the sum being taken over all the lattice-points. To get the intensity, we have to take the square of the modulus of Y, which we do by multiplying the series on the right-hand side of (*1*.23) by the corresponding series in which i is replaced by $-i$. This gives for the intensity J_0 due to the undisturbed lattice the double summation

$$J_0 = \frac{|\Phi_0|^2}{R^2} \sum_n \sum_m e^{i\kappa(\mathbf{r}_n - \mathbf{r}_m \cdot \mathbf{S})}. \qquad (1.24)$$

Each summation has to be extended over all values of n and m, which range from 1 to N, N being the total number of lattice-points. Equation (*1*.24) is, of course, quite general for any array of scattering points, and does not depend on their being arranged in a lattice. For the parallelepipedal space-lattice it readily reduces to the form (*1*.13).

Let us now assume small vector displacements $\mathbf{u}_1, \mathbf{u}_2, \ldots \mathbf{u}_n, \mathbf{u}_m, \ldots$ of the lattice points from the ideal positions. The vectors $\mathbf{r}_n$ and $\mathbf{r}_m$ in (*1*.24) then have to be replaced by $\mathbf{r}_n + \mathbf{u}_n$ and $\mathbf{r}_m + \mathbf{u}_m$, and the expression for the intensity becomes

$$J = \frac{|\Phi_0|^2}{R^2} \sum_n \sum_m e^{i\kappa(\mathbf{r}_n - \mathbf{r}_m \cdot \mathbf{S})}\, e^{i\kappa(\mathbf{u}_n - \mathbf{u}_m \cdot \mathbf{S})}. \qquad (1.25)$$

If we are dealing with oscillations of the points, such as occur in thermal movement, it will be necessary to take the mean of (*1*.25), which represents the intensity due to some instantaneous configuration of points, over a period long compared with the period of vibration of any point. The first factor under the summation signs does not vary with time, and it is the second that has to be averaged. Expression (*1*.25) can only be used if the frequency of oscillation of the points is small compared with that of the incident radiation, so that any given configuration can be considered as persisting over a time long compared with the period of the wave, an assumption which is fully justified in the cases we shall consider.

To discuss the mean of the factor involving the displacements of the atoms n and m, we put, for brevity,

$$\kappa(\mathbf{u}_n - \mathbf{u}_m \cdot \mathbf{S}) = p_{n,m}. \qquad (1.26)$$

If we write, for the moment, p for any of the quantities $p_{n,m}$,

$$\overline{e^{ip}} = 1 + \overline{ip} - \frac{\overline{p^2}}{2!} - \frac{\overline{ip^3}}{3!} + \ldots = 1 - \frac{\overline{p^2}}{2} + \frac{\overline{p^4}}{24} - \ldots; \qquad (1.27)$$

for the mean value of the terms involving odd powers of p will be zero, since positive and negative values of the difference of the displacement of the two points parallel to any given direction will be equally likely.

Equation (*1*.27) may, to a close approximation, be written in the form

$$\overline{e^{ip}} = e^{-\frac{1}{2}\overline{p^2}}, \qquad (1.28)$$

a result given by Debye and by Waller, but first rigorously derived by Ott [9] in 1935.

The mean value of (*1*.25) therefore becomes

$$\bar{J} = \frac{|\Phi_0|^2}{R^2} \sum_n \sum_m e^{i\kappa(\mathbf{r}_n - \mathbf{r}_m \cdot \mathbf{S})}\, e^{-\frac{1}{2}\overline{p^2_{n,m}}}. \qquad (1.29)$$

Now

$$p_{n,m} = \frac{4\pi \sin\theta}{\lambda}(u_{nS} - u_{mS}), \qquad (1.30)$$

where u_{nS} and u_{mS} are the components of the displacements of the two lattice-points n and m parallel to the direction of the vector S defining the reflecting plane. We have therefore to calculate the mean value of $(u_{nS} - u_{mS})^2$. We may write

$$\overline{(u_{nS} - u_{mS})^2} = \overline{u_{nS}^2} + \overline{u_{mS}^2} - 2\overline{u_{nS}u_{mS}}. \qquad (1.31)$$

The assumptions made by Debye in his first papers on the temperature effect were equivalent to the supposition that the oscillations of the different lattice-points were independent, and that all possessed the same mean energy. If this were so, we could put

$$\overline{u_{nS}u_{mS}} = 0;\ \overline{u_{nS}^2} = \overline{u_{mS}^2} = \overline{u_S^2}, \qquad (1.32)$$

where $\overline{u_S^2}$ is the mean-square elongation of any point of the lattice from its mean position in a direction parallel to the vector S. Now, as Debye himself pointed out in a later paper, the assumption of the independence of the lattice-points is not justifiable in considering the thermal vibrations of a real lattice. The atoms of the lattice are coupled together by the lattice forces, and the direction of vibration of one point must influence those of its neighbours. We cannot therefore put $\overline{u_{nS}u_{mS}} = 0$, and the value of $\overline{p^2_{nm}}$ will depend on the pair of lattice-points that are being considered. This leads to important consequences, which will be discussed in detail in Chapter V, but to complete our preliminary account of the geometrical theory of diffraction by a simple lattice we shall consider the case of a set of points all of which do vibrate independently, and in the same way, so that equations (*1*.32) may be taken as applicable.

We return now to equation (*1*.29). The double summation contains N^2 terms, N being the total number of lattice-points. In N of these terms $n = m$, and for each of these the exponential factor is equal to unity. For all terms involving a pair of different lattice-points $\frac{1}{2}\overline{p^2_{nm}}$ is the same, and by (*1*.30), (*1*.31), and (*1*.32) is equal to 2M, if

$$M = 8\pi^2 \overline{u_S^2} (\sin^2\theta)/\lambda^2. \qquad (1.33)$$

Equation (*1*.29) may thus be written

$$\bar{J} = \frac{|\Phi_0|^2}{R^2}\left\{N + e^{-2M} \sum_n{}' \sum_m{}' e^{i\kappa(\mathbf{r}_n - \mathbf{r}_m \cdot \mathbf{S})}\right\}, \qquad (1.34)$$

where the dashes denote that terms for which $n = m$ are not to be included in the summations. If this restriction were removed, the