

$$R = R_0 + b_1 T^{n_1} + b_2 T^{n_2}, \quad (4)$$

where  $b_1 < 0$ .

The presence of a negative term in Eq. (4), if it is supported, creates serious difficulties for the present quantum-mechanical theory of the Hall effect and for the establishment of a relation between  $\rho$  and  $R$ . In particular, it contradicts Eqs. (1) and (2); therefore, further careful investigations are necessary in the region of low temperatures for the resolution of the question of the reality of the existence of the anomalous Hall effect found in Ref. 6.

<sup>1</sup> N. S. Akulov and A. V. Cheremushkina, Dokl. Akad. Nauk SSSR **102**, 45 (1955).

<sup>2</sup> N. S. Akulov and A. V. Cheremushkina, Dokl. Akad. Nauk SSSR **98**, 35 (1954).

<sup>3</sup> R. Karplus and J. Luttinger, Phys. Rev. **95**, 1154 (1954).

<sup>4</sup> A. G. Samoilovich and V. A. Kon'kov, J. Exptl. Theoret. Phys. (U.S.S.R.) **20**, 783 (1950).

<sup>5</sup> J.-P. Jan, Helv. Phys. Acta **25**, 677 (1952).

<sup>6</sup> J.-P. Jan and H. M. Gijssman, Physica **18**, 339 (1952).

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### The Effect of Ordering on the Energy Spectrum of Phonons

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A METHOD was set forth in Ref. 1 for the study of the vibration spectrum of solid solutions of isotopes. The method developed there can be applied to the determination of the spectral density of such solutions in the presence of long-range order. In the case considered, the lattice is divided into two sublattices, for which the probabilities  $P_i^I$  of finding the  $i$ th isotope are different and are given by the values

$$P_1^I = 1 - c + \frac{s}{2}; \quad P_1^{II} = 1 - c - \frac{s}{2}; \quad (1)$$

$$P_2^I = c - \frac{s}{2}; \quad P_2^{II} = c + \frac{s}{2}.$$

The indices I and II denote the types of sites,  $c$  = concentration of the second isotope and the quantity  $s$  characterizes the degree of order. The value  $s = 1$  ( $c = \frac{1}{2}$ ) corresponds to complete ordering of the crystal, the value  $s = 0$  to complete disorder.

To make clear the peculiarities of the spectrum, we consider the case of a small difference in masses of the two isotopes. According to the results obtained<sup>1</sup>, the spectral density of a system with random distribution of masses can be represented in the form

$$\nu(z) = \nu_0(z) - d\xi/dz, \quad (2)$$

where, for small mass differences,

$$\xi(z) = \frac{1}{N} \left\{ z\nu_0(z) \sum_{\mathbf{r}} \bar{\varepsilon}_{\mathbf{r}} \right. \quad (3)$$

$$\left. + z^2 \int_{\omega^2(\mathbf{k})=z} \frac{d\Omega}{|\nabla\omega^2|} \int \frac{dk'}{z - \omega^2(\mathbf{k}')} \times \sum_{\mathbf{r}, \mathbf{r}'} \bar{\varepsilon}_{\mathbf{r}} \bar{\varepsilon}_{\mathbf{r}'} \exp \{2\pi i (\mathbf{k} - \mathbf{k}')(\mathbf{r} - \mathbf{r}')\} + \dots \right\},$$

$$\bar{\varepsilon}_{\mathbf{r}} = (\overline{m_{\mathbf{r}}} - m_{\mathbf{r}}) / \overline{m_{\mathbf{r}}}. \quad (4)$$

Here  $z$  is the square of the frequency,  $m_{\mathbf{r}}$  is the value of the mass at site  $\mathbf{r}$  ( $\mathbf{r} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$ ,  $n_i$  = an integer,  $\mathbf{a}_i$  = lattice constants), the bar denotes averaging,  $N$  = total number of atoms,  $d\Omega$  is an element of area on the surface  $\omega^2(\mathbf{k}) = z$  over which integration is to be carried out,  $\nabla\omega^2$  is the gradient in the space of the wave vector  $\mathbf{k}$ ,  $f$  is the principal value of the integral,  $\nu_0(z)$  is the unperturbed spectral density; the spectral density is normalized to unity. For a crystal with the distribution of Eq. (1), it is natural to use (for the unperturbed case) the spectral density  $\nu_0^{\text{ord}}$  of a lattice with alternating masses

$$\overline{m}_I = \overline{m}(1-x), \quad \overline{m}_{II} = \overline{m}(1+x), \quad (5)$$

which represent the mean masses at sites of type I and II, respectively. Here  $\overline{m} = (1-c)m_1 + cm_2$ ,  $x = s(m_2 - m_1)/2\overline{m} = s\epsilon/2$ . Then

$$\bar{\varepsilon}_I = \bar{\varepsilon}_{II} = 0, \quad \bar{\varepsilon}_I^2 = \left(c - \frac{s}{2}\right) \left(1 - c + \frac{s}{2}\right) \epsilon^2,$$

$$\bar{\varepsilon}_{II}^2 = \left(c + \frac{s}{2}\right) \left(1 - c - \frac{s}{2}\right) \epsilon^2$$

and, in accord with (2) and (3), we have

$$\nu(z) = \nu_{0\text{ord}}(z) - \frac{d}{dz} \xi_{\text{ord}}(z), \quad (6)$$

$$\xi_{\text{ord}}(z) \quad (7)$$

$$= \varepsilon^2 \left\{ c(1-c) - \frac{s^2}{2} \right\} z^2 \nu_{0\text{ord}}(z) \int_0^{z_g^0} \frac{\nu_{0\text{ord}}(z')}{|z-z'|} dz'.$$

Thus the fluctuating addition, defined by the departure of the actual masses from the mean values  $\bar{m}_I$  and  $\bar{m}_{II}$ , is proportional to  $\varepsilon^2$ . It is easy to see that for complete order ( $s = 1$ ,  $c = \frac{1}{2}$ ), the additional contribution is zero.

For three-dimensional crystals and sufficiently small values of mass differences for the isotopes, complete ordering does not in general lead to a discontinuity in the frequencies, and, consequently, Eqs. (2) and (3) have meaning for all values of the frequency except the limit frequency  $z_g^0$ . When a discontinuity appears, (2) and (3) are not valid close to frequencies which bound the forbidden region. Expressions that are valid for all frequencies, and the displacement of the limiting frequencies, are easily determined by means of another decomposition, shown in Ref. 1.

In many cases, as a consequence of the basic symmetry of the coefficients of interaction, the function  $\nu_{0\text{ord}}$  can have singularities. For example, if the interaction is limited to nearest neighbors, the spectral density of a simple cubic lattice, for the sites I and II of which we have, respectively, sites with even and odd values of  $(n_1 + n_2 + n_3)$ ,

has (near the limit frequencies  $z_0$ ) singularities of the form

$$\nu_{0\text{ord}} \sim \sqrt{xz_0 / |z_0 - z|}. \quad (8)$$

The frequency gap in this case is

$$z_0^+ - z_0^- \sim 2xz_0. \quad (9)$$

In spite of the fact that (2) and (3) are not valid near  $z_0$  (because of the singularities of  $\nu_{0\text{ord}}$ ) we can, with their help, still draw some conclusions on the spectrum of the crystal under investigation.

For complete order, according to the relations obtained, the fluctuating term is equal to zero and the behavior of the spectral density near the limiting frequencies  $z_0^\pm$  is given by Eq. (8). The frequency gap is a maximum in this case.

With the appearance of disorder, as a result of the drawing together of  $m_I$  and  $m_{II}$ , the frequency gap decreases. Moreover, the increasing fluctuation contribution can materially affect the course of the spectral density near  $z_0^\pm$ . Near the limiting frequencies, the fluctuating term  $\Delta\nu$ , in accord with (3) and (8), has the form

$$\Delta\nu \sim \frac{\varepsilon}{s} \left\{ c(1-c) - \frac{s^2}{4} \right\} \left( \frac{xz_0}{|z_0 - z|} \right)^{3/2}. \quad (10)$$

Hence it is evident that the role of the added term depends on the degree of order. For  $xz_0 / |z_0 - z| \sim 1$ , when the increase in  $\nu_{0\text{ord}}$  is already considerable, the fluctuating term remains small and cannot compensate for the increase if  $s$  is not small. For small  $s$ , on the other hand, compensation can take place.

In the case of complete disorder,  $x = 0$  and the frequency gap vanishes.

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<sup>1</sup> I. M. Lifshitz and G. I. Stepanova, J. Exptl. Theoret. Phys. (U.S.S.R.) 30, 938 (1956); Soviet Phys. JETP 3, 656 (1956).

Translated by R. T. Beyer  
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