being significantly dependent upon the range of the interatomic potential.

The method of lattice statics, on the other hand, is exact within the harmonic approximation, which is shown to be quite valid for the present calculations. It appears, therefore, that the only consistent method of calculating the direct-space forces due to the defect and hence the strain-field displacements and associated parameters is the method of lattice statics. Certainly, it would seem that any strain-field properties obtained as a result of direct-space calculations in any of the bcc metals should be reappraised using the lattice statics approach.

ACKNOWLEDGMENTS

The author wishes to thank Professor J. R. Hardy for suggesting this problem and Professor R. A. Johnson for providing certain unpublished results of the strain-field configuration about a vacancy.

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PHYSICAL REVIEW B VOLUME 2, NUMBER 6 15 SEPTEMBER 1970

Dynamics of Disordered Alloys and Glasses*

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(Received 26 January 1970)

A formalism is presented for the calculation of the spectrum of normal modes of a disordered solid by means of a perturbation theory that takes a mean-field model as its unperturbed system. A transformation is used that allows the long-range correlations in the low-frequency vibrational modes to be accurately taken into account. In the special case of a random substitutional alloy, a result is found which reduces to those of other workers when the limit of small mass difference of the constituents or low concentration is taken. Some aspects of the application of the theory to amorphous systems are also discussed.

I. INTRODUCTION

The topic of the dynamics of disordered systems is at present a rather fragmented area of theoretical physics, in that the concepts that have been developed to discuss one type of disordered solid are only rarely applicable to other systems. A calculation of the spectrum of vibrational modes of a substitutional alloy, for example, may be attempted in a perturbation theory in which the phonon modes of a pure material form the unperturbed states. The results may then be expressed as a power series in either the concentration of one element of the alloy[1] or the difference in mass of the two elements.[2] Such methods, however, cannot readily be applied to glasses or other materials that are lacking in long-range order, in that there is then no obvious Brillouin zone to limit the wave numbers of whatever phonon spectrum is chosen to represent the unperturbed system; in other words, there is no one-to-one correspondence between the atomic sites in the glass and in any perfect periodic lattice except in the special case of one-dimensional systems. The most fruitful approach to calculating the vibrational spectrum of glasses accordingly starts[3] with the Einstein or mean-field model, in which such a one-to-one correspondence does exist; the unperturbed system then involves the independent motion of the N atoms forming the glass about their equilibrium sites $\vec{l}$. The difficulty here is that in the perturbed modes of lowest frequency there is correlation between the motions of atoms separated by large distances. Perturbation theory must then be used in such a way that various infinite sets of terms must be summed if the spectrum is to display the correct Debye form at low frequencies. In diagrammatic language, the terms of such a series are represented as in Fig. 1 by closed paths linking the various equilibrium sites $\vec{l}$. The difficulty of performing infinite summations of such diagrams with only limited statistical information about the locations of the sites $\vec{l}$ does not need stressing.

The approach adopted in this paper represents an attempt to combine the most useful features of the previous approaches to these problems. We take as our unperturbed system the Einstein model but then perform a transformation which in the limiting case of a perfect crystal would simply be a reduction to phonon modes, and which for a glassy system allows us to incorporate such knowledge as we have about the relative positions of the atoms.

The principal advantage of this approach lies in the fact that some separation is possible between the concepts of *structural disorder* and *dynamical disorder*. Structural disorder is represented by the presence in the perturbation expansions of a function $R_{\vec{q}\vec{q}'}$ that vanishes for the case of a perfect Bravais lattice, but which is nonzero in an amorphous system. Dynamical disorder, on the other hand, arises from the variation from site to site of the masses of the atoms and the forces connecting them, and appears in the perturbation expansions through a function $B(\vec{l},\vec{q},\vec{q}')$: Thus the case of an isotopically disordered alloy can be treated as a power series in B alone. This particular example is treated in some detail for a cubic crystal in Sec. III of this paper, since it yields a very simple result for the frequency spectrum that can be compared with the results of other workers. Section IV is devoted to a discussion of the validity of truncating the renormalized perturbation series for an amorphous solid: The conclusion reached is that the presence of short-range order leads to a rapid convergence of the power series in the structural-disorder function.

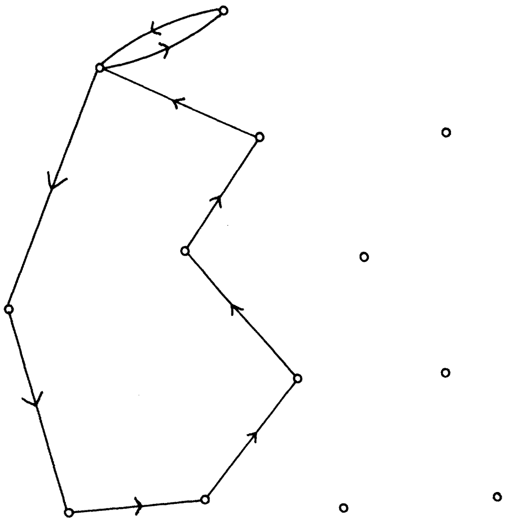

FIG. 1. Typical term in a perturbation theory based on the Einstein model.

II. FORMALISM

We start by considering an array of N atoms whose equilibrium positions are defined by the vectors $\vec{l}$. The classical equations of motion for small oscillations about these sites can be written in the form

$$\frac{d^2 y_i(\vec{l})}{dt^2} = \sum_{\vec{l}',j} K_{ij}(\vec{l},\vec{l}')\,y_j(\vec{l}') \quad , \tag{1}$$

where $y_i(\vec{l})$ is the ith Cartesian component of the displacement of an atom from its site $\vec{l}$ and the $K_{ij}(\vec{l},\vec{l}')$ are a set of coefficients defined by the masses of the atoms and the interatomic forces and are subject to the condition

$$\sum\nolimits_{\vec{l}'} K_{ij}(\vec{l},\vec{l}') = 0 \quad .$$

For a mode of angular frequency ω, Eq. (1) can be written as

$$\sum_{\vec{l}',j} \left[(\omega^2 - T)\delta_{\vec{l}\vec{l}'}\delta_{ij} - V_{ij}(\vec{l},\vec{l}')\right] y_j(\vec{l}') = 0 \tag{2}$$

or more briefly as

$$\sum_{\vec{l}',j} (D^{-1})_{ij}(\vec{l},\vec{l}',\omega^2)\,y_j(\vec{l}') = 0 \quad , \tag{3}$$

where

$$V_{ij}(\vec{l},\vec{l}') = -K_{ij}(\vec{l},\vec{l}') - T\delta_{\vec{l}\vec{l}'}\delta_{ij} \tag{4}$$

and T is some suitably chosen constant. If we define $\mathfrak{N}(\omega^2)$ as the number of modes with frequency less than ω, then it can be shown that the density of modes as a function of ω^2 is given by

$$\frac{d\mathfrak{N}}{d\omega^2} = g(\omega^2) = -\pi^{-1}\,\mathrm{Im}\sum_{\vec{l},i} D_{ii}(\vec{l},\vec{l},\omega^2 + i\eta) \quad , \tag{5}$$

with the Green's function $D_{ij}(\vec{l},\vec{l}',\omega^2)$ defined from Eq. (3) by

$$D^{-1}{}_{ij}(\vec{l},\vec{l}\,',\omega^2)D_{jk}(\vec{l}\,',\vec{l}\,'',\omega^2)=\delta_{\vec{l}\vec{l}''}\delta_{ik}$$

and with η a vanishingly small positive quantity. With the definition

$$D_0=(\omega^2-T)^{-1} \quad ,$$

one may write

$$D_{ij}(\vec{l},\vec{l}\,')=D_0\delta_{\vec{l}\vec{l}'}\delta_{ij}+D_0^2V_{ij}(\vec{l},\vec{l}\,') + D_0^3\sum_{k,\vec{l}''}V_{ik}(\vec{l},\vec{l}\,'')V_{kj}(\vec{l}\,'',\vec{l}\,')+\cdots \quad . \tag{6}$$

The summation of this series forms the major problem to be discussed in this paper.

If we were dealing with the problem of a perfect Bravais lattice, then we could evaluate TrD, the trace of the Green's function, most directly by making a transformation involving the matrix

$$S_{\vec{l}\vec{q}}=N^{-1/2}e^{-i\vec{q}\cdot\vec{l}} \quad , \tag{7}$$

with the N vectors $\vec{q}$ defined to lie within the first Brillouin zone and to satisfy suitable periodic boundary conditions. Under these conditions, the matrix S is unitary and thus has the inverse

$$E_{\vec{q}\vec{l}}=N^{-1/2}e^{i\vec{q}\cdot\vec{l}} \quad . \tag{8}$$

In the more general case of an amorphous solid, S is no longer unitary, and no simply defined Brillouin zone exists. Nevertheless, we shall retain the definitions of S and E given in Eqs. (7) and (8) and also assume periodic boundary conditions to apply over a large volume Ω of the disordered solid, so that the density of allowed values in wavenumber space remains uniform and equal to $\Omega/8\pi^3$. We shall, however, leave open for the time being the question of which N allowed values of $\vec{q}$ we choose when performing summations over this quantity. We look for the inverse of S by introducing a matrix $R_{\vec{q}\vec{q}'}$ defined by the equation

$$(I+R)S^{-1}=E \quad , \tag{9}$$

with I the unit matrix. Multiplication on the right by S then yields the relation

$$R_{\vec{q}\vec{q}'}=N^{-1}\sum_{\vec{l}} e^{i(\vec{q}-\vec{q}')\cdot\vec{l}}-\delta_{\vec{q}\vec{q}'} \quad . \tag{10}$$

The matrix R will now be recognized as being related to the structure factor of the solid. In the special case of a perfect lattice it vanishes for all $\vec{q}$ and $\vec{q}\,'$ within the first Brillouin zone. In the general case we iterate Eq. (9) to find

$$S^{-1}=E-RE+R^2E-\cdots \quad ,$$

with R given by Eq. (10).

We now apply a transformation[4] to the interaction term V and write

$$\begin{aligned} V &= SS^{-1}VSS^{-1} \\ &= S(E-RE+R^2E-\cdots)VS(E-RE+R^2E-\cdots) \; . \end{aligned} \tag{11}$$

This allows Eq. (5) to be rewritten in the form

$$g(\omega^2)=-\pi^{-1}\,\mathrm{Im}\sum_{\vec{q},i}D_{ii}(\vec{q},\vec{q},\omega^2) \quad , \tag{12}$$

with

$$D(\vec{q},\vec{q}\,',\omega^2)=\sum_{p=0}^{\infty}D_0^{p+1}[(S^{-1}VS)^p]_{\vec{q}\vec{q}'} \quad . \tag{13}$$

Further,

$$\begin{aligned}(S^{-1}V_{ij}S)_{\vec{q}\vec{q}'} &= N^{-1}\sum_{\vec{q}'',\vec{l},\vec{l}'}[(I+R)^{-1}]_{\vec{q}\vec{q}''}e^{i\vec{q}''\cdot\vec{l}}V_{ij}(\vec{l},\vec{l}\,')e^{-i\vec{q}'\cdot\vec{l}'} \\ &= N^{-1}\sum_{\vec{q}''}[(I+R)^{-1}]_{\vec{q}\vec{q}''}\sum_{\vec{l}}e^{i(\vec{q}''-\vec{q}')\cdot\vec{l}} \\ &\quad\times\sum_{\vec{L}}V_{ij}(\vec{l},\vec{l}-\vec{L})e^{i\vec{q}'\cdot\vec{L}} \quad , \end{aligned} \tag{14}$$

where in the last line $\vec{L}$ has been written for $\vec{l}-\vec{l}\,'$.

In a perfect Bravais lattice the sum over $\vec{L}$ would be independent of $\vec{l}$, and would thus be a function only of $\vec{q}\,'$. This will also be approximately the case in many disordered systems: One may visualize as an example a glass in which each atom is surrounded by four others in a roughly tetrahedral arrangement. Although the orientation of these tetrahedra may vary from site to site, the sum over $\vec{L}$ may well be only weakly dependent on this orientation. We accordingly consider this sum as being composed of two parts – its average over all $\vec{l}$ and its site-dependent deviation from that average – and write

$$\sum_{\vec{L}} V_{ij}(\vec{l},\vec{l}-\vec{L})e^{i\vec{q}'\cdot\vec{L}}=V_{ij}(\vec{q}\,')+U_{ij}(\vec{l},\vec{q}\,') \; , \tag{15}$$

with

$$\sum_{\vec{l}} U_{ij}(\vec{l},\vec{q}\,')=0 \quad . \tag{16}$$

In terms of these quantities Eq. (14) becomes

$$(S^{-1}V_{ij}S)_{\vec{q}\vec{q}'}=V_{ij}(\vec{q})\delta_{\vec{q}\vec{q}'}+W_{ij}(\vec{q},\vec{q}\,') \quad , \tag{17}$$

with

$$W_{ij}(\vec{q},\vec{q}\,')=\sum_{\vec{q}''}[(I+R)^{-1}]_{\vec{q}\vec{q}''}\sum_{\vec{l}}B_{ij}(\vec{l},\vec{q}\,'',\vec{q}\,') \tag{18}$$

and

$$B_{ij}(\vec{l},\vec{q}\,'',\vec{q}\,')=N^{-1}e^{i(\vec{q}''-\vec{q}')\cdot\vec{l}}U_{ij}(\vec{l},\vec{q}\,') \quad . \tag{19}$$

Substitution of Eq. (17) in Eq. (13) allows us to form an expression for the elements of the Green's function that are diagonal in $\vec{q}$ (although not necessarily diagonal in the Cartesian coordinate system). We find

$$\begin{aligned} D_{ij}(\vec{q},\vec{q},\omega^2) &= D_0\delta_{ij}+D_0^2[V_{ij}(\vec{q})+W_{ij}(\vec{q},\vec{q})] \\ &\quad + D_0^3\sum_{\vec{q}',k}[V_{ik}(\vec{q})\delta_{\vec{q}\vec{q}'}+W_{ik}(\vec{q},\vec{q}\,')] \\ &\quad \times[V_{kj}(\vec{q})\delta_{\vec{q}'\vec{q}}+W_{kj}(\vec{q}\,',\vec{q})]+\ldots \end{aligned}$$

$$= \sum_k \left(\frac{D_0}{1-D_0 V(\vec{q})}\right)_{ik} \left(\delta_{kj} + \sum_{\vec{q}',m} W_{km}(\vec{q},\vec{q}')D_{mj}(\vec{q}',\vec{q},\omega^2)\right).$$

Use of Dyson's equation[5] allows us to express $D_{ij}(\vec{q},\vec{q},\omega^2)$ in terms of the proper self-energy or Dysonian $M_{ij}(\vec{q},\omega^2)$. We have

$$D_{ij}(\vec{q},\vec{q},\omega^2) = \sum_k \left(\frac{D_0}{1-D_0 V(\vec{q})}\right)_{ik} \times \left[\delta_{kj} + \sum_m M_{km}(\vec{q},\omega^2)D_{mj}(\vec{q},\vec{q},\omega^2)\right]$$
$$= \{[\omega^2 - T - V(\vec{q}) - M(\vec{q},\omega^2)]^{-1}\}_{ij}. \qquad (20)$$

The Dysonian $M_{ij}(\vec{q},\omega^2)$ is most simply defined by illustrating its various components in diagrams of the form shown in Fig. 2. This particular diagram represents the product

$$(-R)_{\vec{q}\vec{q}'}(-R)_{\vec{q}'\vec{q}''}B_{ik}(\vec{l},\vec{q}'',\vec{q}''') \times \{[\omega^2 - T - V(\vec{q}''')]^{-1}\}_{km}B_{mj}(\vec{l}',\vec{q}''',\vec{q}).$$

The sum of all such diagrams (the simplest of which are shown in Fig. 3) in which the wave-number index of the propagator $(\omega^2 - T - V)^{-1}$ is not equal to $\vec{q}$ forms $M_{ij}(\vec{q},\omega^2)$. The cross at which each vertical dashed line terminate denote the atomic site $\vec{l}$ appearing in the function B_{ij}.

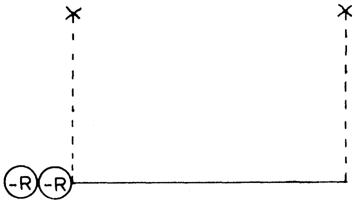

FIG. 2. Typical element of $M_{ij}(\vec{q},\omega^2)$.

III. RANDOM SUBSTITUTIONAL ALLOY

As an illustration of this technique we consider the well-known example of a random substitutional alloy. In the simplest version of this problem the force constants are assumed equal to those in some pure material; the disorder enters the problem only through the possibility of a given site $\vec{l}$ of the Bravais lattice being occupied by an atom of mass either m_a or m_b, with respective probabilities c_a and c_b. If we choose T equal to zero, then Eqs. (15) and (16) tell us that $V_{ij}(\vec{q})$ takes on the value corresponding to a pure lattice of mass m, with m the reciprocal of the average inverse mass:

$$m = m_a m_b/(c_a m_b + c_b m_a).$$

Since R vanishes in this example, Eqs. (18) and (19) tell us that

$$W_{ij}(\vec{q},\vec{q}') = \frac{1}{N}\sum_{\vec{l}} e^{i(\vec{q}-\vec{q}')\cdot\vec{l}}\left(\frac{m}{m_{\vec{l}}}-1\right)V_{ij}(\vec{q}').$$

We form an approximate expression for the Dysonian by evaluating the diagrams shown in Fig. 4. In this figure the occurrence of the same site $\vec{l}$ in two or more factors of $B_{ij}(\vec{l},\vec{q},\vec{q}'')$ is shown by terminating the dashed lines at the same cross. The heavy lines replacing the light horizontal lines of Fig. 2 indicate that the propagator $[\omega^2 - T - V(\vec{q})]^{-1}$ has been replaced by $D(\vec{q},\vec{q},\omega^2)$ in an approximate renormalization, the principal defect of which is the fact that the wave number $\vec{q}$ is not excluded[6] from the terms comprising D. One then has

$$M_{ij}(\vec{q},\omega^2) = \sum_{\vec{l}}\left(\frac{m}{m_{\vec{l}}}-1\right)\frac{V_{ij}(\vec{q})}{N} + \sum_{\vec{l}}\left(\frac{m}{m_{\vec{l}}}-1\right)^2 \sum_{\vec{q}',k,m}\frac{V_{ik}(\vec{q}')}{N}D_{km}(\vec{q}')\frac{V_{mj}(\vec{q})}{N} + \cdots$$
$$= \sum_{\vec{l},k}\left\{\left[1-\left(\frac{m}{m_{\vec{l}}}-1\right)\sum_{\vec{q}'}\frac{V(\vec{q}')}{N}D(\vec{q}')\right]^{-1}\right\}_{ik}\left(\frac{m}{m_{\vec{l}}}-1\right)\frac{V_{kj}(\vec{q})}{N} = \sum_k \sum_{p=a,b}\left(\frac{c_p\gamma_p}{1-\gamma_p J(\omega^2)}\right)_{ik} V_{kj}(\vec{q}),$$

where

$$\gamma_p = m/m_p - 1$$

and

$$J_{ij}(\omega^2) = \frac{1}{N}\sum_{k,\vec{q}'} V_{ik}(\vec{q}')D_{kj}(\vec{q}',\vec{q}',\omega^2).$$

Some further reduction shows that

$$M(\vec{q},\omega^2) = -\frac{\gamma_a\gamma_b J(\omega^2)}{[1-\gamma_a J(\omega^2)][1-\gamma_b J(\omega^2)]}V(\vec{q}), \qquad (21)$$

and so

$$D_{ij}(\vec{q},\vec{q},\omega^2) = \{[\omega^2 - F(\omega^2)V(\vec{q})]^{-1}\}_{ij}, \qquad (22)$$

where

$$F_{ij}(\omega^2) = \delta_{ij} - \left(\frac{\gamma_a\gamma_b J(\omega^2)}{[1-\gamma_a J(\omega^2)][1-\gamma_b J(\omega^2)]}\right)_{ij}. \qquad (23)$$

It is thus only necessary to solve the integral equation

$$J_{ij}(\omega^2) = \frac{1}{N}\sum_{k,\vec{q}} V_{ik}(\vec{q})\left(\frac{1}{\omega^2 - F(\omega^2)V(\vec{q})}\right)_{kj} \qquad (24)$$

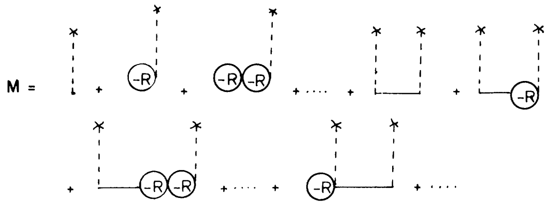

FIG. 3. Expansion of $M_{ij}(\vec{q}, \omega^2)$ in powers of B (represented by vertical dashed lines) and R.

to obtain an expression for $D_{ij}(\vec{q}, \vec{q}, \omega^2)$ and hence the density of states $g(\omega^2)$.

It is interesting to note that if the concentration of one of the elements of the alloy is small, then the Dysonian may be expanded in a power series in c_a, and that if only terms linear in c_a are retained one finds

$$M(\vec{q}, \omega^2) \simeq \{c_a \lambda^2 J(\omega^2)/[1 - \lambda J(\omega^2)]\} V(\vec{q}) \quad ,$$

where $\lambda = (m_b - m_a)/m_a$. This result is identical with that quoted by A. W. B. Taylor.[1] The more general result given in Eqs. (21)–(24), however, satisfies the symmetry criterion noted by D. W. Taylor.[7]

In the special case of a cubic crystal structure, our result simplifies considerably, since then $J_{ij}(\omega^2)$ reduces to a scalar function of ω^2, and so, consequently, does $F_{ij}(\omega^2)$. We then have

$$J(\omega^2) = \frac{1}{3N} \sum_{i,\vec{q}} \left(\frac{V(\vec{q})}{\omega^2 - F(\omega^2) V(\vec{q})} \right)_{ii}$$

$$= \frac{1}{3N} \sum_{\vec{q},\vec{s}} \frac{\Omega^2_{\vec{q}\vec{s}}}{\omega^2 - F(\omega^2)\Omega^2_{\vec{q}\vec{s}}} \quad ,$$

where $\Omega_{\vec{q}\vec{s}}$ is the frequency of the normal mode of wave number $\vec{q}$ and polarization $\vec{s}$ in a perfect crystal of atoms of mass m. If we define $g_0(\Omega^2)$ as the density of normal modes per unit squared frequency in such a crystal, then

$$J(\omega^2) = \frac{1}{3N} \int \frac{\Omega^2}{\omega^2 - F(\omega^2)\Omega^2} g_0(\Omega^2) \, d\Omega^2 \qquad (25)$$

and

$$g(\omega^2) = -\frac{1}{\pi} \operatorname{Im} \int \frac{1}{\omega^2 - F(\omega^2)\Omega^2} g_0(\Omega^2) \, d\Omega^2 \; , \qquad (26)$$

with ω^2 again assumed to have a vanishingly small positive imaginary part. The function $J(\omega^2)$ may then quickly be computed from Eq. (25) and the scalar version of Eq. (23) by an iterative method for any given form of $g_0(\Omega^2)$. The frequency spectrum of the alloy is then determined from Eq. (26).

In his study of the disordered substitutional alloy, Maris[2] has considered the special case where the masses of the two constituents are approximately equal. His method involved a diagrammatic expansion in which those terms of fourth or higher order in the small parameter $\lambda = (m_b - m_a)/m_a$ were ignored. The results of the present paper reduce to those of Maris when the right-hand side of Eq. (23) is rewritten as a power series in λ; this is to be expected, since all the diagrams considered by that author are included in the present approximation.

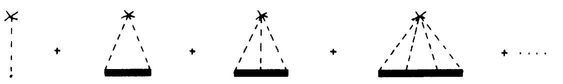

FIG. 4. Approximation for M in the special case of a random substitutional alloy.

IV. AMORPHOUS SYSTEMS

In an amorphous solid the matrix R defined in Eq. (9) will not vanish. The matrix elements $R_{qq'}$ will be functions of $\vec{q} - \vec{q}\,'$ of random and rapidly varying phase, and of a modulus governed by the relation

$$|R_{\vec{q}\vec{q}'}|^2 = N^{-1} \left[\int e^{i(\vec{q}-\vec{q}')\cdot\vec{r}} p(\vec{r}) \, d\vec{r} + 1 \right] \quad ,$$

with $p(\vec{r})$ the probability that any particular atom has a neighbor at a vector distance $\vec{r}$ from it and with $d\vec{r}$ an element of volume. The quantity $|R_{\vec{q}\vec{q}'}|^2$ is directly available for many materials from measurements of the diffraction intensities of neutrons and x rays.

The nature of most glasses and amorphous solids is such that $p(\vec{r})$ tends to have the form shown in Fig. 5; no two atoms have their equilibrium positions closer than some distance a, and there is a

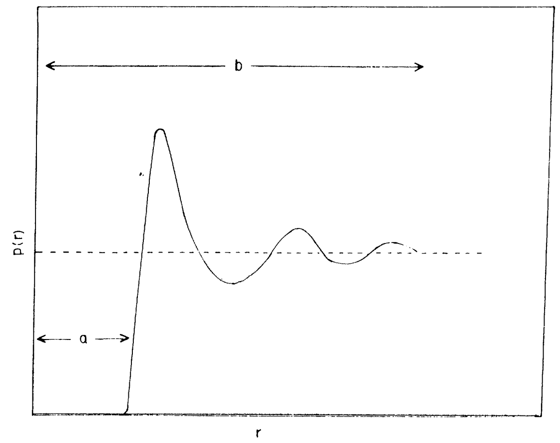

FIG. 5. Pair distribution function $p(\vec{r})$ for a particular direction of $\vec{r}$.

distance b beyond which $p(\vec{r})$ is very close to a value of N/Ω. The quantity $|R_{\vec{q}\vec{q}'}|^2$ accordingly has the form shown in Fig. 6, and exhibits its first maximum when $|\vec{q}-\vec{q}'|$ is of the order of $2\pi(N/\Omega)^{1/3}$. For small values of $|\vec{q}-\vec{q}'|$ this function will vary as

$$|R_{\vec{q}\vec{q}'}|^2 \sim (1/6N)|\vec{q}-\vec{q}'|^2 r_c^2$$

with r_c a length related to b and defined by the relation

$$r_c^2 = \int \vec{r}^{\,2}[N/\Omega - p(\vec{r})]\, d\vec{r}$$

The density fluctuations in many glasses may be thought of as due to regions of compaction in which the atomic density is increased by only a small fraction of its average value while b is only of the order of magnitude of a few interatomic spacings. Let us now choose for our transformation the N allowed wave vectors $\vec{q}$ defined by the condition $|\vec{q}| < (6N\pi^2/\Omega)^{1/3}$. An expression of the Dysonian $M_{ij}(\vec{q}, \omega^2)$ in powers of R now becomes reasonable, since for the most part the wave numbers will be such that $|R_{\vec{q}\vec{q}'}|^2 \ll 1/N$.

This may be illustrated by a consideration of some of the more important terms entering the expansion for $M_{ij}(\vec{q}, \omega^2)$. The sixth diagram in Fig. 3, for example, contains a factor of R^2, the principal contribution of which comes from the diagonal element $(R^2)_{\vec{q}\vec{q}}$. Now

$$\begin{aligned}(R^2)_{\vec{q}\vec{q}} &= N^{-2} \sum_{\vec{l}, \vec{l}', q' (\neq \vec{q})} e^{i(\vec{q}-\vec{q}')\circ(\vec{l}-\vec{l}')} \\ &= \frac{\Omega}{8\pi^3 N^2} \sum_{\vec{l}, \vec{l}'} e^{i\vec{q}\cdot(\vec{l}-\vec{l}')} \int e^{-i\vec{q}'\cdot(\vec{l}-\vec{l}')}\, d\vec{q} - 1 \quad ,\end{aligned}$$

with the integration over the volume element $d\vec{q}\,'$ in wave-number space being limited to a sphere of radius $q_D = (6N\pi^2/\Omega)^{1/3}$. We then find that with the definition of the function

$$\mathcal{G}(x) = 3(\sin x - x\cos x)/x^3$$

we can write

$$\begin{aligned}(R^2)_{\vec{q}\vec{q}} &= N^{-1} \sum_{\vec{l}, \vec{l}'} e^{i\vec{q}\circ(\vec{l}-\vec{l}')} \mathcal{G}(q_D|\vec{l}-\vec{l}'|) - 1 \\ &= \int e^{i\vec{q}\circ\vec{r}} \mathcal{G}(q_D|\vec{r}|) p(\vec{r})\, d\vec{r} \qquad (27)\end{aligned}$$

If we had been considering a perfect Bravais lattice instead of an amorphous solid, we should have found an expression similar to Eq. (27), but with the difference that $\mathcal{G}$ would have been replaced with a function that vanished at every lattice point $\vec{l}$. Since then $p(\vec{r})$ would have been nonzero only at precisely those same points, the integrand [and hence $(R^2)_{\vec{q}\vec{q}}$] would have vanished. In an amorphous solid, on the other hand, there will be a finite overlap of the functions $\mathcal{G}(q_D|\vec{r}|)$ and $p(\vec{r})$, and $(R^2)_{\vec{q}\vec{q}}$ will not vanish. It will, however, in general be small, since the first maximum of $p(\vec{r})$ will still occur close to the value of $|\vec{r}|$ at which $\mathcal{G}(q_D|\vec{r}|)$ first vanishes.

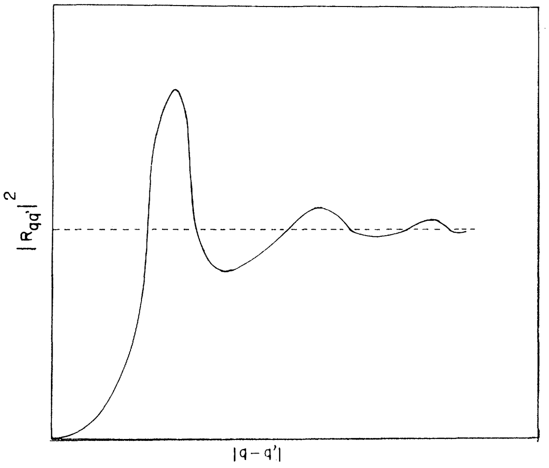

FIG. 6. Function $|R_{\vec{q}\vec{q}'}|^2$ shown here is related to the Fourier transform of $p(\vec{r})$.

The presence of factors of R in the perturbation expansion is not the only consequence of the amorphous nature of the solid that we are considering. We must also take note of the variation with position $\vec{l}$ of the function $U_{ij}(\vec{l}, \vec{q}')$ defined in Eq. (15). Although it is not possible to make many general statements about the form of $U_{ij}(\vec{l}, \vec{q}')$, there are some notable simplifications that appear when specific glassy systems are considered. In a tetrahedrally coordinated glass, for example, $U_{ij}(\vec{l}, \vec{q}')$ will be very small for small $\vec{q}'$ as a consequence of the fact that $U_{ij}(\vec{l}, 0)$ vanishes for an atom in a perfect tetrahedrally symmetric environment. There is also experimental evidence that correlations in $U_{ij}(\vec{l}, \vec{q}')$ do not extend beyond nearest neighbors in some such systems. We shall, however, postpone detailed computations of the form of these spectra to a later publication.

ACKNOWLEDGMENT

This work was completed while one of us (P. L. T.) was a guest of the Aspen Center for Physics.

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*Work supported by the U.S. Atomic Energy Commission under Contract No. AT(11-1)-623.

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