

2.6. *The method of correlators*

In this section we shall discuss a method of describing scattering that differs from the approach on which eq. (2.3) is based. This method takes the scattering perturbation V to be a random function of time and coordinates. Thus, for example, in the Hamiltonian given by eq. (3.1), which represents electron scattering by lattice vibrations, the atomic displacements $\xi_{a\alpha}$ are random time-dependent functions.

Assume that at $t = 0$ the electron is in a certain state $|i\rangle$. According to the general rules of quantum mechanics, the probability that the electron will be in state $|f\rangle$ at the instant t is

$$P_{i \rightarrow f}(t) = \frac{1}{\hbar^2} \left| \int_0^t dt_1 e^{i\omega t_1} M(t_1) \right|^2, \quad (2.101)$$

where $\hbar\omega = \varepsilon_f - \varepsilon_i$ is the change in the electron energy due to the transition and M is the transition matrix element:

$$M(t) = \langle f | V(t) | i \rangle. \quad (2.102)$$

As a rule the perturbation $V(t)$, and together with it the matrix element $M(t)$, are stationary random functions. This means that the average over the time,

$$\frac{1}{t_0} \int_0^{t_0} d\bar{t} M(\bar{t} + t) \equiv \langle M(t) \rangle = \langle M \rangle, \quad (2.103)$$

taken over a sufficiently large averaging interval t_0 , is independent of the length and position of the averaging interval. This also means that the average of the product of two matrix elements, corresponding to different instants of time:

$$\begin{aligned} \frac{1}{t_0} \int_0^{t_0} d\bar{t} M^*(\bar{t} + t) M(\bar{t} + t') &\equiv \langle M^*(t) M(t') \rangle = \langle M^*(0) M(t' - t) \rangle \\ &\equiv K(t' - t), \end{aligned} \quad (2.104)$$

depends only on the interval $t' - t$ between these two instants of time. The function $K(t)$ is called the correlator of the matrix elements.

The random function $M(t)$ is characterized by a correlation time $\bar{\tau}$, such that if $|t - t'| \gg \bar{\tau}$, then the quantities $M(t)$ and $M(t')$ are “statistically independent”, i.e.

$$\langle M^*(t) M(t') \rangle = \langle M^*(t) \rangle \langle M(t') \rangle = |\langle M \rangle|^2. \quad (2.105)$$

To determine the average given by eqs. (2.103) and (2.104) correctly, the interval t_0 must be much greater than $\bar{\tau}$.

It will be assumed in the following that $\langle M \rangle = 0$. Then $K(t) \rightarrow 0$ as $t \rightarrow \pm\infty$, with $K(t)$ becoming small for $|t| \gg \bar{\tau}$.

Let us now represent the probability given by eq. (2.101) in the form

$$P_{i \rightarrow f}(t) = \frac{1}{\hbar^2} \int_0^t dt_1 \int_0^t dt_2 e^{i\omega(t_2 - t_1)} M^*(t_1) M(t_2) \quad (2.106)$$

and go over to integration with respect to the variables

$$\bar{t} = \frac{1}{2}(t_1 + t_2) \quad \text{and} \quad \tilde{t} = t_2 - t_1. \quad (2.107)$$

We then obtain

$$P_{i \rightarrow f}(t) = \frac{1}{\hbar^2} \int_{-t}^t d\tilde{t} e^{i\omega\tilde{t}} \int_{\frac{1}{2}|\tilde{t}|}^{t-\frac{1}{2}|\tilde{t}|} d\bar{t} M^*(\bar{t} - \frac{1}{2}\tilde{t}) M(\bar{t} + \frac{1}{2}\tilde{t}). \quad (2.108)$$

After assuming that $t \gg \bar{\tau}$ and making use of definition (2.104) of a correlator, we have

$$P_{i \rightarrow f}(t) = \frac{t}{\hbar^2} K_\omega, \quad K_\omega = \int_{-\infty}^{\infty} dt e^{i\omega t} K(t). \quad (2.109)$$

Thus, for $t \gg \bar{\tau}$ the transition probability is found to be proportional to t , and we can apply the concept of a transition probability per unit time

$$W_{i \rightarrow f} = \frac{1}{\hbar^2} K_\omega, \quad (2.110)$$

as in eq. (2.3).

Another version of the correlator method emerges when the perturbation V is time-independent, but is a random function in space, for instance, when an electron is scattered by a static potential of randomly distributed centers.

The matrix element of the transition $\mathbf{k} \rightarrow \mathbf{k}'$, calculated with plane waves as the wave functions of the initial and final states, has the form

$$M_{\mathbf{k} \rightarrow \mathbf{k}'} = \frac{1}{L^3} \int_{L^3} d^3r e^{-i\mathbf{q}r} V(\mathbf{r}), \quad \mathbf{q} = \mathbf{k}' - \mathbf{k}, \quad (2.111)$$

and the square of its absolute value can be represented in a form similar to eq. (2.106), viz.

$$|M_{\mathbf{k} \rightarrow \mathbf{k}'}|^2 = \frac{1}{(L^3)^2} \int_{L^3} d^3r_1 \int_{L^3} d^3r_2 e^{-i\mathbf{q}(r_2 - r_1)} V^*(\mathbf{r}_1) V(\mathbf{r}_2). \quad (2.112)$$

After transformation to the integration variables

$$\bar{\mathbf{r}} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) \quad \text{and} \quad \tilde{\mathbf{r}} = \mathbf{r}_2 - \mathbf{r}_1, \quad (2.113)$$

the space average, i.e. the space correlator, is then obtained:

$$\frac{1}{L_0^3} \int_{L_0^3} d^3\bar{r} V^*(\bar{\mathbf{r}} + \mathbf{r}) V(\bar{\mathbf{r}} + \mathbf{r}') \equiv \langle V^*(\mathbf{r}) V(\mathbf{r}') \rangle. \quad (2.114)$$

Here L_0^3 [similar to t_0 in eq. (2.104)] is the volume of the averaging domain. It is assumed that $L_0 \ll L$. If the random potential $V(\mathbf{r})$ is spatially homogeneous, i.e. if the correlator depends only on the relative position of the points \mathbf{r} and \mathbf{r}' , then

$$\langle V^*(\mathbf{r}) V(\mathbf{r}') \rangle = \langle V^*(0) V(\mathbf{r}' - \mathbf{r}) \rangle \equiv K(\mathbf{r}' - \mathbf{r}). \quad (2.115)$$

In the following it is assumed that the average of the potential is

$$\frac{1}{L_0^3} \int_{L_0^3} d^3\bar{r} V(\bar{\mathbf{r}} + \mathbf{r}) = \langle V(\mathbf{r}) \rangle = \langle V \rangle = 0. \quad (2.116)$$

As in the case of time averages, $K(\mathbf{r}) \rightarrow 0$ as $|\mathbf{r}| \rightarrow \infty$. The decrease in the correlator is characterized by the correlation length \bar{l} . The dimension L_0 of the averaging region should be much larger than \bar{l} .

Assuming that $L \gg \bar{l}$, we have

$$|M_{\mathbf{k} \rightarrow \mathbf{k}'}|^2 = \frac{1}{L^3} K_{\mathbf{q}}, \quad K_{\mathbf{q}} = \int_{\infty} d^3 r e^{-i\mathbf{q}\mathbf{r}} K(\mathbf{r}), \quad (2.117)$$

so that the scattering probability per unit time is

$$W_{\mathbf{k} \rightarrow \mathbf{k}'} = \frac{2\pi}{\hbar} \frac{1}{L^3} \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) K_{\mathbf{q}}. \quad (2.118)$$

Finally, if V is a random function of both \mathbf{r} and t , a combined treatment of time and space correlations is feasible. Proceeding as before we have

$$W_{\mathbf{k} \rightarrow \mathbf{k}'} = \frac{1}{\hbar^2} \frac{1}{L^3} K_{\omega\mathbf{q}}, \quad \hbar\omega = \varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}, \quad \mathbf{q} = \mathbf{k}' - \mathbf{k},$$

$$K_{\omega\mathbf{q}} = \int_{-\infty}^{+\infty} dt \int_{\infty} d^3 r e^{i\omega t - i\mathbf{q}\mathbf{r}} K(\mathbf{r}, t), \quad (2.119)$$

which contains the space-time correlator

$$K(\mathbf{r}, t) = \langle V^*(0, 0) V(\mathbf{r}, t) \rangle. \quad (2.120)$$

Here the angular brackets denote averaging over time in accordance with eq. (2.104) and averaging over space in accordance with eq. (2.114). It is assumed that

$$\langle V(\mathbf{r}, t) \rangle = \langle V \rangle = 0. \quad (2.121)$$

Note that if V is independent of t , then, as can readily be seen, eq. (2.119) is transformed into eq. (2.118).

If we discard condition (2.121), then

$$\langle V^*(0, 0) V(\mathbf{r}, t) \rangle_{r \rightarrow \infty} = \langle V^*(0, 0) \rangle \langle V(\mathbf{r}, t) \rangle = |\langle V \rangle|^2 \neq 0, \quad (2.122)$$

i.e. the correlator does not vanish at infinity, but tends to a certain constant value. The presence of a constant nonvanishing term in $K(\mathbf{r}, t)$ leads to a term in $K_{\omega\mathbf{q}}$ that is proportional to $\delta(\omega) \delta(\mathbf{q})$. Therefore, in calculating the scattering probability, for which \mathbf{k}' is never equal to \mathbf{k} , i.e. $\mathbf{q} \neq 0$, we need not satisfy condition (2.121). The aforesaid does not concern eq. (2.110) because the transition probability can also be considered for transitions with $\varepsilon_f = \varepsilon_i$, i.e. with $\omega = 0$.

The Fourier transforms K_{ω} , $K_{\mathbf{q}}$ and $K_{\omega\mathbf{q}}$ of the correlators tend to zero as $\omega \rightarrow \infty$ and $q \rightarrow \infty$. The regions of the variables ω and q , in which these Fourier transforms are not small, are determined by the correlation time and the correlation length: $\omega \sim 1/\bar{\tau}$ and $q \sim 1/\bar{l}$. It should be kept in mind, however, that it is not at all necessary for such energy ($\hbar\omega$) and momentum

($\hbar\mathbf{q}$) to be transferred in a typical transition. In the energy spectrum of the system, for example, there may be no energy difference corresponding to the frequencies of the most intensive Fourier components K_ω in eq. (2.110). In eq. (2.118) the transfer of momentum $\hbar\mathbf{q}$, corresponding to the most intensive Fourier components K_q , may not be in agreement with energy conservation $\varepsilon_k = \varepsilon_{k+q}$.

If the scattering system can be represented as an ideal gas of quasi-particles, then the scattering probability can be calculated also by another method that is described in detail in ch. 3, using the phonon gas as an example. Note, in this connection, that for scattering by an ideal gas, \bar{l} is of the order of the characteristic wavelength of the quasi-particles, whereas $\hbar/\bar{\tau}$ is of the order of their characteristic energy.

As an example let us consider scattering by the deformation potential of long-wavelength acoustic phonons (see sect. 3.4) that are in thermodynamic equilibrium. Here $V(\mathbf{r}, t)$ is to be understood as being the deformation potential at the point \mathbf{r} at the instant t , equal to $\Xi u(\mathbf{r}, t)$, where $u(\mathbf{r}, t)$ is the relative change in volume of the lattice during thermal vibrations. For the correlator $\langle u(0, 0) u(\mathbf{r}, t) \rangle$ the correlation time $\bar{\tau}$ is of the order of \hbar/T , the vibration period of the thermal phonons, and \bar{l} is of the order of the wavelength $\hbar s/T$ of these phonons. However, as has been mentioned previously, typical energy and momentum transfers are not always equal to T and $\hbar s/T$. This is directly confirmed by an analysis of the kinematics of scattering by acoustic phonons, which is carried out in sect. 4.2.2.

The correlator method will be applied in sections 15.2 and 15.3 in order to deal with scattering by spin fluctuations in a magnetic metal and in a semiconductor with magnetic impurities. Of especial importance is the fact that the description of scattering by means of correlators is also valid in the case when the scattering system cannot be replaced by an ideal gas of quasi-particles. This is true, in particular, for a system of spins close to a phase transition point, at which the excitation of the spin-system cannot be described in terms of an ideal gas of magnons.

The scattering probability, expressed in terms of correlators, retains its meaning even in the case when the averaging $\langle \dots \rangle$ is understood as the averaging, not of classical quantities, but of operators. This implies that we begin by quantum averaging over the states of the scattering system, followed by the statistical averaging with respect to the probabilities of occupying these states. If the operators a and b in the correlator $\langle ab \rangle$ are not commutative, it is necessary to make the substitution

$$\langle ab \rangle \rightarrow \frac{1}{2} \langle ab + ba \rangle. \quad (2.123)$$

The size of the domain of integration for K_q in eq. (2.117) is determined by the correlation length \bar{l} . This means that the scattering probability given by eq. (2.118) includes mutual interference of waves scattered by points lying in a

region having the volume \bar{l}^3 . This interference is appreciable if the “wave-length” corresponding to the momentum transfer $\hbar\mathbf{q}$ is not small compared to the size of the region, i.e. $2\pi/q \gtrsim \bar{l}$. If, however, $2\pi/q \ll \bar{l}$, the size of the domain of integration for $K_{\mathbf{q}}$ is reduced, owing to the oscillating factor, to $2\pi/q$ and only those waves interfere that are scattered from points in a region having the volume $(2\pi/q)^3$.

The calculation of a transition probability with the matrix element given by eq. (2.111) is equivalent to the Born approximation which, as is well-known, assumes that in the scattering region there is almost no difference between the exact wave function and the incident wave. When applied to the potential $V(\mathbf{r})$ set up by several centers, this means, among other things, that the rescattering of waves between the centers is not taken into account. In other words, the wave scattered by each center is the same as if there were no other centers. However, the interference of waves scattered by different centers will be taken into consideration.

A random potential $V(\mathbf{r})$ can quite frequently be represented as the superposition of potentials produced by randomly distributed centers:

$$V(\mathbf{r}) = \sum_{\alpha} v(\mathbf{r} - \mathbf{R}_{\alpha}), \quad (2.124)$$

where $v(\mathbf{r})$ is the potential of a single center located at the origin, and \mathbf{R}_{α} are the random points where the centers are situated. The distribution of the centers can be said to be “random” if the possibility of finding a center at a given point does not depend on whether there are centers at neighboring points. In this case, as is shown by probability theory,

$$\langle V(0) V(\mathbf{r}) \rangle = N \int_{\infty} d^3r' v(\mathbf{r}') v(\mathbf{r} + \mathbf{r}'), \quad (2.125)$$

where N is the average number of centers per cm^3 . In other words, the correlation function is completely determined by the form of the potential of a single center. If potentials $v_i(\mathbf{r})$ of various types are possible, and the probability of finding a potential of a certain type at a given point is independent of the types of the neighboring potentials, then the integral in eq. (2.125) should be averaged over all the possible types of potentials.

It follows from eq. (2.125) that the correlation length \bar{l} is always of the order of the range a of the potential. It is important that this is valid independently of whether the centers overlap ($Na^3 \gtrsim 1$) or do not overlap ($Na^3 \ll 1$).

The applicability of the concept of a “random distribution” of impurities in a crystal is limited to concentrations $Na_0^3 \ll 1$, where a_0^3 is the volume of a primitive cell. The point is that no more than a single impurity can occupy one lattice site; hence, for $Na_0^3 \gtrsim 1$, the probability that a given impurity will occupy a given site does depend upon the arrangement of the other impurities.

Fourier component (2.117) of the correlator given by eq. (2.125) is

$$K_{\mathbf{q}} = N |v_{\mathbf{q}}|^2, \quad \text{where} \quad v_{\mathbf{q}} = \int_{\infty} d^3r e^{-i\mathbf{q}\mathbf{r}} v(\mathbf{r}). \quad (2.126)$$

This means that in the case of scattering by randomly distributed impurities, the scattering probability is the sum of the probabilities of scattering by the separate impurities. In other words, waves, scattered by randomly distributed impurities, do not interfere even in the case when their potentials overlap.