assuming $|\Psi_G\rangle$ to be normalized. Therefore, integrating with respect to λ,

$$\Delta E_G = E_G(1) - E_G(0) = \int_0^1 d\lambda \langle \Psi_G(\lambda) | H_1 | \Psi_G(\lambda) \rangle. \tag{1.2.3}$$

The change in ground state energy is thus expressed entirely in terms of a matrix element of the perturbation H_1, but it is necessary to know this matrix element for all values of the coupling constant λ.

The formula (1.2.3) is general. For the lattice problem H_1 is given by Eq. (1.1.6), and thus

$$\Delta E_G = \tfrac{1}{2} M \sum_{i \neq j} D_{ij} \int_0^1 d\lambda \langle \Psi_G(\lambda) | u_i u_j | \Psi_G(\lambda) \rangle. \tag{1.2.4}$$

1.3. THE NEUTRON SCATTERING CROSS-SECTION

The matrix element in (1.2.4), which gives the change in the ground state energy, is a measure of the *correlation* brought about by the interaction between the displacements of two atoms, u_i and u_j. This is an example of a quantum-mechanical *correlation function.* We come across a more complicated, time-dependent, correlation function, which is more directly related to observable phenomena, when we consider the scattering cross-section for plane waves of the lattice of phonons. We shall discuss specifically the coherent inelastic scattering of slow neutrons, but a similar discussion can be given of the scattering of light (x-rays) by a crystal. Our discussion follows that given in Kittel (1963, Chap. 19), where further details can be found. The formulas for the scattering cross-sections are due to van Hove (1954).

We work in the first Born approximation, in which the incident and scattered particles are represented by plane waves $\exp(i\mathbf{K}\cdot\mathbf{x})$ and $\exp(i\mathbf{K}'\cdot\mathbf{x})$. The inelastic differential scattering cross-section per unit solid angle per unit energy range is

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \sum_F \frac{K'}{K} \left(\frac{M}{2\pi}\right)^2 |\langle \mathbf{K}'\psi_F | H' | \mathbf{K}\psi_G \rangle|^2 \, \delta(\omega + E_G - E_F), \tag{1.3.1}$$

where H' is the interaction between particle and target, ω is the energy transfer to the target, and M is the reduced mass of the particle. It is assumed here that the target is initially in its ground state $|\psi_G\rangle$ with energy E_G; $|\psi_F\rangle$ is the final state with energy E_F. Thus we are assuming that the equilibrium state of the target corresponds to zero temperature; the extension to finite temperatures is developed in Chap. 2. If we assume further that H' is the sum of two-particle interactions between the incident particle and the target particles:

$$H' = \sum_j V(\mathbf{x} - \mathbf{X}_j), \qquad j = 1, 2, \ldots, N, \tag{1.3.2}$$

we have

$$\begin{aligned} \langle \mathbf{K}'\psi_F | H' | \mathbf{K}\psi_G \rangle &= \langle \psi_F | \int d^3x \, e^{i\mathbf{q}\cdot\mathbf{x}} H' | \psi_G \rangle \\ &= V_{\mathbf{q}} \sum_j \langle \psi_F | e^{i\mathbf{q}\cdot\mathbf{X}_j} | \psi_G \rangle, \end{aligned} \tag{1.3.3}$$

where $\mathbf{q} = \mathbf{K} - \mathbf{K}'$ is the change in wave-vector of the incident particle and

$$V_{\mathbf{q}} = \int d^3x \, e^{i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x}) \tag{1.3.4}$$

is the Fourier transform of the scattering potential.

We now have

$$\begin{aligned} \frac{d^2\sigma}{d\Omega\, d\omega} = \sum_F \frac{K'}{K} \left(\frac{M}{2\pi}\right)^2 | V_{\mathbf{q}} |^2 \sum_{jl} \langle \psi_G | e^{-i\mathbf{q}\cdot\mathbf{X}_j} | \psi_F \rangle \\ \times \langle \psi_F | e^{i\mathbf{q}\cdot\mathbf{X}_l} | \psi_G \rangle \delta(\omega + E_G - E_F). \end{aligned} \tag{1.3.5}$$

This can be simplified by introducing the Fourier representation of the delta-function:

$$\delta(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \, dt,$$

where t can be interpreted as a time variable. We can now write

$$e^{i(E_G - E_F)t} \langle \psi_G | e^{-i\mathbf{q}\cdot\mathbf{X}_j} | \psi_F \rangle = \langle \psi_G | e^{iHt} e^{-i\mathbf{q}\cdot\mathbf{X}_j} e^{-iHt} | \psi_F \rangle, \tag{1.3.6}$$

where $H = H_0 + \lambda H_1$ is the hamiltonian describing the target. The operator exponential is to be interpreted as an infinite series, and thus Eq. (1.3.6) may be rewritten with the time factors in the exponent:

$$\langle \psi_G | e^{-i\mathbf{q}\cdot\tilde{\mathbf{X}}_j(t)} | \psi_F \rangle, \tag{1.3.7}$$

where the time-dependent quantity

$$\tilde{\mathbf{X}}_j(t) = e^{iHt}\mathbf{X}_j\, e^{-iHt} \tag{1.3.8}$$

is a *Heisenberg operator* (see Sec. 1.4 below).

It is now possible to sum over the final states $|\psi_F\rangle$ in (1.3.5), using the completeness relation

$$\sum_F |\psi_F\rangle\langle\psi_F| = 1. \tag{1.3.9}$$

The differential cross-section is thus given by

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \frac{K'}{2\pi K}\left(\frac{M}{2\pi}\right)^2 |V_{\mathbf{q}}|^2$$

$$\times \int_{-\infty}^{\infty} e^{i\omega t}\, dt \sum_{jl} \langle \psi_G | e^{-i\mathbf{q}\cdot\tilde{\mathbf{X}}_j(t)}\, e^{i\mathbf{q}\cdot\tilde{\mathbf{X}}_l(0)} | \psi_G \rangle. \tag{1.3.10}$$

Note that the operator exponentials do not commute at different times and cannot be combined into a single exponential. We thus see that the cross-section depends upon the two-body potential and upon the time Fourier transform of the time correlation function

$$\sum_{jl} \langle \psi_G | e^{-i\mathbf{q}\cdot\tilde{\mathbf{X}}_j(t)}\, e^{i\mathbf{q}\cdot\tilde{\mathbf{X}}_l(0)} | \psi_G \rangle.$$

Writing $\mathbf{X}_i = \mathbf{R}_i + \mathbf{u}_i$, where $\mathbf{R}_i$ is as before the undisplaced lattice position (not an operator), the correlation function is

$$F(\mathbf{q}, t) = \sum_{jl} e^{i\mathbf{q}\cdot(\mathbf{R}_l - \mathbf{R}_j)} \langle \psi_G | e^{-i\mathbf{q}\cdot\tilde{\mathbf{u}}_j(t)}\, e^{i\mathbf{q}\cdot\tilde{\mathbf{u}}_l(0)} | \psi_G \rangle. \tag{1.3.11}$$

An important application of this expression is to the discussion of recoilless (Mossbauer) emission of γ-rays from nuclei embedded in a crystal [see Kittel (1963), Chap. 20].

We now make an important approximation. We shall see that $F(\mathbf{q}, t)$ describes inelastic scattering in which phonons are emitted or absorbed by the scattered neutron. Usually the one-phonon processes, in which a single phonon is emitted or absorbed, dominate. We shall confine attention to these. This allows us to expand the exponentials in Eq. (1.3.11) and to keep only terms in the matrix element which involve products of two u operators. (The leading term, in which the exponentials are replaced by unity, represents elastic scattering and is of no interest here.) Furthermore, we are only interested in terms which involve u-operators at *different* times (the other terms are time-independent and lead to an overall factor—the "Debye-Waller factor"—multiplying the magnitude of the scattering cross-section. It is also easily seen that the expectation values of *single* u-operators are zero.) The higher-order terms in the expansion of (1.3.11), involving products of more than two u-operators, correspond to multi-phonon processes and will be neglected. Finally, we suppose for simplicity that the polarization of the phonon mode of interest is parallel to $\mathbf{q}$, so that the product $\mathbf{q} \cdot \mathbf{u}_j$ can be replaced by the scalar qu_j.

With all these approximations (and omitting the Debye-Waller factor), the correlation function (1.3.11) reduces to

$$F(\mathbf{q}, t) \simeq q^2 \sum_{jl} e^{i\mathbf{q}\cdot(\mathbf{R}_l - \mathbf{R}_j)} \langle \psi_G | \tilde{u}_j(t) \tilde{u}_l(0) | \psi_G \rangle, \qquad (1.3.12)$$

where $\tilde{u}(t)$ is a Heisenberg operator as in (1.3.8).

1.4. THE GREEN'S FUNCTION AND ITS EQUATION OF MOTION

In Eqs. (1.2.4) and (1.3.12) we now have two examples, one time-independent and the other time-dependent, of correlation functions of interest in the lattice problem. These, and similar correlation functions, are conveniently calculated by means of Green's functions.

First we recall some general quantum-theoretical formulas [see Messiah (1961, Chap. VIII)]. In the Schrödinger picture or "representation" of quantum mechanics the vector $|\Psi_S(t)\rangle$ representing the state of a system at time t evolves in time in accordance with the Schrödinger equation

$$i\frac{\partial |\Psi_S\rangle}{\partial t} = H|\Psi_S\rangle. \qquad (1.4.1)$$