1.2. THE GROUND STATE ENERGY AS AN INTEGRAL OVER COUPLING CONSTANT

An exact solution in closed form, such as can be obtained foı the harmonic oscillator by direct diagonalization of the hamiltonian, is only possible in exceptionally simple cases. We now want to rederive the ground state energy of the harmonic lattice by more general quantum-theoretical methods which, although more complicated, can also be applied to a wide range of problems for which the above type of closed solution cannot be obtained. The method consists of a calculation of ΔE_G using H_1 as a perturbation. Although the strength of the perturbation may be small, it connects together all the particles in the system. It is then not sufficient, as in elementary applications of perturbation theory to one- or two-particle systems, to calculate only the first few terms of the perturbation series and to assume that the higher terms are negligible. In fact the essential features of the perturbation (in the present case the existence of propagating modes) come from the high-order terms in the perturbation series, and we must therefore work to all orders in H_1. For this purpose we use a general formula for ΔE_G which is particularly suitable for perturbation theory. (The formula seems to be due to Pauli, and has been rederived many times.) When the hamiltonian is $H_0 + \lambda H_1$, the ground state energy E_G and the ground state eigenfunction $|\Psi_G\rangle$ are functions of λ, and $E_G(\lambda)$ is the expectation value

$$E_G(\lambda) = \langle \Psi_G(\lambda) | H(\lambda) | \Psi_G(\lambda) \rangle. \qquad (1.2.1)$$

Hence

$$\frac{\partial E_G}{\partial \lambda} = \langle \Psi_G(\lambda) | H_1 | \Psi_G(\lambda) \rangle + \left\langle \frac{\partial \Psi_G}{\partial \lambda} \right| H(\lambda) \left| \Psi_G \right\rangle + \left\langle \Psi_G \right| H(\lambda) \left| \frac{\partial \Psi_G}{\partial \lambda} \right\rangle. \qquad (1.2.2)$$

The last two terms reduce to

$$E_G(\lambda) \left\{ \left\langle \frac{\partial \Psi_G}{\partial \lambda} \middle| \Psi_G \right\rangle + \left\langle \Psi_G \middle| \frac{\partial \Psi_G}{\partial \lambda} \right\rangle \right\} = E_G(\lambda) \frac{\partial}{\partial \lambda} \langle \Psi_G | \Psi_G \rangle = 0,$$

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