THE THERMODYNAMIC AVERAGE OF FUNCTIONS OF THE DISPLACEMENT OF ATOMS IN A NON-IDEAL CRYSTALLINE LATTICE

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It is necessary to obtain the thermodynamic average of the function $\exp i(\mathbf{q}\cdot\mathbf{u_R})$, where $\mathbf{q}$ is a constant vector and $\mathbf{R}$ the displacement of the $\mathbf{R}$-th atom from its equilibrium position, when one studies the scattering of x rays or slow neutrons by atomic systems. In the case of small oscillations the thermodynamic average of any function $F((\mathbf{q}\cdot\mathbf{u_R}))$ is uniquely determined by the mean-square fluctuation $D(\mathbf{n}, \mathbf{R}, T)$ of the displacement of the $\mathbf{R}$-th atom in the direction of the vector $\mathbf{n} = \mathbf{q}/q$ (T is the temperature of the system). A method is given for the evaluation of the quantity $D(\mathbf{n}, \mathbf{R}, T)$ for an infinite perfect lattice with a finite number of localized defects. We have obtained an asymptotic expression for the function $D(\mathbf{n}, \mathbf{R}, T)$ at large distances from the defects. This asymptotic value is determined by the lattice and the nature of the defects. This method of evaluation can also be applied to other problems.

WHEN considering problems connected with small vibrations of crystal lattices it is usually necessary to take the time average of several functions of the displacement of a given atom of the lattice in thermal equilibrium from its equilibrium position. If, for instance, we study the scattering of x rays (or slow neutrons) by a crystal lattice, we must find the time average of the quantity $\exp i(\mathbf{q}\cdot\mathbf{u_R})$, where $\mathbf{q} = (\mathbf{p}-\mathbf{p}')/h$ ($\mathbf{p}$ and $\mathbf{p}'$ are respectively the momenta of the incident and the scattered waves, h is Planck's constant divided by 2π), $\mathbf{u_R}$ is the displacement of the $\mathbf{R}$-th atom in the lattice from its equilibrium position, $\mathbf{R}$ is the radius vector of the equilibrium position of the atom. Another example would be the evaluation of the dispersion of the displacement of the atom from its equilibrium position.

If we use the distribution function for the displacements from its equilibrium position for a one-dimensional oscillator (Bloch,[1] see also reference 2) which is in thermodynamic equilibrium with the surrounding medium, and also use the fact that the motion of any atom can be written as a linear combination of normal vibrations when the atoms in the system execute small vibrations, we can show that the thermodynamic average of any function $F(\mathbf{q}\cdot\mathbf{u_R})$ which depends on the dot product of the constant vector $\mathbf{q}$ and the displacement, $\mathbf{u_R}$, of the $\mathbf{R}$-th atom in the system which executes small vibrations, can be expressed by the formula

$$\langle F(\mathbf{q}\mathbf{u_R})\rangle = \pi^{-1/2}\int_{-\infty}^{\infty} F(xq\sqrt{2}\,D(\mathbf{n}, \mathbf{R}, T))\,e^{-x^2}dx, \qquad (1)$$

where $q = |\mathbf{q}|$, $\mathbf{n} = \mathbf{q}/q$, T is the absolute temperature, and $D(\mathbf{n}, \mathbf{R}, T)$ is the mean-square fluctuation of the displacement of the $\mathbf{R}$-th atom in the direction of the vector $\mathbf{n}$. It is thus sufficient to find the quantity $D(\mathbf{n}, \mathbf{R}, T) = \langle(\mathbf{n}\cdot\mathbf{u_R})^2\rangle^{1/2}$ for the evaluation of $\langle F(\mathbf{q}\cdot\mathbf{u_R})\rangle$ or, in particular, of the quantity $\langle\exp i(\mathbf{q}\cdot\mathbf{u_R})\rangle$.

It is very difficult to evaluate the quantity $D(\mathbf{n}, \mathbf{R}, T)$ for the case of an imperfect crystal lattice. Among the deformations of a crystalline lattice there is, however, one form of deformation which enables us to overcome the difficulties in the calculation of the quantity $D(\mathbf{n}, \mathbf{R}, T)$. We have in mind the so-called localized lattice defects which can be described by a method developed and effectively used by I. M. Lifshitz[3-9] in several of his papers. This method makes it possible to consider such important lattice defects as the substitution of an atom in the lattice by a foreign atom, the occurrence of a vacancy or of the displacement of an atom in the lattice, and other localized irregularities.

In connection with the proposed use of averages of functions of the form $F(\mathbf{q}\cdot\mathbf{u_R})$ (in particular, in the problem of the elastic scattering of slow neutrons by a mixture of light isotopes), we give in the present paper the evaluation of the mean-square fluctuation $D(\mathbf{n}, \mathbf{R}, T)$ of the displacements of

atoms in a given direction $\mathbf{n}$ for an infinite crystal lattice with a finite number of localized defects.

The local character of the perturbations enables us to choose the normal coordinates of the infinite unperturbed lattice in such a special way that they can be divided into two sets, one of which is not changed by the presence of the perturbation. The method of calculation makes use of this fact and can also be used for other problems connected with vibrations of imperfect lattices.

The small-oscillations equation of any system of atoms can be written in the form

$$m_{\mathbf{R}} \frac{d^2 u_{\mathbf{R}}}{dt^2} = - \sum_{\mathbf{R}', \sigma'} A^{\sigma\sigma'}_{\mathbf{R}\mathbf{R}'} \, u^{\sigma'}_{\mathbf{R}'}, \tag{2}$$

where $m_{\mathbf{R}}$ is the mass of the $\mathbf{R}$-th atom in the lattice, $u^{\sigma}_{\mathbf{R}}$ the component of the displacement of the $\mathbf{R}$-th atom from its equilibrium position along the σ-th axis of a Cartesian system of coordinates, and $A^{\sigma\sigma'}_{\mathbf{R}\mathbf{R}'}$ the coefficients of the interaction between the atoms in the system in the linear approximation. The general solution of the set of differential equations (2) is a superposition of normal vibrations $\xi_{\lambda\rho}\chi_{\lambda\rho}(\mathbf{R})$

$$u_{\mathbf{R}} = (m_{\mathbf{R}})^{-1/2} \sum_{\lambda\rho} \xi_{\lambda\rho} \, \chi_{\lambda\rho}(\mathbf{R}), \tag{3}$$

where the $\xi_{\lambda\rho}$ are normal coordinates, satisfying the equations

$$d^2\xi_{\lambda\rho} / dt^2 + \lambda \xi_{\lambda\rho} = 0$$

($\lambda = \omega^2_{\lambda}$ are the squares of the eigen frequencies of the system); the $\chi_{\lambda\rho}(\mathbf{R})$ form a complete orthonormal set of eigenfunctions of the equation

$$L\chi = \lambda\chi; \tag{4}$$

L is a Hermitian operator defined by its matrix elements

$$L^{\sigma\sigma'}_{\mathbf{R}\mathbf{R}'} = A^{\sigma\sigma'}_{\mathbf{R}\mathbf{R}'} (m_{\mathbf{R}} \, m_{\mathbf{R}'})^{-1/2}. \tag{5}$$

The squares of the eigen frequencies of the system are the eigenvalues of the operator L.

Using Eq. (3) and the fact that the distribution function of the displacements of a one-dimensional oscillator in thermodynamic equilibrium with its surrounding medium is a Gaussian distribution (Bloch[1]), we can write the expression for the square of the fluctuation $D^2(\mathbf{n}, \mathbf{R}, T)$ of the displacement of the $\mathbf{R}$-th atom of the system in the form

$$D^2(\mathbf{n}, \mathbf{R}, T) = m_{\mathbf{R}}^{-1} \sum_{\lambda\rho} f(\lambda, T) \, | \, \mathbf{n}\chi_{\lambda\rho}(\mathbf{R}) \, |^2, \tag{6}$$

where

$$f(\lambda, T) = (h/2\sqrt{\lambda}) \coth (h\sqrt{\lambda}/2kT) \tag{7}$$

is the square of the mean square fluctuation of the Gaussian distribution, T the absolute temperature, and k Boltzmann's constant. We note that Eq. (6) for D^2 can be written in the form

$$D^2(\mathbf{n}, \mathbf{R}, T) = m_{\mathbf{R}}^{-1} \sum_{\sigma\sigma'} \{f(L, T)\}^{\sigma\sigma'}_{\mathbf{R}\mathbf{R}'} \, n^{\sigma} n^{\sigma'}, \tag{8}$$

where the $\{f(L, T)\}^{\sigma\sigma'}_{\mathbf{R}\mathbf{R}'}$ are the matrix elements of the operator $f(L, T)$.

The spectrum of the operator L consists for an infinite perfect crystal lattice of several finite sections of the real axis, and every point of the spectrum of the operator L is infinitely degenerate. In that case we can rewrite Eq. (6) as follows

$$D^2(\mathbf{n}, \mathbf{R}, T) = \frac{1}{m_{\mathbf{R}}} \int f(\lambda, T) \{ \sum_{\rho} | \, \mathbf{n}\psi_{\lambda\rho}(\mathbf{R}) \, |^2 \} \, d\lambda. \tag{9}$$

Following Lifshitz,[3,4] we call a localized lattice deformation any defect that can be taken into account in the small-oscillations equations (2) by adding some finite-dimensional Hermitean operator Λ to the operator L of the unperturbed lattice. A whole series of actually existing defects (substitution of an atom of the basic lattice by a foreign one, vacancies, interstitials, and so on) are defects of this kind. It has been shown[4] that when the operator L is bounded and has a continuous spectrum and the operator Λ has a finite number of dimensions, the spectrum of the perturbed operator $\tilde{L} = L + \Lambda$ can differ from the spectrum of L only in a finite number of isolated points. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be all the points of the discrete spectrum of the operator $\tilde{L} = L + \Lambda$. If we denote all quantities referring to the perturbed operator $\tilde{L}$ by a tilde, ($\sim$) we can, according to (9), write down for the quantity $\tilde{D}^2$ of the perturbed problem the following expression

$$\tilde{D}^2(\mathbf{n}, \mathbf{R}, T) = m_{\mathbf{R}} (\tilde{m}_{\mathbf{R}})^{-1} D^2(\mathbf{n}, \mathbf{R}, T) + (m_{\mathbf{R}})^{-1} S(\mathbf{n}, \mathbf{R}, T), \tag{10}$$

$$S(\mathbf{n}, \mathbf{R}, T) = \int f(\lambda, \quad T) \, \{ \sum_{\rho} | \, \mathbf{n}\tilde{\psi}_{\lambda\rho}(\mathbf{R}) |^2 - \sum_{\rho} | \mathbf{n}\psi_{\lambda\rho}(\mathbf{R}) \, |^2 \} \, d\lambda + \sum_{\lambda_k} f(\lambda_k, T) \, | \, \mathbf{n}, \, \tilde{\psi}_{\lambda_k}(\mathbf{R}) \, |^2, \tag{11}$$

where the $\tilde{\psi}_{\lambda\rho}$ and $\tilde{\psi}_{\lambda k}$ are the eigenfunctions of the operator $\tilde{L}$ corresponding respectively to the continuous and the discrete spectra, and $\tilde{m}_{\mathbf{R}}$ is the mass of the $\mathbf{R}$-th atom of the perturbed lattice.

It is necessary, according to (10), to evaluate the quantity $S(\mathbf{n}, \mathbf{R}, T)$ in order to find the quantity $\tilde{D}^2$. It appears that to do this it is necessary to know the complete set of the eigenfunctions of the operator $\tilde{L}$. Since the perturbing operator Λ has a finite number of dimensions, however, the problem of finding the quantity $\tilde{D}^2(\mathbf{n}, \mathbf{R}, T)$ simplifies considerably.

Let us denote by H_λ the eigen-subspace of the operator L corresponding to the spectral point λ. We separate from this subspace the subspace H''_λ spanned by the functions ψ_λ satisfying the equation $\Lambda\psi_\lambda = 0$. It is clear that any solution of the equation $(L-\lambda)\psi_\lambda = 0$ corresponding to the subspace H''_λ is at the same time a solution of the perturbed equation $(\tilde{L}-\lambda)\psi_\lambda = 0$. We denote by H'_λ the subspace orthogonal to H''_λ which with H''_λ makes up the eigen-subspace H_λ. We consider also subspaces H′ and H″ which are the closures respectively of the subspaces H'_λ and H''_λ with all possible λ (it is evident that any space H is the orthogonal sum of subspaces H'_λ and H''_λ).

Let L′ and L″ be the operators produced by the operator L in the subspaces H′ and H″, respectively. Let $\tilde{L}'$ and $\tilde{L}''$ be similarly the operators produced by the operator $\tilde{L}$, also in the subspaces H′ and H″. One shows easily that $\tilde{L}'' = L''$ and $\tilde{L}' = L' + \Lambda$. This last fact enables us to conclude that all physical consequences caused by the localized perturbation Λ must be describable in terms of the subspace H′. In our particular case this means that we can consider in Eq. (11) for $S(\mathbf{n}, \mathbf{R}, T)$ the summation over ρ to extend only over the eigenfunctions of the operators L′ and L′ + Λ defined in H′. One sees easily that the degree of degeneracy of the spectrum of the operators L′ and L′ + Λ is finite.

It will be found convenient to choose as the basis in H′ a complete set of eigenfunctions of the operator L′. We obtain such a basis by constructing a base in the eigen-subspaces H'_λ of the operator L′. To do this we consider the eigenfunctions $\mathbf{g}_i(\mathbf{R})$ of the operator Λ, i.e., let $\Lambda\mathbf{g}_i = \gamma_i\mathbf{g}_i$, where the γ_i are the non-zero eigenvalues of the operator Λ. The number of functions $\mathbf{g}_i$ is equal to the rank r of the operator Λ. We shall assume that the functions $\mathbf{g}_i$ are normalized to $[\mathbf{g}_i\mathbf{g}_k] = \delta_{ik}$ (here and henceforth the square brackets indicate the scalar product in the atomic-displacements space: $[\mathbf{g}_i\mathbf{g}_k] = \sum_{\sigma,\mathbf{R}} g_i^\sigma(\mathbf{R})\,\overline{g_k^\sigma(\mathbf{R})}$.

If we choose for the eigenfunctions of the operator L the usual representation

$$\chi_{k,s}(\mathbf{R}) = \mathbf{e}_{k,s}\exp[ik\mathbf{R}] \tag{12}$$

[here $\mathbf{e}_{k,s}$ is the polarization vector, $\mathbf{k}$ a reciprocal-lattice vector multiplied by 2π, and s the number of the vibration mode; the eigenvalues of the operator L in this representation are functions of $\mathbf{k}$ and s: $\lambda = \lambda_s(\mathbf{k})$], we can write the vectors $\mathbf{g}_i(\mathbf{R})$ in the form

$$g_i(\mathbf{R}) = \int \varphi_{\lambda,i}(\mathbf{R})\,d\lambda, \tag{13}$$

$$\varphi_{\lambda,i} = \sum_s \int \frac{[g_i\chi_{k,s}]\,\chi_{k,s}(\mathbf{R})\,d\Omega}{|\nabla\lambda_s(\mathbf{k})|}. \tag{14}$$

The integrals in (14) [and also those in (17) below] are taken over the surfaces $\lambda_s(\mathbf{k}) = \lambda$.

One can show that the space spanned by all functions $\varphi_{\lambda,i}$ with a given value of λ completely exhausts the subspace H'_λ. From this it follows that the closure of the linear envelope of the functions $\varphi_{\lambda,i}$ with all possible λ and i contains within itself the subspace H′. The functions

$$\psi_{\lambda\rho} = \sum_i c_{\rho i}(\lambda)\,\varphi_{\lambda,i} \tag{15}$$

with the $c_{\rho i}(\lambda)$ satisfying the conditions

$$\sum_{ij} c_{\rho i}(\lambda)\,\overline{c_{\rho' j}(\lambda)}\,\alpha_{ij}(\lambda) = \delta_{\rho\rho'}, \tag{16}$$

where

$$\alpha_{ij}(\lambda) = \sum_s \int \frac{[g_i\chi_{k,s}]\,[g_j\chi_{k,s}]\,d\Omega}{|\nabla\lambda_s(\mathbf{k})|}, \tag{17}$$

form thus an orthonormal basis for the space H′.

We shall look for solutions of the perturbed equation $(L' + \Lambda - \lambda)\tilde{\psi}_\lambda = 0$ in the form of an expansion in terms of the eigenfunctions of the operator L′; to do this we write

$$(L' - \lambda)\tilde{\psi}_\lambda = -\Lambda\tilde{\psi}_\lambda. \tag{18}$$

Since $\Lambda\tilde{\psi}_\lambda$ belongs to the subspace of the functions $\mathbf{g}_i$,

$$(L' - \lambda)\tilde{\psi}_\lambda = \sum_i c_i(\lambda)\,\mathbf{g}_i = \sum_i c_i(\lambda)\int \varphi_{\mu i}\,d\mu.$$

We have thus for the eigenfunctions of the operator L′ + Λ

$$\tilde{\psi}_\lambda = \sum_i c_i(\lambda)\left\{\int \frac{\varphi_{\mu i}\,d\mu}{\mu - \lambda} + A(\lambda)\,\psi_{\lambda,i}\right\}. \tag{19}$$

The symbol $\int$ indicates here the principal-value integral. $A(\lambda)$ is a regularizing function, which depends on λ and which must be determined together with the coefficients $c_i(\lambda)$. It is clear that for the discrete spectrum of the operator L′ + Λ, the integrals in (19) are taken in the usual sense and $A(\lambda) \equiv 0$.

To determine the functions $c_i(\lambda)$ and $A(\lambda)$, we apply to both sides of Eq. (19) the operator Λ and multiply the result by $\mathbf{g}_j$. This leads to a set of r homogeneous linear equations for the $c_i(\lambda)$:

$$\sum_i c_i(\lambda)\left[A(\lambda)\,\alpha_{ij}(\lambda) + \int \frac{\alpha_{ij}(\mu)}{\mu - \lambda}\,d\mu + \delta_{ij}/\gamma_j\right] = 0. \tag{20}$$

If λ belongs to the spectrum of the operator L, the condition that the set (20) be solvable leads to an algebraic equation for $A(\lambda)$ of degree not

greater than r (if λ does not belong to the spectrum of the operator L, this condition gives us an equation for the points of the discrete spectrum of the perturbed operator $L' + \Lambda$). Let $A_\rho(\lambda)$ be the solutions of this equation, and let the $c_{\rho i}(\lambda)$ be the corresponding solutions of the set (20). It is clear that $c_{\rho i}(\lambda)$ with different values of ρ are orthogonal to one another in the metric defined by the matrix $\| \alpha_{ij}(\lambda) \|$ and that they can thus be chosen to satisfy Eq. (16). If we substitute in (19) the values obtained for $A_\rho(\lambda)$ and for the $c_{\rho i}(\lambda)$, normalized according to (16), we find the eigenfunctions of the continuous spectrum of the perturbed problem

$$\tilde{\psi}_{\lambda\rho} = N_\rho(\lambda)\left\{A_\rho(\lambda)\sum_i c_{\rho i}(\lambda)\varphi_{\lambda i} + \sum_i c_{\rho i}(\lambda)\int \frac{\varphi_{\mu i}\, d\mu}{\mu - \lambda}\right\}, \quad (21)$$

where $N_\rho(\lambda)$ is a normalization factor. One can show* that

$$N_\rho(\lambda) = [A_\rho^2(\lambda) + \pi^2]^{-1/2}.$$

If we put

$$\theta_{\lambda\rho} = \frac{1}{\pi}\sum_i c_{\rho i}(\lambda)\int \frac{\varphi_{\mu i}}{\mu - \lambda}\, d\mu, \quad (22)$$

and introduce the function

$$\zeta_\rho(\lambda) = \cot^{-1}(\pi^{-1} A_\rho(\lambda)), \quad (23)$$

we can therefore rewrite Eq. (21) as follows

$$\tilde{\psi}_{\lambda\rho} = \cos\zeta_\rho(\lambda)\,\psi_{\lambda\rho} + \sin\zeta_\rho(\lambda)\,\theta_{\lambda\rho}, \quad (24)$$

where the functions $\psi_{\lambda\rho}$ are given by Eq. (15).

Comparison shows the functions $\zeta_\rho(\lambda)$, defined by Eq. (23) and by the equation for $A_\rho(\lambda)$, to be the same as the shift functions, first obtained by a slightly different method by I. M. Lifshitz for the one-dimensional[4] and the many-dimensional[6] cases. Lifshitz showed (see also a paper by Kreĭn[11]) that if we know the functions $\zeta_\rho(\lambda)$ we can find the difference of the traces of two operators such as $f(L + \Lambda)$ and $f(L)$, where $f(x)$ is one of a very large class of functions. One can show from the asymptotic behavior of the functions $\tilde{\psi}_{\lambda\rho}$ and $\psi_{\lambda\rho}$ at large distances from the lattice defect that the functions $\zeta_\rho(\lambda)$ also determine the phase shift of the wave scattered by the localized defect. This conclusion is a generalization of Lifshitz' result[12] to problems that are not spherically symmetric.

One can use the properties of the functions $\psi_{\lambda\rho}$, $\theta_{\lambda\rho}$, and $\zeta_\rho(\lambda)$ to show that the functions $\tilde{\psi}_{\lambda\rho}$ form a complete orthonormal set of eigenfunctions of the operator $L' + \Lambda$ in the continuous spectrum.

To find the functions $\tilde{\psi}_{\lambda_k}$ of the discrete spectrum of the operator $L' + \Lambda$ we must put $A(\lambda) = 0$ in Eqs. (19) and (20) and write integrals in the usual sense instead of principal-value integrals. The condition that Eqs. (20) be solvable gives us an equation for the eigenvalues λ_k of the operator $L' + \Lambda$ in the discrete spectrum. The expressions for the $\tilde{\psi}_{\lambda_k}$ and the corresponding normalization conditions can easily be obtained and are therefore omitted here.

Having found the eigenfunctions (15) and (24) of the operators L' and $L' + \Lambda$, we can use (11) to evaluate $S(\mathbf{n}, \mathbf{R}, T)$ and thus also $\tilde{D}^2(\mathbf{n}, \mathbf{R}, T)$ from (10). We get for $S(\mathbf{n}, \mathbf{R}, T)$ the following expression

$$S(\mathbf{n}, \mathbf{R}, T) = \frac{h}{2}\int \coth\left(\frac{h\sqrt{\lambda}}{2kT}\right) F(\lambda, \mathbf{R})\,\frac{d\lambda}{\sqrt{\lambda}} + \frac{h}{2}\sum_{\lambda_i} \coth\left(\frac{h\sqrt{\lambda_i}}{2kT}\right)\frac{1}{\sqrt{\lambda_i}}(\mathbf{n}\tilde{\psi}_{\lambda i}(\mathbf{R}))^2; \quad (25)$$

$$F(\lambda, \mathbf{R}) = \sum_\rho \{\sin^2\zeta_\rho(\lambda)\,[|\,\mathbf{n}\theta_{\lambda\rho}(\mathbf{R})\,|^2 - |\,\mathbf{n}\psi_{\lambda\rho}(\mathbf{R})\,|^2] + \tfrac{1}{2}\sin 2\zeta_\rho(\lambda)\,[(\mathbf{n}\theta_{\lambda\rho}(\mathbf{R}))\,\overline{(\mathbf{n}\psi_{\lambda\rho}(\mathbf{R}))} + \overline{(\mathbf{n}\theta_{\lambda\rho}(\mathbf{R}))}\,(\mathbf{n}\psi_{\lambda\rho}(\mathbf{R}))]. \quad (26)$$

Knowing the value of $\tilde{D}^2(\mathbf{n}, \mathbf{R}, T)$ for the perturbed problem we can easily use Eq. (1) to evaluate the time average of any function $F(\mathbf{q}\cdot\mathbf{u}_\mathbf{R})$ when localized defects are present in the crystal lattice. We obtain in that way the complete solution of the problem posed in the present paper.

Expression (25) derived for $S(\mathbf{n}, \mathbf{R}, T)$, along with Eq. (10) for the square of the mean-square fluctuation of the displacements of the atoms of a crystal lattice with a finite number of defects, can be used to draw some conclusions about the behavior of the quantity $\tilde{D}^2$ at large distances from the defects. A detailed analysis of Eqs. (25) and (26) shows that at large distances R from a defect the asymptotic behavior of Eq. (25) for S is determined solely by the long-wave part of the spectrum, so that we can neglect in the expression for S the contribution from the optical modes of vibrations and the contribution from the vibrations corresponding to the discrete spectrum. One can evalu-

*The proof of this statement, as of some other statements about the functions $\tilde{\psi}_{\lambda\rho}$, is omitted here because it is cumbersome. These proofs are based upon a consideration of the asymptotic behavior of the functions $\tilde{\psi}_{\lambda\rho}$ at large distances from the localized defect. Their asymptotic behavior can be found, if one knows the asymptotic behavior of the functions $\varphi_{\lambda i}$. The functions $\varphi_{\lambda i}$ are by (14) expressed as a sum of integrals. Lifshitz[5] and Lifshitz and Peresada[10] have evaluated the asymptotic behavior of similar integrals in connection with other problems.

ate the asymptotic behavior in the general case of an arbitrary lattice and of any localized defect. We shall not perform here the fairly cumbersome and tiresome calculation, but only quote the general result.

For large values of R the asymptotic behavior of S is the sum of a finite number of terms of the form

$$A_i \frac{T}{\Theta}\left(\frac{b}{R}\right)^2 \coth\left(B_i \frac{RT}{b\Theta}\right),$$

where the quantities A_i and B_i can be evaluated in closed form for each given crystal and each given perturbation. They depend on the direction of the radius vector $\mathbf{R}$ at the point of observation, on the differential properties of the surfaces $\lambda_i(\mathbf{k}) = \lambda$ as $\lambda \to 0$, and on the type of the lattice defect. Θ is some characteristic temperature similar to the Debye temperature, and b is a characteristic length of the same order of magnitude as the dimensions of the elementary crystal cell.

It follows from the expression given here for S that at crystal temperatures T and at distances R such that $RT \ll b\Theta$ the asymptotic form of S is

$$A\left(\frac{b}{R}\right)^3 + B\left(\frac{T}{\Theta}\right)^2 \frac{b}{R}$$

where for a given lattice and a given perturbation A and B depend only on the vector $\mathbf{R}/R$. In particular, $S \sim A(b/R)^3$ when $T = 0$, i.e., at absolute zero the extra term in the fluctuation of the displacement decreases in inverse proportion to the cube of the distance from the defect. When $RT \gg b\Theta$ this extra term decreases as $1/R^2$.

Summarizing the results of this paper we can reach the following conclusions:

1. The time average of any function of the dot product of a constant vector $\mathbf{q}$ and the displacement from the equilibrium position $\mathbf{u_R}$ of the $\mathbf{R}$-th atom of any system of atoms which executes small vibrations and which is in thermodynamic equilibrium with the surrounding medium is uniquely determined by the mean square fluctuation $D(\mathbf{n}, \mathbf{R}, T)$ of the displacements of the $\mathbf{R}$-th atom in the direction of the vector $\mathbf{n} = \mathbf{q}/q$.

2. One can evaluate the fluctuation $D(\mathbf{n}, \mathbf{R}, T)$ in closed form in the case of an arbitrary infinite perfect crystal lattice in which there is a finite number of localized defects such as foreign atoms substituted for an atom, interstitials, vacancies, and so on, provided one knows the spectral properties of the corresponding perfect lattice without defects and provided one knows the finite-dimensional operator Λ which describes these defects.

Although the determination of $D(\mathbf{n}, \mathbf{R}, T)$ can be reduced to the evaluation of the trace of an operator, it turns out to be impossible to apply here Lifshitz' results[6] on the evaluation of the difference between traces, since in this case one cannot write the operator whose trace determines the value of $D(\mathbf{n}, \mathbf{R}, T)$ as some function of the operator L.

3. The change in the square of the function $D(\mathbf{n}, \mathbf{R}, T)$, caused by the presence of localized deformations in the crystal lattice, is determined, according to (10), by the function $S(\mathbf{n}, \mathbf{R}, T)$; we suggested in this paper a special method of evaluating this function. This method is based upon the fact that, in the case of localized lattice deformations described by adding a finite-dimensional operator Λ to the operator L, it turns out to be possible to split off from the space H, on which the operator L is determined, a subspace H′ such that all physical consequences caused by the perturbation Λ can be described in terms of the subspace H′. This makes it possible to obtain the closed Eq. (25) for $S(\mathbf{n}, \mathbf{R}, T)$.

4. As expected, the quantities $\zeta_\rho(\lambda)$, first defined by Lifshitz[6] for the case of a three-dimensional lattice and called by him "shifts," occur in the expression for $S(\mathbf{n}, \mathbf{R}, T)$. These quantities determine the phase shifts of the waves scattered by a localized inhomogeneity of the crystal.

5. In the general case of an arbitrary infinite perfect crystal with a finite number of localized defects, one can find the asymptotic behavior of the function at large distances from the defects. The asymptotic expression for S includes the dependence on the form of the localized irregularity of the lattice. The difference between the mean-square fluctuations $\tilde{D}^2$ and D^2 of the perturbed and the unperturbed lattices at absolute zero decreases with the distance R as R^{-3}. At sufficiently low temperatures, there is a region in the crystal where $(\tilde{D}^2 - D^2) \sim AR^{-3} + T^2R^{-1}$. Outside this region $(\tilde{D}^2 - D^2) \sim TR^{-2}$ as $R \to \infty$.

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