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DISCRETE FREQUENCIES IN A LATTICE PERTURBED BY ISOTOPE DEFECTS

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ABSTRACT. An investigation is made of the process of generation of discrete vibration frequencies outside the allowed frequency bands of a lattice when it is perturbed by the change of the mass of an atom. A criterion for monatomic lattices is described which enables one to predict whether in the perturbed state of the lattice, the discrete frequency generated from any branch is independent of the other branches. Finally, the discrete frequencies in the case of several linear lattice models are evaluated

INTRODUCTION

The problem of generation of discrete vibrational frequencies due to isotope defects in a lattice has been studied by Lifshitz (1943a, 1943b, 1944, 1956), and by Montroll and Potts (1955, 1956). The general techniques developed by them have been applied mostly to a lattice model in which there is no coupling between the various components of the displacements of the atoms. Recently, Nardelli (1960) has studied the problem in the case of cubic lattices. The object of this paper is to discuss a few lattice models in which there is coupling between the displacements; but still it is possible to evaluate the discrete frequencies due to an isotope defect exactly.

THE SECULAR EQUATION FOR THE DISCRETE FREQUENCY

We will adopt here the notation of Lifshitz (1943a) with slight changes. The lattice under consideration has N unit cells in each of which there are p atoms, the mass of the s-th atom being m_s. The coordinate of the unit cell is given by the vector q, whose dimension equals the dimension of the lattice. Periodic boundary conditions will be used throughout.

The eigenfrequencies of the unperturbed lattice are the roots of the equation

$$|\hat{A}-\hat{I}\omega^2| = 0 \qquad \dots \quad (1)$$

where the dynamical matrix $\hat{A}$ is determined from the equations of motion of the atoms in the lattice. Each element of $\hat{A}$ has six indices, three for the row and three for the column. The following equation gives the correspondence between this notation and that of Born and Huang (1954);

$$A_{q-q'}(s,j\,|\,s',j') = \frac{1}{\sqrt{m_s m_{s'}}}\;\phi_{jj'}\begin{pmatrix} q-q' \\ s \quad s' \end{pmatrix} \qquad \ldots \quad (2)$$

The index j refers to the component of the displacement of the atoms.

In the presence of an isotope defect of mass m_s' at the s-th position in the q-th unit cell, the eigenfrequencies are the roots of the equation

$$|\hat{I}+\hat{G}(\omega)\hat{\Lambda}\,| = 0 \qquad \ldots \quad (3)$$

where $\hat{G}(\omega) = (\hat{A}-\hat{I}\omega^2)^{-1}$ and $\hat{\Lambda}$ is the perturbation matrix. In this case $\hat{\Lambda}$ is a diagonal matrix whose elements are given by

$$\Lambda_{q'-q''}(s',j'\,|\,s'',j'') = \epsilon_s\omega^2\delta_{j'j''}\delta_{s's}\delta_{q'q}\,\delta_{q''q}\,\delta_{s''s} \qquad \ldots \quad (4)$$

where $$\epsilon_q = 1-\frac{m'_s}{m_s}\,.$$

In a three dimensional lattice, for example, there will be only three nonvanishing elements in $\hat{\Lambda}$, and they will be the diagonal elements characterised by the indices q, s, and the three values of j

The determinant in equation (3) can be reduced to the form

$$\begin{vmatrix} 1+\epsilon_s\omega^2G_0(s,1\,|\,s,1) & \epsilon_s\omega^2G_0(s,1\,|\,s,2) & \epsilon_s\omega^2G_0(s,1\,|\,s,3) \\ \epsilon_s\omega^2G_0(s,2\,|\,s,1) & 1+\epsilon_s\omega^2G_0(s,2\,|\,s,2) & \epsilon_s\omega^2G_0(s,2\,|\,s,3) \\ \epsilon_s\omega^2G_0(s,3\,|\,s,1) & \epsilon_s\omega^2G_0(s,3\,|\,s,2) & 1+\epsilon_s\omega^2G_0(s,3\,|\,s,3) \end{vmatrix} = 0 \qquad \ldots \quad (5)$$

The evaluation of the elements of $\hat{G}$ matrix which occur in equation (5) can be done by the bilinear formula for the matrix elements of a function of an operator. The eigenvectors of $\hat{A}$ span a space of $3pN$ dimensions, and constitute an orthogonal set. (The degenerate eigenvectors can be orthogonalised in the usual way). For convenience we will use the symbol $|k, r>$ for a typical normalised eigenvector of $\hat{A}$, where k can take up N values inside the unit cell of the reciprocal lattice, of volume $(2\pi)^3/N$, and r can take up $3p$ values.

Each eigenvector of $\hat{A}$ has $3pN$ components. We will denote a typical component by the symbol $|k, r; q, s, j>$. These components are known to be of the form (Lifshitz, 1943a)

$$|k, r; q, s, j> = \frac{1}{\sqrt{N}}\,Q_r^{s,j}(k)\exp\left(\frac{2\pi i}{N}\,k.q\right) \qquad \ldots \quad (6)$$

where $Q_r^{s,j}(k)$ is the (s, j)-th component of the r-th eigenvector of a $3p \times 3p$ Hermitean matrix $\hat{a}_k$ which is related to $\hat{A}$ by the equation

$$a_k(s, j \mid s', j') = \sum_q A_q(s, j \mid s', j') \exp\left(\frac{2\pi i}{N} k.q\right) \quad \ldots \quad (7)$$

The eigenvalues of $\hat{a}_k$ are the $3p$ branch (squared) frequencies $\omega_r(k)$ for a given value of k. The branch index r can take up $3p$ values. In each branch there are N frequencies corresponding to the N values of k.

By the bilinear formula, the matrix element of $\hat{G}$ is

$$G_{q-q'}(s, j \mid s', j') = \sum_{k,r} \frac{\langle k, r, q', s', j' \mid k, r; q, s, j \rangle}{\omega_r^2(k) - \omega^2}$$

$$= \frac{1}{(2\pi)^3} \sum_r \int_{V^*} \frac{d^3k Q_r^{s,j}(k) Q^{*}{}_r^{s',j'}(k) \exp\left[2\pi i\, k.(q-q')\right]}{\omega_r^2(k) - \omega^2} \quad \ldots \quad (8)$$

In this, the summation over k has been replaced by an integration. V^* is the volume of the unit cell of the reciprocal lattice*.

In particular, the elements of $\hat{G}$ that occur in equation (5)are given by

$$G_0(s, j \mid s', j') = \frac{1}{(2\pi)^3} \sum_r \int_{V^*} \frac{d^3k\, Q_r^{s,j}(k) Q^{*}{}_r^{s',j'}(k)}{\omega_r^2(k) - \omega^2} \quad \ldots \quad (9)$$

Actual computation of the discrete frequencies has been done in those lattice models in which there is no coupling between the various components of the displacements of the atoms, since the evaluation of the matrix elements of $\hat{G}$ is easy for such models. We will now prove a theorem that if a certain criterion is satisfied in a lattice model, an isotope defect perturbs each frequency branch separately, and evaluation of the matrix elements of $\hat{G}$ is somewhat simpler even in the presence of coupling between the displacement components.

Only monatomic lattices can satisfy this criterion. We will evaluate the discrete frequencies in certain linear lattice models satisfying this criterion, and it will be shown that when this criterion is satisfied, the range of interaction between

In this equation the vector k is normalised in such a way that the volume V equals $(2\pi)^3$.

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the atoms is of no consequence, as far as the solvability of the problem is concerned.

THE CRITERION FOR THE UNMIXING OF THE PERTURBATION IN DIFFERENT BRANCHES

Let us consider a monatomic lattice model ($p = 1$), in which each atom has three degrees of freedom, and in which the elements of $\hat{A}$ satisfy the equation

$$A_{q'-q''}(j' \mid j'') = C_{q'-q''}\alpha(j' \mid j'') \qquad \dots \quad (10)$$

where $\alpha(j' j'')$ is a number independent of q.

The dynamical matrices corresponding to the various branches are obtained by a similarity transformation

$$\hat{P}\ \hat{A}\ \hat{P}^{-1} = \hat{B} \qquad \dots \quad (11)$$

where $\hat{B}$ is a matrix of the form

$$B = \begin{bmatrix} \hat{X} & \hat{0} & \hat{0} \\ \hat{0} & \hat{Y} & \hat{0} \\ \hat{0} & \hat{0} & \hat{Z} \end{bmatrix} \qquad (12)$$

Here $\hat{X}$, $\hat{Y}$, and $\hat{Z}$ are $N \times N$ submatrices.

In this model it is easily shown that the elements of $\hat{P}$ are

$$P_{q'-q''}(j' \mid j'') = \delta_{q'q''}\ \beta(j' \mid j'') \qquad \dots \quad (13)$$

and

$$\begin{aligned} \hat{X} &= x\hat{C} \\ \hat{Y} &= y\hat{C} \\ \hat{Z} &= z\hat{C} \end{aligned} \qquad \dots \quad (14)$$

where x, y, and z are pure numbers and $\hat{C}$ is a $N \times N$ cyclic matrix. x, y and z are, in fact, the eigenvalues of the 3×3 matrix $\hat{\alpha}$ whose elements are $\alpha(j' \mid j'')$. Using equation (11) it can be shown that the 3×3 matrix $\hat{\beta}$ whose elements are $\beta(j' \mid j'')$ diagonalises $\hat{\alpha}$ by the similarity transformation

$$\hat{\beta}\ \hat{\alpha}\ \hat{\beta}^{-1} = \begin{bmatrix} x & o & o \\ o & y & o \\ o & o & z \end{bmatrix} \qquad \dots \quad (15)$$

The wellknown symmetry properties of $\hat{A}$ require that $\hat{\alpha}$ must be a symmetric matrix, so that $\hat{\beta}$ must be an orthogonal matrix satisfying the condition.

$$\sum_{j} \beta(j\,|\,j')\ \beta(j\,|\,j'') = \delta_{j',j''} \qquad \dots \quad (16)$$

The matrix $\hat{\Lambda}$ for isotope defects can be written in the form

$$\hat{\Lambda} = \begin{bmatrix} \hat{S} & \hat{O} & \hat{O} \\ \hat{O} & \hat{S} & \hat{O} \\ \hat{O} & \hat{O} & \hat{S} \end{bmatrix} \qquad \dots \quad (17)$$

where $\hat{S}$ is a $N \times N$ diagonal submatrix. Using equation (16) and the fact that $\hat{S}$ commutes with each of the submatrices of $\hat{P}$ (which are diagonal), it is easily shown that for this model

$$\hat{P}\ \hat{\Lambda}\ \hat{P}^{-1} = \hat{\Lambda} \qquad \dots \quad (18)$$

Therefore, if we perform a similarity transformation with respect to $\hat{P}$ on equation (3), we obtain

$$|\hat{I}+\hat{G}(x)\hat{S}|\ |\hat{I}+\hat{G}(y)\hat{S}|\ |\hat{I}+\hat{G}(z)\hat{S}| = 0 \qquad \dots \quad (19)$$

where all matrices are now $N \times N$, and

$$\begin{aligned} \hat{G}(x) &= [x\hat{C}-\hat{I}\omega^2]^{-1} \\ \hat{G}(y) &= [y\hat{C}-I\omega^2]^{-1} \\ \hat{G}(z) &= [z\hat{C}-\hat{I}\omega^2)^{-1} \end{aligned} \qquad \dots \quad (20)$$

From equation (19) it is apparent that in a monatomic lattice satisfying the criterion of equation (10), the effect of isotope defects on each frequency branch is independent of the other branches.

With a single isotope defect, equation (19) reduces to the three equations

$$1+\frac{\epsilon\omega^2}{(2\pi)^3}\int_{V*} \frac{d^3k}{\omega^2{}_x(k)-\omega^2} = 0 \qquad \dots \quad (21a)$$

$$1+\frac{\epsilon\omega^2}{(2\pi)^3}\int_{V*} \frac{d^3k}{\omega^2{}_y(k)-\omega^2} = 0 \qquad \dots \quad (21b)$$

$$1+\frac{\epsilon\omega^2}{(2\pi)^3}\int_{V*} \frac{d^3k}{\omega^2{}_z(k)-\omega^2} = 0 \qquad \dots \quad (21c)$$

An example

As a simple example of a physical lattice model satisfying the criterion of equation (10), we consider the case of a linear chain with nearest neighbour interactions and three degrees of freedom per atom. If $u_n \exp(i\omega t)$, $v_n \exp(i\omega t)$, and $w_n \exp(i\omega t)$ denote the two transverse and one longitudinal components respectively of the n-th atom from equilibrium, the equations of motion can be written in the form

$$
\begin{aligned}
m\omega^2 u_n &= \gamma_1(2u_n - u_{n-1} - u_{n+1}) + \gamma_2(2v_n - v_{n-1} - v_{n+1}) + \gamma_3(2w_n - w_{n-1} - w_{n+1});\\
m\omega^2 v_n &= \gamma_2(2u_n - u_{n-1} - u_{n+1}) + \gamma_1(2v_n - v_{n-1} - v_{n+1}) + \gamma_3(2w_n - w_{n-1} - w_{n+1}),\\
m\omega^2 w_n &= \gamma_3(2u_n - u_{n-1} - u_{n+1}) + \gamma_3(2v_n - v_{n-1} - v_{n+1}) + \gamma_4(2w_n - w_{n-1} - w_{n+1});
\end{aligned}
\qquad \ldots (22)
$$

Here γ_2 is the coupling between u and v components, and γ_3 is the coupling between u and w or between v and w components respectively.

The matrix $\hat{\alpha}$ in this case is of the form

$$
\hat{\alpha} = \begin{bmatrix}
\frac{\gamma_1}{m} & \frac{\gamma_2}{m} & \frac{\gamma_3}{m}\\[2ex]
\frac{\gamma_2}{m} & \frac{\gamma_1}{m} & \frac{\gamma_3}{m}\\[2ex]
\frac{\gamma_3}{m} & \frac{\gamma_3}{m} & \frac{\gamma_4}{m}
\end{bmatrix} \qquad \ldots (23)
$$

and the $N \times N$ matrix $\hat{C}$ is of the form

$$
\hat{C} = \begin{bmatrix}
2 & -1 & 0 & 0 & \ldots & \ldots & 0 & -1\\
-1 & 2 & -1 & 0 & \ldots & \ldots & 0 & 0\\
0 & -1 & 2 & -1 & \ldots & \ldots & 0 & 0\\
\vdots & \vdots & \vdots & \vdots & & & \vdots & \vdots\\
-1 & 0 & 0 & 0 & & & -1 & 2
\end{bmatrix} \qquad \ldots (25)
$$

The three eigenvalues of $\hat{\alpha}$, which we denote as before by x, y, and z, are easily obtained and are given by the equations

$$x = \frac{1}{m}(\gamma_1 - \gamma_2)$$

$$y = \frac{1}{2m}\left[(\gamma_1+\gamma_2+\gamma_4)+\sqrt{(\gamma_1+\gamma_2-\gamma_4)^2+8\gamma_3^2}\right]$$

$$z = \frac{1}{2m}\left[(\gamma_1+\gamma_2+\gamma_4)-\sqrt{(\gamma_1+\gamma_2-\gamma_4)^2+8\gamma_3^2}\right] \qquad \ldots \quad (25)$$

The eigenfrequencies in the various branches as functions of k(which is a one dimensional vector in this case) is obtained by taking the Fourier transform of $\hat{B}$ in accordance with the formula of equation (7);

$$\begin{aligned} \omega^2_x(k) &= 2x(1-\cos k) \\ \omega^2_y(k) &= 2y(1-\cos k) \\ \omega^2_z(k) &= 2z(1-\cos k) \end{aligned} \qquad \ldots \quad (26)$$

We will discuss the equation for the discrete frequency generated from one of the branches only. Equation (21a) can be written in the following form by substituting for the denominator of the integrand from equation (26);

$$1+\frac{\epsilon\omega^2}{2\pi}\int^{2\pi}\frac{dk}{2x(1-\cos k)-\omega^2} = 0 \qquad \ldots \quad (27)$$

For discrete frequencies we are interested in the region $\omega^2 > \omega^2_{xL}$, where $\omega^2_{xL} = 4x$, the maximum frequency of that branch. In this region equation (27) reduces to the form

$$1-\frac{\epsilon\omega}{\sqrt{\omega^2-\omega^2_{xL}}} = 0 \qquad \ldots \quad (28)$$

A solution of this equation for $\omega > \omega_{xL}$ can exist only for positive ϵ, i.e., for a lighter isotope defect, and this solution is

$$\omega_{x0} = \frac{\omega_{xL}}{\sqrt{1-\epsilon^2}} \qquad \ldots \quad (29)$$

The treatment of the other two secular equations proceeds along identical lines.

Thus, in this example, a single lighter isotope defect generates three discrete frequencies, one from each of the acoustic branches. However, for small ϵ the physical observable discrete frequency is the one, which is above the maximum frequency of the stiffest branch, since the other two discrete frequencies will lie submerged among the quasicontinuum of frequencies of the stiffest branch.

A LINEAR LATTICE WITH LONG RANGE INTERACTIONS

In a linear lattice with long range interactions, the equations of motion can be written in the form (with infinite number of atoms)

$$\begin{aligned} m\omega^2 u_n = \sum_p \big[\Gamma_p^{(u,u)}(2u_n-u_{n-p}-u_{n+p})&+\Gamma_p^{(u,v)}(2v_n-v_{n-p}-v_{n+p}) \\ &+\Gamma_p^{(u,w)}(2w_n-w_{n-p}-w_{n+p})\big]\,; \end{aligned} \qquad \ldots \quad (30)$$

with two similar equations for the other two components. Here $\Gamma_p^{(u,v)}$ is the coupling constant between the u-displacement of an atom and the v-displacement of its p-th neighbour.

A physically reasonable assumption to make on the properties of the coupling constants is that they all depend on the distance of separation of the interacting atoms in accordance with the same law. In that case, one can write

$$\Gamma_p^{(u,v)} = \gamma^{(u,v)} f(p) \qquad \ldots \quad (31)$$

where the function $f(p)$ suitably describes the dependence of the coupling constants on the distance of separation of the atoms.

This model satisfies the criterion of equation (10). The matrix $\hat{\alpha}$ will have the same form as in equation (23), if we use the followsing equivalences ,

$$\gamma^{(u,u)} = \gamma^{(v,v)} = \gamma_1, \qquad \gamma^{(u,v)} = \gamma^{(v,u)} = \gamma_2;$$
$$\gamma^{(u,w)} = \gamma^{(w,u)} = \gamma^{(v,w)} = \gamma^{(w,v)} = \gamma_3; \quad \gamma^{(w,w)} = \gamma_4.$$

The matrix $\hat{C}$ is now of the form

$$\hat{C} = \begin{vmatrix} 2\sum\limits_p f(p) & -f(1) & -f(2) & \ldots\ldots \\ -f(1) & 2\sum\limits_p f(p) & -f(1) & \ldots \\ -f(2) & -f(1) & 2\sum\limits_p f(p) & \ldots\ldots \\ -f(3) & -f(2) & -f(1) & \ldots\ldots \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \end{vmatrix} \qquad \ldots \quad (32)$$

The eigenfrequencies of the various branches are

$$\omega_x^2(k) = 2x \left[\sum_{p=1}^{\infty} f(p) - \sum_{p=1}^{\infty} f(p) \cos pk \right] \qquad \ldots \quad (33)$$

with two similar equations for the other two branches. The maximum frequency of the branch is evidently $4x \left[\sum\limits_{p=0}^{\infty} f(2p+1) \right]$. As before, we will evaluate the discrete frequency generated from one of the branches only. The secular equation is

$$1 + \frac{\epsilon\omega^2}{2\pi} \int_0^{\infty} \frac{dk}{2x \left[\sum\limits_p \{f(p) - f(p) \cos pk\} \right] - \omega^2} = 0 \qquad \ldots \quad (34)$$

The integral in equation (34) can be done exactly for several assumed forms of $f(p)$. We give below the results for the discrete frequency arising outside the band in a few cases.

(i) $$f(p) = \exp(-p\sigma).$$

The integral in equation (34) can be done exactly for $\omega^2 > \omega_{xL}{}^2$, and in terms of a variable $\theta = \cosh^{-1}\omega/\omega_{xL}$, the discrete frequency is the root of the equation

$$\coth\left(\theta + \frac{\sigma}{2}\right) = \frac{1}{\epsilon}\tanh\theta \qquad \dots \quad (35)$$

It is easy to show graphically and otherwise that for values of ϵ in the range $0 < \epsilon < 1$ a solution of this transcendental equation must exist, and hence a discrete frequency must arise. For very small values of ϵ, the discrete frequency is

$$\omega_{xO} \simeq \omega_{xL}\left(1 + \frac{\epsilon^2}{2}\coth^2\frac{\sigma}{2}\right) \qquad \dots \quad (36)$$

(ii) $$f(p) = (p)^{-2r}; \; r = \text{Integer}.$$

The series occurring in the denominator of the integrand in equation (34) can be summed exactly in accordance with the formulae (Jeffreys and Jeffreys, 1956),

$$\sum_{p=1}^{\infty} (p)^{-2r}\cos pk = \frac{(-1)^{r-1}}{2}(4\pi^2)^r\left[P_{2r}\left(\frac{k}{2\pi}\right) + b_{2r}\right]$$

and $$\sum_{p=1} (p)^{-2r} = \zeta(2r)$$

where P_{2r} and b_{2r} are respectively the Bernoulli polynomial and the Bernoulli number of order $2r$ respectively, and $\zeta(2r)$ is the Riemann Zeta function. $\zeta(2r)$ is related to b_{2r} through the equation

$$\zeta(2r) = \frac{(-1)^{r-1}}{2}(4\pi^2)^r\, b_{2r}$$

The first few Bernoulli polynomials are

$$P_2(x) = \tfrac{1}{2}(x^2 - x); \quad P_4(x) = \frac{1}{24}(x^4 - 2x^3 + x^2);$$

$$P_6(x) = \frac{1}{720}\left(x^6 - 3x^5 + \frac{5}{2}x^4 - \frac{1}{2}x^2\right);$$

$$P_8(x) = \frac{1}{40320}\left(x^8 - 4x^7 + \frac{14}{3}x^6 - \frac{7}{3}x^4 + \frac{2}{3}x^2\right).$$

The first few Bernoulli numbers are

$$b_2 = \frac{1}{12}\,; \quad b_4 = -\frac{1}{720}\,; \quad b_6 = \frac{1}{30240}\,; \quad b_8 = -\frac{1}{1209600}\,.$$

The equation for the discrete frequency for $r = 1$ is $\left(\text{with } \eta = \frac{\omega}{\omega_{xL}}\right)$

$$\frac{\eta^2}{\sqrt{\eta^2-1}} \sin^{-1}\frac{1}{\eta} = \frac{1}{\epsilon} \qquad \ldots \text{ (37)}$$

A solution of this equation will always exist for $0 < \epsilon < 1$, and for $\epsilon << 1$, the discrete frequency is

$$\omega_{x0} \simeq \omega_{xL}\left(1+\frac{\epsilon^2\pi^2}{8}\right) \qquad \ldots \text{ (38)}$$

For $r = 2$, the equation for the discrete frequency is

$$\frac{\eta}{4\sqrt{1+\eta}} \log \frac{\sqrt{1+\eta}+1}{\sqrt{1+\eta}-1} + \frac{\eta}{2\sqrt{\eta-1}} \sin^{-1}\frac{1}{\eta} = \frac{1}{\epsilon} \qquad \ldots \text{ (39)}$$

In this case also, a solution will always exist for $0 < \epsilon < 1$, and for $\epsilon<<1$ the discrete frequency is given by

$$\omega_{x0} \cong \omega_{xL}\left(1+\frac{\epsilon^2\pi^2}{16}\right) \qquad \ldots \text{ (40)}$$

CONCLUSION

If the condition described in equation (10) does not hold for any given lattice model, the perturbation due to the isotope defect mixes up the various frequency branches, so that it may not be possible to find a one to one correspondence between the discrete frequencies and the unperturbed frequency branches. The models discussed here are one dimensional, but there is no essential complication in the case of two and three dimensional crystals as long as they satisfy the criterion of equation (10). For three dimensional crystals the evaluation of the integrals in equation (21) can be done numerically if one knows the frequency distribution function of the unperturbed lattice. Whether any actual crystals can be adequately represented by a model satisfying the criterion of equation (10) must remain an open question.

We have seen that the difference between the discrete frequency and the maximum frequency of any branch depends on ϵ^2. This property is related to the existence of the square root singularity in the frequency distribution function of a linear lattice. A simple proof of the fact that for small ϵ one can expect the discrete frequency to depend on ϵ^2 irrespective of the details of the law of interaction between the atoms in a linear lattice is given in the Appendix.

APPENDIX

When ϵ is very small, a solution of equation (34) would exist only if ω is slightly greater than ω_{xL}. Let

$$\sum_{p=1}^{\infty} [f(p)-f(p)\cos pk] = F(k).$$

$F(k)$ has a maximum at $k=\pi$, and evidently

$$\omega^2_{xL} = 2xF(\pi).$$

In the neighbourhood of this maximum we can expand $F(k)$ in a power series in $k' = k-\pi$. Remembering that most of the contribution to the integral comes from the neighbourhood of $k' \cong 0$, we can write the integral in equation (34) in the form

$$-\int_{-\infty}^{\infty} \frac{dk'}{(\omega^2-\omega^2_{xL})+xF''(\pi)k'^2} = -\frac{\pi}{xF''(\pi)} \frac{1}{\sqrt{\omega^2-\omega^2_{xL}}}$$

We thus get the following approximate secular equation for the discrete frequency for small ϵ;

$$1-\frac{\epsilon\omega^2}{2\sqrt{xF''(\pi)}} \frac{1}{\sqrt{\omega^2-\omega^2_{xL}}} \cong 0.$$

The solution of this equation is

$$\omega_{x0} = \omega_{xL}\left[1+\frac{F(\pi)}{4F''(\pi)}\epsilon^2\right].$$

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