

is given by $F=0$, where $F=\tan\beta_2 \sin\alpha_1 - \tan\beta_1 \sin\alpha_2 - \tan\beta_0 \sin(\alpha_2 - \alpha_1)$. Here α_1, α_2 are the projected angles of the two outgoing prongs in the plane of the emulsion, β_1, β_2 , are the corresponding dip angles, and β_0 is the dip angle of the incoming meson.⁸ The deviation from coplanarity $|F|$ is plotted (Fig. 4) versus $|\Theta|$, the deviation from the angular correlation curve for π^+H scattering. $\Theta = (\Delta\theta^2 + \Delta\phi^2)^{1/2}$, where $\Delta\theta$ and $\Delta\phi$ represent the respective angular deviations of each event from the calculated π^+H scattering curve as obtained from Fig. 2.

The distribution of the π^+H scattering between the forward and backward direction in the center-of-mass system is

$$d\sigma_{c.m.} = 2.7 \pm 1.3 \text{ mb/steradian for } \phi_{c.m.} = 35 - 90^\circ,$$

and

$$d\sigma_{c.m.} = 4.4 \pm 1.6 \text{ mb/steradian for } \phi_{c.m.} = 90 - 180^\circ.$$

As the scanning efficiency drops off for recoil prongs shorter than $\sim 50\mu$, a cutoff was taken at a recoil proton

⁸ This relation holds for either the original dip angles or the final dip angles in the shrunk emulsion. In Fig. 4, $|F|$ is plotted in the form using the final dip angles.

length of 100μ , which corresponds to a meson scattering angle of $\phi_{c.m.} = 35^\circ$. The asymmetry of the differential cross section with a peak in the backward direction found by Anderson and co-workers⁹ at π^+ energies of 135 Mev and 110 Mev appears to be still evident in the present work at 75 Mev. From the work of Shutt and co-workers,¹⁰ there is very little asymmetry at 53 Mev. The total cross section for π^+H scattering obtained is 41 ± 15 mb for $\phi_{c.m.} > 35^\circ$. This is in agreement with other measurements.¹¹

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⁹ Anderson, Fermi, Nagle, and Yodh, Phys. Rev. 86, 793 (1952).

¹⁰ Fowler, Fowler, Shutt, Thorndike, and Whittemore, Phys. Rev. 86, 1053 (1952).

¹¹ Anderson, Fermi, Long, and Nagle, Phys. Rev. 85, 936 (1952).

The Occurrence of Singularities in the Elastic Frequency Distribution of a Crystal

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It is shown that for a crystal, under the assumption of harmonicity for the interatomic forces and as a consequence of the periodic structure, the frequency distribution function of elastic vibrations has analytic singularities. In the general case, the nature of the singularities depends only on the number of dimensions of the crystal. For a two-dimensional crystal, the distribution function has logarithmically infinite peaks. In the three-dimensional case, the distribution function itself is continuous whereas its first derivative exhibits infinite discontinuities. These results are elementary consequences of a theorem of Morse on the existence of saddle points for functions defined on a torus.

I. INTRODUCTION

IT is well known that the shape of the frequency distribution function $g(\nu)$ of a crystal (defined as the number of elastic frequencies per unit frequency interval, divided by the total number of frequencies) determines an important part of the thermodynamical properties of the crystal. The frequency distribution of two- and three-dimensional crystals, as predicted by the Born-von Karman theory of crystal dynamics, has been extensively studied by approximate methods based on the use of a finite sample of elastic vibrations.¹ A

smooth distribution function was obtained in all cases, showing for small frequencies a behavior in full agreement with the Debye continuum theory, tending continuously to zero at the maximum frequency and displaying for intermediate frequencies a few finite maxima.²

The analytical nature of the frequency distribution function, or rather of its asymptotic form for a crystal of infinite extension, has recently attracted attention as a consequence of an exact calculation by Montroll for a two-dimensional square lattice.³ As found by

¹ M. Blackman, Repts. Prog. Phys. 8, 11 (1941) and references there quoted; E. Montroll, J. Chem. Phys. 10, 219 (1942); E. Montroll and D. Peaslee, J. Chem. Phys. 12, 98 (1944); H. M. J. Smith, Trans. Phil. Soc. A241, 105 (1948); W. V. Houston, Revs. Modern Phys. 20, 161 (1948); R. B. Leighton, Revs. Modern Phys. 20, 165 (1948).

² The frequency distribution obtained by Leighton (reference 1), has at the maximum frequency of each branch a singularity very similar to some of the singularities we shall show to exist in three dimensions. The singularities obtained by Houston (reference 1) are entirely spurious.

³ E. Montroll, J. Chem. Phys. 15, 575 (1947).

Montroll, for arbitrary values of the constants describing the forces between particles, the frequency distribution function has two logarithmically infinite peaks, one for each branch of the spectrum. These singularities were of course bound to remain undetected in the previous approximate investigations, in which the infinite peaks were approximated by finite maxima. Montroll's result has been extended by Smollett to the case of a two-dimensional ionic lattice, taking into account the long range Coulomb forces between ions.⁴

As noticed by Smollett, the logarithmic peaks obtained for the two-dimensional lattices considered are a simple consequence of the existence of saddle points for the function $\nu(\mathbf{q})$ expressing the frequency of an elastic plane wave in terms of its wave vector. The main object of the present paper is to point out that the existence of such saddle points in the $\nu(\mathbf{q})$ function, far from being accidental, is necessarily implied by the periodic structure of the lattice. According to a general theorem of M. Morse, any function of more than one independent variable which, as $\nu(\mathbf{q})$, is periodic in all its variables has at least a certain number of saddle points; this number is determined by topological considerations and depends only on the number of independent variables. It is this mathematical fact which accounts for the occurrence of logarithmic peaks in the $g(\nu)$ function; it implies that such peaks will appear quite generally for two-dimensional lattices.

For three-dimensional crystals, the theorem of Morse implies again the existence of saddle points in the $\nu(\mathbf{q})$ function. As will be shown below, saddle points of $\nu(\mathbf{q})$ produce, however, weaker singularities in the distribution function, no longer connected with its maxima: $g(\nu)$ remains continuous whereas $dg/d\nu$ has infinite discontinuities. In contradiction with a prediction by Smollett,⁴ no logarithmic infinities are therefore in general to be expected for three-dimensional lattices, although some could possibly occur when the forces between particles satisfy special conditions, not implied by the symmetry properties of the crystal.

II. TYPES OF SINGULARITIES

We shall now analyze in somewhat more detail the two elements which by their combination account for the occurrence of analytic singularities in the frequency distribution $g(\nu)$ of a crystal, namely, the rather elementary fact that saddle points of $\nu(\mathbf{q})$, and more generally points where $\text{grad}\nu(\mathbf{q})=0$, produce singularities in the $g(\nu)$ function, and the more fundamental theorem of Morse according to which the periodicity of the crystal implies the existence of saddle points for $\nu(\mathbf{q})$. The former fact will be discussed in this section, whereas Sec. III will deal with the application of Morse's theorem.

As is known from lattice dynamics,⁵ under the

⁴ M. Smollett, Proc. Phys. Soc. (London) A65, 109 (1952).

⁵ See for example M. Born and M. Goeppert-Mayer, *Handbuch der Physik* (J. Springer, Berlin, 1933), 24, No. 2, Chap. IV.

assumption of harmonicity for the forces between particles, the elastic vibrations of a crystal are superpositions of normal modes, each of which is a plane wave vibration with a definite frequency ν and a wave vector $2\pi\mathbf{q}$ defined up to the addition of an arbitrary vector $2\pi\sum_{\alpha}n_{\alpha}\mathbf{h}_{\alpha}$; here the n_{α} are integers and the \mathbf{h}_{α} are the basic vectors of the reciprocal lattice, related to the basic vectors \mathbf{s}_{β} of the crystal cell by

$$(\mathbf{h}_{\alpha}\cdot\mathbf{s}_{\beta})=\begin{cases} 1 & \text{for } \alpha=\beta \\ 0 & \text{for } \alpha\neq\beta. \end{cases}$$

For a crystal with Z atoms per cell, and in l dimensions (the cases $l=2$ and 3 will be discussed here),⁶ there are lZ independent plane wave vibrations for each wave vector \mathbf{q} , and their frequencies $\nu(\mathbf{q})$ are the positive square roots of the eigenvalues of a positive-definite symmetric matrix with lZ rows and columns; the coefficients of this matrix are periodic functions of \mathbf{q} with the periodicity of the reciprocal lattice. The frequency $\nu(\mathbf{q})$ is therefore an lZ valued function satisfying

$$\nu\left(\mathbf{q}+\sum_{\alpha=1}^l n_{\alpha}\mathbf{h}_{\alpha}\right)=\nu(\mathbf{q}), \quad (n_{\alpha} \text{ integers}). \quad (1)$$

It consists of lZ branches, some of which may become equal for special values of \mathbf{q} . Such equalities will be referred to as contacts between branches. According to (1), it is sufficient to consider $\nu(\mathbf{q})$ as defined in one single cell of the reciprocal lattice.

In terms of the multivalued $\nu(\mathbf{q})$ function, the frequency distribution function $g(\nu)$ for a crystal of infinite extension is given by

$$g(\nu)d\nu=(v_0/Zl)\int d_l\mathbf{q},$$

the integral being extended to the region within one cell of reciprocal space where $\nu\leq\nu(\mathbf{q})\leq\nu+d\nu$; an easy calculation gives then

$$g(\nu)=\frac{v_0}{Zl}\sum\int_{S(\nu)}\left[\sum_{\alpha=1}^l\left(\frac{\partial\nu(\mathbf{q})}{\partial q_{\alpha}}\right)^2\right]^{-\frac{1}{2}}dS; \quad (2)$$

v_0 is the volume of the crystal cell, and the q_{α} 's are the components of \mathbf{q} . The summation \sum extends over all branches of $\nu(\mathbf{q})$. For each of them $S(\nu)$ is the line (for $l=2$) or surface (for $l=3$) of reciprocal space defined by the equation $\nu(\mathbf{q})=\nu$ and limited to one cell of the reciprocal lattice; dS is the length or area of an infinitesimal portion of $S(\nu)$. Equation (2) remains valid after any change of coordinates in \mathbf{q} space leaving invariant the area or volume element $d_l\mathbf{q}$ of reciprocal space.

⁶ In one dimension, $l=1$, the frequency distribution is known to have no singularity apart from infinities at the extreme frequencies of each branch. See F. Seitz, *Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), p. 123.

It is now clear that the analytic singularities of $g(\nu)$ originate from the so-called critical points of $\nu(\mathbf{q})$, i.e., the points where all derivatives $\partial\nu/\partial q_\alpha$ vanish. Let us investigate the singularity produced in $g(\nu)$ by a critical point \mathbf{q}_c of $\nu(\mathbf{q})$, in the general case where the determinant $|\partial^2\nu/\partial q_\alpha\partial q_\beta|$ does not vanish at \mathbf{q}_c (as is usual in mathematics, such a critical point will be called non-degenerate). Putting $\nu(\mathbf{q}_c)=\nu_c$, we may write in first approximation for \mathbf{q} near \mathbf{q}_c , and after a convenient change of coordinates preserving $d\mathbf{q}$,

$$\nu = \nu_c + a \sum_{\alpha=1}^l \epsilon_\alpha \xi_\alpha^2 + \dots, \quad \epsilon_\alpha = \pm 1, \quad \xi = \mathbf{q} - \mathbf{q}_c, \quad a > 0. \quad (3)$$

Restricting the summation in (2) to the branch with the critical point and the integration to a neighborhood of \mathbf{q}_c , we use (3) in (2) and obtain the following singularities in $g(\nu)$ for ν near ν_c .

Two-Dimensional Crystal

$$(M, i=0) \quad \epsilon_1 = \epsilon_2 = -1,$$

$$g(\nu) = \begin{cases} C + (\pi v_0/Zla) + 0(\nu - \nu_c) & \text{for } \nu < \nu_c \\ C + 0(\nu - \nu_c) & \text{for } \nu > \nu_c \end{cases}$$

$$(S, i=1) \quad \epsilon_1 = -\epsilon_2 = \pm 1,$$

$$g(\nu) = C - \frac{v_0}{Zla} \log \left| 1 - \frac{\nu}{\nu_c} \right| + 0(\nu - \nu_c)$$

$$(m, i=2) \quad \epsilon_1 = \epsilon_2 = 1,$$

$$g(\nu) = \begin{cases} C + 0(\nu - \nu_c) & \text{for } \nu < \nu_c \\ C + (\pi v_0/Zla) + 0(\nu - \nu_c) & \text{for } \nu > \nu_c \end{cases}$$

Three-Dimensional Crystal

$$(M, i=0) \quad \epsilon_1 = \epsilon_2 = \epsilon_3 = -1,$$

$$g(\nu) = \begin{cases} C + (2\pi v_0/Zla^{\frac{2}{3}})(\nu - \nu_c)^{\frac{2}{3}} + 0(\nu - \nu_c) & \text{for } \nu < \nu_c \\ C + 0(\nu - \nu_c) & \text{for } \nu > \nu_c \end{cases}$$

$$(S_1, i=1) \quad \epsilon_{\alpha_1} = \epsilon_{\alpha_2} = -\epsilon_{\alpha_3} = -1,$$

$$g(\nu) = \begin{cases} C + 0(\nu - \nu_c) & \text{for } \nu < \nu_c \\ C - (2\pi v_0/Zla^{\frac{2}{3}})(\nu - \nu_c)^{\frac{2}{3}} + 0(\nu - \nu_c) & \text{for } \nu > \nu_c \end{cases}$$

$$(S_2, i=2) \quad \epsilon_{\alpha_1} = \epsilon_{\alpha_2} = -\epsilon_{\alpha_3} = 1,$$

$$g(\nu) = \begin{cases} C - (2\pi v_0/Zla^{\frac{2}{3}})(\nu - \nu_c)^{\frac{2}{3}} + 0(\nu - \nu_c) & \text{for } \nu < \nu_c \\ C + 0(\nu - \nu_c) & \text{for } \nu > \nu_c \end{cases}$$

$$(m, i=3) \quad \epsilon_1 = \epsilon_2 = \epsilon_3 = 1,$$

$$g(\nu) = \begin{cases} C + 0(\nu - \nu_c) & \text{for } \nu < \nu_c \\ C + (2\pi v_0/Zla^{\frac{2}{3}})(\nu - \nu_c)^{\frac{2}{3}} + 0(\nu - \nu_c) & \text{for } \nu > \nu_c \end{cases}$$

The symbols M and m refer to maxima and minima, respectively. S refers to saddle points in the two-

dimensional case, whereas for three dimensions, the saddle points are of two different types, denoted by S_1 and S_2 . The number i is the so-called index of the critical point, to be used later. In all expressions C is a constant and $O(\nu - \nu_c)$ denotes a rest term of the order of $\nu - \nu_c$ for $\nu \rightarrow \nu_c$. Higher singularities would be produced by critical points for which $|\partial^2\nu/\partial q_\alpha\partial q_\beta| = 0$, in particular by a continuous family of critical points. Such cases are to be considered exceptional as compared to the general case just discussed: it can be shown that they occur only when the constants describing the forces between particles satisfy special relations not implied by the crystal symmetries.

III. APPLICATION OF MORSE'S THEOREM

According to the periodicity condition (1), it is natural to consider the $\nu(\mathbf{q})$ function as defined in one cell of the reciprocal lattice, and to identify points \mathbf{q} , \mathbf{q}' of the boundary of the cell for which

$$\mathbf{q}' = \mathbf{q} + \sum_{\alpha=1}^l n_\alpha \mathbf{h}_\alpha, \quad (n_\alpha \text{ integers}).$$

The domain of definition thus obtained for $\nu(\mathbf{q})$ is an l dimensional torus.

We now state the theorem of Morse under elementary and too restrictive assumptions: consider a function f defined on a closed topological manifold satisfying convenient conditions of differentiability and regularity; assume f to be three times continuously differentiable and to have no degenerate critical points. Call index of a nondegenerate critical point the number of positive eigenroots of the quadratic form in the Taylor expansion of f near the critical point [number of positive terms in the sum in (3)]. Under these conditions, the number of critical points of index i is at least equal to the Betti number R_i of the manifold for the dimension i .⁷

For $l=2$, the two-dimensional torus has Betti numbers $R_0=1$, $R_1=2$, $R_2=1$. If a branch of $\nu(\mathbf{q})$ satisfies the above conditions, it has therefore at least one maximum, two saddle points and one minimum. The corresponding singularities in $g(\nu)$ were listed in Sec. II. By reason of symmetry the two saddle points may often correspond to the same value of $\nu(\mathbf{q})$; they will then produce one single logarithmic peak in $g(\nu)$.

In three dimensions, the Betti numbers of the torus are $R_0=1$, $R_1=3$, $R_2=3$, $R_3=1$. For a branch of $\nu(\mathbf{q})$ satisfying the above conditions, there are at least one maximum, three saddle points of each type and one

⁷ For an elementary exposition and examples, see M. Morse, *Am. Math. Monthly* 49, 358 (1942), Sec. 5. For details and proofs, see M. Morse, *Trans. Am. Math. Soc.* 27, 345 (1925); *Calculus of Variations in the Large, Colloquium Lectures* (American Mathematical Society, Providence, 1934), Chap. VI; *Mémoires de Sciences Mathématiques*, "Functional Topology and Abstract Variational Theory" (Gauthier-Villars, Paris, 1939), Fasciule 92. Regarding the definition of the Betti numbers, for our purpose it is sufficient to say that R_i is the maximum number of closed i dimensional surfaces on the manifold which cannot be transformed into one another or into a point by continuous deformation on the manifold.

minimum. Saddle points of the same type will often correspond to the same frequency. The branch considered produces therefore in $g(\nu)$ at least one singularity of each of the four types listed in the previous section for $l=3$.

To determine the net number of singularities to be expected in the frequency distribution $g(\nu)$, one has now to take into account two important factors. Firstly, singularities produced in $g(\nu)$ by various branches may compensate each other. Inspection of the list of singularities in Sec. II shows that for $l=2$ such compensations can occur for the singularities produced in $g(\nu)$ by a maximum and a minimum of $\nu(\mathbf{q})$, whereas cancellations are impossible for the logarithmic peaks resulting from saddle points. For $l=3$ compensations can take place between a maximum and a saddle point of type S_2 (i.e., of index 2), as well as between a minimum and a saddle point of type S_1 (i.e., of index 1).

Secondly, the assumptions made above for the branches of the $\nu(\mathbf{q})$ function are too restrictive: both the behavior of $\nu(\mathbf{q})$ for small ν and certain contacts between branches prevent them from being fulfilled. Before entering into general considerations, let us discuss the region of very small frequencies. It is reached for the l acoustical branches near $\mathbf{q}=0$ (long wavelengths), where the Debye continuum theory of solids is applicable. For each acoustical branch $\nu(\mathbf{q})$ has its absolute minimum $\nu(0)=0$ at $\mathbf{q}=0$. As is well known, this minimum does not have the same properties as the critical points considered up to now. The Taylor expansion (3) is not valid in its neighborhood and is replaced by an expression

$$\nu = |q| \cdot \varphi(\mathbf{q}/|q|) + O(|q|^2) \quad (4)$$

for $|q|$ small; φ is a positive function of the direction of \mathbf{q} , which can be determined from the elastic constants of the crystal.⁸ According to (4), $|\text{grad}\nu(\mathbf{q})|$ does not tend to zero for $\mathbf{q} \neq 0$ tending to zero, although the gradient is undefined at the point $\mathbf{q}=0$ itself. Therefore this minimum of $\nu(\mathbf{q})$ produces no singularity in $g(\nu)$: from (4) follows the familiar behavior of $g(\nu)$ for small frequencies,

$$g(\nu) \sim \nu^{l-1}.$$

In the same way as $\mathbf{q}=0$ is for the acoustical branches what we may call a generalized minimum, other generalized critical points can occur in $\nu(\mathbf{q})$ at the contacts between branches. For our purpose, the concept of generalized critical point \mathbf{q}_c of index i can be described in the following way: for a one-valued function $f(\mathbf{q})$, one branch of $\nu(\mathbf{q})$ for example, it is a point in the neighborhood of which, although $f(\mathbf{q})$ has no Taylor expansion of type (3), the surfaces $f(\mathbf{q})=f_0$, with f_0 constant and near $f(\mathbf{q}_c)$, have the same topological shape as for the nondegenerate critical points of index i considered above. Just as for the generalized minimum (i.e., critical point of index l) discussed above for the

acoustical branches, the generalized critical points to be expected in $\nu(\mathbf{q})$ give rise to an expansion similar to (4)

$$\nu(\mathbf{q}) - \nu(\mathbf{q}_c) = |\xi| \cdot \psi(\xi/|\xi|) + O(|\xi|^2), \quad \xi = \mathbf{q} - \mathbf{q}_c.$$

If the directions in which $\psi(\xi/|\xi|)$ vanishes are discrete for $l=2$ or depend on one continuous parameter for $l=3$, such generalized critical points produce in $g(\nu)$ weaker singularities (discontinuities in higher derivatives) than the conventional critical points of same index; moreover the weaker singularities produced by the various branches in contact are likely to compensate each other. On the other hand, if ψ vanishes identically, the quadratic terms of the expansion have to be used. They have the form

$$\nu(\mathbf{q}) - \nu(\mathbf{q}_c) = |\xi|^2 \psi_1(\xi/|\xi|) + O(|\xi|^3)$$

and, for general values of the forces, they can be shown to produce in $g(\nu)$ the same singularities as the conventional critical points discussed in Sec. II, with again possible compensation between the branches in contact.

The important fact is now that the theorem of Morse is valid under much wider conditions than stated above.⁷ For the functions which, like the branches of $\nu(\mathbf{q})$, may have generalized critical points, its prediction is that the number of critical points of index i , the generalized ones included, is at least equal to the Betti number R_i . We have therefore to discuss under what conditions generalized critical points can occur, and which critical points may be expected not to be of generalized type and hence to produce in $g(\nu)$ the singularities predicted for them in Sec. II. The absolute minimum $\nu=0$ of $\nu(\mathbf{q})$, reached in the acoustical branches, is already known to be of generalized type. Other generalized critical points can be produced only by contacts between branches and will now be discussed for the most common types of contacts.

The condition of having two eigenvalues equal decreases by two the number of parameters on which a real symmetric matrix depends.⁹ For two-dimensional crystals, the contacts between branches occur therefore in general in isolated points of reciprocal space. If we define the various branches $\nu_1(\mathbf{q})$, $\nu_2(\mathbf{q})$, \dots , $\nu_{lZ}(\mathbf{q})$ by the increasing order of their frequencies for each \mathbf{q} :

$$\nu_1(\mathbf{q}) \leq \nu_2(\mathbf{q}) \leq \dots \leq \nu_{lZ}(\mathbf{q}), \quad (5)$$

an algebraic discussion shows that at an isolated point of contact a maximum of one branch can coincide with a minimum of the subsequent branch, and both can be of generalized type. No generalized saddle points are to be expected for arbitrary force constants.

For $l=3$ on the contrary, contacts between branches, occurring along curves or in isolated points of \mathbf{q} space, often affect saddle points as well as extrema. Certain contacts are a consequence of crystal symmetries, others do not follow from symmetry and are therefore

⁸ H. A. Jahn, Proc. Roy. Soc. (London) A179, 320 (1941).

⁹ J. von Neumann and E. Wigner, Physik. Z. 30, 467 (1929).

called accidental. Both types have been carefully discussed for energy bands of electrons in a crystal; this discussion applies without essential change to crystal vibrations.¹⁰ Using again (5), let us consider two branches $\nu_i(\mathbf{q})$ and $\nu_{i+1}(\mathbf{q})$ in contact along a curve C , which is necessarily a closed circuit when taken on the three-dimensional torus. Let the maximum of $\nu_i(\mathbf{q}) = \nu_{i+1}(\mathbf{q})$ on C be reached at \mathbf{q}_1 , its minimum at \mathbf{q}_2 . The point \mathbf{q}_1 can be a maximum of ν_i and a saddle point of index 2 for ν_{i+1} , and these critical points can be of generalized type. The same holds for \mathbf{q}_2 which can be a saddle point of index 1 for ν_i and a minimum for ν_{i+1} .¹¹ For contacts of two or more branches in an isolated point $\mathbf{q} \neq 0$ of reciprocal space, the generalized critical points which are most likely to appear are a generalized maximum for the lower branch and a generalized minimum for the upper branch, although more complicated situations are not excluded.

Apart from the absolute minimum $\nu=0$, the critical points which can be of generalized type are seen to belong to pairs of critical points of equal frequency. The pairs are maximum-minimum for $l=2$ or 3, maximum-saddle point of index 2 and minimum-saddle point of index 1 for $l=3$. Apart from maximum-minimum for $l=3$, these are also the pairs of critical points which can produce compensating singularities in $g(\nu)$. For $l=2$, all saddle points and the absolute maximum of $\nu(\mathbf{q})$ will therefore remain unaffected by the contacts between branches and they will produce in $g(\nu)$ the singularities predicted for them in Sec. II. No compensation can take place between these singularities, but as noted already in Sec. II, the logarithmic peaks resulting from saddle points belonging to the same branch may coincide as a consequence of crystal symmetries. *This gives for the $g(\nu)$ function of a two-dimensional crystal at least one logarithmic peak per branch and at least a finite discontinuity, occurring at the upper end of the spectrum.* The results obtained by Montroll³ and Smollett⁴ clearly illustrate this conclusion.

For $l=3$, according to our discussion of the most common contacts between branches, the only critical points of $\nu(\mathbf{q})$ which are never affected by such contacts are the absolute maximum of $\nu(\mathbf{q})$, the saddle points of index 2 of the branch with lowest maximum frequency and the saddle points of index 1 of the branch with largest minimum frequency. These points contribute to $g(\nu)$ the singularities predicted for them in Sec. II. No compensation is possible between these singularities,

¹⁰ Contacts resulting from symmetry are treated by group-theoretical methods by Bouckaert, Smoluchowski, and Wigner, *Phys. Rev.* **50**, 58 (1936), and by C. Herring, *Phys. Rev.* **52**, 361 (1937). For accidental contacts, see C. Herring, *Phys. Rev.* **52**, 365 (1937). The author is indebted to Dr. C. Herring for bringing to his attention the whole question of contacts between branches.

¹¹ From a mathematical standpoint, the separation of the branches ν_i and ν_{i+1} according to (5) is unnatural: along a path through a point of C , the natural continuation of ν_i is ν_{i+1} and vice versa. This can be avoided by considering the multivalued $\nu(\mathbf{q})$ function as a univalued function on a convenient covering manifold of the torus.

but the crystal symmetries may imply the coincidence of singularities produced by various saddle points belonging to the same branch and having the same index. *The general prediction we can make for three-dimensional crystals is therefore that, $g(\nu)$ being continuous, $dg/d\nu$ has at least two infinite discontinuities, and takes the value $-\infty$ at the upper end of the spectrum.* In many cases, of course, especially when the crystal symmetry is not too high, the number of infinite discontinuities in $dg/d\nu$ will be considerably larger. For the detailed analytical nature of these discontinuities, the reader is referred to the list of singularities in Sec. II, from where it is obtained by mere differentiation of $g(\nu)$ near ν_c .

IV. CONCLUDING REMARKS

As was emphasized several times, the whole discussion carried out in this paper is of a general nature. In each step we tried to handle the case of greatest generality, leaving out various exceptions. Most exceptional cases arise when the force constants strictly satisfy special relations not following from crystal symmetry; hence these cases have no physical interest; they will exhibit in $g(\nu)$ stronger singularities than predicted above, for example logarithmic peaks in three dimensions. The only exceptional case which has not been excluded for general values of the force constants is that of three-dimensional crystals with more complicated contacts between branches than considered above; for them the number or strength of the singularities, if affected at all, could only be reduced.

In regard to the numerical determination of frequency distributions for crystals, the above discussion shows that great attention has to be paid to location and shape of the critical points of $\nu(\mathbf{q})$. This information can be obtained from the shape of the contours of constant frequency in reciprocal space, as was done by Smollett for a two-dimensional ionic lattice.⁴

Finally, it is worth mentioning that the discussion presented in this paper also applies to the Bloch theory of electrons in crystal lattices. The energy of the electron, which is here taking the place of the square of the vibration frequency, is a periodic function of the wave vector and has therefore at least the minimum numbers of critical points predicted by the theorem of Morse, with the same consequences as above for the distribution function (density) of states in energy.¹²

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¹² The density of states of an electron in a two-dimensional layer of graphite has been calculated by C. A. Coulson and R. Taylor, *Proc. Phys. Soc. (London)* **A65**, 815 (1952). In agreement with our predictions, it has two logarithmic infinities for intermediate energies and finite discontinuities at both ends of the energy range.