k_1k_2k} \\
&+ 24\sum_{k_1k_2} C_4(k_1,k_2,-k_2,-q)N_{k_2}\widetilde{G}_{k_1,k}
\end{aligned}
\tag{2.17b}
$$

and,

$$
\omega\widetilde{\Gamma}^{(1)}_{k_1k_2k} = \omega_{k_1}\widetilde{\Gamma}^{(2)}_{k_1k_2k} + \omega_{k_2}\widetilde{\Gamma}^{(3)}_{k_1k_2k}
\tag{2.18a}
$$

$$
\begin{aligned}
\hbar\omega\widetilde{\Gamma}^{(2)}_{k_1k_2k} &= \hbar\omega_{k_2}\widetilde{\Gamma}^{(4)}_{k_1k_2k} + \hbar\omega_{k_1}\widetilde{\Gamma}^{(1)}_{k_1k_2k} + 2C_1(-k_1)\widetilde{G}_{k_2k} + 4\sum_{k_1'} C_2(k_1',-k_1)\widetilde{\Gamma}^{(1)}_{k_1'k_2k} \\
&+ 6\sum_{k_1'} C_3(k_1',-k_1',-k_1)N_{k_1'}\widetilde{G}_{k_2k} + 12\sum_{k_1'} C_3(k_1',-k_2,-k_1)N_{k_2}\widetilde{G}_{k_1'k}
\end{aligned}
\tag{2.18b}
$$

$$
\begin{aligned}
\hbar\omega\widetilde{\Gamma}^{(3)}_{k_1k_2k} &= \hbar\omega_{k_1}\widetilde{\Gamma}^{(4)}_{k_1k_2k} + \hbar\omega_{k_2}\widetilde{\Gamma}^{(1)}_{k_1k_2k} + 2C_1(-k_2)\widetilde{G}_{k_1k} + 4\sum_{k_1'} C_2(k_1',-k_2)\widetilde{\Gamma}^{(1)}_{k_1k_1'k} \\
&+ 6\sum_{k_1'} C_3(k_1',-k_1',-k_2)N_{k_1'}\widetilde{G}_{k_1k} + 12\sum_{k_1'} C_3(k_1',-k_1,-k_2)N_{k_1}\widetilde{G}_{k_1'k}
\end{aligned}
\tag{2.18c}
$$

$$\begin{aligned}\hbar\omega\widetilde{\Gamma}^{(4)}_{k_1k_2k} &= \hbar\omega_{k_1}\widetilde{\Gamma}^{(3)}_{k_1k_2k} + \hbar\omega_{k_2}\widetilde{\Gamma}^{(2)}_{k_1k_2k} + 2C_1(-k_1)\widetilde{G}^{(1)}_{k_2k} + 2C_1(-k_2)\widetilde{G}^{(1)}_{k_1k} \\ &+ 4\sum_{k_1^{'}} C_2\left(k_1^{'},-k_1\right)\widetilde{\Gamma}^{(3)}_{k_1^{'}k_2k} + 4\sum_{k_1^{'}} C_2\left(k_1^{'},-k_2\right)\widetilde{\Gamma}^{(2)}_{k_1k_1^{'}k} \\ &+ 6\sum_{k_1^{'}} C_3\left(k_1^{'},-k_1^{'},-k_2\right)N_{k_1^{'}}\widetilde{G}^{(1)}_{k_1k} + 12\sum_{k_1^{'}} C_3\left(k_1^{'},-k_1,-k_2\right)\left\langle B_{k_1}A^{+}_{k_1}\right\rangle\widetilde{G}_{k_1^{'}k} \\ &+ 6\sum_{k_1^{'}} C_3\left(k_1^{'},-k_1^{'},-k_1\right)N_{k_1^{'}}\widetilde{G}^{(1)}_{k_2k} + 12\sum_{k_1^{'}} C_3\left(k_1^{'},-k_2,-k_1\right)\left\langle A^{+}_{k_2}B_{k_2}\right\rangle\widetilde{G}_{k_1^{'}k}\end{aligned} \tag{2.18d}$$

D. The number density of phonons

From these correlation functions, we calculated the number density of phonons from equations (2.13a) with $k = q$ and $t = t'$:

$$n_k = \left\langle a_k^{+} a_k \right\rangle = \frac{1}{4}\int_{-\infty}^{\infty}\left(1+\frac{\omega}{\omega_k}\right)^2 J_{kk}(\omega)d\omega \tag{2.19}$$

E. The energy of the system

The energy of the system is given by the thermal average of the Hamiltonian

$$E = \left\langle H \right\rangle = \sum_k \hbar\omega_k \left\langle a_k^{+} a_k \right\rangle + \left\langle V_1 \right\rangle + \left\langle V_2 \right\rangle + \left\langle V_3 \right\rangle + \left\langle V_4 \right\rangle \tag{2.20}$$

The usual zero-point energy of the harmonic crystal was ignored, and

$$\left\langle V_1 \right\rangle = \sum_k C_1(k)\left\langle A_k \right\rangle \tag{2.21a}$$

$$\left\langle V_2 \right\rangle = \sum_{k_1,k_2} C_2(k_1,k_2)\left\langle A_{k_1}A_{k_2} \right\rangle \tag{2.21b}$$

$$\left\langle V_3 \right\rangle = \sum_{k_1,k_2,k_3} C_3(k_1,k_2,k_3)\left\langle A_{k_1}A_{k_2}A_{k_3} \right\rangle \tag{2.21c}$$

$$\left\langle V_4 \right\rangle = \sum_{k_1,k_2,k_3,k_4} C_4(k_1,k_2,k_3,k_4)\left\langle A_{k_1}A_{k_2}A_{k_3}A_{k_4} \right\rangle \tag{2.21d}$$

Following Pathak's method [24], the energy of system can be simplified as follows:

$$E = \frac{1}{4}\sum_{k}\hbar\omega_k \int_{-\infty}^{\infty}\left(3\frac{\omega^2}{\omega_k^2} + 2\frac{\omega}{\omega_k} - 1\right)J_{kk}(\omega)d\omega - \langle V_2\rangle - 2\langle V_3\rangle - 3\langle V_4\rangle \tag{2.22}$$

where $\langle V_2\rangle$, $\langle V_3\rangle$ can be obtained from Green's function $\widetilde{G}_{qk}(\omega)$ and $\widetilde{\Gamma}^{(1)}_{k_2k_3k_1}(\omega)$; $\langle V_4\rangle$ are evaluated using the decoupling approximation in Eq. (2.15) and $\widetilde{G}_{qk}(\omega)$. The detailed processes are presented in Supplemental Material [25].

Ⅲ. Applications

In this section, we apply our results detailed in the section Ⅱ to obtain the properties of various cases of the periodic FK models.

A. $a = b$

In this case, the period of the FK potential equals that of the lattice chain, i.e., g is the reciprocal lattice vector. The C_1 and C_3 terms in the FK model vanish, and we get the following:

$$C_2(k_1,k_2) = \frac{\pi^2\hbar V_0}{ma^2}\left(\omega_{k_1}\omega_{k_2}\right)^{-\frac{1}{2}}\Delta(k_1+k_2) \tag{3.1}$$

$$C_4(k_1,k_2,k_3,k_4) = -\frac{\pi^4\hbar^2 V_0}{6m^2a^4N}\left(\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}\right)^{-\frac{1}{2}}\Delta(k_1+k_2+k_3+k_4) \tag{3.2}$$

For this case, solving Eqs. (2.17) for $\widetilde{G}_{q,k}$ yields

$$\widetilde{G}_{q,k} = \frac{\delta_{qk}}{\pi}\frac{\omega_q}{\omega^2 - \omega_q^2 - M_1} \tag{3.3}$$

where,

$$M_1 = \frac{4\pi^2 V_0}{ma^2} - \frac{4\pi^4\hbar V_0}{m^2a^4N}\sum_{k_1}\frac{1}{\omega_{k_1}}\left\langle A_{k_1}^{+}A_{k_1}\right\rangle \tag{3.4}$$

$(M_1)^{\frac{1}{2}}$ is the shift of frequency due to the FK potential. Letting $\tilde{\omega}_k^{(1)} = (\omega_k^2 + M_1)^{\frac{1}{2}}$, we obtain the spectral-density function from Eq. (2.12)

$$J_{kk}(\omega) = \frac{\omega_k}{\tilde{\omega}_k^{(1)}} \frac{\delta(\omega - \tilde{\omega}_k^{(1)}) - \delta(\omega + \tilde{\omega}_k^{(1)})}{e^{\beta\hbar\omega} - 1} \tag{3.5}$$

Using Eq. (3.5), we then get

$$N_k = \langle A_k^+ A_k \rangle = \int_{-\infty}^{\infty} J_{kk}(\omega) d\omega = \frac{\omega_k}{\tilde{\omega}_k^{(1)}} \coth \frac{\beta\hbar\tilde{\omega}_k^{(1)}}{2} \tag{3.6}$$

The number density of phonons is

$$n_k = \frac{1}{4} \int_{-\infty}^{\infty} \left(1 + \frac{\omega}{\omega_k}\right)^2 J_{kk}(\omega) d\omega = \frac{1}{4}\left[\left(\frac{\omega_k}{\tilde{\omega}_k^{(1)}} + \frac{\tilde{\omega}_k^{(1)}}{\omega_k}\right) \coth \frac{\beta\hbar\tilde{\omega}_k^{(1)}}{2} - 2\right] \tag{3.7}$$

The energy of the system then becomes

$$E = \sum_k \hbar\omega_k n_k + \langle V_2 \rangle + \langle V_4 \rangle \tag{3.8}$$

Using a similar method as that detailed in section Ⅱ E, $\langle V_4 \rangle$ is

$$\langle V_4 \rangle = \frac{1}{8} \sum_k \int_{-\infty}^{\infty} \hbar\omega_k \left(\frac{\omega^2}{\omega_k^2} - 1\right) J_{kk}(\omega) d\omega - \frac{1}{2} \langle V_2 \rangle \tag{3.9}$$

$\langle V_2 \rangle$ is obtained from Eqs. (2.9), (2.11), and (2.21b)

$$\langle V_2 \rangle = \sum_k \frac{\pi^2 \hbar V_0}{ma^2} \frac{1}{\omega_k} \int_{-\infty}^{\infty} J_{kk}(\omega) d\omega \tag{3.10}$$

Then,

$$E = -\frac{1}{2} \sum_k \hbar\omega_k + \frac{1}{8} \sum_k \hbar\omega_k \left(\frac{3\tilde{\omega}_k^{(1)}}{\omega_k} + \frac{\omega_k}{\tilde{\omega}_k^{(1)}} + \frac{8\pi^2 V_0}{ma^2 \omega_k \tilde{\omega}_k^{(1)}}\right) \coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(1)}}{2}\right) \tag{3.11}$$

If $M_1 = 0$, i.e., if we ignore the action of the FK on-site potential, we readily find that $N_k = 2n_k + 1$, while n_k and E become the results of the harmonic approximation from Eq. (3.7) and Eq. (3.11). If $M_1 \neq 0$, a shift of frequency will result. In Eq. (3.4), the first term depends only on the amplitude of the FK on-site potential; the second term also will depend on the temperature.

The phonon dispersion for $a = b$ is

$$\tilde{\omega}_k^{(1)} = \left(\omega_k^2 + M_1\right)^{\frac{1}{2}} \tag{3.12}$$

When we continue only up to the quadratic term of the on-site potential, Eq. (3.12) becomes simple because M_1 is a constant. Then, the frequency spectrum has a finite value $\left(M_1\right)^{\frac{1}{2}}$ at $k = 0$, consistent with some previous results [7, 13, 23]. The unperturbed normal mode frequencies for the linear chain are given by

$$\omega_k = \left|\omega_L \sin\left(\frac{k}{2}\right)\right| \tag{3.13}$$

where ω_L is the largest frequency. As an example, Fig.1 shows the results of the dispersion of a monatomic linear chain with $a = b$ calculated using Eqs. (3.12) and (3.13). In this figure, we used the normalized frequency, i.e., let $\omega_L = 1$. We also took the amplitude of the on-site potential to be $\frac{\pi^2 V_0}{ma^2} = 0.1$ in the calculating of Fig. 1.

If the quartic term is retained, and the sum in Eq. (3.4) is replaced by an integral, Eq. (3.12) becomes an integral equation (see Eq. (3.4), (3.6) and (3.12)) that can be written as

$$\left(\tilde{\omega}_k^{(1)}\right)^2 = \omega_k^2 + \frac{4\pi^2 V_0}{ma^2} - \frac{2\pi^3 \hbar V_0}{m^2 a^4} \int_{-\pi}^{\pi} \frac{dk}{\tilde{\omega}_k^{(1)}} \coth \frac{\beta\hbar\tilde{\omega}_k^{(1)}}{2} \tag{3.14}$$

For high temperatures, Eq. (3.14) can be written approximately as [25]

$$\left(\tilde{\omega}_k^{(1)}\right)^2 = \omega_k^2 + \frac{4\pi^2 V_0}{ma^2}\left[1 - \chi(\beta)\right] \tag{3.15}$$

where $\chi(\beta)=\frac{\pi^2\hbar}{ma^2}\left[\frac{\beta\hbar}{6}+\frac{2}{\beta\hbar}\left(\frac{4\pi^2V_0}{ma^2}\right)^{-\frac{1}{2}}\left(\omega_L^2+\frac{4\pi^2V_0}{ma^2}\right)^{-\frac{1}{2}}\right]$. We replaced the $\tilde{\omega}_k^{(1)}$ within the integral sign in the right side of Eq. (3.14) by $\left(\tilde{\omega}_k^{(1)}\right)^2=\omega_k^2+\frac{4\pi^2V_0}{ma^2}$, and $\omega_k=\left|\omega_L\sin\left(\frac{k}{2}\right)\right|$.

Using Eq. (3.15), the effect of temperature can be estimated. For this example, we take $\omega_L\sim 2\times10^{13}\sec^{-1}$, atomic mass $m\sim 5\times10^{-25}kg$, lattice constant $a\sim 0.2nm$, $V_0\sim 0.5eV$, and then $\frac{\pi^2V_0}{ma^2}\approx 0.1\omega_L^2$. At $T=300K$, we obtain $\chi(\beta)\sim 0.01$. In this case, the effect of temperature is very small. But if $V_0\sim 0.05eV$, $\chi(\beta)\sim 0.15$, then the effect of temperature cannot be ignored. If the temperature is high enough, or V_0 is small enough, then the frequency from Eq. (3.15) may become imaginary, and the crystal will become unstable.

For $T\to 0$, substituting $\coth\frac{\beta\hbar\tilde{\omega}_k^{(1)}}{2}=1+2\sum_{n=1}^{\infty}\exp\left(-n\beta\hbar\tilde{\omega}_k^{(1)}\right)$ into Eq. (3.14), and using Laplace's method [27] to calculate the integral in Eq. (3.14) (the detailed processing is shown in Supplemental Material [25]), we have

$$\left(\tilde{\omega}_k^{(1)}\right)^2=\omega_k^2+\frac{4\pi^2V_0}{ma^2}-\frac{4\pi^2\hbar}{ma^3}\left(\frac{V_0}{m}\right)^{\frac{1}{2}}K\left(\left(-\frac{4\pi^2V_0}{ma^2}\right)^{-\frac{1}{2}}\omega_L\right)=\omega_k^2+\left(\Delta\omega_k^{(1)}\right)^2 \tag{3.16}$$

where $K(x)$ is the complete elliptic integral of the first kind. We will use similar methods to detail the number density and energy. Since $\tilde{\omega}_k^{(1)}\neq\omega_k$ from Eq. (3.16), the number density of phonons does not vanish at absolute zero. It is

$$n_k=\frac{\left(\Delta\omega_k^{(1)}\right)^4}{16\omega_k^4} \tag{3.17}$$

Using $\omega_L \sim 2\times10^{13}\sec^{-1}$, atomic mass $m \sim 5\times10^{-25}kg$, lattice constant $a \sim 0.2nm$, $V_0 \sim 0.2eV$, and then $\frac{\pi^2 V_0}{ma^2} \approx 0.04\omega_L^2$, we find that $n_k \sim 0.01\%$. This percentage corresponds to about 10^{20} vibrations per mole.

The zero-point energy is

$$E_0 = \frac{1}{2}\sum_k \hbar\omega_k + \frac{1}{8}\sum_k \left[\frac{8\pi^2\hbar V_0}{ma^2\omega_k} + \left(1 - \frac{4\pi^2 V_0}{ma^2\omega_k^2}\right)\frac{\hbar\left(\Delta\omega_k^{(1)}\right)^2}{\omega_k}\right] \tag{3.18}$$

B. $a = \frac{b}{2}$

For this case, the wave vector of the on-site potential, $g = \frac{\pi}{a}$, is half that of the reciprocal lattice vector. The difference between $k + \frac{\pi}{a}$ and $k - \frac{\pi}{a}$ is a reciprocal lattice vector, meaning that $f\left(k + \frac{\pi}{a}\right) = f\left(k - \frac{\pi}{a}\right)$ for any function of the lattice. Therefore, the contribution of C_1 and C_3 terms in the perturbation Hamiltonian vanish, and

$$C_2(k_1,k_2) = \frac{\pi^2\hbar V_0}{4ma^2}\left(\omega_{k_1}\omega_{k_2}\right)^{-\frac{1}{2}}\Delta\left(k_1 + k_2 - \frac{\pi}{a}\right) \tag{3.19a}$$

$$C_4(k_1,k_2,k_3,k_4) = -\frac{\pi^4\hbar^2 V_0}{96m^2a^4N}\left(\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}\right)^{-\frac{1}{2}}\Delta\left(k_1 + k_2 + k_3 + k_4 - \frac{\pi}{a}\right) \tag{3.19b}$$

Eq. (2.17b) becomes

$$\omega\tilde{G}^{(1)}_{q,k} = \frac{\delta_{qk}}{\pi} + \omega_q\tilde{G}_{q,k} + \left[\frac{\pi^2 V_0}{2ma^2} - \frac{\pi^4\hbar V_0}{4m^2a^4N}\sum_{k_2}\frac{1}{\omega_{k_2}}\left\langle A_{k_2}^{+}A_{k_2}\right\rangle\right]\left(\omega_{q+\frac{\pi}{a}}\omega_q\right)^{-\frac{1}{2}}\tilde{G}_{q+\frac{\pi}{a},k} \tag{3.20}$$

Substituting $q \to q + \frac{\pi}{a}$ in the subscript of Eqs. (3.20a) and (2.17a), we obtain another two equations that are represented in Appendix A.

Combining Eqs. (2.17a), (3.20), (A.1) and (A.2), we obtain

$$\widetilde{G}_{q,k} = \frac{1}{\pi} \frac{\delta_{qk}\omega_q + \delta_{q+\frac{\pi}{a}k} M_2 \left(\omega_q \omega_{q+\frac{\pi}{a}}\right)^{\frac{1}{2}} \left(\omega^2 - \omega^2_{q+\frac{\pi}{a}}\right)^{-1}}{\omega^2 - \omega_q^2 - M_2^2 \left(\omega^2 - \omega^2_{q+\frac{\pi}{a}}\right)^{-1}} \tag{3.21}$$

where,

$$M_2 = \frac{\pi^2 V_0}{ma^2} - \frac{\pi^4 \hbar V_0}{4m^2 a^4 N} \sum_{k_2} \frac{1}{\omega_{k_2}} \left\langle A^+_{k_2} A_{k_2} \right\rangle \tag{3.22}$$

We define

$$\frac{1}{\omega^2 - \omega^2_{q+\frac{\pi}{a}}} = \Delta_{q+\frac{\pi}{a}}(\omega) - i\Gamma_{q+\frac{\pi}{a}}(\omega) \tag{3.23}$$

Here,

$$\Delta_{q+\frac{\pi}{a}}(\omega) = P \frac{1}{\omega^2 - \omega^2_{q+\frac{\pi}{a}}} \tag{3.24a}$$

$$\Gamma_{q+\frac{\pi}{a}}(\omega) = \pi\delta\left(\omega^2 - \omega^2_{q+\frac{\pi}{a}}\right) \tag{3.24b}$$

where P denotes the principal value. From Eq. (3.21) and (2.12), the spectral-density function is

$$J_{kq} = \frac{2M_2\Gamma_{q+\frac{\pi}{a}}}{\pi\left(e^{\beta\hbar\omega} - 1\right)} \cdot \frac{\delta_{qk}\omega_q M_2 + \delta_{q+\frac{\pi}{a}k} \left(\omega_q \omega_{q+\frac{\pi}{a}}\right)^{\frac{1}{2}} \left(\omega^2 - \omega_q^2\right)}{\left(\omega^2 - \omega_q^2 - M_2^2 \Delta_{q+\frac{\pi}{a}}\right)^2 + \Gamma^2_{q+\frac{\pi}{a}} M_2^4} \tag{3.25}$$

From the spectral-density function, we obtain

$$N_k = \frac{2\omega_k}{\pi} \int_{-\infty}^{\infty} \frac{1}{e^{\beta\hbar\omega} - 1} \cdot \frac{M_2^2 \Gamma_{k+\frac{\pi}{a}} d\omega}{\left(\omega^2 - \omega_k^2 - M_2^2 \Delta_{k+\frac{\pi}{a}}\right)^2 + \Gamma_{k+\frac{\pi}{a}}^2 M_2^4} \tag{3.26}$$

and the number density of phonons is

$$n_k = \frac{\omega_k}{2\pi} \int_{-\infty}^{\infty} \left(1 + \frac{\omega}{\omega_k}\right)^2 \frac{1}{e^{\beta\hbar\omega} - 1} \cdot \frac{M_2^2 \Gamma_{k+\frac{\pi}{a}} d\omega}{\left(\omega^2 - \omega_k^2 - M_2^2 \Delta_{k+\frac{\pi}{a}}\right)^2 + \Gamma_{k+\frac{\pi}{a}}^2 M_2^4} \tag{3.27}$$

N_k and n_k can be simplified when the damping, $M_2 \Gamma_{k+\frac{\pi}{a}}$, is small. At this limit, J_{kq} has a steep maximum at $\omega^2 = \omega_k^2 + M_2^2 \Delta_{k+\frac{\pi}{a}}$. The integrals are evaluated approximately by replacing the peak distribution by a Dirac delta function. We then obtain

$$N_k = \frac{\omega_k}{\tilde{\omega}_k^{(2)}} \coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(2)}}{2}\right) \tag{3.28}$$

and,

$$n_k = \frac{1}{4}\left[\left(\frac{\omega_k}{\tilde{\omega}_k^{(2)}} + \frac{\tilde{\omega}_k^{(2)}}{\omega_k}\right) \coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(2)}}{2}\right) - 2\right] \tag{3.29}$$

where $\tilde{\omega}_k^{(2)} = \left(\omega_k^2 + M_2^2 \Delta_{k+\frac{\pi}{a}}\right)^{\frac{1}{2}}$. When ω_k is close to $\tilde{\omega}_k^{(2)}$ we can replace N_k by $2n_k + 1$. We use this limit to check the correctness of our derivation.

The energy of the system from Eq. (3.8) and (3.9) is

$$E = -\frac{1}{2}\sum_k \hbar\omega_k + \frac{1}{8}\sum_k \hbar\omega_k \left(\frac{3\tilde{\omega}_k^{(2)}}{\omega_k} + \frac{\omega_k}{\tilde{\omega}_k^{(2)}} + \frac{\pi^2 V_0}{ma^2} \frac{M_2 \Delta_{k+\frac{\pi}{a}}}{\omega_k \tilde{\omega}_k^{(2)}}\right) \coth\frac{\beta\hbar\tilde{\omega}_k^{(2)}}{2} \tag{3.30}$$

The phonon dispersion for $a=\frac{b}{2}$ can be determined from

$$\left(\tilde{\omega}_k^{(2)}\right)^2 = \omega_k^2 + M_2^2\left[\left(\tilde{\omega}_k^{(2)}\right)^2 - \omega_{k+\frac{\pi}{a}}^2\right]^{-1} \tag{3.31}$$

Solving Eq. (3.31), we then obtain

$$\left(\tilde{\omega}_k^{(2)}\right)^2 = \frac{1}{2}\left(\omega_k^2 + \omega_{k+\frac{\pi}{a}}^2\right) \pm \frac{1}{2}\left(\omega_k^2 - \omega_{k+\frac{\pi}{a}}^2\right)\left[1 + 4M_2^2\left(\omega_k^2 - \omega_{k+\frac{\pi}{a}}^2\right)^{-2}\right]^{\frac{1}{2}} \tag{3.32}$$

The dispersion relation of the normal modes has two branches. Fig. 2 shows the phonon dispersion with normalized frequency $\omega_L = 1$ and $\frac{\pi^2 V_0}{ma^2} = 0.1$ when we ignore the quartic term from the perturbation.

The discussed method of the dispersion dependence on temperature is similar to that for $a=b$ if the quartic term from perturbation is not ignored.

C. $a=\frac{b}{3}$

In this case, the wave vector of the external potential is $g=\frac{2\pi}{3a}$, and the difference between $k+\frac{2\pi}{3a}$ and $k-\frac{2\pi}{3a}$ is not a reciprocal lattice vector. Then, the contribution of the C_1 and C_3 terms in the perturbation Hamiltonian cannot be neglected. To simplify our calculation, we first keep the C_1 and C_2 terms, and ignore the C_3 and C_4 terms. The C_1 term naturally vanishes in this case, and so the Eqs. (2.17) can be written as

$$\omega\tilde{G}_{qk} = \omega_q \tilde{G}_{qk}^{(1)} \tag{3.33a}$$

$$\omega\widetilde{G}^{(1)}_{qk} = \frac{\delta_{qk}}{\pi} + \omega_q \widetilde{G}_{qk} + \alpha_2\left(\omega_{q-\frac{2\pi}{3a}}\omega_q\right)^{-\frac{1}{2}}\widetilde{G}_{q-\frac{2\pi}{3a}k} + \alpha_2\left(\omega_{q+\frac{2\pi}{3a}}\omega_q\right)^{-\frac{1}{2}}\widetilde{G}_{q+\frac{2\pi}{3a}k} \tag{3.33b}$$

Replacing q by $q-\frac{2\pi}{3a}$ and $q+\frac{2\pi}{3a}$ in Eqs. (3.33), we obtain four other equations (Eq. (B.1)~(B.4)) that are shown in Appendix B. Solving the six equations, the Green's function is

$$\widetilde{G}_{qk} = \frac{\frac{\delta_{qk}}{\pi}\omega_q + \phi_{q+\frac{2\pi}{3a}}\Delta_{q+\frac{2\pi}{3a}} + \phi_{q-\frac{2\pi}{3a}}\Delta_{q-\frac{2\pi}{3a}} + i\left(\phi_{q+\frac{2\pi}{3a}}\Gamma_{q+\frac{2\pi}{3a}} + \phi_{q-\frac{2\pi}{3a}}\Gamma_{q-\frac{2\pi}{3a}}\right)}{\omega^2 - \left(\widetilde{\omega}^{(3)}_q\right)^2 + i\left(\varphi_{q+\frac{2\pi}{3a}}\Gamma_{q+\frac{2\pi}{3a}} + \varphi_{q-\frac{2\pi}{3a}}\Gamma_{q-\frac{2\pi}{3a}}\right)} \tag{3.34}$$

where,

$$\phi_{q+\frac{2\pi}{3a}} = \frac{\alpha_2\omega_q^{\frac{1}{2}}}{\pi}\left[\delta_{q+\frac{2\pi}{3a}k}\,\omega^{\frac{1}{2}}_{q+\frac{2\pi}{3a}} - \frac{\alpha_2}{\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}}\left(\delta_{qk}\omega_q^{\frac{1}{2}} - \delta_{q+\frac{2\pi}{3a}k}\,\omega^{\frac{1}{2}}_{q+\frac{2\pi}{3a}} - \delta_{q-\frac{2\pi}{3a}k}\,\omega^{\frac{1}{2}}_{q-\frac{2\pi}{3a}}\right)\right] \tag{3.35a}$$

$$\phi_{q-\frac{2\pi}{3a}} = \frac{\alpha_2\omega_q^{\frac{1}{2}}}{\pi}\left[\delta_{q-\frac{2\pi}{3a}k}\,\omega^{\frac{1}{2}}_{q-\frac{2\pi}{3a}} - \frac{\alpha_2}{\omega^2_{q-\frac{2\pi}{3a}} - \omega^2_{q+\frac{2\pi}{3a}}}\left(\delta_{qk}\omega_q^{\frac{1}{2}} - \delta_{q+\frac{2\pi}{3a}k}\,\omega^{\frac{1}{2}}_{q+\frac{2\pi}{3a}} - \delta_{q-\frac{2\pi}{3a}k}\,\omega^{\frac{1}{2}}_{q-\frac{2\pi}{3a}}\right)\right] \tag{3.35b}$$

$$\varphi_{q+\frac{2\pi}{3a}} = -\left[\alpha_2^2\left(1+\left(\omega^2-\omega_q^2\right)\left(\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}\right)^{-1}\right) + 2\alpha_2^3\left(\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}\right)^{-1}\right] \tag{3.35c}$$

$$\varphi_{q-\frac{2\pi}{3a}} = -\left[\alpha_2^2\left(1+\left(\omega^2-\omega_q^2\right)\left(\omega^2_{q-\frac{2\pi}{3a}} - \omega^2_{q+\frac{2\pi}{3a}}\right)^{-1}\right) + 2\alpha_2^3\left(\omega^2_{q-\frac{2\pi}{3a}} - \omega^2_{q+\frac{2\pi}{3a}}\right)^{-1}\right] \tag{3.35d}$$

$$\alpha_2 = \frac{2\pi^2 V_0}{9ma^2} \tag{3.35e}$$

$$\left(\widetilde{\omega}^{(3)}_q\right)^2 = \omega_q^2 - \varphi_{q+\frac{2\pi}{3a}}\Delta_{q+\frac{2\pi}{3a}} - \varphi_{q-\frac{2\pi}{3a}}\Delta_{q-\frac{2\pi}{3a}} \tag{3.35f}$$

From the Green's function, the spectral-density function is

$$J_{kq} = \frac{2}{e^{\beta\hbar\omega}-1}\frac{\left(\frac{\delta_{qk}}{\pi}\omega_q + \phi_{q+\frac{2\pi}{3a}}\Delta_{q+\frac{2\pi}{3a}} + \phi_{q-\frac{2\pi}{3a}}\Delta_{q-\frac{2\pi}{3a}}\right)\left(\varphi_{q+\frac{2\pi}{3a}}\Gamma_{q+\frac{2\pi}{3a}} + \varphi_{q-\frac{2\pi}{3a}}\Gamma_{q-\frac{2\pi}{3a}}\right) - \left(\omega^2 - \left(\tilde{\omega}_q^{(3)}\right)^2\right)\left(\phi_{q+\frac{2\pi}{3a}}\Gamma_{q+\frac{2\pi}{3a}} + \phi_{q-\frac{2\pi}{3a}}\Gamma_{q-\frac{2\pi}{3a}}\right)}{\left(\omega^2 - \left(\tilde{\omega}_q^{(3)}\right)^2\right)^2 + \left(\varphi_{q+\frac{2\pi}{3a}}\Gamma_{q+\frac{2\pi}{3a}} + \varphi_{q-\frac{2\pi}{3a}}\Gamma_{q-\frac{2\pi}{3a}}\right)^2} \tag{3.36}$$

If $\left(\varphi_{q+\frac{2\pi}{3a}}\Gamma_{q+\frac{2\pi}{3a}} + \varphi_{q-\frac{2\pi}{3a}}\Gamma_{q-\frac{2\pi}{3a}}\right)$ is small, we can replace the Breit-Wigner form of the spectral-density function by a Dirac delta function, and have

$$N_k = \frac{\omega_k}{\tilde{\omega}_k^{(3)}}\left[1 - \frac{\alpha_2^2}{\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}}\left(\Delta_{k+\frac{2\pi}{3a}} - \Delta_{k-\frac{2\pi}{3a}}\right)\right]\coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(3)}}{2}\right) \tag{3.37}$$

and the number density is

$$n_k = \frac{\omega_k}{4\tilde{\omega}_k^{(3)}}\left[1 - \frac{\alpha_2^2\left(\Delta_{k+\frac{2\pi}{3a}} - \Delta_{k-\frac{2\pi}{3a}}\right)}{\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}}\right]\left\{\left[1 + \left(\frac{\tilde{\omega}_k^{(3)}}{\omega_k}\right)^2\right]\coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(3)}}{2}\right) - \frac{2\tilde{\omega}_k^{(3)}}{\omega_k}\right\} \tag{3.38}$$

The energy is

$$\begin{aligned} E = {} & \frac{1}{4}\sum_k \hbar\omega_k \frac{\omega_k}{\tilde{\omega}_k^{(3)}}\left[1 - \frac{\alpha_2^2\left(\Delta_{k+\frac{2\pi}{3a}} - \Delta_{k-\frac{2\pi}{3a}}\right)}{\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}}\right]\left\{\left[3\left(\frac{\tilde{\omega}_k^{(3)}}{\omega_k}\right)^2 - 1\right]\coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(3)}}{2}\right) - \frac{2\tilde{\omega}_k^{(3)}}{\omega_k}\right\} \\ & - \frac{1}{2}\sum_k \hbar\frac{\alpha_2^2}{\tilde{\omega}_k^{(3)}}\coth\left(\frac{\beta\hbar\tilde{\omega}_k^{(3)}}{2}\right)\left[\Delta_{k+\frac{2\pi}{3a}} + \Delta_{k-\frac{2\pi}{3a}} + \frac{2\alpha_2\left(\Delta_{k+\frac{2\pi}{3a}} - \Delta_{k-\frac{2\pi}{3a}}\right)}{\omega^2_{q+\frac{2\pi}{3a}} - \omega^2_{q-\frac{2\pi}{3a}}}\right] \end{aligned} \tag{3.39}$$

If we retain only the C_1 and C_2 terms, the phonon dispersion becomes independent of the temperature. From Eq. (3.35f), the dispersion can be calculated: Fig. 3 shows an example. Three branches are found in this calculation.

Next, we will consider the effect of the terms $C_3(k_1,k_2,k_3)$ and $C_4(k_1,k_2,k_3,k_4)$. Accordingly, we must calculate another kind of Green's functions $\widetilde{\Gamma}^{(1)}_{k_1k_2k}$. The additions are too complicated for the calculation if we do not use approximations. First, we assume that the dispersion of phonons remains centrosymmetric, i.e., $\omega_k = \omega_{-k}$. Then, $C_1(-k_1)\widetilde{G}_{k_2k}$, and $\sum_{k_1'} C_3(k_1',-k_1',-k_1)N_{k_1'}\widetilde{G}_{k_2k}$ in Eq. (2.18) can be ignored. From Figures 1-3, we find that the approximation is reasonable. Second, we retain only the linear term of the FK potential in the calculated $\widetilde{\Gamma}^{(1)}_{k_1k_2k}$. In this case, some equations can be rewritten. Eq. (3.33b) becomes

$$\begin{aligned}\omega\widetilde{G}^{(1)}_{qk} &= \frac{\delta_{qk}}{\pi} + \omega_q\widetilde{G}_{qk} + (\alpha_2+\alpha_4)\left(\omega_{q-\frac{2\pi}{3a}}\omega_q\right)^{-\frac{1}{2}}\widetilde{G}_{q-\frac{2\pi}{3a}k} + (\alpha_2+\alpha_4)\left(\omega_{q+\frac{2\pi}{3a}}\omega_q\right)^{-\frac{1}{2}}\widetilde{G}_{q+\frac{2\pi}{3a}k} \\ &+ \sum_{k_1k_2}\alpha_3\left(\omega_{k_1}\omega_{k_2}\omega_q\right)^{-\frac{1}{2}}\widetilde{\Gamma}^{(1)}_{k_1k_2k}\left[\Delta\left(k_1+k_2-q+\frac{2\pi}{3a}\right)-\Delta\left(k_1+k_2-q-\frac{2\pi}{3a}\right)\right]\end{aligned} \tag{3.40}$$

Using the same method as above, other equations are obtained, as shown in Appendix B (Eq. (B.5) and (B.6)). We first need to know $\widetilde{\Gamma}^{(1)}_{k_1k_2k}$ if we want to obtain $\widetilde{G}_{qk}$ from Eq. (3.40), From Eq. (2.18), we have

$$\omega\widetilde{\Gamma}^{(1)}_{k_1k_2k} = \omega_{k_1}\widetilde{\Gamma}^{(2)}_{k_1k_2k} + \omega_{k_2}\widetilde{\Gamma}^{(3)}_{k_1k_2k} \tag{3.41a}$$

$$\omega\widetilde{\Gamma}^{(2)}_{k_1k_2k} = \omega_{k_1}\widetilde{\Gamma}^{(1)}_{k_1k_2k} + \omega_{k_2}\widetilde{\Gamma}^{(4)}_{k_1k_2k} + \alpha_2\left(\omega_{k_1}\omega_{k_1+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\widetilde{\Gamma}^{(1)}_{k_1+\frac{2\pi}{3a}k_2k} + \alpha_2\left(\omega_{k_1}\omega_{k_1-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\widetilde{\Gamma}^{(1)}_{k_1-\frac{2\pi}{3a}k_2k} + \Phi_1(k_1,k_2,k) \tag{3.41b}$$

$$\omega\tilde{\Gamma}^{(3)}_{k_1k_2k}=\omega_{k_2}\tilde{\Gamma}^{(1)}_{k_1k_2k}+\omega_{k_1}\tilde{\Gamma}^{(4)}_{k_1k_2k}+\alpha_2\left(\omega_{k_2}\omega_{k_2+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(1)}_{k_1k_2+\frac{2\pi}{3a}k}+\alpha_2\left(\omega_{k_2}\omega_{k_2-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(1)}_{k_1k_2-\frac{2\pi}{3a}k}+\Phi_2(k_1,k_2,k) \tag{3.41c}$$

and,

$$\begin{aligned}\omega\tilde{\Gamma}^{(4)}_{k_1k_2k}&=\omega_{k_2}\tilde{\Gamma}^{(2)}_{k_1k_2k}+\omega_{k_1}\tilde{\Gamma}^{(3)}_{k_1k_2k}+\alpha_2\left(\omega_{k_2}\omega_{k_2+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(2)}_{k_1k_2+\frac{2\pi}{3a}k}+\alpha_2\left(\omega_{k_2}\omega_{k_2-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(2)}_{k_1k_2-\frac{2\pi}{3a}k}\\&\quad+\alpha_2\left(\omega_{k_1}\omega_{k_1+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(3)}_{k_1+\frac{2\pi}{3a}k_2k}+\alpha_2\left(\omega_{k_1}\omega_{k_1-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(3)}_{k_1-\frac{2\pi}{3a}k_2k}+\Phi_3(k_1,k_2,k)\end{aligned} \tag{3.41d}$$

Using replacement $q-\dfrac{2\pi}{3a}\rightarrow q$ and $q+\dfrac{2\pi}{3a}\rightarrow q$, other equations about $\tilde{\Gamma}^{(i)}_{k_1k_2k}$ are obtained; they are listed in Supplemental Material [25]. Solving the system of equations, and only keeping the linear terms of the FK on-site potential, $\tilde{\Gamma}^{(1)}_{k_1k_2k}$ becomes

$$\begin{aligned}\tilde{\Gamma}^{(1)}_{k_1k_2k}&=\frac{\alpha_3}{2(\omega_{k_1}\omega_{k_2})^{\frac{1}{2}}}\left[\frac{1}{\omega^2-(\omega_{k_1}+\omega_{k_2})^2}-\frac{1}{\omega^2-(\omega_{k_1}-\omega_{k_2})^2}\right]\\&\quad\times\left[\frac{\omega^2-\omega_{k_1}^2+\omega_{k_2}^2}{\omega_{k_2}}N_{k_2}+\frac{\omega^2+\omega_{k_1}^2-\omega_{k_2}^2}{\omega_{k_1}}N_{k_1}+2\omega\left(N^{(1)}_{k_1}+N^{(2)}_{k_2}\right)\right]\\&\quad\times\left[\left(\omega_{k_1+k_2-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{G}_{k_1+k_2-\frac{2\pi}{3a}k}-\left(\omega_{k_1+k_2+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{G}_{k_1+k_2+\frac{2\pi}{3a}k}\right]\end{aligned} \tag{3.42}$$

Substituting Eq. (3.42) into Eq. (3.40), and using replacement $q-\dfrac{2\pi}{3a}\rightarrow q$ and $q+\dfrac{2\pi}{3a}\rightarrow q$, we have three equations about $\tilde{G}_{qk}$ and $\tilde{G}^{(1)}_{qk}$, viz., Eq. (B.7), (B.12) and (B.13) in Appendix B. Combining Eq. (3.33a), (B.1), (B.3), (B.7), (B.12) and (B.13), and only keeping the squared terms in α_2, α_3, and α_4, then the Green's function $\tilde{G}_{qk}$ can be obtained as follows:

$$\tilde{G}_{qk} = \frac{\frac{\delta_{qk}}{\pi}\omega_q + \mathrm{Re}\,\xi + i\,\mathrm{Im}\,\xi}{\omega^2 - \omega_q^2 + \mathrm{Re}\,\zeta + i\,\mathrm{Im}\,\zeta} \tag{3.43}$$

where ξ and ζ are two functions respectively dependent on vectors k and q. “Re” and “Im” represent their real- and imaginary-parts. The details of ξ and ζ are given in Appendix C, and their real- and imaginary-parts in the Supplemental Material [25]. From the Green’s function, Eqs. (3.43) and (2.12), we obtain the spectral-density function

$$J_{kq} = \frac{2}{\exp(\beta\hbar\omega) - 1} \cdot \frac{\left(\frac{\delta_{qk}}{\pi}\omega_q + \mathrm{Re}\,\xi\right)\mathrm{Im}\,\zeta - \left(\omega^2 - \left(\tilde{\omega}_q^{(3)}\right)^2\right)\mathrm{Im}\,\xi}{\left(\omega^2 - \left(\tilde{\omega}_q^{(3)}\right)^2\right)^2 + (\mathrm{Im}\,\zeta)^2} \tag{3.44}$$

where, $\left(\tilde{\omega}_q^{(3)}\right)^2 = \omega_q^2 - \mathrm{Re}\,\zeta$. Then, the N_k and the number density are

$$N_k = \frac{\omega_k}{\tilde{\omega}_k^{(3)}}\left(1 + \frac{\pi}{\omega_k}\mathrm{Re}\,\xi\right)\coth\frac{\beta\hbar\tilde{\omega}_k^{(3)}}{2} \tag{3.45}$$

$$n_k = \frac{\omega_k}{2\tilde{\omega}_k^{(3)}}\left(1 + \frac{\pi}{\omega_k}\mathrm{Re}\,\xi\right)\left[\left(1 + \left(\frac{\tilde{\omega}_q^{(3)}}{\omega_k}\right)^2\right)\coth\frac{\beta\hbar\tilde{\omega}_q^{(3)}}{2} - 2\frac{\tilde{\omega}_q^{(3)}}{\omega_k}\right] \tag{3.46}$$

The effects of $C_3(k_1,k_2,k_3)$ and $C_4(k_1,k_2,k_3,k_4)$ are included in $\mathrm{Re}\,\zeta$.

The energy of the system calculated from Eq. (2.22) is very complicated for $a = \frac{b}{3}$. It is represented in Supplemental Material [25]. Undoubtedly, when the cubic term is considered into our calculation, it becomes very complicated. However, we emphasize that the cubic term is important to thermal conductivity, even though the influence of the cubic term can exist only for a third-order state or a higher commensurate one [28].

D. $a = s_r b$

s_r is a rational number less than one. In this case, there is an integer n for which $ng = \dfrac{2\pi n s_r}{a}$ is a reciprocal lattice vector. This means $\widetilde{G}_{qk} = \widetilde{G}_{q+ngk}$, $\omega_q = \omega_{q+ng}$. Ignoring the effect of the cubic- and quadratic- terms of the FK model, we have from Eqs. (2.17a) and (2.17b)

$$\left(\omega^2 - \omega_q^2\right)\widetilde{G}_{qk} + \alpha\left(\frac{\omega_q}{\omega_{q+(n-1)g}}\right)^{\frac{1}{2}}\widetilde{G}_{q+(n-1)gk} + \alpha\left(\frac{\omega_q}{\omega_{q+g}}\right)^{\frac{1}{2}}\widetilde{G}_{q+gk} = \frac{\delta_{qk}}{\pi}\omega_q \tag{3.47}$$

Using the substitution $q \to q+g \ldots q \to q+(n-1)g$, we obtain a matrix equation

$$\begin{pmatrix} \omega^2 - \omega_q^2 & \alpha\left(\dfrac{\omega_q}{\omega_{q+g}}\right)^{\frac{1}{2}} & 0 & 0 & \cdots & \alpha\left(\dfrac{\omega_q}{\omega_{q+(n-1)g}}\right)^{\frac{1}{2}} \\ \alpha\left(\dfrac{\omega_{q+g}}{\omega_q}\right)^{\frac{1}{2}} & \omega^2 - \omega_{q+g}^2 & \alpha\left(\dfrac{\omega_{q+g}}{\omega_{q+2g}}\right)^{\frac{1}{2}} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \alpha\left(\dfrac{\omega_{q+(n-1)g}}{\omega_q}\right)^{\frac{1}{2}} & 0 & 0 & \cdots & \alpha\left(\dfrac{\omega_{q+(n-1)g}}{\omega_{q+(n-2)g}}\right)^{\frac{1}{2}} & \omega^2 - \omega_{q+(n-1)g}^2 \end{pmatrix} \begin{pmatrix} \widetilde{G}_{qk} \\ \widetilde{G}_{q+gk} \\ \cdots \\ \widetilde{G}_{q+(n-1)gk} \end{pmatrix} = \begin{pmatrix} \dfrac{\delta_{qk}\omega_q}{\pi} \\ \dfrac{\delta_{q+gk}\omega_{q+g}}{\pi} \\ \cdots \\ \dfrac{\delta_{q+(n-1)k}\omega_{q+(n-1)k}}{\pi} \end{pmatrix} \tag{3.48}$$

where $\alpha = -\dfrac{2\pi^2 V_0}{mb^2}$. If we require solutions accurate only to the squared terms of α, the solution of the equation is

$$\widetilde{G}_{qk} = \frac{1}{\pi}\frac{\delta_{qk}\omega_q - \alpha\eta_1^{(r)} + \alpha^2\left(\eta_2^{(r)} - \eta_3^{(r)}\right)}{\omega^2 - \omega_q^2 - \alpha^2\left(\theta_1^{(r)} + \theta_2^{(r)}\right)} \tag{3.49}$$

where.

$$\eta_1^{(r)} = \delta_{q+gk}\left(\omega_q\omega_{q+g}\right)^{\frac{1}{2}}\left(\Delta_{q+g} - i\Gamma_{q+g}\right) + \delta_{q-gk}\left(\omega_q\omega_{q-g}\right)^{\frac{1}{2}}\left(\Delta_{q-g} - i\Gamma_{q-g}\right) \tag{3.50a}$$

$$\eta_2^{(r)} = \delta_{q+2gk}\frac{\left(\omega_q\omega_{q+2g}\right)^{\frac{1}{2}}}{\omega_{q+g}^2-\omega_{q+2g}^2}\left(\Delta_{q+g}-\Delta_{q+2g}-i\Gamma_{q+g}+i\Gamma_{q+2g}\right)+\delta_{q-2gk}\frac{\left(\omega_q\omega_{q-2g}\right)^{\frac{1}{2}}}{\omega_{q-g}^2-\omega_{q-2g}^2}\left(\Delta_{q-g}-\Delta_{q-2g}-i\Gamma_{q-g}+i\Gamma_{q-2g}\right)$$

(3.50b)

$$\eta_3^{(r)} = \delta_{qk}\omega_q\sum_{s=1}^{n-2}\frac{\Delta_{q+sg}-\Delta_{q+(s+1)g}-i\Gamma_{q+sg}+i\Gamma_{q+(s+1)g}}{\omega_{q+sg}^2-\omega_{q+(s+1)g}^2} \tag{3.50c}$$

$$\theta_1^{(r)} = \Delta_{q-g}-i\Gamma_{q-g}+\Delta_{q+g}-i\Gamma_{q+g} \tag{3.50d}$$

$$\theta_2^{(r)} = \left(\omega^2-\omega_q^2\right)\sum_{s=1}^{n-2}\frac{\Delta_{q+sg}-\Delta_{q+(s+1)g}-i\Gamma_{q+sg}+i\Gamma_{q+(s+1)g}}{\omega_{q+sg}^2-\omega_{q+(s+1)g}^2} \tag{3.50e}$$

The Δ and Γ are similar, respectively, to the definition in Eq. (3.24a) and (3.24b). The spectral-density function can be obtained from the Green's function

$$J_{kq} = -\frac{2}{\pi\left[\exp(\beta\hbar\omega)-1\right]}$$
$$\times\frac{\alpha^2\,\mathrm{Im}\left(\theta_1^{(r)}+\theta_2^{(r)}\right)\left\{\delta_{qk}\omega_q+\mathrm{Re}\left[\alpha\eta_1^{(r)}+\alpha^2\left(\eta_2^{(r)}-\eta_3^{(r)}\right)\right]\right\}+\left[\omega^2-\left(\widetilde{\omega}_q^{(r)}\right)^2\right]\mathrm{Im}\left[\alpha\eta_1^{(r)}+\alpha^2\left(\eta_2^{(r)}-\eta_3^{(r)}\right)\right]}{\left[\omega^2-\left(\widetilde{\omega}_q^{(r)}\right)^2\right]^2+\alpha^4\left[\mathrm{Im}\left(\theta_1^{(r)}+\theta_2^{(r)}\right)\right]^2}$$

(3.51)

where $\left(\widetilde{\omega}_q^{(r)}\right)^2 = \omega_q^2+\alpha^2\,\mathrm{Re}\left(\theta_1^{(r)}+\theta_2^{(r)}\right)$.

Next, we use the J_{kq} to evaluate some physical properties. First, the correlation function N_k is

$$N_k = \frac{\omega_q}{\widetilde{\omega}_q^{(r)}}\coth\frac{\beta\hbar\widetilde{\omega}_q^{(r)}}{2}\left(1-\alpha^2\sum_{s=1}^{n-2}\frac{\Delta_{q+sg}-\Delta_{q+(s+1)g}}{\omega_{q+sg}^2-\omega_{q+(s+1)g}^2}\right) \tag{3.52}$$

The number density of phonons is

$$n_k = \frac{1}{4}\left[\left(\frac{\omega_k}{\widetilde{\omega}_k^{(r)}}+\frac{\widetilde{\omega}_k^{(r)}}{\omega_k}\right)\coth\frac{\beta\hbar\widetilde{\omega}_k^{(r)}}{2}-2\right]\left(1-\alpha^2\sum_{s=1}^{n-2}\frac{\Delta_{k+sg}-\Delta_{k+(s+1)g}}{\omega_{k+sg}^2-\omega_{k+(s+1)g}^2}\right) \tag{3.53}$$

To calculate the energy of the system, we first must evaluate $\langle V_2\rangle$

$$\langle V_2 \rangle = \frac{\hbar\alpha^2}{2}\sum_k \frac{\coth\frac{\beta\hbar\tilde{\omega}_k^{(r)}}{2}}{\tilde{\omega}_k^{(r)}}\left(\Delta_{k-g}+\Delta_{k+g}\right) \tag{3.54}$$

Using Eq. (3.54) and Eq. (2.22) and ignoring $\langle V_3 \rangle$ and $\langle V_4 \rangle$, the energy of the system is

$$\begin{aligned} E = {} & \frac{1}{4}\sum_k \hbar\omega_k \left[\left(\frac{3\omega_k}{\tilde{\omega}_k^{(r)}} - \frac{\tilde{\omega}_k^{(r)}}{\omega_k}\right)\coth\frac{\beta\hbar\tilde{\omega}_k^{(r)}}{2} - 2\right]\left(1-\alpha^2\sum_{s=1}^{n-2}\frac{\Delta_{k+sg}-\Delta_{k+(s+1)g}}{\omega_{k+sg}^2-\omega_{k+(s+1)g}^2}\right) \\ & -\frac{\hbar\alpha^2}{2}\sum_k \frac{\coth\frac{\beta\hbar\tilde{\omega}_k^{(r)}}{2}}{\tilde{\omega}_k^{(r)}}\left(\Delta_{k-g}+\Delta_{k+g}\right) \end{aligned} \tag{3.55}$$

E. $a = s_i b$

For this case, s_i is an irrational number less than one, meaning that that our system is incommensurate, and $g = \frac{2\pi s_i}{a}$. Any integer multiple of g is not a reciprocal lattice vector. To simplify our calculation, we also ignored the effect of the cubic- and quartic-terms of the FK on-site potential. Combining Eq. (2.17a) and (2.17b), we obtain

$$\left(\omega^2-\omega_q^2\right)\tilde{G}_{qk} + \alpha\left(\frac{\omega_q}{\omega_{q-g}}\right)^{\frac{1}{2}}\tilde{G}_{q-gk} + \alpha\left(\frac{\omega_q}{\omega_{q+g}}\right)^{\frac{1}{2}}\tilde{G}_{q+gk} = \frac{\delta_{qk}}{\pi}\omega_q \tag{3.56}$$

Eq. (3.56) can be written in a matrix form

$$\begin{pmatrix} \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \cdots & \omega^2-\omega_{q-2g}^2 & \alpha\left(\dfrac{\omega_{q-2g}}{\omega_{q-g}}\right)^{\frac{1}{2}} & 0 & 0 & 0 & 0 \\ 0 & \alpha\left(\dfrac{\omega_{q-g}}{\omega_{q-2g}}\right)^{\frac{1}{2}} & \omega^2-\omega_{q-g}^2 & \alpha\left(\dfrac{\omega_{q-g}}{\omega_{q}}\right)^{\frac{1}{2}} & 0 & 0 & 0 \\ 0 & 0 & \alpha\left(\dfrac{\omega_{q}}{\omega_{q-g}}\right)^{\frac{1}{2}} & \omega^2-\omega_{q}^2 & \alpha\left(\dfrac{\omega_{q}}{\omega_{q+g}}\right)^{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 0 & \alpha\left(\dfrac{\omega_{q+g}}{\omega_{q}}\right)^{\frac{1}{2}} & \omega^2-\omega_{q+g}^2 & \alpha\left(\dfrac{\omega_{q+g}}{\omega_{q+2g}}\right)^{\frac{1}{2}} & 0 \\ 0 & 0 & 0 & 0 & \alpha\left(\dfrac{\omega_{q+2g}}{\omega_{q+g}}\right)^{\frac{1}{2}} & \omega^2-\omega_{q+2g}^2 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & \cdots \end{pmatrix} \begin{pmatrix} \cdots \\ \widetilde{G}_{q-2gk} \\ \widetilde{G}_{q-gk} \\ \widetilde{G}_{qk} \\ \widetilde{G}_{q+gk} \\ \widetilde{G}_{q+2gk} \\ \cdots \end{pmatrix} = \begin{pmatrix} \cdots \\ \dfrac{\delta_{q-2gk}\omega_{q-2g}}{\pi} \\ \dfrac{\delta_{q-gk}\omega_{q-g}}{\pi} \\ \dfrac{\delta_{qk}\omega_{q}}{\pi} \\ \dfrac{\delta_{q+gk}\omega_{q+g}}{\pi} \\ \dfrac{\delta_{q+2gk}\omega_{q+2g}}{\pi} \\ \cdots \end{pmatrix}$$

(3.57)

where $\alpha = -\dfrac{2\pi^2 V_0}{mb^2}$. In principle, the extent of this set of equations is infinite. We cannot solve them accurately, but since we only require accuracy to quadratic terms in α, $\widetilde{G}_{qk}$ can be written as

$$\widetilde{G}_{qk} = \frac{1}{\pi}\frac{\delta_{qk}\omega_q + \alpha\eta_1^{(i)} + \alpha^2\left(\eta_2^{(i)} - \eta_3^{(i)}\right)}{\omega^2 - \omega_q^2 - \alpha^2\left(\theta_1^{(i)} + \theta_2^{(i)}\right)} \tag{3.58}$$

where $\eta_1^{(i)}$, $\eta_2^{(i)}$, and $\theta_1^{(i)}$ have same form as $\eta_1^{(r)}$, $\eta_2^{(r)}$, and $\theta_1^{(r)}$ in Eq. (3.50a), (3.50b) and (3.50d), respectively. $\eta_3^{(i)}$ and $\theta_2^{(i)}$ are

$$\eta_3^{(i)} = \delta_{qk}\omega_q \sum_{s=1}^{\infty}\left[\frac{\Delta_{q-sg} - \Delta_{q-(s+1)g} - i\Gamma_{q-sg} + i\Gamma_{q-(s+1)g}}{\omega_{q-sg}^2 - \omega_{q-(s+1)g}^2} + \frac{\Delta_{q+sg} - \Delta_{q+(s+1)g} - i\Gamma_{q+sg} + i\Gamma_{q+(s+1)g}}{\omega_{q+sg}^2 - \omega_{q+(s+1)g}^2}\right] \tag{3.59a}$$

$$\theta_2^{(i)} = \left(\omega^2 - \omega_q^2\right)\sum_{s=1}^{\infty}\left[\frac{\Delta_{q-sg} - \Delta_{q-(s+1)g} - i\Gamma_{q-sg} + i\Gamma_{q-(s+1)g}}{\omega_{q-sg}^2 - \omega_{q-(s+1)g}^2} + \frac{\Delta_{q+sg} - \Delta_{q+(s+1)g} - i\Gamma_{q+sg} + i\Gamma_{q+(s+1)g}}{\omega_{q+sg}^2 - \omega_{q+(s+1)g}^2}\right]$$

(3.59b)

The spectral-density function is obtained from the Green’s function

$$J_{kq} = -\frac{2}{\pi\left[\exp(\beta\hbar\omega)-1\right]} \times \frac{\alpha^2\,\mathrm{Im}\left(\theta_1^{(i)}+\theta_2^{(i)}\right)\left\{\delta_{qk}\omega_q + \mathrm{Re}\left[\alpha\eta_1^{(i)}+\alpha^2\left(\eta_2^{(i)}-\eta_3^{(i)}\right)\right]\right\} + \left[\omega^2-\left(\tilde{\omega}_q^{(i)}\right)^2\right]\mathrm{Im}\left[\alpha\eta_1^{(i)}+\alpha^2\left(\eta_2^{(i)}-\eta_3^{(i)}\right)\right]}{\left[\omega^2-\left(\tilde{\omega}_q^{(i)}\right)^2\right]^2+\alpha^4\left[\mathrm{Im}\left(\theta_1^{(i)}+\theta_2^{(i)}\right)\right]^2} \tag{3.60}$$

where $\left(\tilde{\omega}_q^{(i)}\right)^2 = \omega_q^2 + \alpha^2\,\mathrm{Re}\left(\theta_1^{(i)}+\theta_2^{(i)}\right)$. From the J_{kq}, the correlation function N_k is obtained:

$$N_k = \frac{\omega_q}{\tilde{\omega}_q^{(i)}}\coth\frac{\beta\hbar\tilde{\omega}_q^{(i)}}{2}\left\{1-\alpha^2\sum_{s=1}^{\infty}\left[\frac{\Delta_{q-sg}-\Delta_{q-(s+1)g}}{\omega_{q-sg}^2-\omega_{q-(s+1)g}^2}+\frac{\Delta_{q+sg}-\Delta_{q+(s+1)g}}{\omega_{q+sg}^2-\omega_{q+(s+1)g}^2}\right]\right\} \tag{3.61}$$

The number density of phonons then is

$$n_k = \frac{1}{4}\left[\left(\frac{\omega_k}{\tilde{\omega}_k^{(i)}}+\frac{\tilde{\omega}_k^{(i)}}{\omega_k}\right)\coth\frac{\beta\hbar\tilde{\omega}_k^{(i)}}{2}-2\right]\left\{1-\alpha^2\sum_{s=1}^{\infty}\left[\frac{\Delta_{k-sg}-\Delta_{k-(s+1)g}}{\omega_{k-sg}^2-\omega_{k-(s+1)g}^2}+\frac{\Delta_{k+sg}-\Delta_{k+(s+1)g}}{\omega_{k+sg}^2-\omega_{k+(s+1)g}^2}\right]\right\} \tag{3.62}$$

Similar to our description in Section D, the energy of the system is

$$E = \frac{1}{4}\sum_k\hbar\omega_k\left[\left(\frac{3\omega_k}{\tilde{\omega}_k^{(i)}}-\frac{\tilde{\omega}_k^{(i)}}{\omega_k}\right)\coth\frac{\beta\hbar\tilde{\omega}_k^{(i)}}{2}-2\right]\left\{1-\alpha^2\sum_{s=1}^{\infty}\left[\frac{\Delta_{k-sg}-\Delta_{k-(s+1)g}}{\omega_{k-sg}^2-\omega_{k-(s+1)g}^2}+\frac{\Delta_{k+sg}-\Delta_{k+(s+1)g}}{\omega_{k+sg}^2-\omega_{k+(s+1)g}^2}\right]\right\} - \frac{\hbar\alpha^2}{2}\sum_k\frac{\coth\frac{\beta\hbar\tilde{\omega}_k^{(i)}}{2}}{\tilde{\omega}_k^{(i)}}\left(\Delta_{k-g}+\Delta_{k+g}\right) \tag{3.63}$$

We can obtain the respective phonon dispersions of the commensurate- and incommensurate-structures from the coefficient matrix of Eq. (3.48) and (3.57). If we ignore the effect of the cubic- and quartic-terms of the FK on-site potential, the phonon dispersion is independent of temperature. Comparing the two coefficient matrices, the only difference between the commensurate and incommensurate states is the finite number of coupled wave vectors in the former case, and the infinite number in the latter. The normal modes of the commensurate structure will be divided into finite branches and those of the incommensurate structure will be infinite branches.

To intuitively understand the difference between the phonon dispersions of the commensurate- and incommensurate-lattices, we give, in Fig. 4, some calculated examples with close values of $\frac{a}{b}$. For the infinite number of coupled wave vectors in the incommensurate state, we must make some approximations to calculate the dispersion of the incommensurate structure. We only keep $q \pm 30g$ or less from the center of the wave vectors, such that the coefficient matrix of Eq. (3.57) becomes a 61×61 dynamical matrix centered about wave vector, q. Figs. 4 (a)~(c) respectively show the dispersion for the commensurate case of $b = \frac{7}{6}a$ and the incommensurate cases of $b = 1.17a$ and $b = 1.167a$, with normalized frequency $\omega_L = 1$ and the amplitude of the FK on-site potential $\frac{\pi^2 V_0}{ma^2} = 0.1$. We note (see Figs. 4 (a) and (c)) that the plots become similar when the value of $\frac{b}{a}$ for the commensurate- and incommensurate-states are very close, as in the present calculation. However, we believe that the plots will be quite different when we increase the size of the coefficient matrix of Eq. (3.57).

Novaco [23] did not realize this problem, i.e., that the dispersion curves of commensurate- and incommensurate-states will display large differences if the order of the coefficient matrix of Eq. (3.57) is large enough. His results probably were constrained by computing conditions at that time. We point out that the approximation of using a simplified truncation to calculate the dispersion for the incommensurate state is not sufficient because we cannot judge which of the summation limits of $s \to \infty$ in Eq. (3.59) is convergent, i.e., convergence of the infinite matrix.

Thus, we reached a different conclusion from Novaco [23], and it is not reasonable to expect to find the dynamical structure of an incommensurate state closely resembling that of “nearby” commensurate states, provided that both are described in a way that does not explicitly distinguish between them. The result obtained will affect the nature of incommensurate-commensurate phase transition.

In addition, our calculation indicates that the commensurate case has a definite gap at zero wave vector, while the incommensurate case shows a branch that goes to zero, and the various gaps in the commensurate case are true gaps wherein there is zero density of states. In the incommensurate case, there exist some gaps similar to those of the commensurate state, but there are some modes inside these gaps, although their density is very low. These results are consistent with those of Novaco [23]. The phonon density of states shown in Fig. 4 (d)~(f) clearly reveal these results.

Sutherland [21, 22] studied the dispersion of the incommensurate state in the continuum limit. He found that the spectrum separates into two branches. The lower branch represents the collective motions of the lattice dislocations, as “acoustical” phonons, and the upper branch corresponds to renormalized “optic” phonons [13, 23]. We cannot readily distinguish the two phonons in our calculation; perhaps this is a limitation of the continuum limit approximation.

As mentioned when we keep up only to squared terms of the FK on-site potential model; the phonon dispersion is independent of temperature. In this approximation, the number density and energy of the system for the commensurate- and incommensurate-state have a simple relationship for the dependence on temperature (see Eqs. (3.53), (3.55), (3.62) and (3.63).

To discuss incommensurate-commensurate phase transitions, we need to compare the energy of incommensurate and commensurate structures. From a mathematical point of view, we always can find a rational number that is indefinitely close to an irrational number. Therefore, the energy obtained from Eq. (3.55) and (3.63) can be indefinitely close when rational values of a/b in a commensurate state are indefinitely close to an irrational number a/b in an incommensurate state. For this case, the incommensurate-commensurate phase transition is continuous. We cannot analytically describe the sum upon s in Eqs. (3.55) and (3.63), and hence, the incommensurate-commensurate phase transition is a continuous transition with an unusual nonanalytic nature, described as a "devil's staircase". This agrees with Aubry's result [29], but is only valid at zero Kelvin. Here, we need to emphasize, from Eqs. (3.55) and (3.63), that our result shows that this devil's staircase also can exist at finite temperature. In real crystals, a/b always is a truncated number with a limited number of decimal places. When we compare a commensurate structure of a rational fraction with an incommensurate structure of a truncated irrational number, the energy of the commensurate and incommensurate structures will become discontinuous. Therefore, it implies that the incommensurate-commensurate phase transition in real crystals may be a discontinuous- or first order-one.

Ⅳ. Summary and Conclusions

In this work, we analyzed the lattice vibrations in the FK model using the technique of thermodynamic Green's functions based on field-theoretic methods. We treated the FK model as an external on-site potential, and expanded the external-potential into four terms. When the FK model potential is considered as a perturbation, we analyzed its solution for the phonon dispersion, number of density of phonons, and energy of the system. We first discussed several low-order commensurate states, and found that the cubic terms of the FK on-site potential could only affect only the third-order state or higher commensurate ones. When the cubic- and quartic-terms of the on-site potential are considered, the calculation becomes very complicated. Based on the results of these low-order commensurate states, we analyzed the arbitrary orders of commensurate states and the incommensurate state were analyzed. When we ignored the terms above the quadratic in the displacement in the FK on-site potential, then the phonon dispersion is independent of temperature. Therefore, the energy of the system has a simple relation with temperature from which, we find that the incommensurate-commensurate phase transition is a non-analytic devil's staircase at finite temperature.

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Appendix A

Using replacement $q \to q + \frac{\pi}{a}$ in the subscript of Eqs. (2.20a) and (3.20), we obtain another two equations.

$$\omega \widetilde{G}_{q+\frac{\pi}{a},k} = \omega_{q+\frac{\pi}{a}} \widetilde{G}^{(1)}_{q+\frac{\pi}{a},k} \tag{A.1}$$

$$\begin{aligned} \omega \widetilde{G}^{(1)}_{q+\frac{\pi}{a},k} &= \frac{\delta_{q+\frac{\pi}{a}k}}{\pi} + \omega_{q+\frac{\pi}{a}} \widetilde{G}_{q+\frac{\pi}{a},k} \\ &+ \left[\frac{\pi^2 V_0}{2ma^2} - \frac{3\pi^4 \hbar V_0}{4m^2 a^4 N} \sum_{k_2} \frac{1}{\omega_{k_2}} \left\langle A^+_{k_2} A_{k_2} \right\rangle \right] \left(\omega_{q+\frac{\pi}{a}} \omega_q \right)^{-\frac{1}{2}} \widetilde{G}_{q,k} \end{aligned} \tag{A.2}$$

Eqs. (2.17a), (3.20), (A.1) and (A.2) constitute a system of equations. $\widetilde{G}_{q,k}$ can be solved from it.

Appendix B

1) Only the effects of $C_1(k)$ and $C_2(k_1, k_2)$ are considered

Using replacement $q - \frac{2\pi}{3a} \to q$ in Eqs. (3.33), we have

$$\omega \widetilde{G}_{q-\frac{2\pi}{3a}k} = \omega_{q-\frac{2\pi}{3a}} \widetilde{G}^{(1)}_{q-\frac{2\pi}{3a}k} \tag{B.1}$$

$$\omega \widetilde{G}^{(1)}_{q-\frac{2\pi}{3a}k} = \frac{\delta_{q-\frac{2\pi}{3a}k}}{\pi} + \omega_{q-\frac{2\pi}{3a}} \widetilde{G}_{q-\frac{2\pi}{3a}k} + \alpha_2 \left(\omega_{q+\frac{2\pi}{3a}} \omega_{q-\frac{2\pi}{3a}} \right)^{-\frac{1}{2}} \widetilde{G}_{q+\frac{2\pi}{3a}k} + \alpha_2 \left(\omega_q \omega_{q-\frac{2\pi}{3a}} \right)^{-\frac{1}{2}} \widetilde{G}_{qk} \tag{B.2}$$

and $q + \frac{2\pi}{3a} \to q$

$$\omega \widetilde{G}_{q+\frac{2\pi}{3a}k} = \omega_{q+\frac{2\pi}{3a}} \widetilde{G}^{(1)}_{q+\frac{2\pi}{3a}k} \tag{B.3}$$

$$\omega \widetilde{G}^{(1)}_{q+\frac{2\pi}{3a}k} = \frac{\delta_{q+\frac{2\pi}{3a}k}}{\pi} + \omega_{q+\frac{2\pi}{3a}} \widetilde{G}_{q+\frac{2\pi}{3a}k} + \alpha_2 \left(\omega_q \omega_{q+\frac{2\pi}{3a}} \right)^{-\frac{1}{2}} \widetilde{G}_{qk} + \alpha_2 \left(\omega_{q-\frac{2\pi}{3a}} \omega_{q+\frac{2\pi}{3a}} \right)^{-\frac{1}{2}} \widetilde{G}_{q-\frac{2\pi}{3a}k} \tag{B.4}$$

2) Including the effects of $C_3(k_1, k_2, k_3)$ and $C_4(k_1, k_2, k_3, k_4)$

Using replacement $q - \frac{2\pi}{3a} \to q$ in Eqs. (3.40), we have

$$\begin{aligned}\omega\tilde{G}^{(1)}_{q-\frac{2\pi}{3a}k} &= \frac{\delta_{q-\frac{2\pi}{3a}k}}{\pi} + \omega_{q-\frac{2\pi}{3a}}\tilde{G}_{q-\frac{2\pi}{3a}k} + (\alpha_2+\alpha_4)\left(\omega_{q+\frac{2\pi}{3a}}\omega_{q-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{G}_{q+\frac{2\pi}{3a}k} \\ &+ (\alpha_2+\alpha_4)\left(\omega_q\omega_{q-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{G}_{qk} \\ &+ \sum_{k_1k_2}\alpha_3\left(\omega_{k_1}\omega_{k_2}\omega_{q-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(1)}_{k_1k_2k}\left[\Delta\left(k_1+k_2-q-\frac{2\pi}{3a}\right)-\Delta(k_1+k_2-q)\right]\end{aligned} \tag{B.5}$$

and $q+\frac{2\pi}{3a}\rightarrow q$

$$\begin{aligned}\omega\tilde{G}^{(1)}_{q+\frac{2\pi}{3a}k} &= \frac{\delta_{q+\frac{2\pi}{3a}k}}{\pi} + \omega_{q+\frac{2\pi}{3a}}\tilde{G}_{q+\frac{2\pi}{3a}k} + (\alpha_2+\alpha_4)\left(\omega_{q-\frac{2\pi}{3a}}\omega_{q+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{G}_{q-\frac{2\pi}{3a}k} \\ &+ (\alpha_2+\alpha_4)\left(\omega_q\omega_{q+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{G}_{qk} \\ &+ \sum_{k_1k_2}\alpha_3\left(\omega_{k_1}\omega_{k_2}\omega_{q+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\tilde{\Gamma}^{(1)}_{k_1k_2k}\left[\Delta(k_1+k_2-q)-\Delta\left(k_1+k_2-q+\frac{2\pi}{3a}\right)\right]\end{aligned} \tag{B.6}$$

Substituting Eq.(3.42) into Eq. (3.40) yields

$$\begin{aligned}\omega\tilde{G}^{(1)}_{qk} &= \frac{\delta_{qk}}{\pi} + \frac{\omega_q^2-\alpha_3^2F\left(q-\frac{2\pi}{3a}\right)-\alpha_3^2F\left(q+\frac{2\pi}{3a}\right)}{\omega_q}\tilde{G}_{qk} \\ &+ \left(\alpha_2+\alpha_4+\alpha_3^2F\left(q-\frac{2\pi}{3a}\right)\right)\left(\omega_{q-\frac{2\pi}{3a}}\omega_q\right)^{-\frac{1}{2}}\tilde{G}_{q-\frac{2\pi}{3a}k} \\ &+ \left(\alpha_2+\alpha_4+\alpha_3^2F\left(q+\frac{2\pi}{3a}\right)\right)\left(\omega_{q+\frac{2\pi}{3a}}\omega_q\right)^{-\frac{1}{2}}\tilde{G}_{q+\frac{2\pi}{3a}k}\end{aligned} \tag{B.7}$$

where,

$$F(q)=\sum_k f(q,k)\left[\frac{1}{\omega^2-(\omega_k+\omega_{q-k})^2}-\frac{1}{\omega^2-(\omega_{k_1}-\omega_{q-k})^2}\right] \tag{B.8}$$

$$f(q,k)=\sum_k \frac{1}{2\omega_k\omega_{q-k}}\left[\frac{\omega^2-\omega_k^2+\omega_{q-k}^2}{\omega_{q-k}}N_{q-k}+\frac{\omega^2+\omega_k^2-\omega_{q-k}^2}{\omega_k}N_k+2\omega\left(N_k^{(1)}+N_{q-k}^{(2)}\right)\right] \tag{B.9}$$

$$\alpha_3=-\frac{\pi^3 iV_0}{27a^3}\left(\frac{2\hbar}{m^3N}\right)^{\frac{1}{2}} \tag{B.10}$$

and,

$$\alpha_4=-\frac{2\pi^4\hbar V_0}{81m^2a^4N}\sum_k\frac{N_k}{\omega_k} \tag{B.11}$$

From Eq. (B.7), using $q-\frac{2\pi}{3a}$ or substituting $q+\frac{2\pi}{3a}$ for q, two other equations were

$$\begin{aligned}\omega\widetilde{G}^{(1)}_{q-\frac{2\pi}{3a}k} &= \frac{\delta_{q-\frac{2\pi}{3a}k}}{\pi}+\frac{\omega^2_{q-\frac{2\pi}{3a}}-F\left(q+\frac{2\pi}{3a}\right)-F(q)}{\omega_{q-\frac{2\pi}{3a}}}\widetilde{G}_{q-\frac{2\pi}{3a}k}\\ &+\left(\alpha_2+\alpha_4+F\left(q+\frac{2\pi}{3a}\right)\right)\left(\omega_{q+\frac{2\pi}{3a}}\omega_{q-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\widetilde{G}_{q+\frac{2\pi}{3a}k}\\ &+\left(\alpha_2+\alpha_4+F(q)\right)\left(\omega_q\omega_{q-\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\widetilde{G}_{qk}\end{aligned} \tag{B.12}$$

$$\begin{aligned}\omega\widetilde{G}^{(1)}_{q+\frac{2\pi}{3a}k} &= \frac{\delta_{q+\frac{2\pi}{3a}k}}{\pi}+\frac{\omega^2_{q+\frac{2\pi}{3a}}-F(q)-F\left(q-\frac{2\pi}{3a}\right)}{\omega_{q+\frac{2\pi}{3a}}}\widetilde{G}_{q+\frac{2\pi}{3a}k}\\ &+\left(\alpha_2+\alpha_4+F(q)\right)\left(\omega_q\omega_{q+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\widetilde{G}_{qk}\\ &+\left(\alpha_2+\alpha_4+F\left(q-\frac{2\pi}{3a}\right)\right)\left(\omega_{q-\frac{2\pi}{3a}}\omega_{q+\frac{2\pi}{3a}}\right)^{-\frac{1}{2}}\widetilde{G}_{q-\frac{2\pi}{3a}k}\end{aligned} \tag{B.13}$$

Appendix C

$$\begin{aligned}\zeta &= \alpha_3^2\left[F\left(q-\frac{2\pi}{3a}\right)+F\left(q+\frac{2\pi}{3a}\right)\right]+\alpha_3^2\,\frac{\omega^2-\omega_q^2}{\omega^2-\omega^2_{q+\frac{2\pi}{3a}}}\left[F(q)+F\left(q-\frac{2\pi}{3a}\right)\right]\\ &\quad+\alpha_3^2\,\frac{\omega^2-\omega_q^2}{\omega^2-\omega^2_{q-\frac{2\pi}{3a}}}\left[F(q)+F\left(q+\frac{2\pi}{3a}\right)\right]\\ &\quad-(\alpha_2+\alpha_4)^2\left[\frac{1}{\omega^2-\omega^2_{q+\frac{2\pi}{3a}}}+\frac{1}{\omega^2-\omega^2_{q-\frac{2\pi}{3a}}}+\frac{\omega^2-\omega_q^2}{\omega^2_{q+\frac{2\pi}{3a}}-\omega^2_{q-\frac{2\pi}{3a}}}\left(\frac{1}{\omega^2-\omega^2_{q+\frac{2\pi}{3a}}}-\frac{1}{\omega^2-\omega^2_{q-\frac{2\pi}{3a}}}\right)\right]\end{aligned}\tag{C.1}$$

$$\begin{aligned}\xi &= (\alpha_2+\alpha_4)\left[\frac{\frac{\delta_{q+\frac{2\pi}{3a}k}}{\pi}\left(\omega_q\omega_{q+\frac{2\pi}{3a}}\right)^{\frac{1}{2}}}{\omega^2-\omega^2_{q+\frac{2\pi}{3a}}}+\frac{\frac{\delta_{q-\frac{2\pi}{3a}k}}{\pi}\left(\omega_q\omega_{q-\frac{2\pi}{3a}}\right)^{\frac{1}{2}}}{\omega^2-\omega^2_{q-\frac{2\pi}{3a}}}\right]\\ &\quad+\alpha_3^2\,\frac{\delta_{qk}}{\pi}\left[\frac{F(q)+F\left(q-\frac{2\pi}{3a}\right)}{\omega^2-\omega^2_{q+\frac{2\pi}{3a}}}+\frac{F(q)+F\left(q+\frac{2\pi}{3a}\right)}{\omega^2-\omega^2_{q-\frac{2\pi}{3a}}}\right]\\ &\quad-(\alpha_2+\alpha_4)^2\,\frac{\frac{\delta_{qk}}{\pi}\omega_q-\frac{\delta_{q+\frac{2\pi}{3a}k}}{\pi}\left(\omega_q\omega_{q+\frac{2\pi}{3a}}\right)^{\frac{1}{2}}-\frac{\delta_{q-\frac{2\pi}{3a}k}}{\pi}\left(\omega_q\omega_{q-\frac{2\pi}{3a}}\right)^{\frac{1}{2}}}{\omega^2_{q+\frac{2\pi}{3a}}-\omega^2_{q-\frac{2\pi}{3a}}}\left(\frac{1}{\omega^2-\omega^2_{q+\frac{2\pi}{3a}}}-\frac{1}{\omega^2-\omega^2_{q-\frac{2\pi}{3a}}}\right)\end{aligned}\tag{C.2}$$

Using $F(q)$ expression in Eqs. (B.8) and (B.9). The whole representation of ζ 's and ξ 's real and imaginary parts are shown in Supplemental Material [25].

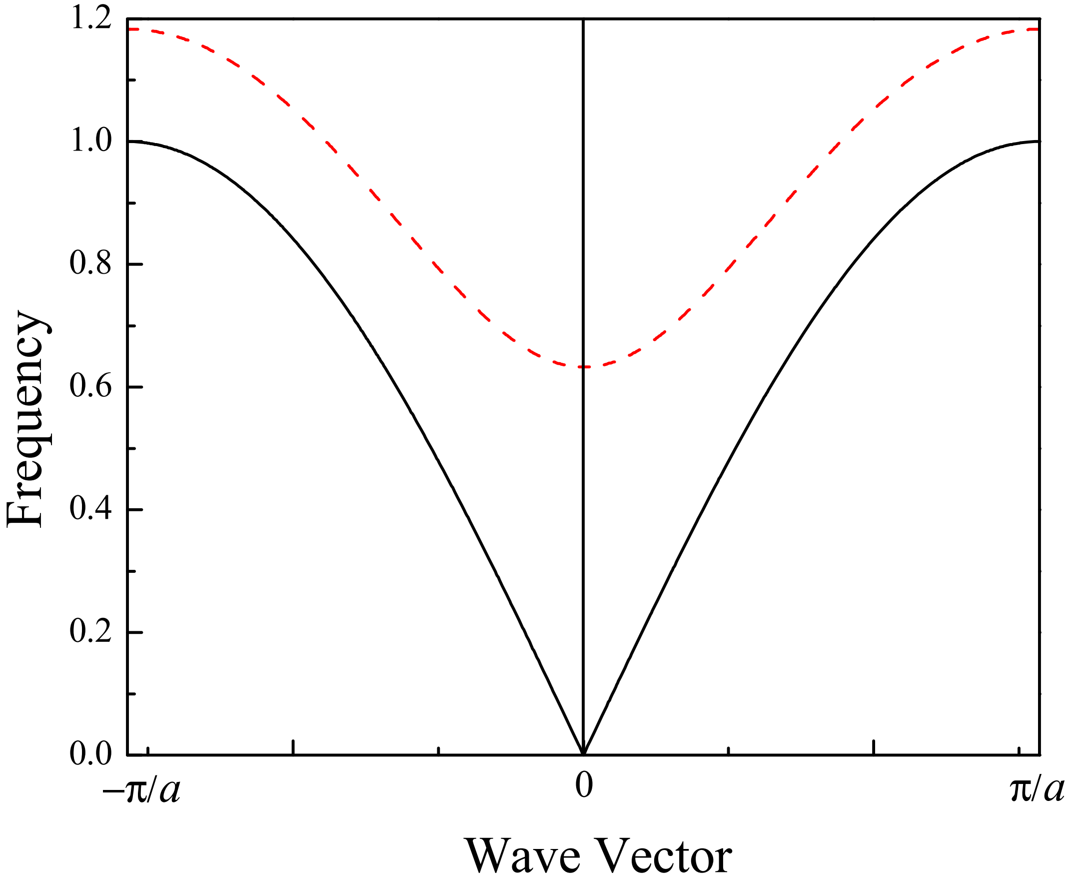

Fig.1. Phonon dispersion for $a = b$ without the FK on-site potential (black solid line), and including the FK on-site potential (red dashed line). $\omega_L = 1$ and $\frac{\pi^2 V_0}{ma^2} = 0.1$ are used in the calculation.

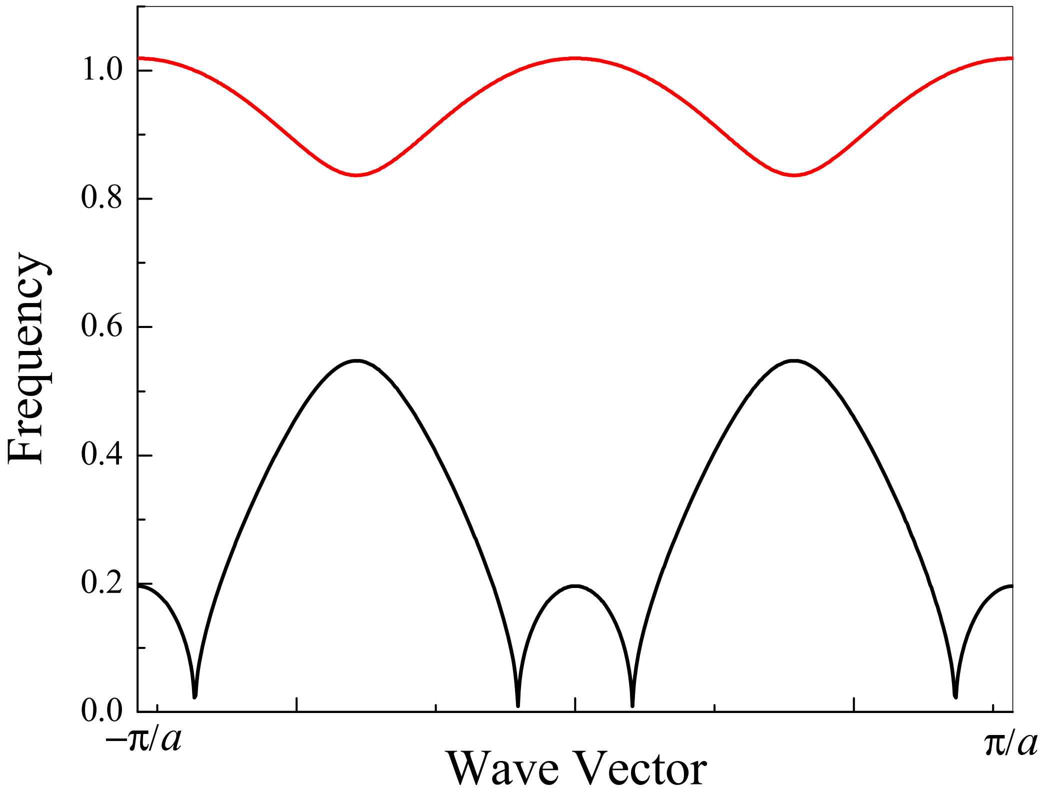

Fig. 2. Phonon dispersion for $a = \frac{b}{2}$ with the FK potential. Two branches are shown using a black line and a red line. The parameters used in the calculation are same as those in Fig.1.

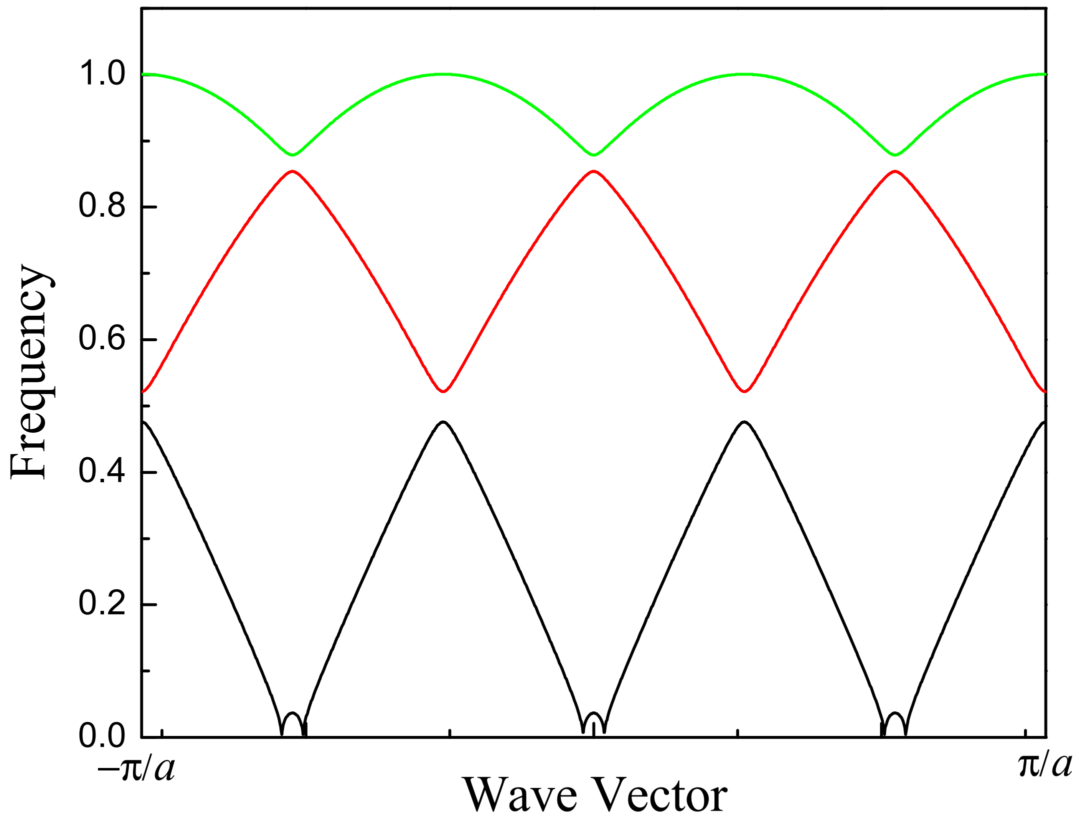

Fig. 3. Phonon dispersion for $a = \frac{b}{3}$ with the FK on-site potential. Three branches are shown using black, red and green lines. The parameters used in the calculation are same as those in Fig.1.

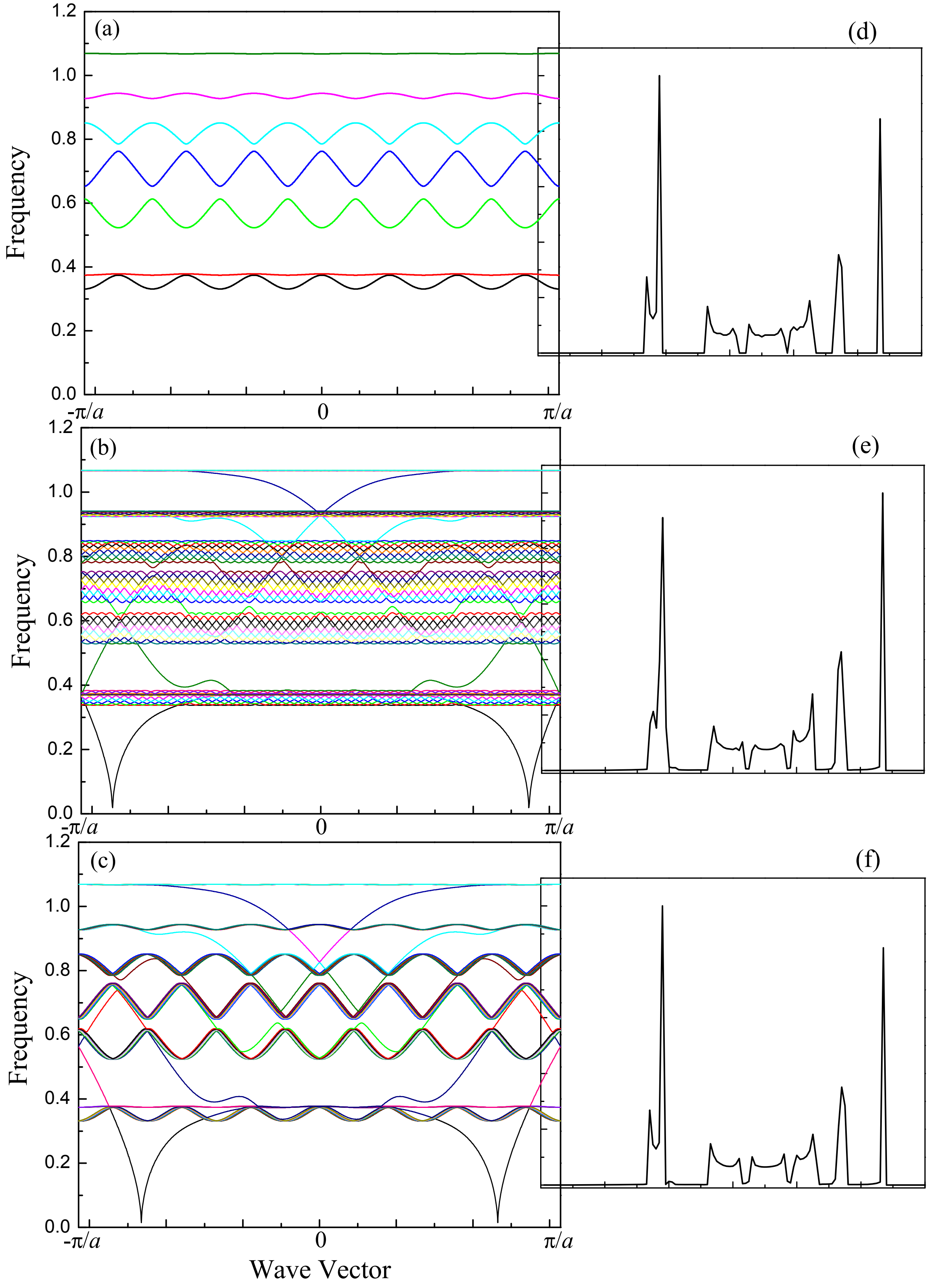

Fig. 4. The phonon dispersions of a commensurate chain (a) with $b=\frac{7}{6}a$, that of incommensurate chains (b), with $b=1.17a$, and (c) with $b=1.167a$. The curves (d), (e), and (f) on the right correspond to the phonon density of state. The parameters used in the calculations are same as those in Fig.1.