Force constants and dispersion relations for the zincblende and diamond structures revisited

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The bulk atomic equations of motion are revisited in order to show explicitly, for high symmetry directions, the transformation of this three-dimensional problem into decoupled one-dimensional problems. The force constants of the corresponding one-dimensional equations are related to a larger number of force constants of the bulk problem. We illustrate how the three-dimensional force constants (and consequently the whole dynamical matrix) can be estimated from a few either experimental or theoretical points for semiconductors in the zincblende and diamond structures.

Keywords: Force constants; zincblende; diamond.

Las ecuaciones del movimiento en materiales masivos son retomadas para mostrar explícitamente, para direcciones de alta simetría, las transformaciones de este problema tridimensional en problemas unidimensionales desacoplados. Las constantes de fuerza de las correspondientes ecuaciones unidimensionales son relacionadas a un número mayor de constantes de fuerzas en el material masivo. Se ilustra como las constantes de fuerza tridimensionales (y consecuentemente la matriz dinámica) pueden ser estimadas a partir de unos pocos puntos experimentales o teóricos, para semiconductores de las estructuras blenda de zinc y diamante.

Descriptores: Constantes de fuerza; blenda de zinc; diamante.

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1. Introduction

Many properties of solids depend on the dynamics of the crystal lattice. Though the current interest of most researchers is mainly focused on phonons in heterostructures, some problems still demand an appreciable knowledge of the bulk atomic oscillations. Examples are phonon imaging [1,2] and the reduction of thermal conductivity in superlattices in comparison to bulk materials [3–5].

It is worth recalling that, along high symmetry directions such as either the [001] or the [111] direction, and for semiconductors with both the zincblende and diamond structures, the three-dimensional (3D) equations of motion are decoupled into one longitudinal and two transverse oscillations which are described by linear chain models (see [6] and references therein). This exact result for the bulk is useful for the study of heterostructures. In fact, for heterostructures grown along high symmetry directions, it is usually assumed that the force constants in each constituent layer are equal to the bulk force constants. These bulk values are estimated either from experimental dispersion relations or from theoretical calcu-

lations, and linear chain models are employed in studying the phonon modes of this more complex system. Early works considered only interaction with a few neighbors [7–9]. More elaborate linear models were later developed, such as the planar bond-charge model [10]. Other authors simply take the bulk force constants from first principles calculations [11,12].

For less symmetric directions, there is no simple treatment at hand. From the theoretical viewpoint, even though atomic equations of motion have been known for a long time [13], the huge number of atoms in bulk materials makes their numerical solution an unaffordable task. Thus, the above-mentioned examples demand simpler phonon models. Among these we find, for example, phenomenological models like the rigid-ion model [13, 14], the shell model [15, 16], and the bond-charge model [17, 18]. However, the numerical implementation of these is not straightforward; therefore, analytical results are always of interest.

In this paper the phonon equations of motion for bulk semiconductors are revisited. Instead of finding the irreducible representation for a given direction, as for example in Ref. 6, we consider a given number of atoms and assume

harmonic interaction between a limited number of neighbors. The dynamical matrix is then constructed, taking into account the symmetry of the underlying lattice. Interesting properties of the equations are found in this way. In particular, we check explicitly how the 3D problem reduces to decoupled linear chain equations for high symmetry directions, with the aim of obtaining the relation between the 3D and one-dimensional (1D) force constants. To the best of our knowledge, this relation has not been explored so far. Our study helps to understand better the richness of the linear chain models. We also show how to fit the 3D bulk force constants (and consequently the whole dynamical matrix) from a few points, either experimental or theoretical. We focus our study on both the zincblende and diamond structures, which are examples of a diatomic basis in a crystal lattice. We also find it useful to consider the monatomic face-centered-cubic (fcc) lattice, for it is an illustrative example where analytical calculations are easier than in the rest of the treated problems dealt with.

This paper is organized as follows: in the next section we enumerate the properties of the equations of motion that are needed in this paper. In Sec. III, we consider the face-centered-cubic (fcc) lattice with a monatomic basis. In Sec. IV, we study both the diamond and zincblende structures. At the end, our main conclusions are summarized.

2. Atomic equations of motion

In the harmonic approximation the crystal hamiltonian reads [13]

$$
H = \sum_{l\kappa\alpha} \frac{p_\alpha^2(l\kappa)}{2M_\kappa}
$$
$$
+ \frac{1}{2} \sum_{l\kappa\alpha, l'\kappa'\beta} \Phi_{\alpha\beta}(l\kappa, l'\kappa') u_\alpha(l\kappa) u_\beta(l'\kappa'), \quad (1)
$$

where $l, l' = 1, 2, \ldots, N$ label the elementary cells, $\kappa, \kappa' = 1, 2, \ldots, r$ label the atoms in the basis, $\alpha, \beta = x, y, z$ represent the coordinate axis, M_κ is the mass of the κ-atom, $p_\alpha(l\kappa)$ is the linear momentum of the $l\kappa$-atom in the α direction, $u_\alpha(l\kappa)$ represents the displacement from the equilibrium position of the $l\kappa$-atom in the α direction, and $\Phi_{\alpha\beta}(l\kappa, l'\kappa')$ are the force constants. The force constants are symmetric in the indices l, κ, α

$$
\Phi_{\alpha\beta}(l\kappa, l'\kappa') = \Phi_{\beta\alpha}(l'\kappa', l\kappa). \quad (2)
$$

The hamiltonian is invariant under an infinitesimal translation of the whole crystal; this yields the following relation between the force constants

$$
\sum_{l\kappa} \Phi_{\alpha\beta}(l\kappa, l'\kappa') = \sum_{l'\kappa'} \Phi_{\beta\alpha}(l'\kappa', l\kappa) = 0. \quad (3)
$$

From the crystal invariance under translations in a lattice vector, we find that

$$
\Phi_{\alpha\beta}(l\kappa, l'\kappa') = \Phi_{\alpha\beta}((l - l')\kappa, 0\kappa'), \quad (4)
$$

i.e., the force constants are functions of the relative position of lth and l'th cells. The equations of motion in the reciprocal space are of the form

$$
\omega^2 e_\alpha(\kappa) = \sum_{\kappa'\beta} D_{\alpha\beta}(\kappa\kappa', \mathbf{q}) e_\beta(\kappa'), \quad (5)
$$

where $e_\alpha(\kappa)$ is the polarization vector and D is the dynamical matrix given by

$$
D_{\alpha\beta}(\kappa\kappa', \mathbf{q}) = \frac{1}{\sqrt{M_\kappa M_{\kappa'}}} \sum_{l'} \Phi_{\alpha\beta}(l\kappa, l'\kappa')
$$
$$
\times \exp(-i\mathbf{q} \cdot [\mathbf{x}(l) - \mathbf{x}(l')]), \quad (6)
$$

where $\mathbf{x}(l)$ is the vector position of the elementary cell. The dynamical matrix is hermitian

$$
D_{\alpha\beta}(\kappa\kappa', \mathbf{q}) = D_{\beta\alpha}^*(\kappa'\kappa, \mathbf{q}), \quad (7)
$$

and has the property

$$
D_{\alpha\beta}(\kappa\kappa', -\mathbf{q}) = D_{\alpha\beta}^*(\kappa\kappa', \mathbf{q}). \quad (8)
$$

The invariance of the force constants under a symmetry operation S (S is represented by a unitary matrix) is written in matrix form as

$$
S\Phi S^\dagger = \Phi. \quad (9)
$$

From this relation, the dependence between the matrix elements of the force constant matrix can be established. The dagger ($\dagger$) means the hermitian conjugate.

3. Monatomic crystal

We first consider a fcc lattice with a monatomic basis. This simple case helps to understand the properties of the force constants in more complicated situations. For our purpose it is sufficient to consider the [100] direction. The structure has a fourth-order symmetry axis in this direction [19]. The C_4 symmetry operation can be represented by the matrix

$$
C_4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (10)
$$

Employing (9), the force constant matrix is written as

$$
\Phi = \begin{pmatrix} \Phi_{11} & 0 & 0 \\ 0 & \Phi_{22} & \Phi_{23} \\ 0 & -\Phi_{23} & \Phi_{22} \end{pmatrix}. \quad (11)
$$

Considering also the symmetry properties (2) and (4), the matrix is reduced to the diagonal form

$$
\Phi = \begin{pmatrix} \Phi_{11} & 0 & 0 \\ 0 & \Phi_{22} & 0 \\ 0 & 0 & \Phi_{22} \end{pmatrix}. \quad (12)
$$

TABLE I. Position and distance from the origin of the first 14th neighbors for the monatomic fcc lattice.

neighbor	$\mathbf{n}$	$|\mathbf{n}|$
1	$(\pm a/2, 0, \pm a/2)$; $(\pm a/2, \pm a/2, 0)$; $(0, \pm a/2, \pm a/2)$	$\frac{\sqrt{2}}{2}a$
2	$(\pm a, 0, 0)$; $(0, \pm a, 0)$; $(0, 0, \pm a)$	a
3	$(\pm a, \pm a/2, \pm a/2)$; $(\pm a/2, \pm a, \pm a/2)$; $(\pm a/2, \pm a/2, \pm a)$	$\frac{\sqrt{6}}{2}a$
4	$(\pm a, \pm a, 0)$; $(0, \pm a, \pm a)$; $(\pm a, 0, \pm a)$	$\sqrt{2}a$
5	$(\pm a, \pm a, \pm a)$	$\sqrt{3}a$
6	$(\pm 3a/2, \pm a/2, \pm a/2)$; $(\pm a/2, \pm 3a/2, \pm a/2)$; $(\pm a/2, \pm a/2, \pm 3a/2)$	$\frac{\sqrt{11}}{2}a$
7	$(\pm 3a/2, \pm a, \pm a/2)$; $(\pm a, \pm 3a/2, \pm a/2)$; $(\pm a/2, \pm a, \pm 3a/2)$; $(\pm 3a/2, \pm a/2, \pm a)$; $(\pm a/2, \pm 3a/2, \pm a)$; $(\pm a, \pm a/2, \pm 3a/2)$	$\frac{\sqrt{14}}{2}a$
8	$(\pm 2a, 0, 0)$; $(0, \pm 2a, 0)$; $(0, 0, \pm 2a)$	$2a$
9	$(\pm 2a, \pm a/2, \pm a/2)$; $(\pm a/2, \pm 2a, \pm a/2)$; $(\pm a/2, \pm a/2, \pm 2a)$; $(\pm 3a/2, 0, \pm 3a/2)$; $(\pm 3a/2, \pm 3a/2, 0)$; $(0, \pm 3a/2, \pm 3a/2)$	$\frac{3\sqrt{2}}{2}a$
10	$(\pm 2a, \pm a, 0)$; $(0, \pm 2a, \pm a)$; $(\pm 2a, 0, \pm a)$; $(\pm a, \pm 2a, 0)$; $(0, \pm a, \pm 2a)$; $(\pm a, 0, \pm 2a)$	$\sqrt{5}a$
11	$(\pm 2a, \pm a, \pm a)$; $(\pm a, \pm 2a, \pm a)$; $(\pm a, \pm a, \pm 2a)$	$\sqrt{6}a$
12	$(\pm 2a, \pm 3a/2, \pm a/2)$; $(\pm 2a, \pm a/2, \pm 3a/2)$; $(\pm 3a/2, \pm 2a, \pm a/2)$; $(\pm a/2, \pm 2a, \pm 3a/2)$; $(\pm a/2, \pm 3a/2, \pm 2a)$; $(\pm 3a/2, \pm a/2, \pm 2a)$	$\frac{\sqrt{26}}{2}a$
13	$(\pm 2a, \pm 2a, 0)$; $(0, \pm 2a, \pm 2a)$; $(\pm 2a, 0, \pm 2a)$	$2\sqrt{2}a$
14	$(\pm 2a, \pm 2a, \pm 2a)$	$2\sqrt{3}a$

TABLE II. Relation between the number of force constants (number of neighbors) in the linear chain and in the 3D problem.

linear chain	Bulk (3D)
1	1
2	2
3	6
4	8
5	15

Thus, the motion is decoupled into a longitudinal (L) and two degenerate transverse (T) oscillations. The dynamical matrix (6) has also this property. For the sake of simplicity we limit our study to the longitudinal phonons. The dispersion relation (5) is quite simple in this case:

$$\omega^2 = D_{11}(\mathbf{q}). \qquad (13)$$

In the rest of this section we omit the coordinate axis label. Employing (2), (3), and (4) the following expression for the dynamical matrix D is obtained:

$$D(\mathbf{q}) = -\frac{2}{M}\sum_n \Phi(n)\sin^2\left(\frac{\mathbf{q}\cdot\mathbf{n}}{2}\right), \qquad (14)$$

where $\mathbf{n} = \mathbf{x}(l) - \mathbf{x}(l')$. Thus equation (13) yields the known dispersion relation for the monatomic linear chain [20]

$$\omega^2 = \frac{4}{M}\sum_{m>0}^{f} K_m \sin^2\left(\frac{mqa}{2}\right), \qquad (15)$$

where K_m are the force constants of the linear chain. We computed the dynamical matrix (14) considering the first 14th neighbors. In Table I, the position of these atoms and their distance from the origin are presented. Replacing the values of $\mathbf{n}$ from the table in the expression (14), substituting the resulting expression in (13), and comparing with (15), we obtain the following relation between the 3D force constants and the linear chain force constants. Note that for the linear chain the lattice constant $a_0/2$ should be employed.

$$K_1 = -(4\Phi_1 + 8\Phi_3 + 8\Phi_6 + 16\Phi_7 + 8\Phi_9 + 8\Phi_{12})$$

$$K_2 = -(\Phi_2 + 4\Phi_3 + 4\Phi_4 + 4\Phi_5 + 4\Phi_{10} + 8\Phi_{11})$$

$$K_3 = -(4\Phi_6 + 8\Phi_7 + 4\Phi_9^* + 8\Phi_{12})$$

$$K_4 = -(\Phi_8 + 4\Phi_9 + 4\Phi_{10} + 4\Phi_{11} + 8\Phi_{12}$$
$$+ 4\Phi_{13} + 4\Phi_{14})$$

$$\vdots \qquad\qquad (16)$$

Table II shows that few neighbors in the linear chain correspond to a larger number of neighbors in the 3D case. Of course, in the bulk there is a larger number of neighbors at some distance from an arbitrary atom. This simple case illustrates why the linear chain with interaction with a few neighbors fits well with the experimental results in a variety of situations.

TABLE III. Position and distance from the origin of the first three nearest neighbors for both the diamond and zincblende structures.

Neighbor	$\mathbf{x}(l)$	$\lvert\mathbf{r}\rvert$
1	$l_0 = (0,0,0)$; $l_1 = (a_0/2, -a_0/2, 0)$;	$\frac{\sqrt{3}}{4}a_0$
	$l_2 = (0, -a_0/2, -a_0/2)$; $l_3 = (a_0/2, 0, -a_0/2)$	
2	$L_0 = (a_0/2, a_0/2, 0)$; $L_1 = (-a_0/2, a_0/2, 0)$;	$\frac{\sqrt{2}}{2}a_0$
	$L_2 = (-a_0/2, -a_0/2, 0)$; $L_3 = (a_0/2, -a_0/2, 0)$;	
	$L_4 = (0, a_0/2, a_0/2)$; $L_5 = (0, -a_0/2, a_0/2)$;	
	$L_6 = (0, -a_0/2, -a_0/2)$; $L_7 = (0, a_0/2, -a_0/2)$;	
	$L_8 = (a_0/2, 0, a_0/2)$; $L_9 = (-a_0/2, 0, a_0/2)$;	
	$L_{10} = (-a_0/2, 0, -a_0/2)$; $L_{11} = (a_0/2, 0, -a_0/2)$	
3	$L'_0 = (0, a_0/2, -a_0/2)$; $L'_1 = (a_0/2, 0, a_0/2)$; $L'_2 = (a_0/2, a_0/2, 0)$;	$\frac{\sqrt{11}}{4}a_0$
	$L'_3 = (0, -a_0/2, a_0/2)$; $L'_4 = (-a_0/2, 0, -a_0/2)$; $L'_5 = (-a_0/2, -a_0/2, 0)$;	
	$L'_6 = (a_0, -a_0/2, -a_0/2)$; $L'_7 = (a_0/2, -a_0, -a_0/2)$; $L'_8 = (a_0/2, -a_0/2, -a_0)$;	
	$L'_9 = (a_0, 0, 0)$; $L'_{10} = (0, -a_0, 0)$; $L'_{11} = (0, 0, -a_0)$	

4. Diatomic crystal: zincblende and diamond structures

We consider here the elementary cell of a fcc structure with lattice constant a_0 and a two-atom basis. The basis atom located at the lattice point is labeled κ, and the other one is shifted $\mathbf{x}(\kappa') = (-a_0/4, a_0/4, a_0/4)$, and labeled κ'. If the two atoms are different, we have the zincblende structure, whereas if the two basis atoms are equal we have the diamond structure. We study the equations of motion with third-nearest neighbors interaction, and then we consider some particular directions. We should note that the first and third neighbors are κ' atoms, located at $\mathbf{r} = \mathbf{x}(l) + \mathbf{x}(\kappa')$. Second neighbors are κ atoms, located at $\mathbf{r} = \mathbf{x}(l)$. Only the coordinates $\mathbf{x}(l)$ are needed to compute $D(\kappa\kappa', \mathbf{q})$ after (6). The position of all the atoms $(\mathbf{x}(l))$ and their distance from the origin are found in Table III.

We first compute $D(\kappa\kappa', \mathbf{q})$. The first nearest neighbors are 4 atoms, which are invariant under the operations of the group C_{3v} [19]. For example, we have the following representation for the combined operation of third order rotation and inversion acting on the atom located at $l_0 + x(\kappa')$ (see Table III).

$$C_3 = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \sigma_v = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (17)$$

The force matrix Φ is invariant under this transformation (9), *i.e.*

$$\sigma_v C_3 \Phi C_3^t \sigma_v^t = \Phi. \quad (18)$$

In this way we find the independent elements. For the other three first neighbors, we use the symmetry operations which transform the matrix Φ_{l0} at the point l_0 into matrices Φ_{li} at the points l_i, $i = 1, 2, 3$, *i.e.* C_4^z for Φ_{l1}, $\sigma_v^{xy} C_4^z$ for Φ_{l2} and $\sigma_v^{xy} C_4^z$ for Φ_{l3}. The results are summarized in the following. Note that only two independent force constants are needed.

$$\Phi_{l0}^{(1)} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{12} \\ \alpha_{12} & \alpha_{11} & -\alpha_{12} \\ \alpha_{12} & -\alpha_{12} & \alpha_{11} \end{pmatrix}, \quad (19)$$

$$\Phi_{l1}^{(1)} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & -\alpha_{12} \\ \alpha_{12} & \alpha_{11} & \alpha_{12} \\ -\alpha_{12} & \alpha_{12} & \alpha_{11} \end{pmatrix}, \quad (20)$$

$$\Phi_{l2}^{(1)} = \begin{pmatrix} \alpha_{11} & -\alpha_{12} & -\alpha_{12} \\ -\alpha_{12} & \alpha_{11} & -\alpha_{12} \\ -\alpha_{12} & -\alpha_{12} & \alpha_{11} \end{pmatrix}, \quad (21)$$

$$\Phi_{l3}^{(1)} = \begin{pmatrix} \alpha_{11} & -\alpha_{12} & \alpha_{12} \\ \alpha_{12} & \alpha_{11} & \alpha_{12} \\ -\alpha_{12} & \alpha_{12} & \alpha_{11} \end{pmatrix}. \quad (22)$$

Using these expressions in (6), we obtain the dynamical matrix for the first neighbors

$$D^{(1)}(\kappa\kappa', \mathbf{q}) = \frac{1}{\sqrt{M_\kappa M_{\kappa'}}} \left[\Phi_{l0}^{(1)} + \Phi_{l1}^{(1)} \exp\left(i\frac{a_0(q_x - q_y)}{2}\right) \right.$$
$$+ \Phi_{l2}^{(1)} \exp\left(-i\frac{a_0(q_y + q_z)}{2}\right)$$
$$+ \left. \Phi_{l3}^{(1)} \exp\left(i\frac{a_0(q_x - q_z)}{2}\right) \right]. \quad (23)$$

The force constant matrices are invariant under translation $x(\kappa')$. Then the difference between the first and third neighbors is just a labeling convention, as can be seen in the following:

$$\Phi_{L'_9}^{(3)} = \Phi_{L'_{10}}^{(3)} = \Phi_{L'_{11}}^{(3)} = \Phi_{l0}^{(3)},$$
$$\Phi_{L'_2}^{(3)} = \Phi_{L'_5}^{(3)} = \Phi_{L'_8}^{(3)} = \Phi_{l1}^{(3)},$$
$$\Phi_{L'_0}^{(3)} = \Phi_{L'_3}^{(3)} = \Phi_{L'_6}^{(3)} = \Phi_{l2}^{(3)},$$
$$\Phi_{L'_1}^{(3)} = \Phi_{L'_4}^{(3)} = \Phi_{L'_7}^{(3)} = \Phi_{l3}^{(3)}. \quad (24)$$

And we have for the corresponding dynamical matrix (6),

$$D^{(3)}\left(\kappa\kappa',\mathbf{q}\right)=\frac{1}{\sqrt{M_\kappa M_{\kappa'}}}\left[2\Phi^{(3)}_{l_1}\cos\left(q_x+q_y\right)\frac{a_0}{2}\right.$$

$$+2\Phi^{(3)}_{l_2}\cos\left(q_y-q_z\right)\frac{a_0}{2}+2\Phi^{(3)}_{l_3}\cos\left(q_x+q_z\right)\frac{a_0}{2}$$

$$+\exp\left(iq_x a_0\right)\left(\Phi^{(3)}_{l_0}+\Phi^{(3)}_{l_2}\exp\left(-i\left(q_y+q_z\right)\frac{a_0}{2}\right)\right)$$

$$+\exp\left(-iq_y a_0\right)\left(\Phi^{(3)}_{l_0}+\Phi^{(3)}_{l_3}\exp\left(i\left(q_x-q_z\right)\frac{a_0}{2}\right)\right)$$

$$+\exp\left(-iq_z a_0\right)\left(\Phi^{(3)}_{l_0}+\Phi^{(3)}_{l_1}\exp\left(i\left(q_x-q_y\right)\frac{a_0}{2}\right)\right)\right].\quad(25)$$

To calculate $D\left(\kappa\kappa',\mathbf{q}\right)$, we only need in our case the second neighbors. These atoms are invariant under operations of the group C_{2v} [19]. Following the same method as before, we arrive at the representation

$$\Phi^{(2)}_{L_0}=\begin{pmatrix}\beta_{11}&\beta_{12}&0\\\beta_{12}&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix},\quad(26)$$

$$\Phi^{(2)}_{L_1}=\begin{pmatrix}\beta_{11}&-\beta_{12}&0\\-\beta_{12}&\beta_{11}&0\\0&0&\beta_{33}\end{pmatrix},\quad(27)$$

$$\Phi^{(2)}_{L_2}=\Phi^{(2)}_{L0},\quad(28)$$

$$\Phi^{(2)}_{L_3}=\Phi^{(2)}_{L_1},\quad(29)$$

$$\Phi^{(2)}_{L_4}=\begin{pmatrix}\beta_{33}&0&0\\0&\beta_{11}&\beta_{12}\\0&\beta_{12}&\beta_{11}\end{pmatrix},\quad(30)$$

$$\Phi^{(2)}_{L_5}=\begin{pmatrix}\beta_{33}&0&0\\0&\beta_{11}&-\beta_{12}\\0&-\beta_{12}&\beta_{11}\end{pmatrix},\quad(31)$$

$$\Phi^{(2)}_{L_6}=\Phi^{(2)}_{L_4},\quad(32)$$

$$\Phi^{(2)}_{L_7}=\Phi^{(2)}_{L_5},\quad(33)$$

$$\Phi^{(2)}_{L_8}=\begin{pmatrix}\beta_{11}&0&-\beta_{12}\\0&\beta_{33}&0\\-\beta_{12}&0&\beta_{11}\end{pmatrix},\quad(34)$$

$$\Phi^{(2)}_{L_9}=\begin{pmatrix}\beta_{11}&0&\beta_{12}\\0&\beta_{33}&0\\\beta_{12}&0&\beta_{11}\end{pmatrix},\quad(35)$$

$$\Phi^{(2)}_{L_{10}}=\Phi^{(2)}_{L_8},\quad(36)$$

$$\Phi^{(2)}_{L_{11}}=\Phi^{(2)}_{L_9},\quad(37)$$

where we use the symmetry operations which transform the matrix Φ_{L_0} at the point L_0 into the matrices Φ_{L_i} at the points L_i, $i=1,2,\cdots,11$, i.e. C^z_4 for Φ_{L_1}, C^z_2 for Φ_{L_2}, C^{-z}_4 for Φ_{L_3}, C^{-y}_4 for Φ_{L_4}, $C^x_4 C^{-y}_4$ for Φ_{L_5}, $C^x_2 C^{-y}_4$ for Φ_{L_6}, $C^{-x}_4 C^{-y}_4$ for Φ_{L_7}, C^x_4 for Φ_{L_8}, $C^{-y}_4 C^x_4$ for Φ_{L_9}, $C^y_2 C^x_4$ for $\Phi_{L_{10}}$, and $C^y_4 C^x_4$ for $\Phi_{L_{11}}$.

Property (3) helps to obtain the diagonal elements of the force constant matrix

$$\Phi\left(l\kappa,l\kappa\right)=-4\left(\alpha_{11}+3\gamma_{11}+2\beta_{11}+\beta_{33}\right)\hat{I},\quad(38)$$

where $\hat{I}$ is the identity matrix of order 3.

We obtain $D\left(\kappa\kappa,\mathbf{q}\right)$ from (6):

$$D\left(\kappa\kappa,\mathbf{q}\right)=\frac{1}{M_\kappa}\left(\Phi\left(l\kappa,l\kappa\right)+4A\right),\quad(39)$$

$$A=\begin{pmatrix}A_{xx}&-\beta_{12}S_xS_y&\beta_{12}S_xS_z\\-\beta_{12}S_xS_y&A_{yy}&-\beta_{12}S_yS_z\\\beta_{12}S_xS_z&-\beta_{12}S_yS_z&A_{zz}\end{pmatrix},$$

$$A_{xx}=\beta_{11}C_x\left(C_y+C_z\right)+\beta_{33}C_yC_z,$$

$$A_{yy}=\beta_{11}C_y\left(C_x+C_z\right)+\beta_{33}C_xC_z,$$

$$A_{zz}=\beta_{11}C_z\left(C_x+C_y\right)+\beta_{33}C_xC_y,$$

where $C_x=\cos\left(q_x a_0/2\right)$, $S_x=\sin\left(q_x a_0/2\right)$, etc...

Given that κ and κ' have the same symmetry, we could write for $D\left(\kappa'\kappa',\mathbf{q}\right)$

$$D\left(\kappa'\kappa',\mathbf{q}\right)=\frac{1}{M_\kappa}\left(\Phi\left(l\kappa',l\kappa'\right)+4A\right),\quad(40)$$

$$A=\begin{pmatrix}A_{xx}&-\delta_{12}S_xS_y&\delta_{12}S_xS_z\\-\delta_{12}S_xS_y&A_{yy}&-\delta_{12}S_yS_z\\\delta_{12}S_xS_z&-\delta_{12}S_yS_z&A_{zz}\end{pmatrix}.$$

In order to estimate the 3D force constants, we proceed as follows. We consider the decoupled L and T modes in the [100] direction, and the decoupled T modes in the [110] direction. The equations of motion in these directions are equivalent to linear chains, as in the preceding section. We fit the linear chain dispersion relation to the experimental values reported for Ge in Ref. 21. As we only need a few constants, we calculate the analytical expressions for frequencies both at the edge and at the center of the BZ for the linear chain model (for the acoustical branch, we calculate the expression of the sound velocity). From the expressions obtained, we compute the values of the linear chain force constants. For these decoupled oscillations, planes of atoms are oscillating with the same frequency. For this reason, it is usual to speak about planar vibrations. We will use this terminology below. With the help of the planar force constants, we compute the 3D force constants. We will see that, for Ge, all the 3D force constants up to the third-neighbor approximation are estimated straightforwardly. We first study the L and T modes in the [100] direction, and then the decoupled T modes in the [110] direction.

Employing (23), (25), (39), and (40), it is possible to write the equation of motion in the [001] direction. In this direction, the structure has C_{2v} symmetry [19]. It is straightforward enough to compute the irreducible representation for the atomic oscillations along this direction:

$$D^u_\Delta=\Delta_1\oplus\Delta'_2\oplus 2\Delta_5,\quad(41)$$

where we use the notation from [19]. We find the longitudinal oscillations are decoupled from the transverse ones. For the longitudinal case, the equations of motion are

$$\omega^2 e_1\left(\kappa\right) = -\frac{4}{M_\kappa}\left(\alpha_{11}+2\gamma_{11}+\gamma_{11}+4\beta_{11}\sin^2\frac{qa_0}{4}\right)e_1\left(\kappa\right)$$
$$+\frac{1}{\sqrt{M_\kappa M_{\kappa'}}}\left((2\alpha_{11}+4\gamma_{11})\left(1+\exp\left(iqa_0/2\right)\right)\right.$$
$$+2\gamma_{11}\left(\exp\left(-iqa_0/2\right)+\exp\left(iqa_0\right)\right)\big) e_1\left(\kappa'\right),\qquad(42)$$

$$\omega^2 e_1\left(\kappa'\right) = -\frac{4}{M_{\kappa'}}\left(\alpha_{11}+2\gamma_{11}+\gamma_{11}+4\delta_{11}\sin^2\frac{qa_0}{4}\right)e_1\left(\kappa'\right)$$
$$+\frac{1}{\sqrt{M_\kappa M_{\kappa'}}}\left((2\alpha_{11}+4\gamma_{11})\left(1+\exp\left(iqa_0/2\right)\right)\right.$$
$$+2\gamma_{11}\left(\exp\left(-iqa_0/2\right)+\exp\left(iqa_0\right)\right)\big) e_1\left(\kappa\right),\qquad(43)$$

These expressions are equivalent to a diatomic linear chain with second-neighbor interactions (See [20] and Appendix 5.). The substitutions presented in Table IV are needed.

TABLE IV. Relation between the 3D bulk and the linear chain with second neighbor interaction for the [001] direction: longitudinal oscillations. For the diamond structure, $\beta_{11}=\delta_{11}$ ($\gamma_a=\gamma_c$), and $M_\kappa=M_{\kappa'}$.

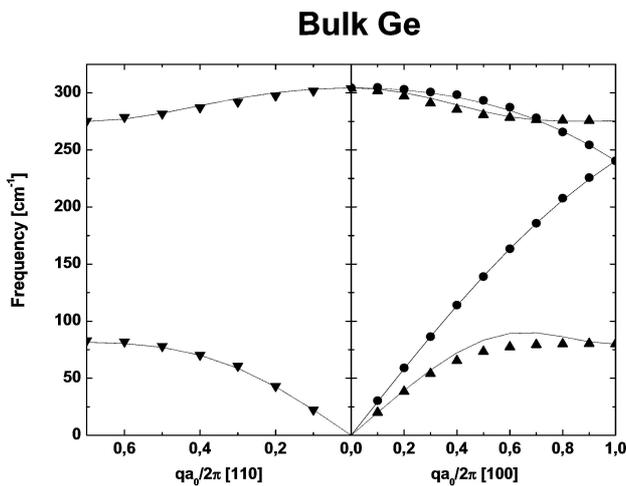| Bulk (3D)		linear chain
a_0	$\rightarrow$	$2a$
$-\left(2\alpha_{11}+4\gamma_{11}\right)$	$\rightarrow$	γ_{ca}
$-2\gamma_{11}$	$\rightarrow$	γ_{ca1}
$-4\beta_{11}$	$\rightarrow$	γ_a
$-4\delta_{11}$	$\rightarrow$	γ_c

Bulk Ge

FIGURE 1. Calculated bulk Ge frequencies (in cm^{-1}) as a function of the normalized wave vector for the [100] and [110] directions are represented with solid lines. Experimental values from [21] for [100] longitudinal modes (circles), [100] transverse modes (up triangles), and [110] transverse modes (down triangles) are given for comparison. See text for details.

In Table VII, the planar force constants fitted to [21] are presented. The results from the first principles calculations of Ref. 11 are shown in parentheses. The dispersion relation in this direction is represented in Fig. 1 with a solid line. The experimental values of Ref. 21 are also included in this figure. A good agreement is found. Employing the relations presented in Table IV, it is possible to estimate the values of the 3D force constants α_{11}, β_{11} and γ_{11}, which are reported in Table VII.

In the [100] direction we have the following characteristic equations for the transverse oscillations:

$$\omega^2\left(e_2\left(\kappa\right)\right)-e_3(\kappa) = -\frac{4}{M_\kappa}\left(\alpha_{11}+3\gamma_{11}+2(\beta_{11}+\beta_{33})\right.$$
$$\times\sin^2 qa_0/4\right)\left(e_2\left(\kappa\right)-e_3(\kappa)\right)$$
$$+\frac{1}{\sqrt{M_\kappa M_{\kappa'}}}\big((2\alpha_{11}+4\gamma_{11}+4\gamma_{12}-2\alpha_{12})$$
$$+(2\gamma_{11}-2\gamma_{12})\exp(-iqa_0/2)$$
$$+(2\alpha_{11}+4\gamma_{11}+2\alpha_{12}-4\gamma_{12})\exp(iqa_0/2)$$
$$+(2\gamma_{12}+2\gamma_{11})\exp(iqa_0)\big)\left(e_2(\kappa')-e_3(\kappa')\right),\qquad(44)$$

$$\omega^2\left(e_2(\kappa')-e_3(\kappa')\right) = -\frac{4}{M_{\kappa'}}\left(\alpha_{11}+3\gamma_{11}+2(\delta_{11}+\delta_{33})\right.$$
$$\times\sin^2 qa_0/4\right)\left(e_2(\kappa')-e_3(\kappa')\right)$$
$$+\frac{1}{\sqrt{M_\kappa M_{\kappa'}}}\big((2\alpha_{11}+4\gamma_{11}+4\gamma_{12}-2\alpha_{12})$$
$$+(2\gamma_{11}-2\gamma_{12})\exp(-iqa_0/2)$$
$$+(2\alpha_{11}+4\gamma_{11}+2\alpha_{12}-4\gamma_{12})\exp(iqa_0/2)+(2\gamma_{12}$$
$$+2\gamma_{11})\exp(iqa_0)\big)(e_2(\kappa)-e_3(\kappa)).\qquad(45)$$

This problem is again equivalent to a diatomic linear chain, and the replacements shown in Table VI are needed. However, in this case, the force between neighboring atoms depends on whether they are in the same cell or in different cells, as shown in Appendix A. This situation is also discussed in Ref. 20.

TABLE V. Relation between the 3D bulk and the linear chain for the [001] direction: transverse modes. For the diamond structure, $\beta_{11}+\beta_{33}=\delta_{11}+\delta_{33}$ ($\gamma_a=\gamma_c$), and $M_\kappa=M_{\kappa'}$.

Bulk (3D)		linear chain
$e_2\left(\kappa\right)-e_3\left(\kappa\right)$	$\rightarrow$	$e\left(\kappa\right)$
$e_2\left(\kappa'\right)-e_3\left(\kappa'\right)$	$\rightarrow$	$e\left(\kappa'\right)$
a_0	$\rightarrow$	$2a$
$-\left(2\alpha_{11}+4\gamma_{11}+4\gamma_{12}-2\alpha_{12}\right)$	$\rightarrow$	γ_{ca}
$-\left(2\alpha_{11}+4\gamma_{11}+2\alpha_{12}-4\gamma_{12}\right)$	$\rightarrow$	γ_{ca1}
$-\left(2\gamma_{11}-2\gamma_{12}\right)$	$\rightarrow$	γ_{ca2}
$-\left(2\gamma_{11}+2\gamma_{12}\right)$	$\rightarrow$	γ_{ca3}
$-\left(2\beta_{11}+2\beta_{33}\right)$	$\rightarrow$	γ_a
$-\left(2\delta_{11}+2\delta_{33}\right)$	$\rightarrow$	γ_c

Given the C_{2v} symmetry for the direction [110], it is straightforward to compute the irreducible representation for the atomic oscillations along this direction:

$$D_{\Sigma}^{u} = 2\Sigma_1 \oplus \Sigma_2 \oplus 2\Sigma_3 \oplus \Sigma_4, \qquad (46)$$

where one of the transverse oscillations is decoupled from the other, with the following equations of motion:

$$\omega^2(e_1(\kappa) - e_2(\kappa)) = -\frac{4}{M_\kappa}[\alpha_{11} + 3\gamma_{11}$$

$$+ 2(\beta_{11} + \beta_{33})\sin^2 qa_0/2)$$

$$+ (\beta_{11} - \beta_{12})\sin^2 qa_0/4](e_1(\kappa) - e_2(\kappa))$$

$$- \frac{1}{\sqrt{M_\kappa M_{\kappa'}}}[2\alpha_{11} - 2\alpha_{12} + 2\gamma_{11} - 2\gamma_{12}$$

$$+(\alpha_{11}+\alpha_{12}+3\gamma_{11}+3\gamma_{12})(\exp(iqa_0/2)+\exp(-iqa_0/2))$$

$$+ (2\gamma_{11} - 2\gamma_{12})(\exp(iqa_0)$$

$$+ \exp(-iqa_0))](e_1(\kappa') - e_2(\kappa')), \qquad (47)$$

$$\omega^2(e_1(\kappa') - e_2(\kappa')) = -\frac{4}{M_{\kappa'}}[\alpha_{11} + 3\gamma_{11}$$

$$+ 2(\delta_{11} + \delta_{33})\sin^2 qa_0/2)$$

$$+ (\delta_{11} - \delta_{12})\sin^2 qa_0/4](e_1(\kappa') - e_2(\kappa'))$$

$$- \frac{1}{\sqrt{M_\kappa M_{\kappa'}}}[2\alpha_{11} - 2\alpha_{12} + 2\gamma_{11} - 2\gamma_{12}$$

$$+(\alpha_{11}+\alpha_{12}+3\gamma_{11}+3\gamma_{12})(\exp(iqa_0/2)+\exp(-iqa_0/2))$$

$$+ (2\gamma_{11} - 2\gamma_{12})(\exp(iqa_0) + \exp(-iqa_0))]$$

$$\times (e_1(\kappa) - e_2(\kappa)). \qquad (48)$$

TABLE VI. Relation between the 3D bulk and the linear chain with fourth neighbor interaction for the [110] direction: transverse modes. For the diamond structure, $\beta_{11} - \beta_{12} = \delta_{11} - \delta_{12}(\gamma_a = \gamma_c)$, $\beta_{11} + \beta_{33} = \delta_{11} + \delta_{33}(\gamma_{a1} = \gamma_{c1})$, and $M_\kappa = M_{\kappa'}$.

Bulk (3D)		linear chain
$e_1(\kappa) - e_2(\kappa)$	$\rightarrow$	$e(\kappa)$
$e_1(\kappa') - e_2(\kappa')$	$\rightarrow$	$e(\kappa')$
a_0	$\rightarrow$	$2a$
$-(2\alpha_{11} + 4\gamma_{11} - 2\alpha_{12})$	$\rightarrow$	γ_{ca}
$-(\alpha_{11} + 2\gamma_{11} + \alpha_{12} + 2\gamma_{12})$	$\rightarrow$	$\gamma_{ca1} = \gamma_{ca2}$
$-(2\gamma_{11} - 2\gamma_{12})$	$\rightarrow$	$\gamma_{ca3} = \gamma_{ca4}$
$-(\beta_{11} - \beta_{12})$	$\rightarrow$	γ_a
$-(\delta_{11} - \delta_{12})$	$\rightarrow$	γ_c
$-(2\beta_{11} + 2\beta_{33})$	$\rightarrow$	γ_{a1}
$-(2\delta_{11} + 2\delta_{33})$	$\rightarrow$	γ_{c1}

These equations are equivalent to those obtained for the linear chain with fourth-neighbor interaction, shown in Appendix A. The substitutions shown in Table VI are needed.

Employing the relations presented in both Tables V and VI, it is possible to fit the remaining bulk force constants. The numerical values are presented in Table VII. The calculated dispersion relation (solid line) and the experimental points of Ref. 21 are shown in Fig. 1. The agreement with the experimental values for almost all the BZ could be used as an additional check of the calculations. Note that some $1D$ force constants are fixed by previous fitted $3D$ force constants, reducing the freedom to fit some experimental points with the linear chains. For this reason, a good agreement with the experimental results for some T modes in the [001]

TABLE VII. Planar and 3D force constants for Germanium (in 10^5 din cm $^{-1}$). In parentheses, the value reported in Ref. 11 for the planar force constants.

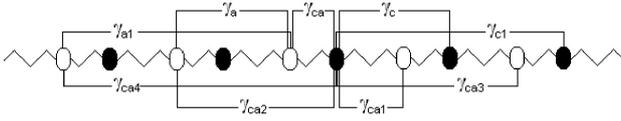| Bulk (3D)		linear chain		
α_{11}	-0.4928	L [100]	γ_{ca}	-0.9867 (-0.941)
$\beta_{11} = \delta_{11}$	-0.0305		$\gamma_a = \gamma_c$	-0.1221 (-0.130)
γ_{11}	-0.0002		γ_{ca1}	-0.0005 (0.000)
α_{12}	0.3682	T [100]	γ_{ca}	-1.72546
$\beta_{33} = \delta_{33}$	0.0582		$\gamma_a = \gamma_c$	0.05537
γ_{12}	-0.0005		γ_{ca1}	-0.24806
$\beta_{12} = \delta_{12}$	-0.0195		γ_{ca2}	0.00066
			γ_{ca3}	-0.00162
		T [110]	γ_{ca}	-1.7232
			$\gamma_a = \gamma_c$	-0.0109
			$\gamma_{ca1} = \gamma_{ca2}$	-0.1263
			$\gamma_{ca3} = \gamma_{ca4}$	0.00066
			$\gamma_{a1} = \gamma_{c1}$	0.05537

FIGURE 2. A representation of a diatomic linear chain with 4 neighbor interaction.

direction of the BZ is not observed. In order to improve this calculation, more neighbors should be considered; but this is beyond the scope of the present work.

5. Conclusions

We have explicitly shown the transformation of the 3D bulk oscillation equations of motion into 1D problems for high symmetry directions for diamond and zincblende lattices.

Instead of following the more traditional way of finding the irreducible representation for a given direction, we consider a given number of atoms and limit ourselves to the harmonic interaction between a limited number of neighbors. The dynamical matrix is then constructed taking into account the symmetry of the underlying lattice. In this way, we found that the force constants in these decoupled 1D equations are related to a larger number of force constants in the whole 3D

problem. We report for the first time the explicit relationships between 3D and 1D parameters.

3D force constants can then be estimated from a few either experimental or theoretical points, which in general are most frequently available for high symmetry directions. At this stage, the frequency at a general point of the Brillouin Zone can be found.

We illustrate the calculation for Ge which crystallizes in the diamond structure, and excellent agreement is found with the experimental data.

Acknowledgements

Appendix A: Linear chains

The most general linear chain we consider for the fcc structure has an interaction with up to 4 neighbors. The force constants are sketched in Fig. 2. Simpler linear chains are obtained as a particular case, when the right force constants tend to zero. To fit the experimental values, only the frequencies at the center and edge of the Brillouin zone, and the sound velocity of the acoustic phonons are needed. These expressions are written as

$$\omega(\Gamma) = \sqrt{\frac{\Lambda}{\mu}},$$

$$\omega_{op}(X) = \sqrt{\frac{m_c\left(2\gamma_a + \Lambda\right) + m_a\left(2\gamma_c + \Lambda\right) + \sqrt{2m_am_c\Upsilon^2 + \left(m_c\left(2\gamma_a + \Lambda\right) - m_a\left(2\gamma_c + \Lambda\right)\right)^2}}{m_am_c}},$$

$$\omega_{ac}(X) = \sqrt{\frac{m_c\left(2\gamma_a + \Lambda\right) + m_a\left(2\gamma_c + \Lambda\right) - \sqrt{2m_am_c\Upsilon^2 + \left(m_c\left(2\gamma_a + \Lambda\right) - m_a\left(2\gamma_c + \Lambda\right)\right)^2}}{m_am_c}},$$

$$v_s = \sqrt{\frac{a_0^2q^2}{M\Lambda}\left[\Lambda\left(\gamma_a + \gamma_c + 4\gamma_{a1} + 4\gamma_{c1}\right) - 2\left(\gamma_{ca1} - \gamma_{ca2} + 2\gamma_{ca3} - 2\gamma_{ca4}\right)^2\right]}, \qquad (49)$$

where $\mu = (m_a + m_c)/m_am_c$ is the reduced mass, $M = m_a + m_c$ is the total mass, $\Lambda = \gamma_{ca} + \gamma_{ca1} + \gamma_{ca2} + \gamma_{ca3} + \gamma_{ca4}$, and $\Upsilon = \gamma_{ca} - \gamma_{ca1} - \gamma_{ca2} + \gamma_{ca3} + \gamma_{ca4}$.

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