ANALYTICAL REPRESENTATION OF THE DISTRIBUTION FUNCTION OF OSCILLATION FREQUENCIES OF AN IDEAL CRYSTAL LATTICE

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A new method is proposed for analytic approximation of the distribution function of the squared harmonic oscillation frequencies of an ideal crystal lattice on the basis of the force constants. The Montroll method for analytic approximation of the distribution function on basis of given numerical values of some of the first distribution function moments is improved. The method is illustrated in a concrete case.

MANY properties of crystals, connected with lattice vibrations, are determined in the harmonic approximation by the distribution function $g(\omega)$ of the natural frequencies ω of the crystal lattice. The distribution function $g(\omega)$ is determined uniquely by the microscopic model of the crystal lattice, but apparently cannot be obtained in explicit form. For concrete calculations of $g(\omega)$ it is necessary therefore to use approximate methods.

A large number of studies of the theory of crystal lattice have made use either of the Debye approximation of the function $g(\omega)$, or of the Einstein approximation. On the other hand, in cases when allowance for the details of the function $g(\omega)$ is important, one resorts to various numerical methods.

In connection with the foregoing, many efforts have been expended to find analytic approximations of $g(\omega)$. One of the methods of such an approximation is the method of moments, proposed by Montroll[1,2]. This method consists of finding several first terms of the expansion of the function $g(\omega)$ in Legendre polynomials, using for this purpose the numerical values of a finite number of moments of the distribution function $g(\omega)$. A practical application of this method, however, leads to the conclusion that the successive approximations fluctuate quite strongly relative to one another. In 1954–55, Rosenstock[3,4] and Lebowitz and Lax[5] proposed a method for analytically approximating $g(\omega)$, in which account is taken also of the singularities of the Van Hove spectrum. This method calls for a preliminary determination of the positions of the singularities and to a determination of their form.

In the present article we propose a method that differs from the foregoing. It is based on the possibility of representing the distribution function of the squares of the lattice vibration frequencies in the form of the arithmetic mean of the spectral densities of several Jacobi matrices (see[6]), and on the asymptotic properties of these matrices.

1. CONCERNING ONE NEW REPRESENTATION OF THE DISTRIBUTION FUNCTION OF THE FREQUENCIES OF AN IDEAL LATTICE

It will henceforth be more convenient for us to deal with the distribution function of the squares of the frequencies $\rho(\lambda)$, $\lambda = \omega^2$, which is simply connected with the function $g(\omega)$:

$$g(\omega) = 2\omega\rho(\omega^2) = 2\sqrt{\lambda}\rho(\lambda).$$

We shall prove in this section that the function $\rho(\lambda)$ can be represented in simple fashion in terms of quantities determined by a finite number of several self-adjoint operators with nondegenerate spectra, and we report certain properties of these operators; these properties will be needed later on.

We consider an ideal infinite crystal lattice with n atoms per unit cell. The equations of the harmonic oscillations of the lattice can be written in the form

$$(L - \lambda)\chi = 0, \tag{1}$$

where L is an operator whose matrix elements in the coordinate representation are very simply connected with the force constants and with the masses of the lattice atoms, χ is an infinite-dimensional vector in the space H of the displacement of the lattice atoms from their equilibrium positions. The eigenvalues λ of the operator L are the squares of the natural frequencies of the crystal lattice. The operator L is Hermitian.

Using the translational symmetry of the lattice, we can write the solutions of (1) in the form of plane modulated waves in such a way that the "components" of the vector χ take the form

$$\chi_{k,s}(\mathbf{R} + \mathbf{r}) = \mathbf{e}_{k,s}(\mathbf{r})\exp(2\pi i\mathbf{k}\mathbf{R}). \tag{2}$$

Here $\mathbf{R} + \mathbf{r}$ are the radius vectors of the average positions of the atoms ($\mathbf{R}$—radius vectors of the sites of one of the Bravais lattices, $\mathbf{r}$—radius vectors of the atoms in the unit cell of the crystal). $\mathbf{k}$—vector of principal cell of the reciprocal lattice, s—number of oscillation branch ($s = 1, 2, \ldots, 3n$). The vector $\mathbf{e}_{k,s}(\mathbf{r})$ belongs to the usual three-dimensional space. The eigenvalues $\lambda_s(\mathbf{k})$ of the operator L are obtained from the solution of the secular equation; the eigenvectors of the operator L will be assumed to be normalized by the condition

$$[\chi_{k,s}, \chi_{k',s'}] = \delta_{ss'}\delta(\mathbf{k} - \mathbf{k}'), \tag{3}$$

where the square brackets denote the scalar product[1] in the space H. A consequence of the condition (3) is

$$\sum_{\mathbf{r}} |\mathbf{e}_{\mathbf{k},s}(\mathbf{r})|^2 = 1. \tag{4}$$

As is well known, the distribution function $\rho(\lambda)$ of the squares of the frequencies can be represented in the form[7]

$$\rho(\lambda) = \frac{V}{3n} \sum_{s=1}^{3n} \int \frac{d\Omega_s}{|\nabla\lambda_s(\mathbf{k})|}, \tag{5}$$

where V is the volume of the unit cell of the crystal, $d\Omega_S$ is the area element of the surface $\lambda_S(\mathbf{k}) = \lambda$, the symbol ∇ denotes the operator of the gradient in k-space. The integrals in (5) are taken over the surfaces $\lambda_S(\mathbf{k}) = \lambda$. For our purpose, we should obtain for $\rho(\lambda)$ a new representation, different from (5). It is therefore necessary to introduce for the operator L eigenfunctions that differ from their tradiational representation (2).

Let h be an arbitrary real vector from the space H, normalized to unity. With the aid of the vector h we form the subspace of vectors

$$\mathbf{h},\ L\mathbf{h},\ L^2\mathbf{h}, \ldots \tag{6}$$

We denote this subspace by H(h). It is easy to verify that the subspace H(h) is invariant against the operator L, i.e., any vector from this subspace cannot be derived from it by the operator L. From the invariance of the subspace (6) it follows that the operator L induces in this subspace a certain operator, which we shall denote by L_h. The vector h is called the vector generating the operator L_h. According to the theory of linear operators (see, for example,[8]), the spectrum of the operator L_h is nondegenerate.

We choose in H(h) a basis by successive orthogonalization of the vectors (6). We denote the corresponding vectors of the basis by $\mathbf{h}_0 \equiv \mathbf{h}, \mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \ldots$. On this basis, as is well known[8], the operator is represented in the form of a Jacobi matrix

$$(L_h) = \begin{pmatrix} (L_h)_{00} & (L_h)_{01} & 0 & 0 & \ldots \\ (L_h)_{10} & (L_h)_{11} & (L_h)_{12} & 0 & \ldots \\ 0 & (L_h)_{21} & (L_h)_{22} & (L_h)_{23} & \ldots \\ 0 & 0 & (L_h)_{32} & (L_h)_{33} & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}. \tag{7}$$

The eigenfunctions of the operator L_h can be shown shown[6] to be of the form

$$\psi_h(\lambda) = \sqrt{\rho_h(\lambda)} \sum_{k=0}^{\infty} P_k^{(h)}(\lambda)\, \mathbf{h}_k, \tag{8}$$

where $P_k^{(h)}(\lambda)$ are polynomials of λ, satisfying the recurrence relations

$$\lambda P_k^{(h)}(\lambda) = L_{k,k-1} P_{k-1}^{(h)}(\lambda) + L_{k,k} P_k^{(h)}(\lambda) + L_{k,k+1} P_{k+1}^{(h)}(\lambda), \tag{9}$$

subject to the initial conditions $P_0^{(h)} = 1$, $P_1^{(h)} = (\lambda - L_{00})/L_{01}$, and $\rho_h(\lambda)$ is a wave function, with respect to which the polynomials $P_k^{(h)}(\lambda)$ are orthogonal:

$$\int P_k^{(h)}(\lambda)\, P_l^{(h)}(\lambda)\, \rho_h(\lambda)\, d\lambda = \delta_{kl}. \tag{10}$$

The function $\rho_h(\lambda)$ is called the spectral density of the operator L_h. It follows from (10) that

$$\sqrt{\rho_h(\lambda)\rho_h(\lambda')} \sum_{k=0}^{\infty} P_k^{(h)}(\lambda)\, P_k^{(h)}(\lambda') = \delta(\lambda - \lambda'), \tag{11}$$

and from (8) we get

$$\rho_h(\lambda) = [\psi_h(\lambda), \mathbf{h}_0]^2. \tag{12}$$

The vectors $\mathbf{h}_k$ can be represented in the form[8]

$$\mathbf{h}_k = P_k^{(h)}(L)\,\mathbf{h}, \tag{13}$$

making it possible to write down the eigenfunctions (8) of the operator L in the form

$$\psi_h(\lambda) = \sqrt{\rho_h(\lambda)} \left(\sum_{k=0}^{\infty} P_k^{(h)}(\lambda)\, P_k^{(h)}(L) \right) \mathbf{h}. \tag{14}$$

We shall now show that the distribution function $\rho(\lambda)$ of the squares of the frequencies of an ideal lattice can be written in the form of the arithmetic mean of several spectral densities $\rho_h(\lambda)$ with a special choice of the generating vectors h. To this end, we expand the function (14) in terms of the eigenfunctions (2):

$$\psi_h(\lambda) = V \sum_{s=1}^{3n} \int [\psi_h(\lambda),\ \chi_{\mathbf{k},s}]\, \chi_{\mathbf{k},s}\, d\mathbf{k}, \tag{15}$$

and substitute to the function $\psi_h(\lambda)$ in the right side of (15) the expression (14). Using the Hermitian character of the operator L, also Eq. (11), we can easily transform (15) into

$$\psi_h(\lambda) = V \sum_{s=1}^{3n} \int \frac{[\mathbf{h}, \chi_{\mathbf{k},s}]\, \chi_{\mathbf{k},s}}{\sqrt{\rho_h(\lambda_s(\mathbf{k}))}}\, \delta(\lambda - \lambda_s(\mathbf{k}))\, d\mathbf{k}$$

or, what is the same,

$$\psi_h(\lambda) = \frac{V}{\sqrt{\rho_h(\lambda)}} \sum_{s=1}^{3n} \int_{\lambda_s(\mathbf{k})=\lambda} \frac{[h,\ \chi_{\mathbf{k},s}]\, \chi_{\mathbf{k},s}}{|\nabla\lambda_s(\mathbf{k})|}\, d\Omega_s. \tag{16}$$

Multiplying both sides of this equation by h and using (12), we get

$$\rho_h(\lambda) = V \sum_{s=1}^{3n} \int_{\lambda_s(\mathbf{k})=\lambda} \frac{|[\mathbf{h}, \chi_{\mathbf{k},s}]|^2\, d\Omega_s}{|\nabla\lambda_s(k)|}. \tag{17}$$

We now take the vectors h to be the vectors $\mathbf{e}_i(\mathbf{r})$, which are unit vectors collinear with the displacement of the r-th atom of the principal unit cell along the i-th axis of the Cartesian coordinate system. From (2) and from the definition of the vectors $\mathbf{e}_i(\mathbf{r})$ it is obvious that

$$[\mathbf{e}_i(\mathbf{r}),\ \mathbf{e}_{\mathbf{k},s}(\mathbf{r})] = \overline{\mathbf{e}^i_{\mathbf{k},s}(\mathbf{r})}. \tag{18}$$

We put in (17) $\mathbf{h} = \mathbf{e}_i(\mathbf{r})$ and sum the obtained expression over i and r. This yields

$$\sum_{i,\mathbf{r}} \rho_{\mathbf{e}_i(\mathbf{r})}(\lambda) = V \sum_{s=1}^{3n} \int \frac{\sum_{\mathbf{r}} |\mathbf{e}_{\mathbf{k},s}(\mathbf{r})|^2\, d\Omega_s}{|\nabla\lambda_s(\mathbf{k})|}$$

or, according to (4),

$$\sum_{i,\mathbf{r}} \rho_{\mathbf{e}_i(\mathbf{r})}(\lambda) = V \sum_{s=1}^{3n} \int \frac{d\Omega_s}{|\nabla\lambda_s(\mathbf{k})|}.$$

Comparing this expression with (5), we can write for

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[1] The scalar product in space H is defined by the equation

$$[\psi, \chi] = \sum_{\mathbf{R}+\mathbf{r}} \sum_{i=1}^{3} \overline{\chi^i(\mathbf{R}+\mathbf{r})}\, \psi^i(\mathbf{R}+\mathbf{r}).$$

The bar denotes complex conjugation, and the index i denotes the projection of the component of the vector in the R + r-th site of the lattice by the i-th axis of the Cartesian coordinate system.

the distribution function $\rho(\lambda)$

$$\rho(\lambda)=\frac{1}{3n}\sum_{i,r}\rho_{e_i(r)}(\lambda). \tag{19}$$

We have thus shown that the distribution function of the squares of the frequencies can be represented in the form of the arithmetic mean of the spectral densities of 3n Hermitian operators with nondegenerate spectra. In the particular case of a single-atom cubic lattice, formula (19) reduces to the simple equation

$$\rho(\lambda)=\rho_e(\lambda), \tag{20}$$

where e is a unit vector collinear with the displacement of one of the atoms of the lattice along one of the fourfold axes.

It follows from the representation (19) that to find the function $\varphi(\lambda)$ in the general case of an arbitrary lattice it suffices to obtain the 3n functions $\rho_{e_i(r)}(\lambda)$. The functions $\rho_{e_i(r)}$ can apparently not be obtained in explicit form. However some rather general regularities of the Jacobi matrices (7) make it possible to obtain analytic approximations of these functions, and with them also the analytic approximation of the distribution function of the squares of the frequencies $\rho(\lambda)$. The next section is devoted to this question.

We note here that the eigenvectors $\psi_h(\lambda)$ of the operator L describe certain special types of oscillations. These types of oscillations, as was already noted by one of us[6], are of independent interest in the theory of crystal-lattice vibrations (thus, in particular, it is relatively easy to express in terms of these functions such microscopic characteristics of the lattice as the mean-squared displacement of the lattice atoms from the equilibrium position, the correlation functions for the displacements of the atoms, etc.).

2. ANALYTIC APPROXIMATION OF THE FUNCTION $\rho_h(\lambda)$

As shown in the preceding section, the distribution function of the squares of the frequencies can be expressed in a simple manner in terms of the spectral densities of several operators L_h. Therefore, by finding the analytic approximation of these spectral densities, we determine by the same token the analytic approximation of the distribution function.

For simplicity, let us consider a single-atom crystal lattice. At the end of this section we shall generalize the results of the case of an arbitrary crystal lattice.

For a single-atom lattice, the distribution function of the squares of the frequencies is equal to the arithmetic mean of the three spectral densities $\rho_1(\lambda)$, $\rho_2(\lambda)$, and $\varphi_3(\lambda)$, where $\rho_i(\lambda)$ is the spectral density of the operator generated by a unit displacement of one of the atoms of the lattice along the i-th axis of a Cartesian coordinate system.

The spectrum of the operator L_h for a single-atom lattice is continuous and lies in the interval $(0, \lambda^h_{max})$, where λ^h_{max} is the maximum eigenvalue of the operator L_h. The value of λ^h_{max} can be obtained without particular difficulty.

As is well known (see, for example[9],) the matrix elements of the matrix (7) satisfy in this case the following limiting conditions:

$$\lim_{k\to\infty}(L_h)_{k,k}=\frac{\lambda^h_{max}}{2},\quad \lim_{k\to\infty}(L_h)_{k,k-1}=\frac{\lambda^h_{max}}{4}. \tag{21}$$

In the case of rapid convergence of the indicated matrix elements, the matrix (7) for single-atom lattices can be regarded as a perturbation of the operator of the type

$$(L^0_h)=\lambda^h_{max}\begin{pmatrix} 1/2 & 1/4 & 0 & 0 & \dots \\ 1/4 & 1/2 & 1/4 & 0 & \dots \\ 0 & 1/4 & 1/2 & 1/4 & \dots \\ 0 & 0 & 1/4 & 1/2 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \tag{22}$$

The properties of the matrix (22) and its eigenvector have been sufficiently well investigated. The spectral density of the operator (22) is given by

$$\rho^{(0)}(\lambda)=\frac{8}{\pi(\lambda^h_{max})^2}\sqrt{\lambda(\lambda^h_{max}-\lambda)}. \tag{23}$$

We introduce the operators $L^{(m)}_h$, defined in the following manner: when $i, k \le m-1$ all the matrix elements $(L^{(m)}_h)_{i,k}$ coincide with the corresponding matrix elements of the operator L_h, and when $i, k \ge m$ we get the equality

$$(L^{(m)}_h)_{k,k}=\frac{\lambda^h_{max}}{2},\quad (L^{(m)}_h)_{k,k-1}=\frac{\lambda^h_{max}}{4}.$$

From the definition of the operator $L^{(m)}_h$ and from the asymptotic properties of (21) we get

$$L_h=\lim_{m\to\infty}L^{(m)}_h, \tag{24}$$

and consequently also

$$\rho_h=\lim_{m\to\infty}\rho^{(m)}_h, \tag{25}$$

where ρ_h and $\rho^{(m)}_h$ are the spectral densities of the operators L_h and $L^{(m)}_h$.

It follows from (25) that in the case of sufficiently rapid convergence of the matrix elements L_h to the limiting values, the spectral densities $\rho^{(m)}_h$ can be regarded as approximate expressions for ρ_h. It turns out that the $\rho^{(m)}_h$ can be obtained relatively easily. (Henceforth, to abbreviate the notation, we shall omit the index h.) We put

$$\rho^{(m)}(\lambda)=\rho^{(0)}(\lambda)/S^{(m)}(\lambda), \tag{26}$$

where $S^{(m)}(\lambda)$ is a certain unknown function, and $\rho^{(0)}(\lambda)$ is given by (23). Since the polynomials $P^{(m)}_s(\lambda)$ generated by the operator $L^{(m)}$ form a complete set of functions, the function $S^{(m)}$ can be expanded in terms of these polynomials:

$$S^{(m)}(\lambda)=\sum_{s=0}^{\infty}A^{(m)}_s P^{(m)}_s(\lambda). \tag{27}$$

From (26) and (27) it follows that

$$\rho^{(m)}(\lambda)\sum_{s=0}A^{(m)}_s P^{(m)}_s(\lambda)=\rho^{(0)}(\lambda). \tag{28}$$

Since the polynomials $P^{(m)}_s$ are orthogonal with weight $\rho^{(m)}(\lambda)$, we get from (28)

$$A^{(m)}_s=\int_0^{\lambda_{max}}P^{(m)}_s\rho^{(0)}(\lambda)\,d\lambda. \tag{29}$$

The polynomials $P_s^{(m)}$ can be expanded in terms of the polynomials $P_s^{(0)}$, which are orthogonal with weight $\rho^{(0)}(\lambda)$. It is easy to verify that when $n \geq 2m$ there is an equality

$$P_n^{(m)} = \sigma_0 P_n^{(0)} + \sigma_1 P_{n-1}^{(0)} + \ldots + \sigma_{2m-1} P_{n-2m+1}^{(0)}, \qquad (30)$$

where the coefficients σ_i do not depend on the number n. It follows from (29) that the $A_s^{(m)}$ are equal to the coefficients of $P_0^{(0)}$ in the expansion of $P_s^{(m)}$ in terms of $P_i^{(0)}$. Consequently, taking (30) into account, we can state that all the $A_s^{(m)}$ with $s \geq 2m$ are equal to zero. Thus,

$$\rho^{(m)}(\lambda) = \rho^{(0)}(\lambda) \Big/ \sum_{s=0}^{2m-1} A_s^{(m)} P_s^{(m)}(\lambda) \qquad (31)$$

with $A_s^{(m)}$ as defined in (29).

Expression (31) is the sought approximation of the spectral densities in the case of a single-atom lattice. In terms of these expressions we can approximate by means of formula (9) the distribution function of the squares of the frequencies of an ideal lattice. Besides the representation (31), other representations are also possible. Thus, it can be shown that

$$\sum_{s=0}^{2m-1} A_s^{(m)} P_s^{(m)}(\lambda) = (P_m^{(m)})^2 + (P_{m-1}^{(m)})^2 - P_1^{(0)} P_m^{(m)} P_{m-1}^{(m)}, \qquad (32)$$

where $P_1^{(0)} = 4\lambda - 2$.

In the general case of a lattice with an arbitrary basis, we encounter the fact that the spectrum of the operator L_h consists of several non-intersecting segments of the number axis. It turns out that, having information concerning the locations of these segments and their lengths, it is impossible to indicate a general regularity in the behavior of the matrix elements of the operator L_h, and each concrete case has its own regularity. Thus, it is known, for example (see[10]) that the character of the behavior of these matrix elements depends on the arithmetic nature of the numbers which determine the ends of the intervals of the spectrum of the operator L_h. Nonetheless, the general idea of finding the approximation remains the same as before. If the spectrum is contained in p intervals

$$[0, \lambda_0], [\lambda_1, \lambda_1'], \ldots, [\lambda_{p-1}, \lambda_{p-1}'], \qquad (33)$$

Then we can take as the approximation of the spectral function of the operator L_h the function

$$\rho^{(0)}(\lambda) \Big/ \sum A_s P_s(\lambda), \qquad (34)$$

where

$$\rho^{(0)}(\lambda) = \begin{cases} 0, & \text{if } \lambda \text{ does not belong to any of the intervals (33),} \\ \dfrac{8}{\pi p} \dfrac{\sqrt{(\lambda - \lambda_k)(\lambda_k' - \lambda)}}{(\lambda_k' - \lambda_k)^2}, & \text{if } \lambda_k \leqslant \lambda \leqslant \lambda_k'; \end{cases} \qquad (35)$$

$P_S(\lambda)$ are polynomials generated by a specified Jacobi matrix of the operator L_h, while the coefficients A_S are determined from formula (29) with $\rho^{(0)}(\lambda)$ from (35). The matrix elements of the Jacobi matrix for the spectral density (35) coincide asymptotically with the corresponding matrix elements of the matrix of the operator L_h. A similar asymptotic behavior of possessed by the matrix generated by the spectral density (34).

The approximation obtained by this method has the following advantages. It yields exact values of $2m - 1$ moments of the spectral density, and the succeeding ones with a high accuracy. As shown by our experience, the matrix elements converge rapidly to the limiting values (21). Therefore, even at small values of m (order of approximation) the approximation describes well the spectral density. On the edges of the intervals $\rho^{(m)}$ there are root singularities, as follows indeed from the general theory of motion of a crystal lattice.

To estimate the errors of the approximation in practice, it is apparently necessary to compare two neighboring approximations. For integral characteristics of the type $\int f(\lambda)\rho(\lambda)\,d\lambda$, nonetheless, it can be shown that in the general case replacement of this integral by the integral $\int f(\lambda)\rho^{(m)}(\lambda)\,d\lambda$ yields an error which is much smaller than double the maximum deviation on the spectrum of the operator L of the best-approximation polynomial of degree $2m - 1$ of the average function $f(\lambda)$.

3. APPROXIMATION OF THE DISTRIBUTION FUNCTION BY MEANS OF THE MOMENTS

In the calculation of the total dynamic characteristics of a crystal, one resorts very frequently to the calculation with the aid of the moments of the distribution function of the oscillation frequency (the Thirring method). The procedure for calculating the moments from the known matrix of the force constants has been developed in considerable detail (see, for example,[7,11]).

Specifying a finite number of moments itself leaves a great leeway in the reconstruction of the distribution function (see[12]). However, additional information concerning the region in which the distribution function is defined and concerning its continuity impose significant limitations on the character of the behavior of the distribution function, something not utilized in the cited papers of Montroll[1,2]. Thus, for example, the approximation of the spectrum, proposed by Montroll, sometimes leads to negative values of the frequency distribution function. We shall show in this section that the aforementioned information concerning the moments and the region in which the distribution function is defined makes it possible to obtain a much better analytic approximation. For simplicity, we confine ourselves again to the case of a Bravais lattice.

Thus, assume that the moments $\mu_0 = 1$, μ_1, $\mu_2, \ldots, \mu_n$ of the sought distribution function of the squares of the frequencies of a single-atom crystal lattice are specified. Assume also that it is known that the spectrum lies in the interval $[0, \lambda_{max}]$, and the distribution function of the frequencies is continuous in this interval. We introduce formally a certain basis $g_0, g_1, g_2, \ldots$, and a Hermitian operator L with a simple spectrum such that (i) the operator L is represented by a Jacobi matrix in the indicated basis and (ii) the spectral function of this operator coincides with the distribution function of the squares of the frequencies of the ideal lattice. It is easy to show that such an operator exists. (In the general case such an operator is not directly connected with the lattice vibrations, and therefore its eigenfunctions apparently have no physical meaning. On the other hand, in the

case of a cubic lattice, by virtue of (20), the eigenfunctions of the operator L describe oscillations in the subspace generated by the displacement of one of the lattice atoms along one of the fourfold axes.)

From the definition of the spectral function it follows[8] that the moments in such a case are expressed in terms of the matrix elements of the powers of the operator L:

$$\mu_k = (L^k)_{00} = [g_0, L^k g_0]. \quad (36)$$

Knowing n such matrix elements and using the Hermitian character and the Jacobian form of the matrix L in our basis, we can easily find successively n first matrix elements $L_{ik} = [g_i, L g_k]$. In addition to this information, we know also the asymptotic behavior of the matrix elements at large i and k.

Thus, specification of a finite number of moments makes it possible to construct several successive operators $L^{(m)}$, defined in the preceding section. Knowledge of these operators make it possible to find the spectral functions $\rho^{(m)}(\lambda)$, which are analytic approximations of the spectral function $\rho(\lambda)$.

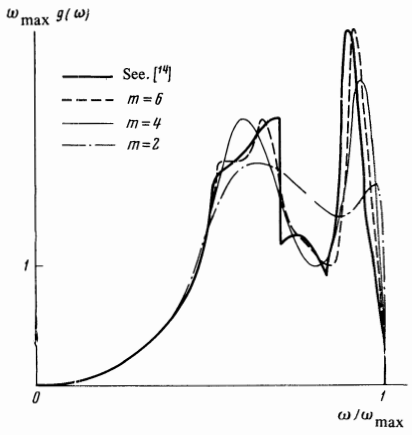
4. ILLUSTRATION OF THE METHOD

By way of an example we present the results of an approximate calculation of the distribution function of the frequencies for one of the simplest models of a crystal lattice. The figure shows plots of the second, fourth, and sixth approximations of the distribution function of the frequencies $g(\omega) = 2\omega\rho(\omega^2)$ for a cubic face-centered lattice with a central interaction of the nearest neighbors. The solid line shows the distribution function of the frequencies for this model, obtained by Leighton[14] (see also the new paper by Gordon[13]).

Owing to the cubic symmetry of the problem, the calculations reduce to finding only one Jacobi matrix. The first matrix elements are $L_{00} = 0.5$, $L_{01} = 0.25$, $L_{11} = 0.5625$, $L_{12} = 0.2339$, $L_{22} = 0.4509$, $L_{23} = 0.2423$, $L_{33} = 0.5075$, $L_{34} = 0.2605$, $L_{44} = 0.5129$, $L_{45} = 0.2473$, and $L_{55} = 0.4958$.

We find it necessary to call attention to the fact that the presented plots of the approximations are equivalent to the use of the information contained respectively in the third, seventh, and eleventh moments of the distribution function.

In conclusion, we are grateful to L. A. Postur, who called our attention to the proof in[9] of the theorem concerning the asymptotic behavior of the matrix elements of the Jacobi matrices, to I. M. Lifshitz and N. I. Akhiezer for a useful discussion of certain problems, and to V. P. Tolstouzhskiĭ, who helped with the numerical computer calculations.



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