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DYNAMICS OF POLYATOMIC CRYSTALS AND IMPERFECT CRYSTALS

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The dynamics of crystals with isolated impurity atom chains and planes is considered within the framework of the general problem of oscillations of binary crystalline systems.[1] The total system spectrum and oscillation spectrum of the separate atoms are expressed in terms of suitably defined spectral functions for the initial "reference" lattice by means of the same type of functionals as those defining the spectral properties of crystals with isolated impurity atoms.

1. INTRODUCTION

In an earlier paper[1] we considered the dynamic problem for binary crystalline compounds of type AB_{r-1} with r atoms per unit cell, constructed by periodic filling the sites of the same Bravais lattice with atoms A and B. Under the simplified but frequently not wholly justified assumption that the force constants depend only on the difference between the radius vectors of the atoms in the lattice, but not on the type of atom, it was possible to solve the indicated problem in terms of the dynamic problem for a certain "standard" monatomic lattice and to consider in unified fashion the problem of the oscillations of systems which, at first glance, are as different as the diatomic crystals of the NaCl and CsCl type,[2] crystals of the type of fully ordered alloys ($AuCu_3$, $AlFe_3$, etc.), and a monatomic lattice with isolated impurity atoms.[3-5]

Further analysis has shown that the results of [1] can also be used directly to determine the oscillation of crystal lattices containing very simple extended defects—arbitrary oriented chains, and also plane clusters of impurity atoms.1)

The present paper is devoted to a general analysis of the dynamics of such systems. A large number of aspects of dynamics of crystals with extended defects of very general type (dislocations, stacking faults) were considered recently in the long-wave approximation by I. Lifshitz and Kosevich.[7] In this paper, unlike in [7], we consider defects with simpler structure, so that we can analyze the entire frequency spectrum within the framework of microscopic lattice dynamics, without resorting to the elasticity-theory approximation. Together with the complete frequency spectrum we consider here also the spectrum of oscillations of individual atoms (both impurity and host), knowledge of which is essential, for example, to determine the probability of the Mossbauer effect and other dynamic effects connected with the interaction between radiation and crystals.

2. SPECTRUM OF OSCILLATIONS OF INDIVIDUAL ATOMS AND COMPLETE FREQUENCY SPECTRUM

We start from the general solution obtained in [1] for the dynamic problem for compounds of the AB_{r-1} type. Namely, if some of the initial lattice points $\mathbf{x}_\mathbf{n}$, forming a regular sublattice ξ_ν, is occupied by atoms of species A with mass M_0, and the remaining lattice points $\mathbf{x}_\mathbf{n}$ are occupied by atoms of a different species B with mass M, and if the force constants depend only on the difference between the radius vectors of the atoms in the lattice, then the dynamic problem for such a structure reduces to a system of equations

$$M_\mathbf{n}\omega^2(\mathbf{f}, \sigma)\,\psi_{\mathbf{f}\sigma}{}^{i}(\mathbf{x}_\mathbf{n}) = \sum_{\mathbf{n}}{}' A^{ii'}(\mathbf{x}_\mathbf{n} - \mathbf{x}_{\mathbf{n}'})\,\psi_{\mathbf{f}\sigma}{}^{i'}(\mathbf{x}_{\mathbf{n}'}), \qquad (2.1)$$

$$M_\mathbf{n} = M\Big(1 - \lambda\sum_{\nu}\delta_{\mathbf{x}_\mathbf{n}-\mathbf{x}_{\mathbf{n}_0},\,\xi_\nu}\Big),$$

$$\lambda = 1 - \frac{M_0}{M} \quad (-\infty < \lambda < 1) \qquad (2.2)$$

[1)] Localized oscillations of the impurity atoms proper, forming isotopic defects of this type, were considered by Kobori[6] for an artificial model of a simple cubic lattice, in which account is taken of the interaction only between nearest neighbors, and the constants of the central and noncentral interactions are assumed equal. In his paper, the problem of finding the spectrum of the impurity atoms reduces to a solution of certain equations containing elliptic integrals of the first kind. The equations are analyzed for the case of a small difference between the masses M_0 and M. However, this analysis is in error: singularities that do not vanish in the limit as $M_0 \to M$ were obtained in the spectrum.

and has solutions determined by the following relations:

$$\psi_{\mathbf{f}\sigma}{}^{i}(\mathbf{x_n}) = \sqrt{r/N}\, v_{\mathbf{f}\sigma}{}^{i}(\mathbf{x_n}) \exp\{i\mathbf{f}(\mathbf{x_n} - \mathbf{x_{n_0}})\},$$

$$v_{\mathbf{f}\sigma}{}^{i}(\mathbf{x_n} + \boldsymbol{\xi}_{\mathbf{v}}) = v_{\mathbf{f}\sigma}{}^{i}(\mathbf{x_n}); \tag{2.3}$$

$$\sum_{j=0}^{r-1} M_{\mathbf{n}_j} v^{i*}_{\mathbf{f}\sigma}(\mathbf{x}_{\mathbf{n}_j})\, v^{i}_{\mathbf{f}\sigma'}(\mathbf{x}_{\mathbf{n}_j}) = \delta_{\sigma\sigma'},$$

$$\sum_{\sigma=1}^{3r} v_{\mathbf{f}\sigma}{}^{i*}(\mathbf{x}_{\mathbf{n}_j})\, v_{\mathbf{f}\sigma}{}^{i'}(\mathbf{x}_{\mathbf{n}_{j'}}) = \frac{1}{M_{\mathbf{n}_j}}\delta_{jj'}\delta^{ii'}; \tag{2.4}$$

$$j^{i} = D^{ik}(\omega^2, \mathbf{f})\, j^{k}; \tag{2.5}$$

$$D^{ik}(\omega^2, \mathbf{f}) \equiv \frac{\lambda\omega^2}{r} \sum_{\mu}{}^{(0)} \sum_{s=1}^{3} \frac{e^{i}(\mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu}, s)\, e^{k}(\mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu}, s)}{\omega^2 - \omega_0{}^2(\mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu}, s)}; \tag{2.6}$$

$$\Delta(\omega^2, \mathbf{f}) \equiv \det\{\delta^{ik} - D^{ik}(\omega^2, \mathbf{f})\} = 0; \tag{2.7}$$

$$v_{\mathbf{f}\sigma}{}^{i}(\mathbf{x}_{\mathbf{n}_0}) = \frac{1}{\sqrt{M}}\left[\frac{d\ln\omega^2(\mathbf{f}, \sigma)}{d\lambda}\right]^{1/2} j_{\mathbf{f}\sigma}{}^{i} \neq 0; \tag{2.8}$$

the connection between the lattices

$$x_{\mathbf{n}}{}^{i} = \sum_{p=1}^{3} a_p{}^{i} n_p \quad (X), \qquad \xi_{\mathbf{v}}{}^{i} = \sum_{p=1}^{3} \alpha_p{}^{i}\nu_p \quad (\Xi),$$

$$y_{\mathbf{m}}{}^{i} = \sum_{p=1}^{3} b_p{}^{i} m_p \quad (Y), \qquad \eta_{\mu}{}^{i} = \sum_{p=1}^{3} \beta_p{}^{i}\mu_p \quad (\mathrm{H}) \tag{2.9}$$

(X and Ξ are the space lattices, and Y and H are the corresponding reciprocal lattices) is given by the relation between their basis vectors $\mathbf{a}_p$, $\boldsymbol{\alpha}_p$, $\mathbf{b}_p$, and $\boldsymbol{\beta}_p$:

$$\hat{\alpha} = \hat{P}\hat{a}, \qquad \hat{b} = \tilde{\hat{a}}^{-1} = \tilde{\hat{P}}\tilde{\hat{\alpha}}^{-1} = \tilde{\hat{P}}\hat{\beta},$$

$$\hat{\beta} = \tilde{\hat{\alpha}}^{-1} = \tilde{\hat{P}}^{-1}\hat{b} \tag{2.10}$$

$a_{pi} \equiv a_p^i$ etc.; the tilde over the letter denotes the transpose).

We shall use essentially the same notation as in [1]: superior Latin indices are Cartesian; n_p, ν_p, m_p, and μ_p—arbitrary integers; $P_{pp'}$—specified integer coefficients; $v_X = \det\hat{\alpha}$ and $v_\xi = \det\hat{\alpha}$—volumes of the unit cells of lattices X and Ξ; $r = \det\hat{P}$—number of atoms in the unit cell of structure Ξ; $\omega^2(\mathbf{f}, \sigma)$—the exact solutions of (2.7), which is of the order 3r; $\sigma = 1, 2, \ldots, 3r$—number of such a solution (number of the branch); $\mathbf{f}$—wave vector, which takes on N/r values in the region $W_\xi \equiv (2\pi)^3/v_\xi$ (for example, of the corresponding unit cell or the first Brillouin zone of the H lattice); N—total number of lattice points (the number of unit cells is N/r); the index j numbers the atoms in the initial and final unit cell of the structure Ξ; j = 0 (x_{n_0}) corresponds to atoms of species A; $j_{\mathbf{f}\sigma}$—real unit vector; $\sum_{\mu}^{(0)}$—summation over r points of the lattice H, belonging to the fundamental cell or to the Brillouin zone of the lattice Y; $\omega_0^2(\mathbf{f}, s)$ and $e^{i}(\mathbf{f}, s)$—solution of the dynamic problem for the "standard" monatomic crystal X, i.e., the problem (2.1) with $M_n = M$ ($\lambda = 0$);

$$M\omega_0{}^2(\mathbf{f}, s)\, e^{i}(\mathbf{f}, s) = G^{ii'}(\mathbf{f})\, e^{i'}(\mathbf{f}, s) \quad (s = 1, 2, 3),$$

$$G^{ii'}(\mathbf{f}) = \sum_{\mathbf{n}} A^{ii'}(\mathbf{x_n}) \exp(-i\mathbf{f}\mathbf{x_n});$$

$$e^{i}(\mathbf{f}, s)\, e^{i}(\mathbf{f}, s') = \delta_{ss'}, \qquad \sum_{s=1}^{3} e^{i}(\mathbf{f}, s)\, e^{i'}(\mathbf{f}, s) = \delta^{ii'} \tag{2.11}$$

(in (2.11) $\mathbf{f}$ varies in the region $w_X \equiv (2\pi)^3/v_X$ corresponding to the fundamental cell of the lattice Y). Putting in the first relation of (2.4) $\sigma = \sigma'$, and in the second $j = j'$ and $i = i'$, we obtain for arbitrary $\mathbf{f}$, with allowance for (2.8),

$$M\sum_{j=1}^{r-1} |\mathbf{v}_{\mathbf{f}\sigma}(\mathbf{x}_{\mathbf{n}_j})|^2 = 1 - (1 - \lambda)\frac{d\ln\omega^2(\mathbf{f}, \sigma)}{d\lambda},$$

$$(1 - \lambda)\sum_{\sigma=1}^{3r} \frac{d\ln\omega^2(\mathbf{f}, \sigma)}{d\lambda}(j_{\mathbf{f}\sigma}{}^{i})^2 = 1,$$

$$\frac{1}{3}(1 - \lambda)\sum_{\sigma=1}^{3r} \frac{d\ln\omega^2(\mathbf{f}, \sigma)}{d\lambda} = 1 \tag{2.12}$$

Besides the amplitude of the displacement of atoms A (2.8), we obtained in [1] a general expression for the amplitude of the displacement of any atom. However, to describe the oscillations of the individual atoms it turns out to be more convenient to introduce in lieu of the amplitudes $\mathbf{v}_{\mathbf{f}\sigma}(\mathbf{x_n})$ the tensor quantity[2)]

$$g^{ik}_{(j)}(\omega^2) = \lim_{\substack{N\to\infty \\ \tau\to 0}} \frac{r}{\pi N}\operatorname{Im}\sum_{\mathbf{f}}\sum_{\sigma=1}^{3r} \frac{M_j v_{\mathbf{f}\sigma}{}^{i*}(\mathbf{x}_{\mathbf{n}_j})\, v_{\mathbf{f}\sigma}{}^{k}(\mathbf{x}_{\mathbf{n}_j})}{\omega^2 - \omega^2(\mathbf{f}, \sigma) - i\tau} \tag{2.13}$$

(at first $N \to \infty$, and then $\tau \to 0$; $M_j \equiv M_{nj}$), which, in accordance with (2.4), is normalized by the condition

$$\int_0^{\omega_m{}^2} g^{ik}_{(j)}(\omega^2)\, d\omega^2 = \delta^{ik} \tag{2.14}$$

(ω_m is the limiting oscillation frequency of the crystal Ξ) and determines the spectral distribution of the oscillations of the j-th atom with allowance for the spatial anisotropy. Starting with (2.13), (2.13), the sum over $\mathbf{f}$ denotes summation over the region $w_\xi \equiv (2\pi)^3/v_\xi$; summation over the re-

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[2)] We shall henceforth use the equivalent notation

$$\lim_{N\to\infty}\frac{1}{N}\sum_{\mathbf{f}} F(\mathbf{f}) \equiv \frac{v_x}{(2\pi)^3}\int d^3f\, F(\mathbf{f}) \equiv \frac{v_\xi}{r(2\pi)^3}\int d^3f\, F(\mathbf{f}).$$

gion $w_X \equiv (2\pi)^3/v_X$ will be denoted by a sum over **f** with index $^{(0)}$. Inasmuch as $v^{i*}_{\mathbf{f}\sigma}(\mathbf{x}_{\mathbf{n}_j} = v^{i}_{-\mathbf{f}\sigma}(\mathbf{x}_{\mathbf{n}_j})$ and $\omega^2(-\mathbf{f}, \sigma) = \omega^2(\mathbf{f}, \sigma)$, the real function $g^{ik}_{(j)}(\omega^2)$ is symmetrical in the indices.

Averaging of (2.13) over the directions of the oscillations leads to the spectral function

$$g_{(j)}(\omega^2) \equiv \frac{1}{3} g^{ii}_{(j)}(\omega^2) = \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{r}{3\pi N} \sum_{\mathbf{f}} \sum_{\sigma=1}^{3r} \frac{M_j \,|\, \mathbf{v}_{\mathbf{f}\sigma}(\mathbf{x}_{\mathbf{n}_j})\,|^2}{\omega^2 - \omega^2(\mathbf{f}, \sigma) - i\tau} \times \int_0^{\omega_m^2} g_{(j)}(\omega^2)\, d\omega^2 = 1. \tag{2.15}$$

If we further average (2.15) over all the atoms in the unit cell, with allowance for (2.4), we immediately obtain the usual definition of the distribution function of the squares of the frequencies of the entire crystal, in the form

$$g(\omega^2) \equiv \frac{1}{r} \sum_{j=0}^{r-1} g_{(j)}(\omega^2) = \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{1}{3\pi N} \sum_{\mathbf{f}} \sum_{\sigma=1}^{3r} \frac{1}{\omega^2 - \omega^2(\mathbf{f}, \sigma) - i\tau},$$

$$\int_0^{\omega_m^2} g(\omega^2)\, d\omega^2 = 1. \tag{2.16}$$

It is significant that the functions (2.15) and (2.16) can be directly expressed in terms of the secular determinant $\Delta(\omega^2, \mathbf{f})$ (2.7), namely

$$g(\omega^2) = g_0(\omega^2) + \frac{\partial}{\partial\omega^2} \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{1}{3\pi N} \operatorname{Im} \sum_{\mathbf{f}} \ln \Delta(\omega^2 - i\tau, \mathbf{f}), \tag{2.17}$$

$$g_A(\omega^2) \equiv g_{(0)}(\omega^2) = -\frac{r(1-\lambda)}{\omega^2} \times \frac{\partial}{\partial\lambda} \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{1}{3\pi N} \operatorname{Im} \sum_{\mathbf{f}} \ln \Delta(\omega^2 - i\tau, \mathbf{f}), \tag{2.18}$$

$$g_B(\omega^2) \equiv \frac{1}{r-1} \sum_{j=1}^{r-1} g_{(j)}(\omega^2) = \frac{1}{r-1} [r g(\omega^2) - g_A(\omega^2)] = \frac{r}{r-1} \Big\{ g_0(\omega^2) + \Big(\frac{\partial}{\partial\omega^2} + \frac{1-\lambda}{\omega^2} \frac{\partial}{\partial\lambda} \Big) \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{1}{3\pi N} \operatorname{Im} \sum_{\mathbf{f}} \ln \Delta(\omega^2 - i\tau, \mathbf{f}) \Big\}, \tag{2.19}$$

where

$$g_0(\omega^2) = \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{1}{3\pi N} \sum_{\mathbf{f}}^{(0)} \sum_{s=1}^{3} \frac{1}{\omega^2 - \omega_0^2(\mathbf{f}, s) - i\tau},$$

$$\int_0^{\omega_{0m}^2} g_0(\omega^2)\, d\omega^2 = 1 \tag{2.20}$$

is the distribution function of the squares of the frequencies of the "standard" lattice, normalized to unity (ω_{0m}—limiting frequency). We recall that the sum over **f** with index $^{(0)}$ denotes summation over the region w_X.

Expression (2.17) was obtained in [1]. The validity of expression (2.18) for the spectral function of the atom A can be directly verified by comparing it with (2.15) at j = 0, where $\mathbf{v}_{\mathbf{f}\sigma}(\mathbf{x}_{\mathbf{n}_0})$ is replaced by its value in (2.8). Inasmuch as the summation over **f** and over σ is actually carried out at constant $\omega^2(\mathbf{f}, \sigma) = \omega^2$, expression (2.15) assumes after such a substitution the form

$$g_{(0)}(\omega^2) = \frac{r(1-\lambda)}{\omega^2} \lim_{\substack{N\to\infty\\ \tau\to 0}} \frac{1}{3\pi N} \operatorname{Im} \sum_{\mathbf{f}} \sum_{\sigma=1}^{3r} \frac{d\omega^2(\mathbf{f}, \sigma)}{d\lambda} \frac{1}{\omega^2 - \omega^2(\mathbf{f}, \sigma) - i\tau}.$$

Exactly the same expression is obtained from (2.18) by writing the determinant $\Delta(\omega^2, \mathbf{f})$ in the form[1]

$$\Delta(\omega^2, \mathbf{f}) = (1-\lambda)^3 \prod_{\sigma=1}^{3r} (\omega^2 - \omega^2(\mathbf{f}, \sigma)) \times \Big[\prod_{\mu}^{(0)} \prod_{s=1}^{3} (\omega^2 - \omega_0^2(\mathbf{f} + 2\pi\eta_\mu, s)) \Big]^{-1} \tag{2.21}$$

and taking account of the fact that the denominator in (2.21) does not depend on λ, while the factor $(1-\lambda)^3$ makes no contribution to (2.18), owing to the sign of the imaginary part. (We use here the symbol $\partial/\partial\lambda$ and not $d/d\lambda$, since in addition to λ there is another independent variable ω^2 on which $\Delta(\omega^2 - i\tau, \mathbf{f})$ depends.) In the derivation of (2.19) we used the normalization condition (2.12) (the first relation).

The function $g_B(\omega^2)$ characterizes the spectrum of the oscillations of atoms of species B, averaged over all such atoms. If all the atoms B occupy in the crystal equivalent positions, which can be obtained from one another by symmetry transformations, then (2.19) characterizes the oscillations of each individual atom B.

Expressions (2.17)–(2.19) make it possible, in principle, to obtain the corresponding spectral functions directly in terms of the solution of the dynamic problem (2.11) for a "standard" lattice.

All the obtained results pertain to binary compounds AB_{r-1} with arbitrary r and arbitrary form of unit cell. In particular, putting $\alpha_p \to \infty$ (p = 1, 2, 3), and taking into account the fact that in this case $r \to \infty$ ($1 \ll r \ll N$), $\beta_p \to 0$ ($p = 1, 2, 3$), and the region of permissible values of $\mathbf{f}$—the volume of the unit cell (or of the Brillouin zone) of the lattice H—also tends to zero at the same time (i.e., $\mathbf{f} \to 0$), we obtain directly the most important spectral function for the monatomic lattice with isolated impurity atoms ($1/r$—impurity concentration):

$$g(\omega^2) = \frac{1}{3}\sum_{\alpha=1}^{3} g^{(\alpha)}(\omega^2), \qquad g_0(\omega^2) = \frac{1}{3}\sum_{\alpha=1}^{3} g_0^{(\alpha)}(\omega^2),$$

$$g_A{}^{\alpha\beta}(\omega^2) = g_A^{(\alpha)}(\omega^2)\,\delta^{\alpha\beta}, \qquad g_B{}^{\alpha\beta}(\omega^2) = g_B^{(\alpha)}(\omega^2)\,\delta^{\alpha\beta}; \tag{2.22}$$

$$g^{(\alpha)}(\omega^2) - g_0^{(\alpha)}(\omega^2) = \frac{1}{\pi r}\frac{\partial}{\partial\omega^2}\lim_{\tau\to 0}\operatorname{Im}\ln\Delta_0^{(\alpha)}(\omega^2 - i\tau, 0), \tag{2.23}$$

$$g_A^{(\alpha)}(\omega^2) = -\frac{1-\lambda}{\pi\omega^2}\frac{\partial}{\partial\lambda}\lim_{\tau\to 0}\operatorname{Im}\ln\Delta_0^{(\alpha)}(\omega^2 - i\tau, 0), \tag{2.24}$$

$$g_B^{(\alpha)}(\omega^2) = \frac{1}{r-1}[rg^{(\alpha)}(\omega^2) - g_A^{(\alpha)}(\omega^2)] \approx g^{(\alpha)}(\omega^2)$$

$$+\frac{1}{r}[g_0^{(\alpha)}(\omega^2) - g_A^{(\alpha)}(\omega^2)],$$

$$\lim_{\tau\to 0}\operatorname{Im}\ln\Delta_0^{(\alpha)}(\omega^2 - i\tau, 0) = -\tan^{-1}\Bigl\{\pi\lambda\omega^2 g_0^{(\alpha)}(\omega^2)\cdot \tag{2.25}$$

$$\Bigl[1 - \lambda\omega^2\int_0^{\omega_{0m}^{(\alpha)2}}\frac{g_0^{(\alpha)}(\omega_0^2)\,d\omega_0^2}{\omega^2 - \omega_0^2}\Bigr]^{-1}\Bigr\}, \tag{2.26}$$

where

$$g_0^{(\alpha)}(\omega^2) = \lim_{\tau\to 0}\frac{v_x}{\pi(2\pi)^3}\operatorname{Im}\sum_{s=1}^{3}\int_{\{w_x\}} d^3f\,\frac{(e^{\alpha}(\mathbf{f}, s))^2}{\omega^2 - \omega_0^2(\mathbf{f}, s) - i\tau},$$

$$\int_0^{\omega_{0m}^{(\alpha)2}} g_0^{(\alpha)}(\omega^2)\,d\omega^2 = 1. \tag{2.27}$$

We took account here of the fact that the tensor $D^{ik}(\omega^2, 0)$, as follows from symmetry consideration, reduces to diagonal form in the crystallographic coordinate system with unit vectors $\mathbf{j}_\alpha$ (for the sake of simplicity, crystals of triclinic and monoclinic symmetry are excluded from consideration), so that[3]

$$\Delta_0(\omega^2 - i\tau, 0) = \prod_{\alpha=1}^{3}\Delta_0^{(\alpha)}(\omega^2 - i\tau, 0),$$

$$\Delta_0^{(\alpha)}(\omega^2 - i\tau, 0) = 1 - \lambda\omega^2\int_0^{\omega_{0m}^{(\alpha)2}}\frac{g_0^{(\alpha)}(\omega_0^2)\,d\omega_0^2}{\omega^2 - \omega_0^2 - i\tau},$$

$$j^{\,i}_{0,\sigma_0,\alpha} = j_\alpha{}^i = \delta^{i\alpha}, \quad \sigma \equiv (\sigma_0, \alpha) \tag{2.28}$$

(the lower index, in this case zero (Δ_0), denotes the dimensionality of the defects).

All the functions having a single index α are normalized to unity and correspond to oscillations in the direction of the α-th crystallographic axis, and $g_0^{(\alpha)}(\omega^2)$ (2.27) is the spectrum of such oscillations in the "standard" lattice. Expression (2.23) corresponds to the well known formula of I. Lifshitz;[3] relation (2.24) was used in [4, 5], and (2.25) describes the matrix-oscillation spectrum altered by the impurities, and has apparently not been presented before. We note that expressions (2.23) and (2.24) also include automatically the discrete level (for $\lambda > \lambda_{cr} > 0$). It is certainly located in a region where $g_0^{(\alpha)}(\omega^2) \equiv 0$ ($\omega^2 > \omega_{0m}^{(\alpha)2}$). Therefore, letting $g_0^{(\alpha)}(\omega^2)$ approach zero, we obtain

$$g^{(\alpha)}(\omega^2) = \frac{1}{r}\delta(\omega^2 - \omega_{\mathrm{loc}}^{(\alpha)2}),$$

$$g_A{}^{(\alpha)}(\omega^2) = (1-\lambda)\frac{d\ln\omega_{\mathrm{loc}}^{(\alpha)2}}{d\lambda}\delta(\omega^2 - \omega_{\mathrm{loc}}^{(\alpha)2}),$$

where $\omega_{\mathrm{loc}}^{(\alpha)2}$—root of the equation[3]

$$1 - \lambda\omega^2\int_0^{\omega_{0m}^{(\alpha)2}}\frac{g_0{}^{(\alpha)}(\omega_0^2)\,d\omega_0^2}{\omega^2 - \omega_0^2} = 0,$$

$$\lambda > \lambda_{cr} = \Bigl[\int_0^{\omega_{0m}^{(\alpha)2}}\frac{g_0{}^{(\alpha)}(\omega_0^2)\,d\omega_0^2}{1 - \omega_0^2/\omega_{0m}{}^{(\alpha)2}}\Bigr]^{-1},$$

and

$$\frac{d\ln\omega_{\mathrm{loc}}^{(\alpha)2}}{d\lambda} = \Bigl\{\lambda^2\omega_{\mathrm{loc}}^{(\alpha)4}\int_0^{\omega_{0m}^{(\alpha)2}}\frac{g_0{}^{(\alpha)}(\omega_0^2)\,d\omega_0^2}{(\omega_{\mathrm{loc}}^{(\alpha)2} - \omega_0^2)^2} - \lambda\Bigr\}^{-1}.$$

In the case of cubic-symmetry crystals, it is necessary to put $g_0^{(\alpha)}(\omega^2) = g_0(\omega^2)$ in all the formulas.

3. CHAIN OF IMPURITY ATOMS

We choose the basis vector a_p such that the unit cell has the form of a thin "plate." Without loss of generality, we put $a_1, a_2 \gg a_3$. In the limit as

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[3] When $r \to \infty$ ($1 \ll r \ll N$) we have the relation

$$\lim_{r\to\infty}\frac{1}{r}\sum_{\mu}{}^{(0)} F(2\pi\eta_\mu) = \frac{v_x}{(2\pi)^3}\int_{\{w_x\}} d^3f\;F(\mathbf{f}).$$

In the derivation of (2.23)–(2.25) we also took account of the fact that

$$\frac{1}{N}\sum_{\mathbf{f}}\ln\Delta_0^{(\alpha)}(\omega^2 - i\tau,\;0) = \frac{1}{\tau}\ln\Delta_0^{(\alpha)}(\omega^2 - i\tau,\;0).$$

$$\alpha_1 \to \infty, \qquad \alpha_2 \to \infty, \qquad \alpha_3 = \text{const} < \infty \tag{3.1}$$

we obtain a lattice with isolated chains of impurity atoms in the α_3 direction. Inasmuch as

$$\boldsymbol{\beta}_1 = \frac{[\boldsymbol{\alpha}_2\boldsymbol{\alpha}_3]}{\alpha_1[\boldsymbol{\alpha}_2\boldsymbol{\alpha}_3]}, \quad \boldsymbol{\beta}_2 = \frac{[\boldsymbol{\alpha}_3\boldsymbol{\alpha}_1]}{\alpha_1[\boldsymbol{\alpha}_2\boldsymbol{\alpha}_3]}, \quad \boldsymbol{\beta}_3 = \frac{[\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2]}{\alpha_1[\boldsymbol{\alpha}_2\boldsymbol{\alpha}_3]}, \tag{3.2*}$$

in the limit of (3.1) we get

$$\boldsymbol{\beta}_1 \to 0, \qquad \boldsymbol{\beta}_2 \to 0, \qquad \boldsymbol{\beta}_3 \neq 0. \tag{3.1'}$$

The latter denotes that the solution of the corresponding dynamic problem is obtained by assuming that $\mathbf{f}$ coincides in direction with α_3:

$$\mathbf{f} = \mathbf{i}_3 f_3, \qquad \mathbf{i}_3 = \boldsymbol{\alpha}_3 / \alpha_3, \tag{3.3}$$

so that $\mathbf{f}\cdot\boldsymbol{\beta}_1/\beta_1 = \mathbf{f}\cdot\boldsymbol{\beta}_2/\beta_2 = 0$ (we recall that $\mathbf{f}$ varies in the region $w_\xi \equiv (2\pi)^3\boldsymbol{\beta}_1[\boldsymbol{\beta}_2 \times \boldsymbol{\beta}_3]$).

Taking (3.3) into account, as well as the fact that $r \to \infty$ $(1 \ll r \ll N)$, let us consider the determinant $\Delta_1(\omega^2 - i\tau, \mathbf{f})$ (2.7). The lower subscript 1 is introduced to denote the dimensionality of the defect), which according to the results of the preceding section determines completely the spectral properties of the entire system and of the individual atoms.

We introduce a Cartesian coordinate system with z axis along $\boldsymbol{\alpha}_3$ (see (3.3)) and denote the projections of the vector $2\pi(\boldsymbol{\beta}_1\mu_1 + \boldsymbol{\beta}_2\mu_2)$ on the unit vectors $\mathbf{i}_1$ and $\mathbf{i}_2$ by f_1' and f_2', so that

$$2\pi(\boldsymbol{\beta}_1\mu_1 + \boldsymbol{\beta}_2\mu_2) = \mathbf{i}_1 f_1' + \mathbf{i}_2 f_2'. \tag{3.3'}$$

We introduce also the abbreviated notation

$$\mathbf{f}' \equiv \mathbf{i}_1 f_1' + \mathbf{i}_2 f_2' + \mathbf{i}_3 f_3 \equiv \mathbf{i}_1 f_1' + \mathbf{i}_2 f_2' + \mathbf{f},$$

$$\mathbf{f}'' \equiv \mathbf{f} + 2\pi\boldsymbol{\eta}_\mu \equiv \mathbf{f}' + 2\pi\boldsymbol{\beta}_3\mu_3, \qquad \mathbf{f}''' \equiv \mathbf{f} + 2\pi\boldsymbol{\beta}_3\mu_3. \tag{3.3''}$$

Then the transition from summation over μ_1 and μ_2 to integration is in accordance with the relation

$$\frac{1}{r}\sum_{\mu_1\mu_2}^{(0)} F(\mathbf{f} + 2\pi\boldsymbol{\eta}_\mu) = \frac{v_x}{(2\pi)^2\alpha_3}\int_{\{w_x\}} df_1' df_2' \, F(\mathbf{f}' + 2\pi\boldsymbol{\beta}_3\mu_3)$$

($F(\mathbf{f}'')$ is an arbitrary function), where account is taken of the fact that

$$\frac{1}{r}\Delta\mu_1\Delta\mu_2 = \frac{1}{r}\,\frac{\Delta f_1'\Delta f_2'}{(2\pi)^2|[\boldsymbol{\beta}_1\boldsymbol{\beta}_2]|} = \frac{v_x}{(2\pi)^2\alpha_3}\Delta f_1'\,\Delta f_2'.$$

Accordingly, we introduce spectral functions normalized to δ^{ik}

$$g_0^{ik}(\omega^2, \mathbf{f}) = \frac{1}{r_3}\sum_{\mu_3}^{(0)} \mathcal{G}_0^{ik}(\omega^2, \mathbf{f} + 2\pi\boldsymbol{\beta}_3\mu_3); \tag{3.4}$$

$$\mathcal{G}_0^{ik}(\omega^2, \mathbf{f} + 2\pi\boldsymbol{\beta}_3\mu_3)$$

$$= \lim_{\substack{r\to\infty\\ \tau\to 0}} \frac{r_3}{\pi r}\,\mathrm{Im}\sum_{\mu_1\mu_2}^{(0)}\sum_{s=1}^{3}\frac{e^i(\mathbf{f}'', s)\,e^k(\mathbf{f}'', s)}{\omega^2 - \omega_0^2(\mathbf{f}'', s) - i\tau}$$

$$= \frac{r_3 v_x}{\pi(2\pi)^2\alpha_3}\lim_{\tau\to 0}\mathrm{Im}\sum_{s=1}^{3}\int_{\{w_x\}} df_1'\, df_2'\,\frac{e^i(\mathbf{f}'', s)\,e^k(\mathbf{f}'', s)}{\omega^2 - \omega_0^2(\mathbf{f}'', s) - i\tau}$$

$$= \frac{r_3 v_x}{(2\pi)^2\alpha_3}\sum_{s=1}^{3}\int_L \frac{e^i(\mathbf{f}'', s)\,e^k(\mathbf{f}'', s)\,dl}{|\nabla_2'\omega_0^2(\mathbf{f}'', s)|}$$

$$(\nabla_2' = \mathbf{i}_1\partial/\partial f_1' + \mathbf{i}_2\partial/\partial f_2'); \tag{3.5}$$

$$\int_{\Omega_1^2(\mathbf{f}''')}^{\Omega_2^2(\;''')} \mathcal{G}_0^{ik}(\omega^2, \mathbf{f}''')\,d\omega^2 = \int_{\omega_1^2(\mathbf{f})}^{\omega_2^2(\mathbf{f})} g_0^{ik}(\omega^2, \mathbf{f})\,d\omega^2 = \delta^{ik}, \tag{3.6}$$

In the last expression of (3.5),[4] the integration is over the sections of the equal-frequency curve L, located within the limits of the region w_x; the curve is defined by the system of equations

$$\omega_0^2(\mathbf{f}'', s) = \omega^2, \tag{3.7'}$$

$$\mathbf{f}''\mathbf{i}_3 = f_3 + 2\pi\mu_3/\alpha_3 = \text{const}. \tag{3.7''}$$

Here r_3 is the number of values which μ_3 can assume in the region corresponding to $1/v_x$. The summation or integration, as before, is carried out in such a way that the summary vector $\mathbf{f}''$ does not go beyond the limits of the first Brillouin zone of the lattice Y. Ω_1, Ω_2, and ω_1, ω_2 are the limiting frequencies of the functions $\mathcal{G}_0^{ik}$ and g_0^{ik} (see below).

We see that the function $\mathcal{G}_0^{ik}(\omega^2, \mathbf{f} + 2\pi\boldsymbol{\beta}_3\mu_3)$ describes the frequency distribution (with account of spatial anisotropy of the displacement of the atoms) of the normal oscillations of the "standard" lat-

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$*[\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2] \equiv \boldsymbol{\alpha}_1 \times \boldsymbol{\alpha}_2$.

[4] To derive (3.5) it is necessary first to integrate over the ring located between curves $\omega_0^2(\mathbf{f}'', s) = \omega_0^2$ and $\omega_0^2(\mathbf{f}'', s) = \omega_0^2 + d\omega_0^2$ (in the plane (3.7")) and then with respect to $d\omega_0^2$. The thickness of such a ring $h(\mathbf{f}'', s)$ at each point is determined from the condition

$$\omega_0^2\left(\mathbf{f}'' + h(\mathbf{f}'', s)\frac{\nabla_2'\omega_0^2(\mathbf{f}'', s)}{|\nabla_2'\omega_0^2(\mathbf{f}'', s)|}, s\right) = \omega_0^2(\mathbf{f}'', s) + d\omega_0^2.$$

Hence

$$d\omega_0^2 = \nabla_2'\omega_0^2\cdot h\nabla_2'\omega_0^2\cdot|\nabla_2'\omega_0^2|^{-1},$$

so that

$$h(\mathbf{f}'', s) = d\omega_0^2 / |\nabla_2'\omega_0^2(\mathbf{f}'', s)|$$

and we obtain directly the final expression (3.5) tice with wave vectors $\mathbf{f}''$ whose ends are on the plane (3.7″) (f_3 and μ_3 are fixed); $g_0^{ik}(\omega^2, \mathbf{f})$ corresponds to additional averaging over such planes with different μ_3. (It must be borne in mind that in the general case $\boldsymbol{\beta}_3$ does not coincide in direction with $\boldsymbol{\alpha}_3$.) Since at specified f_3 and μ_3 the indicated plane does not cross all the surfaces (3.7′), but only those that correspond to ω^2 inside a certain frequency interval, which generally speaking differs from $(0, \omega_{0m}^2)$, the function (3.5) vanishes identically both when $\omega^2 < \Omega_1^2$ and $\omega^2 > \Omega_2^2$. Choosing

$$\omega_1^2(\mathbf{f}) = \min\{\Omega_1^2(\mathbf{f} + 2\pi\boldsymbol{\beta}_3\mu_3)\},$$
$$\omega_2^2(\mathbf{f}) = \max\{\Omega_2^2(\mathbf{f} + 2\pi\boldsymbol{\beta}_3\mu_3)\},$$

we obviously obtain the limiting values of $g_0^{ik}(\omega^2, \mathbf{f})$. If μ_3 can assume only one value $\mu_3 = 0$, then $g_0^{ik}(\omega^2, \mathbf{f})$, in any case, vanishes if ω^2 is sufficiently small and f_3 is large.

We note also that, in accordance with the definition (3.4) and (3.5), $g_0^{ik}(\omega^2, -\mathbf{f}) = g_0^{ik}(\omega^2, \mathbf{f})$ and depends only on the orientation of the chain relative to the crystallographic axes and on $|\mathbf{f}| = f_3$.

Taking (3.4) and (3.5) into account, we obtain

$$\Delta_1(\omega^2 - i\tau, \mathbf{f}) = \det\left\{ \delta^{ik} - \lambda\omega^2 \int\limits_{\omega_1^2(\mathbf{f})}^{\omega_2^2(\mathbf{f})} \frac{g_0^{ik}(\omega_0^2, \mathbf{f})\, d\omega_0^2}{\omega^2 - \omega_0^2 - i\tau} \right\}, \tag{3.8}$$

so that, for example, we have in accord with (2.17)

$$g(\omega^2) - g_0(\omega^2) = \frac{1}{3\pi r} \frac{\partial}{\partial\omega^2} \lim_{\tau\to 0} \operatorname{Im} \frac{\alpha_3}{2\pi} \int\limits_{2\pi\beta_3} df_3 \ln \Delta_1(\omega^2 - i\tau, \mathbf{f}). \tag{3.9}$$

In the derivation of (3.9) we went over to integration with respect to d^3f in accordance with footnote 2), and integrated with respect to f_1 and f_2, obtaining $(2\pi)^2 S(f_3)$, where $S(f_3)$ is the area of the section of the unit cell (or Brillouin zone) of lattice H in the plane f_3 = const. When $r \to \infty$ this cell has the form of a thin "rod" elongated in the direction of $\boldsymbol{\beta}_3$ (see (3.1′)), and it can be assumed that $S(f_3) = |\boldsymbol{\beta}_1 \times \boldsymbol{\beta}_2| = \alpha_3/v_\xi$ independently of f_3.

We note that, within the framework of the first relation in (2.10), $\boldsymbol{\alpha}_3$ can be arbitrary both in direction and in magnitude. The impurity chain itself need not necessarily consist of atoms A only.

Assume, for example, that the impurity chain is located in the "close packing" direction, i.e., in the direction of one of the basis vectors of lattice X, namely $\boldsymbol{\alpha}_3 = r_3\mathbf{a}_3$. If $r_3 > 1$, then such a chain has a periodic structure determined by the formula AB_{r_3-1}. If on the other hand $r_3 = 1$, then the chain consists entirely of atoms A. In this case $1/r$ has the meaning of the concentration of the impurity chains, i.e., the ratio of the number of such chains to the total number of all the chains crossing the plane of the vectors $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$ in the direction of $\boldsymbol{\alpha}_3$. In this case μ_3 can assume only one value, $\mu_3 = 0$, in all the sums considered above.

All the general properties of the dynamic problem, considered in [1], are obviously fully applicable also to the particular case considered here. Thus, if the atoms A are sufficiently light $(1 - \lambda \ll 1)$ and do not interact directly with one another (for example, if they are not nearest neighbors, and the more remote interactions are small), then in first approximation they oscillate like isolated impurities. However, there are essential differences here, too, connected with the concrete form of the spectral functions and with the conditions for the appearance of local and quasi-local oscillations.

Let us consider the simplest case, when $\boldsymbol{\alpha}_3$ coincides with one of the principal crystallographic axes.[5] Then the tensor function $g_0^{ik}(\omega^2, \mathbf{f})$ (3.4) reduces to diagonal form in the crystallographic coordinate system:

$$g_0^{\alpha\beta}(\omega^2, \mathbf{f}) = g_0^{(\alpha)}(\omega^2, \mathbf{f})\,\delta^{\alpha\beta}, \quad g_0^{(\alpha)}(\omega^2, \mathbf{f}) \equiv g_0^{\alpha\alpha}(\omega^2, \mathbf{f}) \tag{3.10}$$

(no summation over α), so that

$$\Delta_1(\omega^2 - i\tau, \mathbf{f}) = \prod_{\alpha=1}^{3} \Delta_1^{(\alpha)}(\omega^2 - i\tau, \mathbf{f}),$$
$$\Delta_1^{(\alpha)}(\omega^2 - i\tau, \mathbf{f}) = 1 - \lambda\omega^2 \int\limits_{\omega_1^{(\alpha)2}(\mathbf{f})}^{\omega_2^{(\alpha)2}(\mathbf{f})} \frac{g_0^{(\alpha)}(\omega_0^2, \mathbf{f})\, d\omega_0^2}{\omega^2 - \omega_0^2 - i\tau} \tag{3.11}$$

(the integration limits are marked with the index α, on which, generally speaking, they can depend).

Using (3.11), we obtain in complete analogy with the corresponding results for isolated impurity atoms (2.22)–(2.26)

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[5] For example, in the case of a face-centered cubic lattice this means that

$$\boldsymbol{\alpha}_p = r'_p\left(-2\mathbf{a}_p + \sum_{s=1}^{3}\mathbf{a}_s\right), \quad P_{pp'} = \begin{pmatrix} -r_1' & r_1' & r_1' \\ r_2' & -r_2' & r_2' \\ r_3' & r_3' & -r_3' \end{pmatrix},$$

$$r = \det \hat{P} = 4r_1'r_2'r_3'$$

(the second factor in $\mathbf{a}_p$ is the edge of the unit cube), with $r_1', r_2' \gg r_3'$.

$$g(\omega^2)=\frac{1}{3}\sum_{\alpha=1}^{3}g^{(\alpha)}(\omega^2), \qquad g_0(\omega^2)=\frac{1}{3}\sum_{\alpha=1}^{3}g_0{}^{(\alpha)}(\omega^2),$$

$$g_A(\omega^2)=\frac{1}{3}\sum_{\alpha=1}^{3}g_A{}^{(\alpha)}(\omega^2), \qquad g_B(\omega^2)=\frac{1}{3}\sum_{\alpha=1}^{3}g_B{}^{(\alpha)}(\omega^2), \tag{3.12}$$

$$g^{(\alpha)}(\omega^2)=\frac{\alpha_3}{2\pi}\int_{2\pi\beta_3} df_3\, g^{(\alpha)}(\omega^2, \mathbf{f}),$$

$$g_0{}^{(\alpha)}(\omega^2)=\frac{\alpha_3}{2\pi}\int_{2\pi\beta_3} df_3 g_0{}^{(\alpha)}(\omega^2, \mathbf{f}),$$

$$g_A{}^{(\alpha)}(\omega^2)=\frac{\alpha_3}{2\pi}\int_{2\pi\beta_3} g_A{}^{(\alpha)}(\omega^2, \mathbf{f})\, df_3,$$

$$g_B{}^{(\alpha)}(\omega^2)=\frac{\alpha_3}{2\pi}\int_{2\pi\beta_3} g_B{}^{(\alpha)}(\omega^2, \mathbf{f})\, df_3;$$

$$g^{(\alpha)}(\omega^2, \mathbf{f})-g_0{}^{(\alpha)}(\omega^2, \mathbf{f})=\frac{1}{\pi r}\,\frac{\partial}{\partial\omega^2}\lim_{\tau\to 0}\operatorname{Im}\ln\Delta_1{}^{(\alpha)}(\omega^2-i\tau, \mathbf{f}); \tag{3.13}$$

$$g_A{}^{(\alpha)}(\omega^2, \mathbf{f})=-\frac{1-\lambda}{\pi\omega^2}\,\frac{\partial}{\partial\lambda}\lim_{\tau\to 0}\operatorname{Im}\ln\Delta_1{}^{(\alpha)}(\omega^2-i\tau, \mathbf{f}); \tag{3.14}$$

$$g_B{}^{(\alpha)}(\omega^2, \mathbf{f})=\frac{1}{r-1}[rg^{(\alpha)}(\omega^2, \mathbf{f})-g_A{}^{(\alpha)}(\omega^2, \mathbf{f})]\approx$$

$$\approx g^{(\alpha)}(\omega^2, \mathbf{f})+\frac{1}{r}[g_0{}^{(\alpha)}(\omega^2, \mathbf{f})-g_A{}^{(\alpha)}(\omega^2, \mathbf{f})]. \tag{3.15}$$

$$\lim_{\tau\to 0}\operatorname{Im}\ln\Delta_1{}^{(\alpha)}(\omega^2-i\tau, \mathbf{f})=-\tan^{-1}\Biggl\{\pi\lambda\omega^2 g_0{}^{(\alpha)}(\omega^2, \mathbf{f})$$

$$\times\left[1-\lambda\omega^2 \mathop{-\!\!\!\!\!\!\int}_{\omega_1^{(\alpha)2}(\mathbf{f})}^{\omega_2^{(\alpha)2}(\mathbf{f})}\frac{g_0{}^{(\alpha)}(\omega_0{}^2, \mathbf{f})\, d\omega_0{}^2}{\omega^2-\omega_0{}^2}\right]^{-1}\Biggr\}. \tag{3.16}$$

Here, just as in (3.9), we use for $S(f_3)$ the expression α_3/v_ξ; $g_0^{(\alpha)}(\omega^2)$ is given by (2.27). All the functions with a single index are normalized to unity. The function $g_A(\omega^2)$ describes oscillations of the atoms A on the defect line.

The function $g_0^{(\alpha)}(\omega^2, \mathbf{f})$ has all the singularities characteristic of the "two-dimensional" distribution function of the oscillation frequency[8] (see also [9]). This leads to the absence of a "critical" value of λ, necessary for the appearance of the local level (see [3] and also Sec. 2). The equation

$$1-\lambda\omega^2\int_{\omega_1^{(\alpha)2}(\mathbf{f})}^{\omega_2^{(\alpha)2}(\mathbf{f})}\frac{g_0{}^{(\alpha)}(\omega_0{}^2, \mathbf{f})\, d\omega_0{}^2}{\omega^2-\omega_0{}^2}=0 \tag{3.17}$$

for $\omega^2 < \omega_1^{(\alpha)2}(\mathbf{f})$ or $\omega^2 > \omega_2^{(\alpha)2}(\mathbf{f})$ has a solution for arbitrary λ: for $\lambda < 0$ we obtain the solution

$$\omega_{1\,\mathrm{loc}}{}^2(\mathbf{f}, \alpha) < \omega_1{}^{(\alpha)2}(\mathbf{f}),$$

and for $\lambda > 0$

$$\omega_{2\,\mathrm{loc}}{}^2(\mathbf{f}, \alpha) > \omega_2{}^{(\alpha)2}(\mathbf{f}).$$

The low frequency oscillations do not differ in character from the high frequency ones—both are truly local. The corresponding oscillation amplitude does not contain the small parameter $1/\sqrt{r}$.

Nonetheless, in order for a gap to appear between ω_{0m}^2 and the impurity band $\omega_{2\mathrm{loc}}^2(\mathbf{f}, \alpha)$, the parameter λ must exceed a certain critical value λ_{cr}, determined from the condition $\min\{\omega_{2\mathrm{loc}}^2(\mathbf{f}, \alpha)\} > \omega_{0m}^2$.

We note that everything stated with respect to $g_0^{(\alpha)}(\omega^2, \mathbf{f})$ and Eq. (3.17) remains in force, of course, also for $g_0^{ik}(\omega^2, \mathbf{f})$ and the equation $\Delta_1(\omega^2, \mathbf{f}) = 0$ in the general case (see (3.8)).

In the case when $1 - \lambda \ll 1$, Eq. (3.17) can be solved explicitly by expanding the integrand in powers of ω_0^2/ω^2. As a result we get

$$\omega_{2\,\mathrm{loc}}^2(\mathbf{f}, \alpha)=\frac{\langle\omega_0{}^2\rangle_{\mathbf{f}}{}^{(\alpha)}}{1-\lambda}+\frac{\langle\omega_0{}^4\rangle_{\mathbf{f}}{}^{(\alpha)}-\langle\omega_0{}^2\rangle_{\mathbf{f}}{}^{(\alpha)2}}{\langle\omega_0{}^2\rangle_{\mathbf{f}}{}^{(\alpha)}}+\cdots, \tag{3.18}$$

where in accord with formula (3.1) of [1] (in which we must put $\mathbf{f} = \mathbf{i}_3 f_3$ (3.3)),

$$\langle\omega_0{}^{2m}\rangle_{\mathbf{f}}{}^{(\alpha)}\equiv\int_{\omega_1^{(\alpha)2}(\mathbf{f})}^{\omega_2^{(\alpha)2}(\mathbf{f})}\omega_0{}^{2m}g_0{}^{(\alpha)}(\omega_0{}^2, \mathbf{f})\, d\omega_0{}^2=\langle\omega_0{}^{2m}\rangle^{(\alpha)}+\frac{1}{M^m}$$

$$\times\sum_{\nu_3\neq 0}\sum_{\mathbf{n}_1\mathbf{n}_2\ldots\mathbf{n}_m}A^{\alpha i_1}(\mathbf{x}_{\mathbf{n}_1})\, A^{i_1 i_2}(\mathbf{x}_{\mathbf{n}_2})\ldots A^{i_{m-1}\alpha}(\mathbf{x}_{\mathbf{n}_m})\, e^{-if_3\alpha_3\nu_3}\,\delta_{\Sigma,\, \alpha_3\nu_3},$$

$$\langle\omega_0{}^{2m}\rangle^{(\alpha)}=\int_0^{\omega_{0m}^{(\alpha)2}}\omega_0{}^{2m}\, g_0{}^{(\alpha)}(\omega_0{}^2)\, d\omega_0{}^2, \qquad \Sigma=\sum_{t=1}^{m}\mathbf{x}_{\mathbf{n}_t}. \tag{3.19}$$

This is perfectly analogous to the corresponding expression for the local frequency in the case of an isolated impurity atom.[4, 5]

4. ISOLATED IMPURITY PLANE

We choose the basis vectors such that the unit cell has the form of a long "rod." Without loss of generality we put $\alpha_3 \gg \alpha_1, \alpha_2$. In the limit

$$\alpha_3\to\infty, \qquad \alpha_1<\infty, \qquad \alpha_2<\infty \tag{4.1}$$

we obtain a lattice with isolated planes of impurity atoms, parallel to the vectors $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$. In view of the relation (3.2), we have here

$$\beta_1\neq 0, \qquad \beta_2\neq 0, \qquad \beta_3\to 0. \tag{4.1'}$$

The latter denotes that the solution of the corresponding dynamic problem is obtained from the formulas of Sec. 2 in which we put

$$\mathbf{f} = \mathbf{i}_1 f_1 + \mathbf{i}_2 f_2, \quad f_3 = 0, \tag{4.2}$$

where $\mathbf{i}_p$ are unit vectors: $\mathbf{i}_1$ and $\mathbf{i}_2$ lie in the plane of the vectors $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$, and $\mathbf{i}_3 \parallel \boldsymbol{\beta}_3$.

The transformation of the indicated formulas is similar to that used in the preceding section. In view of the smallness of β_3, in calculating $\Delta_2(\omega^2 - i\tau, \mathbf{f})$ by means of (2.6) and (2.7) (the lower index 2 corresponds to the two-dimensional defect), the summation over μ_3 is replaced by integration in accordance with the equation

$$\frac{1}{r}\sum_{\mu_3}^{(0)} F(\mathbf{f} + 2\pi\boldsymbol{\eta}_\mu) = \frac{v_x}{2\pi\,|[\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2]|}\int_{2\pi\beta_3} df_3'\, F(\mathbf{f}' + 2\pi\boldsymbol{\eta}_{\mu'}).$$

Here and throughout in this section we use, besides (4.2), the notation

$$\begin{gathered}\mathbf{f}' \equiv \mathbf{i}_1 f_1 + \mathbf{i}_2 f_2 + \mathbf{i}_3 f_3', \qquad f_3' \equiv 2\pi\beta_3\mu_3, \\ \mathbf{f}'' \equiv \mathbf{f} + 2\pi\boldsymbol{\eta}_\mu \equiv \mathbf{f}' + 2\pi\boldsymbol{\eta}_{\mu'}, \qquad \boldsymbol{\eta}_{\mu'} \equiv \boldsymbol{\beta}_1\mu_1 + \boldsymbol{\beta}_2\mu_2 \\ \mathbf{f}''' = \mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu'}\end{gathered} \tag{4.2$'$}$$

We introduce spectral functions normalized to δ^{ik}:

$$g_0^{ik}(\omega^2, \mathbf{f}) = \frac{1}{r'}\sum_{\mu_1\mu_2}^{(0)} \mathcal{G}_0^{ik}(\omega^2, \mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu'}); \tag{4.3}$$

$$\begin{aligned}\mathcal{G}_0^{ik}&(\omega^2, \mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu'}) \\ &= \lim_{\substack{r\to\infty \\ \tau\to 0}} \frac{r'}{\pi r}\,\mathrm{Im}\sum_{\mu_3}^{(0)}\sum_{s=1}^{3}\frac{e^i(\mathbf{f}'', s)\,e^k(\mathbf{f}'', s)}{\omega^2 - \omega_0^2(\mathbf{f}'', s) - i\tau} \\ &= \lim_{\tau\to 0}\frac{r' v_x}{2\pi^2\,|[\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2]|}\,\mathrm{Im}\sum_{s=1}^{3}\int df_3'\,\frac{e^i(\mathbf{f}'', s)\,e^k(\mathbf{f}'', s)}{\omega^2 - \omega_0^2(\mathbf{f}'', s) - i\tau} \\ &= \frac{r' v_x}{2\pi\,|[\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2]|}\sum_{s=1}^{3}\sum_a\frac{e^i(\mathbf{f}_a'', s)\,e^k(\mathbf{f}_a'', s)}{|\partial\omega_0^2(\mathbf{f}_a'', s)/\partial f_{3a}'|};\end{aligned} \tag{4.4}$$

$$\int_{\Omega_1^2(f''')}^{\Omega_2^2(f''')} \mathcal{G}_0^{ik}(\omega^2, \mathbf{f}''')\,d\omega^2 = \int_{\omega_1^2(f)}^{\omega_2^2(f)} g_0^{ik}(\omega^2, \mathbf{f})\,d\omega^2 = \delta^{ik},$$

$$\omega_1^2(\mathbf{f}) = \min\{\Omega_1^2(\mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu'})\},\ \omega_2^2(\mathbf{f}) = \max\{\Omega_2^2(\mathbf{f} + 2\pi\boldsymbol{\eta}_{\mu'})\}. \tag{4.5}$$

Here

$$\mathbf{f}''\mathbf{i}_1 = f_1 + 2\pi\boldsymbol{\eta}_{\mu'}\mathbf{i}_1 = \mathrm{const}_1,\ \mathbf{f}''\mathbf{i}_2 = f_2 + 2\pi\boldsymbol{\eta}_{\mu'}\mathbf{i}_2 = \mathrm{const}_2; \tag{4.6$'$}$$

$$\omega_0^2(\mathbf{f}'', s) = \omega^2; \tag{4.6$''$}$$

$$\mathbf{f}_a'' \equiv \mathbf{i}_1 f_1 + \mathbf{i}_2 f_2 + \mathbf{i}_3 f_{3a} + 2\pi\boldsymbol{\eta}_{\mu'}; \tag{4.7}$$

in the summation or integration, the vector argument $\mathbf{f}''$ must not go beyond the limits of the Brillouin zone of the lattice Y; the sum over a denotes summation over the points of intersection (4.7) of the line (4.6′) (parallel to the z axis) with the surface (4.6″) (μ_1 and μ_2 are fixed; in the general case $\mathbf{i}_p$, with p = 1 and 2, do not coincide in direction with either $\boldsymbol{\alpha}_p$ or $\boldsymbol{\beta}_p$). The fact that the functions $\mathcal{G}_0^{ik}(\omega^2, \mathbf{f} + 2\pi\eta_{\mu'})$ and $g_0^{ik}(\omega^2, \mathbf{f})$ have lower limits (Ω_1^2 and ω_1^2) and upper limits (Ω_2^2 and ω_2^2) that differ in the general case from zero and ω_{0m}^2 is obvious, because the indicated line and surface do not have intersection points for all arbitrary ω^2. We have denoted by r′ the number of values which the vector $2\pi\eta_{\mu'}$ can assume in the region w_x.

In the simplest case, when

$$\alpha_p = r_p \mathbf{a}_p, \quad r = r_1 r_2 r_3, \quad r_1 < \infty, \quad r_2 < \infty, \quad r_3 \to \infty,$$

it is obvious that $r' = r_1 r_2$. If $r' = r_1 = r_2 = 1$, then the impurity plane consists entirely of atoms A, with $1/r = 1/r_3$ having the meaning of the concentration of such planes. On the other hand, if $r_1 r_2 > 1$, the impurity plane has a periodic structure determined by formula $AB_{r'-1}$. For example, by choosing $r_1 = 1$ and $r_2 > 1$ we obtain in the ($\mathbf{a}_1$, $\mathbf{a}_2$) plane a structure consisting of parallel linear chains extending in the direction of the vector $\mathbf{a}_1$ and alternating in the direction of the vector $\mathbf{a}_2$ in accord with the formula AB_{r_2-1}.

Taking (4.3) and (4.4) into account, the determinant $\Delta_2(\omega^2 - i\tau, \mathbf{f})$ (2.6) can be written in the form

$$\Delta_2(\omega^2 - i\tau, \mathbf{f}) = \det\left\{\delta^{ik} - \lambda\omega^2\int_{\omega_1^2(\mathbf{f})}^{\omega_2^2(\mathbf{f})}\frac{g_0^{ik}(\omega_0^2\mathbf{f})\,d\omega_0^2}{\omega^2 - \omega_0^2 - i\tau}\right\}, \tag{4.8}$$

so that, for example, by virtue of (2.17)

$$g(\omega^2) - g_0(\omega^2) = \frac{1}{3\pi r}\frac{\partial}{\partial\omega^2}\lim_{\tau\to 0}\mathrm{Im}\frac{|[\alpha_1\alpha_2]|}{(2\pi)^2}\cdot \int_{(2\pi)^2|[\beta_1\beta_2]|}\ln\Delta_2(\omega^2 - i\tau, \mathbf{f})\,df_1 df_2. \tag{4.9}$$

This result follows directly from (2.17), if we integrate in the latter with respect to f_3 (see footnote [2]):

$$\int_{2\pi\beta_3} df_3 = 2\pi\beta_3 \equiv \frac{2\pi\,|[\alpha_1\alpha_2]|}{v_\xi}.$$

If the vector $\boldsymbol{\alpha}_3$ coincides with a principal crystallographic axis, and α_1 and α_2 are perpendicular to $\boldsymbol{\alpha}_3$, then we have in the crystallographic coordinate frame

$$g_0^{\alpha\beta}(\omega^2,\ \mathbf{f}) = g_0^{\alpha\beta}(\omega^2,\ \mathbf{f}) \sum_{\alpha_1=1}^{2} \sum_{\beta_1=1}^{2} \delta^{\alpha\alpha_1}\delta^{\beta\beta_1} + g_0^{(3)}(\omega^2,\ \mathbf{f})\,\delta^{\alpha 3}\delta^{\beta 3}.$$

By virtue of this, at least for the functions $g^{(3)}(\omega^2, \mathbf{f})$ and $g^{(3)}_{A,\,B}(\omega^2, \mathbf{f})$, which determine the oscillations of the system and of individual atoms in the α_3 direction, we obtain directly formulas of the type (3.13)–(3.16), where we need only make the substitution $\Delta_1^{(\alpha)} \to \Delta_2^{(\alpha)}$ and take (4.2) into account. We then get

$$g^{(3)}(\omega^2) = \frac{|[\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2]|}{(2\pi)^2} \int\limits_{(2\pi)^2\,|\,[\beta_1\beta_2]\,|} df_1\, df_2\, g^{(3)}(\omega^2, \mathbf{f}) \quad \text{etc.}$$

The function $g_0^{ik}(\omega^2, \mathbf{f})$ determines the frequency distribution of the "standard" lattice oscillations corresponding to a fixed projection of the wave vector on the $(\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2)$ plane. It has all the singularities of "one-dimensional" distribution functions,[8, 9] leading to the absence of a "critical" value λ_{cr} necessary for the appearance of local oscillations. Just as in the case of an impurity chain, for arbitrary λ (both $\lambda < 0$ and $\lambda > 0$), local oscillations arise with an amplitude that decreases with increasing distance from the impurity plane (see also [7]). However, if $1 - \lambda \ll 1$ ($\lambda > 0$), a gap between the impurity band and ω_{0m}^2 arises only for sufficiently light atoms A, so that for the occurrence of such a gap it is necessary to have $\lambda > \lambda_{cr}$, where λ_{cr} is determined from the condition $\min\{\omega_{2\,\mathrm{loc}}^2(\mathbf{f}, \sigma)\} > \omega_{0m}^2$.

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