1.6. SUMMATION OF THE ITERATION SERIES

Having seen how to obtain all the terms in the iteration series, we now show that in the present case the series can be summed exactly in closed form. It is simplest to return to the integral equation (1.5.13). The equation is exactly soluble because of the *convolution* form of the last term: if we introduce the time Fourier transforms of the functions involved, defined by the reciprocal formulas

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega)\, e^{-i\omega t}\, d\omega, \qquad G(\omega) = \int_{-\infty}^{\infty} G(t)\, e^{i\omega t}\, dt, \quad (1.6.1)$$

and take the Fourier transform of the integral equation, the last term splits into a product of factors. The transformed equation is

$$G_{ij}(\omega) = G^0(\omega)\,\delta_{ij} + \lambda M G^0(\omega) \sum_k D_{ik} G_{kj}(\omega). \qquad (1.6.2)$$

This can again be solved by iteration, the terms in the iteration series being the Fourier transforms of the terms in Eq. (1.5.14). Thus (1.5.14) transforms to

$$\begin{aligned} G_{ij}(\omega) &= G^0(\omega)\,\delta_{ij} + \lambda M G^0(\omega) D_{ij} G^0(\omega) \\ &\quad + (\lambda M)^2 \sum_{i'} G^0(\omega) D_{ii'} G^0(\omega) D_{i'j} G^0(\omega) + \cdots. \end{aligned} \qquad (1.6.3)$$

Because of the translational invariance of the lattice the terms in this series can be simplified by making a further transformation to **k** space. We introduce a Fourier expansion of $G_{ij}(\omega)$ in the lattice space, analogous to the Fourier expansion, Eqs. (1.1.9) and (1.1.10), of D_{ij},

$$G_{ij}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} G_{\mathbf{k}}(\omega)\, e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)},$$

$$G_{\mathbf{k}}(\omega) = \sum_i G_{ij}(\omega)\, e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}. \qquad (1.6.4)$$

This uncouples the summations in Eq. (1.6.3), and the transformed series is

$$G_{\mathbf{k}}(\omega) \doteq G^0(\omega) + \lambda M G^0(\omega) D_{\mathbf{k}} G^0(\omega) + (\lambda M)^2 G^0(\omega) D_{\mathbf{k}} G^0(\omega) D_{\mathbf{k}} G^0(\omega) + \cdots . \tag{1.6.5}$$

This is now a simple geometric series, with sum to infinity

$$G_{\mathbf{k}}(\omega) = \frac{G^0(\omega)}{1 - \lambda M G^0(\omega) D_{\mathbf{k}}} . \qquad (1.6.6)^2$$

In the three-dimensional case, when $D_{\mathbf{k}}$ is the 3×3 matrix $D_{\mathbf{k}}^{\alpha\beta}$, Eq. (1.6.6) involves a matrix inversion which can be performed by diagonalizing $D_{\mathbf{k}}^{\alpha\beta}$ with normalized eigenvectors $\epsilon^{\alpha}(\mu, \mathbf{k})$ (μ a polarization index)

$$\sum_{\beta} D_{\mathbf{k}}^{\alpha\beta} \epsilon^{\beta}(\mu, \mathbf{k}) = D_{\mathbf{k}}{}^{\mu} \epsilon^{\alpha}(\mu, \mathbf{k}). \tag{1.6.7}$$

Thus the three-dimensional analog of Eq. (1.6.6) is

$$G_{\mathbf{k}}^{\alpha\beta}(\omega) = \sum_{\mu=1}^{3} G_{\mathbf{k}}{}^{\mu}(\omega)\, \epsilon^{\alpha}(\mu, \mathbf{k})\, \epsilon^{\beta}(\mu, \mathbf{k}),$$

where

$$G_{\mathbf{k}}{}^{\mu}(\omega) = G^0(\omega)/(1 - \lambda M G^0(\omega) D_{\mathbf{k}}{}^{\mu}). \tag{1.6.8}$$

We continue to discuss the simpler form (1.6.6).

We now have to evaluate the Fourier transform $G^0(\omega)$. This requires some care if we are to obtain well-defined results. The function $G^0(t)$, Eq. (1.5.11), is a wave of constant amplitude, and the Fourier transform of this does not exist for real ω. We therefore work with the *complex* Fourier transform [Titchmarsh (1937)], and regard ω as a complex variable with a non-zero (but infinitesimal) imaginary part. The imaginary part must be chosen negative for $t < 0$ and positive for $t > 0$, and thus we write

$$G^0(\omega) = -\frac{i}{2M\Omega_0} \int_{-\infty}^{0} e^{i(\omega + \Omega_0 - i\eta)t}\, dt - \frac{i}{2M\Omega_0} \int_{0}^{\infty} e^{i(\omega - \Omega_0 + i\eta)t}\, dt,$$

[2] We can easily check in this case, by direct solution of Eq. (1.6.2) in closed form, that this result is in fact valid for all λ.

where η is a positive infinitesimal. These integrals now converge, and we obtain

$$G^0(\omega) = -\frac{1}{2M\Omega_0}\frac{1}{\omega+\Omega_0-i\eta}+\frac{1}{2M\Omega_0}\frac{1}{\omega-\Omega_0+i\eta}$$
$$=\frac{1}{M(\omega^2-\Omega_0{}^2+i\eta)} \qquad (\eta>0). \tag{1.6.9}$$

We note that the singularities of $G^0(\omega)$ in the complex ω plane are two poles at the unperturbed frequencies $\omega = \pm(\Omega_0 - i\eta)$, one lying just above and the other just below the real axis, as indicated in Fig. 1.2.

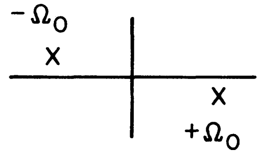

Fig. 1.2. Poles of the Fourier transform of the time-ordered Green's function in the ω plane.

To regain the t-dependent Green's function from Eq. (1.6.9), the Fourier integral is evaluated by contour integration. For $t>0$, the contour consists of the real axis and a large semicircle in the lower half-plane. By Jordan's lemma, the integral over the semicircle tends to zero as the radius tends to infinity. The contour is described in the negative sense, and by the residue theorem the required integral is thus equal to $-2\pi i$ times the residue of the integrand at the pole $\omega = \Omega_0 - i\eta$ which lies inside the contour. This leads at once to the expression (1.5.9). For $t<0$ the contour must be closed in the upper half-plane; we then pick up the pole at $\omega = -\Omega_0 + i\eta$ and regain Eq. (1.5.10).

With the value (1.6.9) for $G^0(\omega)$ we now at once have the exact result

$$G_{\mathbf{k}}(\omega) = \frac{1}{(G^0)^{-1}-\lambda MD_{\mathbf{k}}} = \frac{1}{M(\omega^2-\Omega_0{}^2-\lambda D_{\mathbf{k}}+i\eta)}$$
$$=\frac{1}{M(\omega^2-\Omega_{\mathbf{k}}{}^2+i\eta)}, \tag{1.6.10}$$

so that to obtain $G_{\mathbf{k}}$ from G^0 we simply have to replace Ω_0 by $\Omega_{\mathbf{k}}$, where $\Omega_{\mathbf{k}}{}^2 = \Omega_0{}^2 + \lambda D_{\mathbf{k}}$. This agrees with the result (1.1.11) given by the classical normal mode analysis.

A number of comments are worth making on the calculation which led to Eq. (1.6.10) and on the result:

(i) We see that the effect of the interaction on $G(\omega)$ is to shift the position of the poles from the unperturbed frequencies $\pm\Omega_0$ to the frequencies $\pm\Omega_{\mathbf{k}}$ of the phonon modes. This is a special case of a general property of the function $G_{\mathbf{k}}(\omega)$, valid also for fermion systems: $G_{\mathbf{k}}(\omega)$ is a meromorphic function with simple poles at the excitation frequencies (or energies) of the interacting system corresponding to wave-vector **k**. In the case of the phonon Green's function these excitation energies are of magnitude $\hbar\Omega_{\mathbf{k}}$ because the matrix elements connecting excited states with the ground state vanish unless the number of phonons changes by one.

(ii) The t-dependent Green's function $G_{\mathbf{k}}(t)$, obtained by contour integration from Eq. (1.6.10), is clearly an undamped wave

$$G_{\mathbf{k}}(t) = -\frac{i}{2M\Omega_{\mathbf{k}}}\, e^{-i\Omega_{\mathbf{k}}|t|} \tag{1.6.11}$$

at the new frequency $\Omega_{\mathbf{k}}$. We see from the series (1.6.5) that, if it is broken off after any *finite* number of terms, $G_{\mathbf{k}}(\omega)$ will be a *polynomial* in $G^0(\omega)$ instead of a rational function, and its poles are then still at $\pm\Omega_0$. Thus, in any finite order (however large) of perturbation theory, $G_{\mathbf{k}}(t)$ still has the unperturbed frequency Ω_0. This demonstrates that, in order to obtain the propagating lattice modes and the phonon frequencies $\Omega_{\mathbf{k}}$, the perturbation theory must be taken to infinite order.

(iii) In the present problem the poles of $G_{\mathbf{k}}(\omega)$ lie just off the real axis in the ω plane, and $G_{\mathbf{k}}(t)$ represents undamped propagation. In more general cases (for example the problem of anharmonic phonons) a new phenomenon appears: the poles of $G_{\mathbf{k}}(\omega)$ may be situated at a *finite* distance from the real axis. Suppose there is a pole at $\Omega_{\mathbf{k}} - i\Gamma_{\mathbf{k}}$ in the lower half-plane ($\Gamma_{\mathbf{k}} > 0$): inverting the Fourier transform it is then seen that for $t > 0$ $G_{\mathbf{k}}(t)$ acquires a real exponential factor $\exp(-\Gamma_{\mathbf{k}}t)$. [If there are several poles in the lower half-plane, the dominant term in $G_{\mathbf{k}}(t)$ for large t arises from the pole which lies nearest to the real axis.] Thus $G_{\mathbf{k}}(t)$ has acquired a damping factor, and the excitation of frequency $\Omega_{\mathbf{k}}$ now has a finite lifetime $\Gamma_{\mathbf{k}}^{-1}$. In this way the Green's function can describe damping phenomena and finite lifetime effects. We shall encounter such phenomena in later chapters in connection with the electrical conductivity (Chap. 5) and the magnetic susceptibility (Chap. 7). The way in which the theory can lead to a modified analytic form of $G_{\mathbf{k}}(\omega)$ possessing finite damping is discussed further in Chap 5.

(iv) The poles of $G_{\mathbf{k}}(\omega)$, like those of $G^0(\omega)$, lie one just above and one just below the real axis. This analytic behavior corresponds to our definition of G as a causal (time-ordered) Green's function. We could equally well have worked with the retarded or advanced Green's functions, Eqs. (1.4.8) and (1.4.9), and we would then have obtained instead of Eq. (1.6.10) the expressions

$$G_{\mathbf{k}}{}^R(\omega) = \frac{1}{M(\omega^2 - \Omega_{\mathbf{k}}{}^2 + i\eta\omega)}\,, \qquad G_{\mathbf{k}}{}^A(\omega) = \frac{1}{M(\omega^2 - \Omega_{\mathbf{k}}{}^2 - i\eta\omega)}\,, \tag{1.6.12}$$

where η is again a positive infinitesimal. (We note that, for real ω, G^A is the complex conjugate of G^R.) These functions also have poles at the frequencies $\pm\Omega_{\mathbf{k}}$, but these poles now lie, in the case of $G^R(\omega)$, both just *below* the real axis, and, in the case of $G^A(\omega)$, both just *above* the real axis. Thus $G^R(\omega)$ is regular (free from singularities) in the whole upper half of the ω plane, and $G^A(\omega)$ is regular in the whole lower half of the ω plane. This is a general property of retarded and advanced Green's functions. It has the advantage in general that, if the function $G^R(\omega)$ is known in the lower half-plane, it can be obtained for all complex ω by the process of analytic continuation; similarly for $G^A(\omega)$.

(v) In the present problem the k-dependent Green's functions $G_{\mathbf{k}}(\omega)$, $G_{\mathbf{k}}(t)$ are given by simple expressions, of the same form as the unperturbed Green's functions but containing the phonon frequencies $\Omega_{\mathbf{k}}$. We do not calculate the lattice Green's function

$$G_{ij}(t) = \frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}}(t)\, e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \tag{1.6.13}$$

explicitly; evaluation of the sum over **k** would require knowledge of the phonon dispersion law giving the frequencies $\Omega_{\mathbf{k}}$ as functions of **k**. In fact explicit knowledge of the form of $G_{ij}(t)$ is not needed for the discussion of the physical quantities which will be considered in the next section.

1.7. CALCULATION OF THE GROUND STATE ENERGY AND THE NEUTRON CROSS-SECTION IN TERMS OF THE PHONON GREEN'S FUNCTION

We can now use the exact Green's function (1.6.10) to calculate the correlation functions (1.4.10) and (1.4.11) which determine the change in ground state energy and the neutron scattering. Using the **k**-space transformation (1.6.4) for $G_{ij}(t)$ we have

$$\Delta E_G = \lim_{t \to 0+} \tfrac{1}{2} iM \sum_{i \neq j} D_{ij} \int_0^1 d\lambda \frac{1}{N} \sum_{\mathbf{k}} G_{\mathbf{k}}(t)\, e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)},$$

and

$$\frac{1}{N} \sum_{i \neq j} D_{ij}\, e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} = \frac{1}{N} \sum_{j} D_{\mathbf{k}} = D_{\mathbf{k}};$$

hence

$$\Delta E_G = \lim_{t \to 0+} \tfrac{1}{2} iM \int_0^1 d\lambda \sum_{\mathbf{k}} D_{\mathbf{k}} G_{\mathbf{k}}(t). \tag{1.7.1}$$

But, from Eq. (1.6.11),

$$\lim_{t \to 0+} G_{\mathbf{k}}(t) = -\frac{i}{2M\Omega_{\mathbf{k}}};$$

hence

$$\begin{aligned} \Delta E_G &= \tfrac{1}{4} \int_0^1 d\lambda \sum_{\mathbf{k}} D_{\mathbf{k}}/\Omega_{\mathbf{k}} \\ &= \tfrac{1}{4} \sum_{\mathbf{k}} D_{\mathbf{k}} \int_0^1 \frac{d\lambda}{\sqrt{(\Omega_0{}^2 + \lambda D_{\mathbf{k}})}} \\ &= \tfrac{1}{2} \sum_{\mathbf{k}} \{\sqrt{(\Omega_0{}^2 + D_{\mathbf{k}})} - \Omega_0\}, \end{aligned} \tag{1.7.2}$$