Calculation of phonon dispersion in superlattices using the matching procedure

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A method for calculating phonon dispersion curves of three-dimensional superlattices is presented. The eigenvalues of the dynamical matrix are obtained by matching the eigenvectors of two adjacent media along their common interface. The dispersion curves are obtained by solving a polynomial equation, the degree of which does *not* depend on the thickness of each medium, but is determined only by the range of interlayer coupling. This makes this method very competitive for large-period superlattices. The formalism is applied to the linear superlattice with two kinds of atoms coupled by nearest-neighbor interactions, for which the dispersion equation can be solved analytically. A formula for sound velocity is also included.

I. INTRODUCTION

A superlattice consists of the periodic stacking of different slabs having the same periodicity along the plane parallel to every interface. Viewed as a crystal, its lattice parameter in the stacking direction is much bigger than the two others normal to it. Hence, as the unit cell comprises a lot of atoms, solving the secular equation amounts to diagonalizing a big matrix.

Several methods have been devised to overcome this difficulty. Their common feature is to use the crystalline nature of each layer in the stacking direction. Some use a Green's function formalism;[1–3] the separation between bulk and interface regions is then achieved as in the problem of surface phonons.[4]

Another one starts with the dynamical matrix of the entire unit cell and simplifies the calculation of its determinant using mathematical tricks.[5,6] Finally, a method involving the matching of "bulk" eigenvectors has been used for specific semiconductor superlattices.[7,8]

The goal of this work is to work out a version of the matching procedure[9–11] well suited to studying any three-dimensional (3D) superlattice. Our interest in this method comes from its simplicity and the physical meaning conveyed by this approach.

In this first paper, we present the theory together with an illustrative application. In a second paper, the calculations for an fcc-fcc superlattice will be reported. The outline of this first paper is the following: Sec. II is devoted to the presentation of the model and notations. In Sec. III, the problem is presented, and the equations of motion are classified in two sets: "bulk" equations and interface equations. In Sec. IV, the bulk equations are first solved. The number of coordinates is thus reduced, which constitutes the crucial advantage of this technique. Then, the interface equations are written in terms of these new coordinates, which provides the searched dispersion equation. General properties of the dispersion curves are deduced in Sec. V. An example is dealt with in detail in Sec. VI. The whole work is finally summarized in Sec. VII.

II. MODEL AND NOTATION

The most general superlattice is made of N different materials referred to by the index n ($1 \le n \le N$). It consists of the stacking of identical slices B_i, each one made of N slabs S_n. For each S_n, we define p_n as the number of layers contained in S_n, l_n as the range of the interlayer interaction in S_n, and M_n as the set of the atoms of S_n interacting only with atoms of S_n.

For two adjacent slabs S_n and S_{n+1}, we define the interface $I_{n,n+1}$ made of the layers of S_n (S_{n+1}) containing atoms that interact with atoms of S_{n+1} (S_n), and we assume that $I_{n,n+1}$ contains l_n layers of S_n and l_{n+1} layers of S_{n+1}. These definitions and properties are summarized on Fig. 1.

As all slabs have the same periodicity perpendicular to the stacking direction, we introduce the 2D Brillouin Zone, and the eigenproblem can be solved separately for each $\mathbf{q}_\parallel$ in the 2D Brillouin zone. In all that follows, we shall give the solution for a given $\mathbf{q}_\parallel$ and, if the associated dynamical matrix has other symmetry properties, for a given irreducible representation of the symmetry group.

We now define c_n as the number of coordinates in a 3D unit cell of S_n, and $u_n^i(j,l)$, $1 \le j \le c_n$, as the coordinates describing layer l of S_n in the unit cell of slice B_i.

Although c_n and $u_n^i(j,l)$ depend on $\mathbf{q}_\parallel$, we shall omit this dependence in the notation for simplicity.

III. THE PROBLEM

To obtain the dispersion equation, we need to introduce $\mathbf{q}_\perp$. According to Bloch's theorem, the displacement associated with a given frequency ω is looked for in the form

$$u_n^i(j,l,\omega,q_\perp) = u_n^0(j,l,\omega,q_\perp) Z^i , \tag{1}$$

where

$$Z = e^{iq_\perp L} \tag{2}$$

(L is the period along the stacking direction).

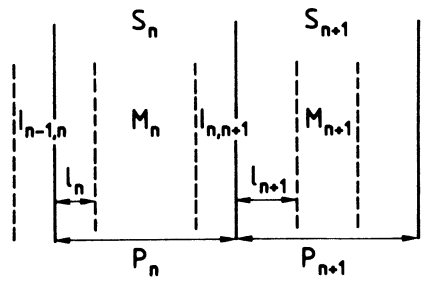

FIG. 1. Schematic representation of the slabs of two adjacent media. The solid lines separate different media, the dashed lines separate the interfaces from the bulk part of the media.

One then just has to satisfy the equations of motion of one unit cell. They constitute a homogeneous linear system in the unknowns $u_1^i(1,1),\ldots,u_1^i(c_1,p_1),\ldots,u_n^i(1,1),\ldots,u_n^i(c_n,p_n)$. Denoting by $\underline{D}$ the associated matrix, the dispersion equation can be written

$$\det(\underline{D})=0 . \tag{3}$$

Solving this equation is cumbersome because of the large size of the matrix $\underline{D}$. The number of unknowns of the preceding system is $\sum_n c_n p_n$, which may equal 100 for large-period superlattices.

In writing Eq. (3), we did not explicitly take advantage of the finite length of the interaction. As a consequence, the nonvanishing matrix elements of $\underline{D}$ are concentrated on both sides of the main diagonal.

This is turned into profit by dividing the equations of motion in two sets, depending upon whether $u_n^i(j,l)$ is relative to an atom of M_n or $I_{n,n+1}$. This is meaningful if M_n is not empty, which supposes $p_n \geq 2l_n$, a hypothesis assumed hereafter. It is easy to deduce from the definitions of Sec. II that $I_{n,n+1}$ involves $c_n l_n + c_{n+1} l_{n+1}$ coordinates, while M_n involves $c_n(p_n - 2l_n)$ coordinates. Hence, we get $\sum_{n=1}^N 2c_n l_n$ interface equations and $\sum_{n=1}^N c_n(p_n - 2l_n)$ "bulk" equations.

The interesting feature of the bulk equations is that the equations of two $u_n^i(j,l)$ and $u_n^i(j,l')$ relative to a given coordinate of two different layers in the same S_n are identical; it is possible to solve these equations before writing down the dispersion equation, whereby the number of coordinates is considerably reduced.

IV. THE DISPERSION EQUATION

As S_n is periodic along the stacking direction, we can apply Bloch's theorem and look for a solution of the equations of motion of M_n in the form

$$u_n^i(j,l)=\sum_k A_n(j,k) z_n(k)^{l-1} R_n^i(k) . \tag{4}$$

The $z_n(k)$'s are the solutions of the secular equation, and the $A_n(j,k)$'s are defined by the condition that the displacement field $A_n(j,k) z_n(k)^{l-1}$ satisfies the bulk equations in S_n. As the slab S_n is of finite thickness, every solution $z_n(k)$ of the secular equation enters the expansion in Eq. (4), whence the number of solutions is exactly $2c_n l_n$.

For a unit cell i, the displacement field of Eq. (4) is thus defined by $\sum_{n=1}^N 2c_n l_n$ coordinates, the $R_n^i(k)$'s. In terms of these new coordinates Eq. (1) reads

$$\sum_k A_n(j,k) z(k)^{l-1}[R_n^i(k) - R_n^0(k) Z^i] = 0 . \tag{5}$$

This equation must hold for any j and l, which implies

$$R_n^i(k) = R_n^0(k) Z^i . \tag{6}$$

The bulk equations being automatically satisfied by the displacement field of Eq. (4), we must only pay attention to the interface equations. Written in terms of the $R_n^i(k)$'s, they yield a problem formally identical to the initial one. Denoting by $\underline{E}$ the associated matrix, we now can write the dispersion equation as

$$\det(\underline{E})=0 . \tag{7}$$

This equation constitutes the main result of this work. Its advantage with respect to (3) lies in the dimension of the matrices: $\underline{D}$ is $\sum_{n=1}^N c_n p_n \times \sum_{n=1}^N c_n p_n$, while $\underline{E}$ is $(\sum_{n=1}^N 2c_n l_n \times \sum_{n=1}^N 2c_n l_n)$. Whereas p_n can take arbitrarily large values depending on the superlattice, l_n depends only on the constitutive materials and can be taken ≤ 2 with a very good accuracy for most metals. The simplification for superlattices with large periods in the stacking direction is thus considerable.

V. PROPERTIES OF THE DISPERSION CURVES WITH RESPECT TO $q_\perp$

The secular equation is an algebraic equation in Z. What is of significance here is its degree, as it determines the maximum number of $q_\perp$'s for a given ω. It can be very easily deduced from a schematic representation of the matrix $\underline{E}$ (Fig. 2). The lines labeled by $2l_n c_n$ represent the interface equations of S_n, while the columns labeled by $2l_n c_n$ represent the coefficients of the coordinates of S_n in the equations of the unit cell i. The dashed blocks are the loci of the only *a priori* nonvanishing coefficients.

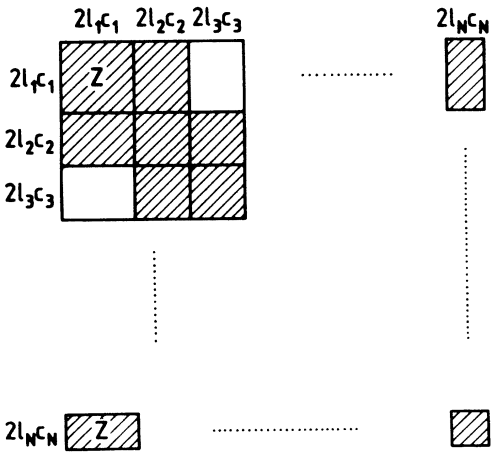

FIG. 2. Schematic representation of the matrix $\underline{E}$ of Eq. (7). The explanations are given in the main text.

The presence of Z in a dashed block means that its coefficients are polynominals of degree 1 in Z. To avoid the appearance of Z^{-1} in the matrix, we have written the equations for the set of interfaces shown in Fig. 3.

From Fig. 2, we see that Z appears only in the $2c_1l_1$ first columns, whereas it appears in $2c_1l_1+2c_nl_n$ lines. A development along the columns thus shows that the determinant of $\underline{E}$ is a polynomial of degree $2l_1c_1$.

The fact that the result depends only on the parameters of S_1 is puzzling, as the choice of the first material in the unit cell 0 is arbitrary. This paradox can be solved in the following manner.

Let us denote by P_n the polynominal of degree $2c_nl_n$ equal to the determinant of the matrix $\underline{E}_n$ obtained by starting the unit cell 0 with the material n.

Multiplying the first $2c_1l_1$ columns of $\underline{E}_1$ by Z^{-1}, then the lines labeled by $2c_2l_2$ by Z, we obtain a matrix that differs from $\underline{E}_2$ only by the order of the columns. Hence, we have

$$P_1=\pm Z^{2l_2c_2-2l_1c_1}P_2 \tag{8}$$

from which we deduce

$$Z^{2l_nc_n}P_n=\pm Z^{2l_mc_m}P_m \tag{9}$$

whatever n and m.

Hence, putting $r=\min_n(2c_nl_n)$, the secular equation relative to $\underline{E}_n$ contains the nonsignificant factor $Z^{2c_nl_n-r}$ whenever $r<2c_nl_n$, and the effective degree of the secular equation is $r=\min_n(2c_nl_n)$.

In a plot of ω as a function of $q_\perp$ for $0\le q_\perp\le\pi/L$, the preceding result means that for a given ω we shall find at most $r/2=\min_n(c_nl_n)q_\perp$'s satisfying Eq. (7).

The other interesting property is the number of branches of the spectrum, i.e., the number of ω's for a given $q_\perp$. As $\underline{D}$ is hermitic, it is equal to the degree in ω^2 of the secular equation, which is easily inferred from Eq. (3) to be $\sum_{n=1}^{N}c_np_n$.

VI. APPLICATION: THE LINEAR SUPERLATTICE

We apply the previous theory to the case of a linear chain with two kinds of atoms coupled by nearest-neighbor interaction. The unit cell is made of p_1 successive atoms of mass m_1 followed by p_2 atoms of mass m_2. The dynamics of the system is defined by three force constants: k_1 (k_2) between two atoms of mass m_1 (m_2), k between an atom of mass m_1 and an atom of mass m_2. The total length of the unit cell is denoted by L (see Fig. 4).

To make the link with the notation of Sec. II, we note that $l_1=l_2=1$ (nearest-neighbor interactions), $c_1=c_2=1$ (one atom per unit cell for each medium), and $I_{1,2}$ and $I_{2,1}$ contains one atom of each type.

As $c_1=c_2=1$, we can drop the index j from the notation $u_n^i(j,l)$; the displacements in the cell i thus are $u_1^i(1),\ldots,u_1^i(p_1)$, $u_2^i(1),\ldots,u_2^i(p_2)$. $\mathbf{q}_\parallel$ is of course irrelevant.

According to Sec. IV, insofar as $p_1,p_2\ge 2$, the $u_1^i(l)$, $1\le l\le p_1$, can be replaced by $2l_1c_1=2$ coordinates. The secular equation of medium 1 is easily derived:

$$m_1\omega^2=k_1(2-z-z^{-1})\ . \tag{10}$$

If z is a solution, z^{-1} is also a solution. We denote the two solutions by z_1 and z_1^{-1}. Then, we can write for $1\le l\le p_1$

$$u_1^i(l)=R_1^i(z_1)z_1^{l-1}+R_1^i(z_1^{-1})z_1^{-l+1}\ , \tag{11}$$

which defines the two coordinates of medium 1.

The situation is similar for medium 2. The secular equation reads

$$m_2\omega^2=k_2(2-z-z^{-1}) \tag{12}$$

and we write for $1\le l\le p_2$

$$u_2^i(l)=R_2^i(z_2)z_2^{l-1}+R_2^i(z_2^{-1})z_2^{-l+1}\ . \tag{13}$$

The interface equations involve $2l_1c_1+2l_2c_2=4$ coordinates. Written in terms of $u_1^i(p_1)$, $u_1^i(1)$, $u_2^i(p_2)$, and $u_1^{i+1}(1)$, they read

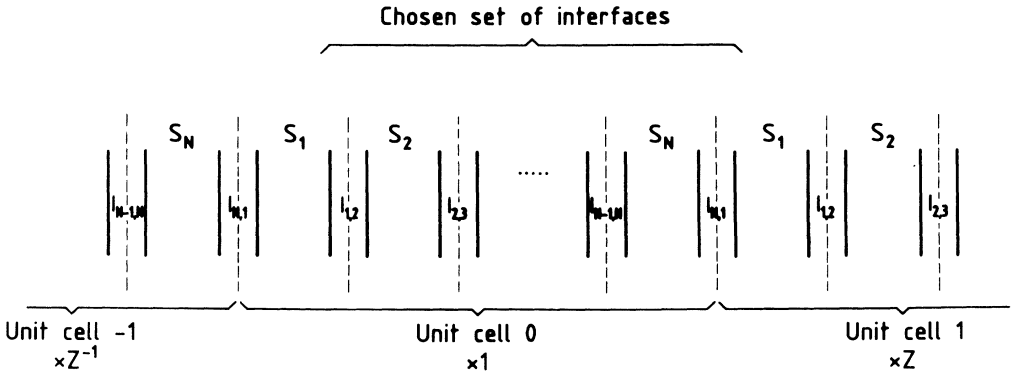

FIG. 3. Schematic representation of a unit cell with parts of the neighboring cells. The multiplying factor depicted below the number of the cell is that of Eq. (6). The chosen set of interfaces corresponds to the matrix of Fig. 2.

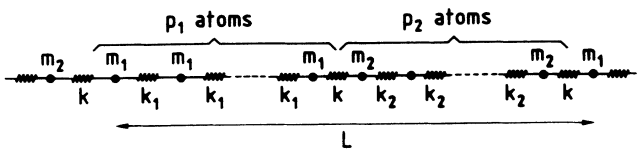

FIG. 4. Illustration of the notations used for the linear superlattice.

$$m_2\omega^2 u_2^i(p_2)=k_2[u_2^i(p_2)-u_2^i(p_2-1)] +k[u_2^i(p_2)-u_1^{i+1}(1)] , \tag{14a}$$

$$m_1\omega^2 u_1^{i+1}(1)=k[u_2^{i+1}(1)-u_2^i(p_2)] +k_1[u_1^{i+1}(1)-u_1^{i+1}(2)] , \tag{14b}$$

$$m_1\omega^2 u_1^i(p_1)=k_1[u_1^i(p_1)-u_1^i(p_1-1)] +k[u_1^i(p_1)-u_2^i(1)] , \tag{14c}$$

$$m_2\omega^2 u_2^i(1)=k[u_2^i(1)-u_1^i(p_1)] +k_2[u_2^i(1)-u_2^i(2)] . \tag{14d}$$

The next step consists of writing this system in terms of the coordinates defined by Eqs. (11) and (13). Remembering that $R_n^{i+1}(z_k)=R_n^i(z_k)Z$ (where $Z=e^{iq_\perp L}$), we get a closed system. The vanishing of its determinant provides the dispersion equation.

In accordance with the general formula derived in Sec. V, this equation is of degree 2 in Z. To solve it explicitly, it is convenient to deal with a real matrix, which is achieved by expressing the previous system in terms of α_j and γ_j given by

$$\alpha_j=R_j(z_j)+R_j(z_j^{-1}) , \qquad \gamma_j=\epsilon_j[R_j(z_j)-R_j(z_j^{-1})] , \tag{15}$$

where

$$\epsilon_j=\begin{cases}1 & \text{if } \mathrm{Im}(z_j)=0\\ i & \text{if } \mathrm{Im}(z_j)\neq 0 .\end{cases} \tag{16}$$

Introducing

$$C_j(l)=\frac{z_j^{l-1}+z_j^{-l+1}}{2}, \quad S_j(l)=\frac{z_j^{l-1}-z_j^{-l+1}}{2\epsilon_j} ,$$

the (4×4) real matrix $\underline{F}$ defined by

$$\begin{aligned}
F_{11}&=k ,\\
F_{12}&=0 ,\\
F_{13}&=(m_2\omega^2-k_2-k)C_2(p_2)+k_2C_2(p_2-1) ,\\
F_{14}&=(m_2\omega^2-k_2-k)S_2(p_2)+k_2S_2(p_2-1) ,\\
F_{21}&=m_1\omega^2-k_1-k+k_1C_1(2) ,\\
F_{22}&=k_1S_1(2) ,\\
F_{23}&=kC_2(p_2) ,\\
F_{24}&=kS_2(p_2) ,
\end{aligned} \tag{17}$$

$$\begin{aligned}
F_{31}&=(m_1\omega^2-k_1-k)C_1(p_1)+k_1C_1(p_1-1) ,\\
F_{32}&=(m_1\omega^2-k_1-k)S_1(p_1)+k_1S_1(p_1-1) ,\\
F_{33}&=k ,\\
F_{34}&=0 ,\\
F_{41}&=kC_1(p_1) ,\\
F_{42}&=kS_1(p_1) ,\\
F_{43}&=m_2\omega^2-k-k_2+k_2C_2(2) ,\\
F_{44}&=k_2S_2(2) ,
\end{aligned}$$

and the (4×4) matrix $\underline{G}$ defined by

$$G_{ij}=ZF_{ij}, \quad i \text{ and } j\leq 2 \tag{18a}$$

$$G_{ij}=F_{ij}, \quad i \text{ or } j\geq 3 \tag{18b}$$

where $Z=e^{iq_\perp L}$, the interface equations read

$$\underline{G}\begin{bmatrix}\alpha_1\\ \gamma_1\\ \alpha_2\\ \gamma_2\end{bmatrix}=0 , \tag{19}$$

and the dispersion equation $\det(\underline{G})=0$ is written

$$AZ^2+BZ+C=0 , \tag{20}$$

where A, B, C are functions of ω given by

$$A=-F_{11}F_{22}F_{33}F_{44} , \tag{21a}$$

$$\begin{aligned}B=&(F_{32}F_{43}-F_{42}F_{33})(F_{14}F_{21}-F_{24}F_{11})\\ &-F_{14}F_{22}(F_{31}F_{43}-F_{41}F_{33})\\ &+F_{44}F_{11}F_{32}F_{23}-F_{44}F_{13}(F_{21}F_{32}-F_{31}F_{22}) ,\end{aligned} \tag{21b}$$

$$C=(F_{14}F_{23}-F_{24}F_{13})(F_{31}F_{42}-F_{41}F_{32}) . \tag{21c}$$

It is readily verified that $A=C$, which ensures that if Z is a solution, Z^{-1} is also a solution.

Finally, the equation of the dispersion curves for $q_\perp\geq 0$ is

$$\text{if } B^2-4A^2\geq 0, \quad \text{no } q_\perp$$

$$\text{if } B^2-4A^2\leq 0, \quad q_\perp=\frac{1}{L}\cos^{-1}(-B/2A) . \tag{22}$$

We now briefly discuss the nature of the dispersion curves. Two limiting cases are particularly important. On one hand, if $k_1=k_2=k$ and $m_1=m_2$, the superlattice is in fact a monoatomic linear chain. Denoting by a its lattice parameter, the dispersion curve is given by

$$\omega=2\left[\frac{k_1}{m_1}\right]^{1/2}\sin(qa/2) \tag{23}$$

for $0\leq q\leq \pi/a$.

With the notation of the superlattice, $L=(p_1+p_2)a$ and q is restricted to $0\leq q\leq \pi/L$. The p_1+p_2 dispersion

curves are obtained from the curve of Eq. (23) by a mere folding procedure.

On the other hand, if $k=0$, the superlattice is a collection of independent finite linear chains of two types. The system is dispersionless, and its frequencies are those of the two finite linear chains with free ends. They are given by

$$\omega_l^1=2\left[\frac{k_1}{m_1}\right]^{1/2}\sin(l\pi/2p_1),\quad l=0,1,\ldots,p_1-1 \tag{24a}$$

for the atoms 1 and

$$\omega_l^2=2\left[\frac{k_2}{m_2}\right]^{1/2}\sin(l\pi/2p_2),\quad l=0,1,\ldots,p_2-1 \tag{24b}$$

for the atoms 2 (see the Appendix). The frequency $\omega=0$ is doubly degenerated; this corresponds to the translational motion of each chain. Hence, the dispersion curves of the general superlattice can be interpreted in the following two ways.

The perturbation due to $k_1\neq k_2\neq k$ and $m_1\neq m_2$ opens gaps at the zone boundaries in the dispersion curves obtained by folding the dispersion curve of the monoatomic linear chain.[12]

The nonvanishing value of k introduces a dispersion in the dispersionless spectrum of the two independent finite linear chains.

We exemplify those remarks with the help of Eq. (22) by plotting two series of dispersion curves relative to superlattices with $p_1=p_2=5$.

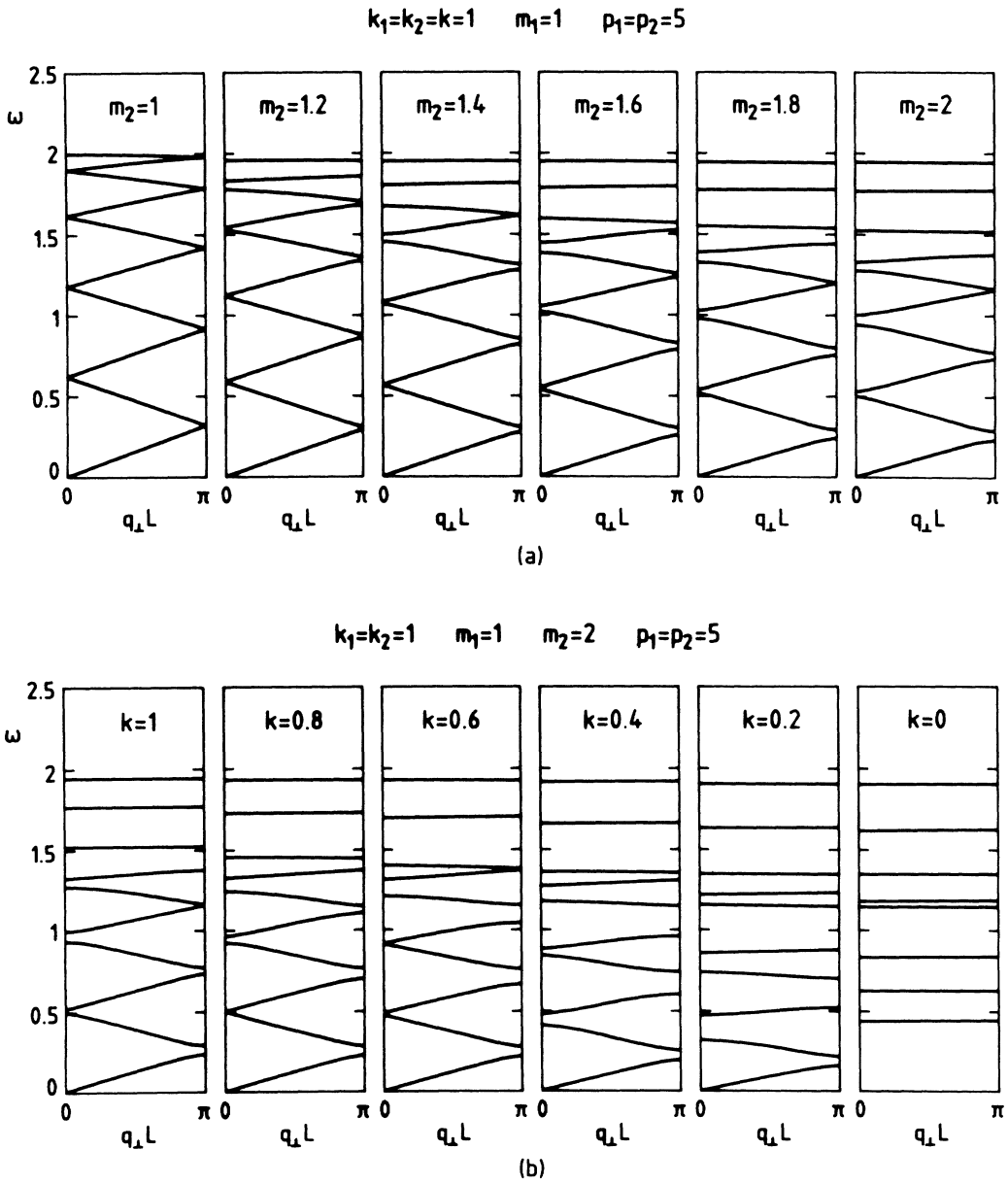

FIG. 5. Plots of dispersion curves for the linear superlattice for (a) various values of m_2, and (b) various values of k. All other parameters keep the value indicated above the figures.

In Fig. 5(a), we start from a monoatomic chain ($k_1=k_2=k=1$, $m_1=m_2=1$) and we increase m_2 while keeping all other parameters constant. This opens nine gaps between the ten dispersion curves, as previously argued.

In Fig. 5(b), we start from the last curve of Fig. 5(a) ($k_1=k_2=k=1$, $m_1=1$, $m_2=2$), and we decrease k from 1 to 0 (all the other parameters remaining constant). Two features appear clearly. Firstly, the gaps increase, or equivalently the dispersion decreases in each band, until $k=0$ where the curves are dispersionless. Secondly, the two lowest curves decrease constantly and both finally give $\omega=0$, the translational motions of the constitutive chains.

Let us emphasize the fact that Eq. (22) gives *explicitly* the equation of the dispersion curves. We chose relatively small values of p_1 and p_2 ($p_1=p_2=5$) for the clarity of the figures, but the treatment is exactly as simple for any p_1 and p_2. This is of course not the case if one deals with Eq. (4), as the coefficients A, B, and C of Eq. (20) would require the development of a $(p_1+p_2)\times(p_1+p_2)$ determinant, a task already hopeless for $p_1=p_2=5$.

Finally, a simple formula for the second velocity can be obtained:

$$\omega=\frac{L}{\left[(p_1m_1+p_2m_2)\dfrac{p_1-1}{k_1}+\dfrac{p_2-1}{k_2}+\dfrac{2}{k}\right]^{1/2}}q_\perp . \quad (25)$$

The derivation will be given elsewhere[13] in a more general context.

VII. CONCLUSION

The calculation of phonon dispersion curves for the most general superlattice by the matching procedure comprises two main steps: (i) to solve the bulk secular equation for each constitutive medium, which produces a new set of coordinates, and (ii) to write the interface equations in terms of these new coordinates.

The degree of the determinantal secular equation of the dispersion curves depends only on the number of atoms per unit cell and on the interaction range in the constitutive media. This degree is equal to the maximum number of wave vectors associated with a given frequency which is thus shown to be independent of the thickness of the layers.

For the linear superlattice with two kinds of atoms and nearest-neighbor interaction, the dispersion equation can be solved analytically. This result is used to illustrate the two possible interpretations of the dispersion curves of a superlattice.

APPENDIX

This result was previously proved through the use of a Green's function analysis.[14] We derive it here by using the matching procedure.

The equations of a monoatomic linear chain (mass m, force constant k, p atoms) with free ends read

$$(m\omega^2-k)u_1+ku_2=0 , \quad (A1)$$

$$(m\omega^2-2k)u_l+ku_{l-1}+ku_{l+1}=0, \quad 2\le l\le p-1 \quad (A2)$$

$$(m\omega^2-k)u_p+ku_{p-1}=0 . \quad (A3)$$

Equations (A2) are satisfied if we look for a solution of the form

$$u_l=\alpha z^{l-1}+\beta z^{-l+1} , \quad (A4)$$

where z is solution of the secular equation

$$m\omega^2=k(2-z-z^{-1}) . \quad (A5)$$

With the help of (A4) and (A5), we can rewrite (A1) and (A3) as

$$(1-z^{-1})\alpha+(1-z)\beta=0 , \quad (A6)$$

$$(z^{p-1}-z^p)\alpha+(z^{-p+1}-z^{-p-1})\beta=0 . \quad (A7)$$

A necessary condition for (α,β) to be nonvanishing is that the determinant vanishes, which leads to

$$z^{2p}=1 . \quad (A8)$$

The solutions are $z=e^{\pm il\pi/p}$, $0\le l\le p$. $z=-1$ gives $\alpha=-\beta$ and must be rejected as the displacement field of (A4) vanishes.

Putting the remaining solutions in (A5), we find p frequencies ($e^{+il\pi/p}$ and $e^{-il\pi/p}$ give the same frequency)

$$\omega_l=2\left[\frac{k}{m}\right]^{1/2}\sin(l\pi/2p) , \quad (A9)$$

where $l=0,1,\ldots,p-1$.

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