frequency for the upper transverse branch is responsible for another weak singularity (see Figs. 3 and 9) slightly above the first true c.p.

In Figs. 11 and 12 the behavior of the $\Theta_D(T)$ and $\omega_D(m)$ curves as a function of **q** vector sample density is demonstrated for the DDNN results. It is evident that the $\Theta_D(T)$ curve is established with virtually no computational uncertainty down to $T\approx 2°\text{K}$. Indeed, the computed values are unchanged by the final subdivision of **q** space ($2^6\times 10^3$ to $2^9\times 10^3$) for temperatures above 2°K. Thus, since we can compute Θ_0 directly from the *theoretical* elastic constants, we can construct the whole curve.

The moment function is less well defined, but the error is only significant for $m\leq -2.5$. Again, as we know that the limiting value[29] for $m=-3$ is $k\Theta_0/h$, we can interpolate and fix the values of $\omega_D(m)$ for $m=-2.5$ to three figures with an uncertainty $\sim\pm 1$ in the last figure.

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Vibrational Spectrum of a One-Dimensional Chain with Randomly Distributed Impurity Springs*†

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The frequency spectrum of a one-dimensional lattice containing randomly distributed impurity springs has been evaluated to first order in the concentration q of impurity springs. It is shown that, with some mathematical manipulation, the solution can be placed into correspondence with the solution of Langer for the analogous problem of isotopic impurities. The virtual crystal approximation which yields the correct elastic constants requires an effective spring constant $\bar{\gamma}$ which is given, in terms of normal spring constant γ and the impurity spring constant γ' by the relation $1/\bar{\gamma}=[(1-q)/\gamma]+q/\gamma'$.

I. INTRODUCTION

IN recent years, considerable progress has been made in the calculation of the vibrational properties of solids with isotopic impurities.[1] For a variety of reasons, however, there has been less consideration of problems in which the interatomic force constants are varied.

Such problems appear, at first, to be unrelated to actual physical situations. In the disordering of two alloys of the beta-brass type, CuZn and CoFe, however, the constituents have almost identical atomic masses. The primary result of disordering appears to be a change of force constants. Since the change of the vibrational spectrum with order influences the equilibrium state or order, it will be necessary to understand these changes before a complete understanding of the order-disorder process is possible.

First steps in this direction have been made by Wojtowicz and Kirkwood[2] as well as Oguchi and Hiroike.[3] In both cases, however, there are approximations which considerably limit the applicability of the results. While it is highly likely that any solution of these problems will be approximate, there is reason to believe that more satisfactory approaches may be found. For that reason, we have turned our attention to the formal solutions of certain simplified problems. It is hoped that these solutions will lead to some insight that will, in turn, lead to better approximations. This first solution of a one-dimensional problem has been solved to develop useful mathematical procedure. Solutions of problems of higher dimensionality have been obtained. They will be presented when they are understood.

The problem which is treated here is that of a linear chain of atoms with the same mass and nearest-neigh-

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[1] For a review of the literature in this field, see A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Theory of Lattice Dynamics in the Harmonic Approximation* (Academic Press Inc., New York, 1963), Chap. 5.

[2] J. Wojtowicz and J. G. Kirkwood, J. Chem. Phys. 33, 37 (1950).

[3] T. Oguchi and K. Hiroike, Busseiron Kenkyu 33, 37 (1950).

bor interactions. Randomly positioned springs are replaced by springs which have a different force constant, and the spectral distribution function is calculated to first order in the concentration of the impurity springs. The mathematical techniques used are almost identical to those of Langer[4] who obtained an exact solution, to first order in the concentration, for the spectral density function of a one-dimensional chain of identical atoms into which isotopic impurities are randomly placed. Indeed, we proceed by showing that the problem considered here can be placed in the same form as the problem which Langer considered, and then use his results.

The corresponding order-disorder problem is both simple and uninteresting. Consider a chain consisting of two distinct chemical species, A and B, of the same mass, which alternate in position in the ordered ground state. Let the ordering process and the vibrational spectrum be controlled by nearest-neighbor interactions, such that the spring constant between A-B pairs is different from that between A-A and B-B nearest-neighbor pairs. Let the force constants between A-A and B-B pairs be identical. Such a situation would be obtained from the polar model of Mott[5] or Harrison and Paskin[6] if their interactions were of sufficiently short range (which they are not) and if the repulsive interactions were all the same. The first configurational excited state of such a system is one in which there is an A-A or B-B pair somewhere along the chain, but perfect short-range order elsewhere. That is, there is a simple antiphase boundary. The corresponding vibrational spectrum would be one for an isolated single-impurity spring constant placed at random in the chain. The next excited state which maintained the composition would consist of two such antiphase boundaries. One would be between an A-A pair and another between a B-B pair, so that they would be separated from one another by more than a nearest-neighbor distance. (This restriction can be lifted by the choice of a suitable grand canonical ensemble.) It follows that the randomly placed impurity-spring-constant problem can be brought into close analogy with the one-dimensional order-disorder problem where the concentration of impurity springs is analogous to the decrease of the short-range order parameter from unity.

It should be noted that the choice of randomly positioned impurity springs makes this solution applicable to the order-disorder problem, rather than the impurity problem. That is, one might be concerned with the effect of randomly distributed impurity atoms on the vibrational spectrum. The major feature of these impurities might very well be the changing of force constants, rather than the changing of the mass. To treat this problem, however, one would be obliged to consider randomly distributed pairs of impurity springs on the sides of the impurity atom, rather than randomly distributed single springs.

II. FORMULATION OF THE PROBLEM

The formulation of the problem presented here is similar to and, whenever possible and practical, identical to that presented by Langer.[4] We consider a very long chain in which every atom has the same mass. There are two types of force constants present in the chain, γ and γ'. The concentration of impurity force constants γ' is q, where $q \ll 1$. The unperturbed chain has $q=0$.

For a particular distribution of springs γ and γ' along the chain, the equations of motion are

$$m\ddot{x}_l=\gamma_{l,l-1}(x_{l-1}-x_l)+\gamma_{l,l+1}(x_{l+1}-x_l)\,. \tag{1}$$

Here x_l is the displacement of the atom at the site l, and $\gamma_{l,l-1}$ is the force constant acting between atoms at site l and $l-1$. The equations of motion can be rewritten as

$$\begin{aligned} m\ddot{x}_l-\gamma(x_{l-1}-x_l)-\gamma(x_{l+1}-x_l) \\ =(\gamma_{l,l-1}-\gamma)(x_{l-1}-x_l)+(x_{l,l+1}-\gamma)(x_{l+1}-x_l)\,. \end{aligned} \tag{2}$$

The transformation to the normal coordinates Q_k of the unperturbed lattice is

$$x_l=\frac{1}{(Nm)^{1/2}}\sum_{k=-N/2}^{N/2} Q_k \exp\left(\frac{2\pi ikl}{N}-i\omega t\right), \tag{3}$$

where N is the number of atoms in the chains. Substitution of Eq. (3) into Eq. (2) yields

$$(\omega_k{}^2-\omega^2)Q_k=-\sum_{k'}\Phi_{k,k'}Q_{k'}\,, \tag{4}$$

where

$$\omega_k=\omega_m|\sin(\pi k/N)|\,,\quad \omega_m=(4\gamma/m)^{1/2}, \tag{5}$$

and

$$\begin{aligned}\Phi_{k,k'}=\frac{(-2i)\sin(\pi k'/N)}{Nm}\sum_l \exp[2\pi i(k'-k)l/N] \\ \times[(\gamma_{l,l+1}-\gamma)\exp(\pi ik'/N) \\ -(\gamma_{l,l-1}-\gamma)\exp(-\pi ik'/N)]\,. \end{aligned} \tag{6}$$

Equation (4) is identical in form to Langer's Eq. (4). The entire difference between the two problems is contained in the explicit form of the $\Phi_{k,k'}$, as expressed in Eq. (6).

For a particular configuration of springs, we can write

$$[D^{-1}(\omega^2)]_{k,k'}=(\omega_k{}^2-\omega^2)\delta_{k,k'}+\Phi_{k,k'}\,, \tag{7}$$

such that Eq. (4) becomes

$$\sum_{k'}(D^{-1})_{k,k'}Q_{k'}=0\,. \tag{8}$$

Following Langer, the spectral distribution function for this configuration, defined by

$$g(\omega)=\lim_{N\to\infty}\frac{2\omega}{N}\sum_n \delta(\Omega_n{}^2-\omega^2)\,, \tag{9}$$

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[4] J. S. Langer, J. Math. Phys. **2**, 584 (1961).

[5] R. J. Harrison and A. Paskin, J. Phys. Radium **23**, 613 (1962).

[6] N. F. Mott, Proc. Phys. Soc. (London) **49**, 258 (1937).

where the Ω_n are the exact eigenfrequencies for the particular configuration of springs, is given by

$$\bar{g}(\omega)=\frac{2\omega}{\pi}\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\frac{1}{N}\,\mathrm{Im}\,\mathrm{Tr}D(\omega^2+i\epsilon)\,. \tag{10}$$

To obtain the spectral distribution function for the random distribution of springs $\bar{g}(\omega)$, we must average over all configurations which are consistent with a fixed value of q. As shown by Langer, it is sufficient to take the configuration average, $\bar{D}(\omega^2+i\epsilon)$, of $D(\omega^2+i\epsilon)$. This average $\bar{D}(\omega^2+i\epsilon)$ is diagonal in k, so that

$$\bar{g}(\omega)=\frac{2\omega}{\pi}\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\frac{1}{N}\,\mathrm{Im}\sum_{k}\bar{D}_k(\omega^2+i\epsilon)\,. \tag{11}$$

III. CONFIGURATION AVERAGE

Following Langer, we obtain from Eq. (7), for a particular configuration,

$$D_{k,k'}(\omega^2)=\frac{\delta_{k,k'}}{\omega_k{}^2-\omega^2}-\frac{1}{\omega_k{}^2-\omega^2}\sum_{k''}\Phi_{k,k''}D_{k'',k'}(\omega^2)\,, \tag{12}$$

which may be iterated to yield

$$D_{k,k'}(\omega^2)=\frac{1}{\omega_k{}^2-\omega^2}\Bigg[\delta_{k,k'}-\frac{\Phi_{k,k'}}{\omega_{k'}{}^2-\omega^2}+\sum_{k_1}\frac{\Phi_{k,k_1}\Phi_{k_1,k'}}{(\omega_{k_1}{}^2-\omega^2)(\omega_{k'}{}^2-\omega^2)}+\cdots\Bigg]. \tag{13}$$

The average over configurations is performed at this point. Since the ω_k's are properties of the unperturbed lattice, it is only necessary to obtain configurational averages of the products $\Phi_{k,k_1}\Phi_{k_1,k_2}\cdots\Phi_{k_n,k'}$. We proceed to obtain these averages. The first, $\langle\Phi_{k,k'}\rangle$ may be obtained in the same manner as Langer obtained his Eq. (19). We get

$$\langle\Phi_{k,k'}\rangle=\frac{(-2i)\sin(\pi k'/N)}{Nm}\Big\langle\sum_{l}\exp[2\pi i(k'-k)l/N]\times[(\gamma_{l,l+1}-\gamma)\exp(i\pi k'/N)-(\gamma_{l,l-1}-\gamma)\exp(-i\pi k'/N)]\Big\rangle. \tag{14}$$

This expression is evaluated by keeping l fixed while summing over configurations. We get zero contribution from any configuration in which $\gamma_{l,l+1}$ or $\gamma_{l,l-1}=\gamma$. Since $\gamma_{l,l+1}=\gamma'$ with frequency q, one obtains

$$\langle\gamma_{l,l+1}-\gamma\rangle=\langle\gamma_{l,l-1}-\gamma\rangle=q(\gamma'-\gamma)\,, \tag{15}$$

and

$$\langle\Phi_{k,k'}\rangle=\frac{4\sin^2(\pi k'/N)}{Nm}q(\gamma'-\gamma)\times\sum_{l}\exp[2\pi il(k'-k)/N]=q\omega_{k'}{}^2\lambda\delta_{k,k'}\,, \tag{16}$$

where

$$\lambda=(\gamma'/\gamma)-1\,. \tag{17}$$

Next consider the second-order term,

$$\langle\Phi_{k,k_1}\Phi_{k_1,k'}\rangle=(-4/N^2m^2)\sin(\pi k_1/N)\sin(\pi k'/N)\times\Big\langle\sum_{l_1,l_2}\{\exp(2\pi i(k_1-k)l_1/N)\exp(2\pi i(k'-k_1)l_2/N)[(\gamma_{l_1,l_1+1}-\gamma)\exp(\pi ik_1/N)-(\gamma_{l_1,l_1-1}-\gamma)\exp(-\pi ik_1/N)]\times[(\gamma_{l_2,l_2+1}-\gamma)\exp(\pi ik'/N)-(\gamma_{l_2,l_2-1}-\gamma)\exp(-\pi ik'/N)]\}\Big\rangle. \tag{18}$$

Terms which are first order in q appear in the configuration average of the four terms represented by the product of the square brackets whenever the two springs of one of the four terms are identical. That is, when $l_2=l_1$, $l_2=l_1-1$, or $l_2=l_1+1$. This complication distinguishes the problem considered here from that of Langer, in which only the terms $l_1=l_2$ contribute to first order in q. This extra complication forces us to use a slightly different approach in the evaluation of the general product of the Φ's. For the second-order term, however, it is easy to sum the appropriate terms.

For terms with $l_1=l_2$, we obtain

$$(-4/Nm^2)\sin(\pi k_1/N)\sin(\pi k'/N)\delta_{k,k'}q(\gamma'-\gamma)^2\{\exp[\pi i(k_1+k')/N]+\exp[-\pi i(k_1+k')/N]\}\,. \tag{19}$$

Terms with $l_2=l_1-1$ yield

$$(4/Nm^2)\sin(\pi k_1/N)\sin(\pi k'/N)\delta_{k,k'}q(\gamma'-\gamma)^2\exp[\pi i(k_1-k')/N]\,, \tag{20}$$

while terms with $l_2=l_1+1$ yield

$$(4/Nm^2)\sin(\pi k_1/N)\sin(\pi k'/N)\delta_{k,k'}q(\gamma'-\gamma)^2\exp[-\pi i(k_1-k')/N]\,. \tag{21}$$

Summing the contributions from (19), (20), and (21), we obtain

$$\langle\Phi_{k,k_1}\Phi_{k_1,k'}\rangle=(\omega_{k'}{}^2\omega_{k_1}{}^2/N)q\lambda^2\delta_{k,k'}+O(q^2)\,. \tag{22}$$

It should be noted that although the intermediate steps are different, the result is identical to Langer's equation (22).

We now proceed to evaluate the configuration average of the general product,

$$\begin{aligned}\langle\Phi_{k,k_1}\Phi_{k_1,k_2}\cdots\Phi_{k_{n-1},k_n}\rangle=&\frac{(-2i)^n}{N^nm^n}\sin\left(\frac{\pi k_1}{N}\right)\sin\left(\frac{\pi k_2}{N}\right)\cdots\sin\left(\frac{\pi k_{n-1}}{N}\right)\sin\left(\frac{\pi k_n}{N}\right)\\ &\times\Big\langle\sum_{l_1}\sum_{l_2}\cdots\sum_{l_n}\exp\left(\frac{2\pi i}{N}\right)[(k_1-k)l_1+(k_2-k_1)l_2+\cdots+(k_n-k_{n-1})l_n]\\ &\times[(\gamma_{l_1,l_1+1}-\gamma)\exp(\pi ik_1/N)-(\gamma_{l_1,l_1-1}-\gamma)\exp(-\pi ik_1/N)]\\ &\times[(\gamma_{l_2,l_2+1}-\gamma)\exp(\pi ik_2/N)-(\gamma_{l_2,l_2-1}-\gamma)\exp(-\pi ik_2/N)]\cdots\\ &\qquad\times[(\gamma_{l_n,l_n+1}-\gamma)\exp(\pi ik_n/N)-(\gamma_{l_n,l_n-1}-\gamma)\exp(-\pi ik_n/N)]\Big\rangle,\end{aligned}\tag{23}$$

where $k_n=k'$. Equation (23) can be written in the form

$$\begin{aligned}\langle\Phi_{k,k_1}\cdots\Phi_{k_{n-1},k_n}\rangle=&\frac{(-2i)^n}{N^nm^n}\prod_{j=1}^{n}\sin\left(\frac{\pi k_j}{N}\right)\\ &\times\Big\langle\sum_{l_1\cdots l_n}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_n=\pm1}\Big\{\exp\frac{2\pi i}{N}[(k_1-k)l_1+\cdots+(k_n-k_{n-1})l_n]\prod_{j=1}^{n}[\sigma_j(\gamma_{l_j,l_j+\sigma_j}-\gamma)\exp(\pi i\sigma_jk_j/N)]\Big\}\Big\rangle.\end{aligned}\tag{24}$$

Let us fix our attention on a particular l_1. For $\sigma_1=+1$, Eq. (24) will yield terms of order q only if, for all values of $s=2, 3,\cdots, n$, $l_s=l_1$ and $\sigma_s=+1$, or $l_s=l_1+1$ and $\sigma_s=-1$. Similarly, for $\sigma_1=-1$, terms of order q will be obtained only if $l_s=l_1$ and $\sigma_s=-1$ or $l_s=l_1-1$ and $\sigma_s=+1$. These restrictions are summarized by the condition that

$$l_s=l_1+\tfrac{1}{2}(\sigma_1-\sigma_s).\tag{25}$$

Thus, we may obtain all the terms of order q in Eq. (24) by substituting Eq. (25) into it, dropping the summations over all l_j but $l_j=l_1$, but retaining the summations over the σ_j. The result is

$$\begin{aligned}\langle\Phi_{k,k_1}\cdots\Phi_{k_{n-1},k_n}\rangle=&\frac{(-2i)^n}{N^nm^n}q(\gamma'-\gamma)^n\left[\prod_{j=1}^{n}\sin\left(\frac{\pi k_j}{N}\right)\right]\times\sum_{l_1}\exp\left[\frac{2\pi i}{N}(k_n-k)l_1\right]\\ &\times\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_n=\pm1}\sigma_1\exp\left(\frac{i\pi\sigma_1k_1}{N}\right)\prod_{j=2}^{n}\sigma_j\exp\left[\frac{\pi i}{N}(k_j-k_{j-1})(\sigma_1-\sigma_j)+\sigma_jk_j\right].\end{aligned}\tag{26}$$

The summation over l_1 in Eq. (26) can be performed immediately. This leaves the summations over the σ variables. The coefficient of k_s in the exponents which remain are

$$\begin{aligned}\{i\pi[\sigma_1-(\sigma_1-\sigma_2)]/N\}&=(i\pi\sigma_2/N), &&\text{for}\quad s=1,\\ \{i\pi[(\sigma_1-\sigma_s)+\sigma_s-(\sigma_1-\sigma_{s+1})]\}&=(i\pi\sigma_{s+1}/N), &&\text{for}\quad s=2,\cdots,n-1,\\ \{i\pi[(\sigma_1-\sigma_n)+\sigma_n]/N\}&=(i\pi\sigma_1/N), &&\text{for}\quad s=n.\end{aligned}\tag{27}$$

Therefore, Eq. (26) can be rewritten as

$$\begin{aligned}\langle\Phi_{k,k_1}\cdots\Phi_{k_{n-1},k_n}\rangle=&\frac{(-2i)^n}{N^{n-1}m^n}\left[\prod_{j=1}^{n}\sin\left(\frac{\pi k_j}{N}\right)\right]\times\delta_{k,k_n}q(\gamma'-\gamma)^n\\ &\times\sum_{\sigma_1\cdots\sigma_n}\left(\prod_{j=1}^{n}\sigma_j\right)\exp\left[\frac{\pi i}{N}(\sigma_2k_1+\sigma_3k_2+\cdots+\sigma_nk_{n-1}+\sigma_1k_n)\right].\end{aligned}\tag{28}$$

Since the σ_j are equivalent variables of summation, Eq. (28) can be rewritten as

$$\langle\Phi_{k,k_1}\cdots\Phi_{k_{n-1},k_n}\rangle=\frac{(-2i)^n}{N^{n-1}m^n}q(\gamma'-\gamma)^n\left(\prod_{j=1}^{n}\sin\frac{\pi k_j}{N}\right)\sum_{\sigma_1\cdots\sigma_n}\prod_{j=1}^{n}\sigma_j\exp\left(\frac{\pi i\sigma_jk_j}{N}\right)\delta_{k,k_n}.\tag{29}$$

In this form, the sums can be performed readily. Using Eq. (5), the average becomes

$$\langle \Phi_{k,k_1}\cdots\Phi_{k_{n-1},k_n}\rangle = \delta_{k,k_n} q\lambda^n \omega_k{}^2\omega_{k_1}{}^2\cdots\omega_{k_{n-1}}{}^2/N^{n-1}. \quad (30)$$

Equation (30) is completely equivalent to the term which is linear in q in Langer's Eq. (25).

IV. THE VIBRATIONAL SPECTRUM

Because of the equivalence presented above, it is possible to use Langer's results directly. He finds vibrational modes associated with each value of k, and with frequency given by

$$\omega=\omega_k+\Delta_k-i\Gamma_k. \quad (31)$$

Here,

$$\Delta_k=(\omega_k/2)[q\kappa(\omega_m{}^2-\omega_k{}^2)]/[\omega_m{}^2-\omega_k{}^2(1-\kappa^2)], \quad (32)$$

and

$$\Gamma_k=(\omega_k/2)[q\kappa^2\omega_k(\omega_m{}^2-\omega_k{}^2)^{1/2}]/[\omega_m{}^2-\omega_k{}^2(1-\kappa^2)], \quad (33)$$

where

$$\kappa=\lambda/(1+\lambda)=1-(\gamma/\gamma'). \quad (34)$$

In these expressions, Γ_k is a measure of the width associated with each phonon of wave vector k due to the lattice disorder.

In addition, the density of states is given by

$$\bar{g}(\omega)=\frac{2}{\pi}\,\mathrm{Re}\left[\omega_m{}^2-\omega^2+\frac{\omega_m{}^2q\kappa(\omega_m{}^2-\omega^2)^{1/2}}{(\omega_m{}^2-\omega^2)^{1/2}+i\kappa\omega}\right]^{-1/2}. \quad (35)$$

Since Langer has discussed his results extensively and carefully, we shall only draw attention to certain aspects of the results which were not, apparently, of primary interest to him, or are unique to the problem considered.

It should be noted, however, that it is $1/\gamma$ and $1/\gamma'$ in this work which correspond to Langer's M and M', respectively. This correspondence becomes obvious when the different definitions of λ are examined.

In the long-wavelength limit, and with $\gamma'\approx\gamma$,

$$\omega^2\approx 4\sin\left(\frac{\pi k}{N}\right)\Big/ M\left[(1-q)\frac{1}{\gamma}+\frac{q}{\gamma'}\right]. \quad (36)$$

Thus, in the elastic limit, an average spring constant can be defined by

$$\frac{1}{\bar{\gamma}}=\frac{(1-q)}{\gamma}+\frac{q}{\gamma'}. \quad (37)$$

The frequency spectrum is, in this limit, identical to that which would be obtained if all the springs were replaced by the correctly averaged spring.

It is important to note, however, that this correct averaging, to obtain a virtual crystal approximation, is of $1/\gamma$, rather than γ itself.

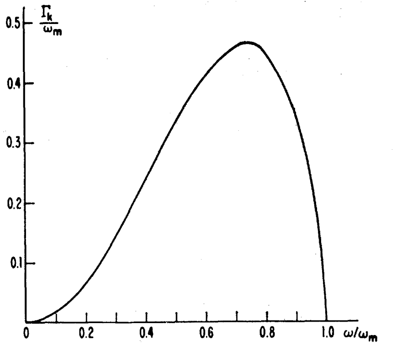

FIG. 1. The functional form of Γ_k for the case of $\kappa=\frac{2}{3}$, $q=\frac{1}{10}$.

While this result might be expected, its application as an approximation to a two- or three-dimensional system is highly suspect. The obvious reason for this is as follows: When the linear chain is placed in tension, the atoms adjacent to the impurity springs are constrained to move along the line of tension. The analogous situation in three dimensions is one in which tension is applied in a manner which corresponds to the limit of a pure longitudinal mode of the unperturbed lattice. When the impurity springs are introduced, however, equilibrium may be reached by displacements which have components normal to the direction of the tension. In this case, Eq. (3.7) is not valid.

It is also of some interest to examine the form of Γ_k, as given in Eq. (33). It is easily seen that $\Gamma_k=0$ for $\omega_k=0$ or $\omega_k=\omega_m$. Since Γ_k is positive, it must have a maximum somewhere in between these two points. That maximum occurs for

$$\omega_k{}^2=\omega_m{}^2\left[\frac{3-(1+8\kappa^2)^{1/2}}{2(1-\kappa^2)}\right], \quad (38)$$

for all possible values of κ^2. The functional form of Γ_k is shown in Fig. 1. The maximum is quite evident. In the paragraphs which follow, an attempt is made to explain this behavior.

The mathematical origin of these widths is discussed by Langer. Each member of the ensemble is not periodic, and k does not label an eigenvector. Thus, a measurement which fixes k will yield a spread in frequencies. Although k becomes, in a certain sense, a good label for the ensemble average, the spread in frequencies must remain. Mathematically, we see the spread in the form of the average spectral distribution function,

$$\bar{g}(\omega)=\frac{2\omega}{\pi}\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\frac{1}{N}\,\mathrm{Im}\sum_k D_k(\omega^2+i\epsilon). \quad (39)$$

For the unperturbed chain,

$$D_k(\omega^2+i\epsilon)=1/(\omega_k{}^2-\omega^2-i\epsilon). \quad (40)$$

The poles of $D_k(\omega^2)$ occur at the eigenvalues associated with k. Langer's results may be paraphased as follows. For the perturbed problem, there are a number of frequencies, denoted $\omega_{k,i}$, which are positions of the poles of each $D_k(\omega^2+i\epsilon)$. These poles lie at the solutions of

$$\omega_k^2-\omega_{k,i}^2+G_k(\omega_{k,i}^2)=0\,, \tag{41}$$

where, from Langer's work,

$$G_k(\omega^2)=q\kappa\omega_k^2\bigg/\left(1+\frac{\kappa\omega^2}{N}\sum_{k'}\frac{1}{\omega_{k'}^2-\omega^2}\right) \tag{42}$$

to first order in q.

The contribution to $\bar{g}(\omega)$ from any one of the frequencies associated with k is proportional to the residue at the corresponding pole of $D_k(\omega^2)$, which is

$$\begin{aligned}&\mathrm{Res}_{\omega=\omega_{k,i}}\{D_k(\omega^2)\}\\&\qquad=[-2\omega_{k,i}+(\partial/\partial\omega)G_k(\omega^2)\,|_{\omega=\omega_{k,i}}]^{-1}\end{aligned} \tag{43}$$

As indicated in Fig. 2, this residue is largest for $\omega_{k,i}$ in the vicinity of ω_k and diminishes rapidly on either side of this point as

$$(\partial G/\partial\omega_k)\,|_{\omega=\omega_{k,i}}$$

becomes large.

With these results of Langer, the mathematical origin of the form of Fig. 1 is readily visualized For each k, Γ_k. is proportional to the range in ω over which the $\omega_{k,i}$ have appreciable residues. Let n_k be the number of modes for which the residues associated with the $\omega_{k,i}$ are appreciable, and ρ_k be the density of modes of the unperturbed system. Then

$$\Gamma_k\propto n_k/\rho_k\propto n_k(\omega_m^2-\omega_k^2)^{1/2}. \tag{44}$$

Thus, it is the singularity in the density of states which causes the vanishing of Γ_k for $\omega_k=\omega_m$. That is, although n_k may be large for $k=k_{\max}$, the infinite density of states causes the total energy spread to be very small.

It is evident that $\Gamma_k=0$ for $k=0$. The form of the increase of Γ_k with increasing k, up to the maximum, is shown more explicitly, however, by an examination of Figs. 2 and 3. In these figures, $G_k(\omega^2)$ and $(\omega^2-\omega_k^2)$ are plotted versus ω^2 for the cases $\omega_k^2\ll\omega_m^2$ and $\omega_k^2\approx\omega_m^2$. The intersections of $G_k(\omega^2)$ with $(\omega^2-\omega_k^2)$ occur at the values of ω^2 equal to the $\omega_{k,i}^2$. The residue associated with these $\omega_{k,i}^2$ are appreciable, however, only at those values of $\omega_{k,i}^2$, such that $\partial G/\partial\omega$ is small. In Fig. 2, only the central $\omega_{k,i}$ satisfies this condition, while in Fig. 3, there are a number of terms for which the residue is appreciable. Thus, in the form of Eq. (44), the maximum in Γ_k may be pictured as a competition between the slowly increasing n_k and the ρ_k which increases more slowly for small k, but increases rapidly near $k_{\max}$.

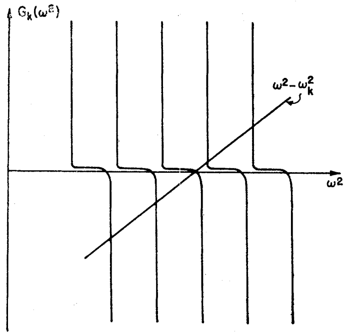

FIG. 2. $G_k(\omega^2)$ and $(\omega^2-\omega_k^2)$ versus ω^2 for $\omega_k^2\ll\omega_m^2$.

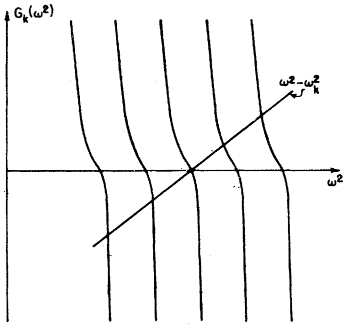

FIG. 3. $G_k(\omega^2)$ and $(\omega^2-\omega_k^2)$ versus ω^2 for $\omega_k^2\approx\omega_m^2$.