

QUANTUM THEORY OF X-RAY SCATTERING. I. ELASTIC SCATTERING BY PERFECT CRYSTAL

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A quantum field theoretical method is applied to the kinematic theory of X-ray diffraction. The present work deals with the quantum theory of elastic X-ray scattering by a perfect crystal.

Generally, the kinematic theory of X-ray diffraction is treated classically. A quantum field theoretical method is applied to the problem of X-ray diffraction in the present work. The scattering of X-rays by perfect crystal is described by a Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}. \quad (1)$$

where \hat{H}_0 are the sum of the Hamiltonians of the crystal $\hat{H}_0^{(1)}$ and the electromagnetic field $\hat{H}_0^{(2)}$, \hat{H}_{int} — is the Hamiltonian of the interaction between the electromagnetic field and the electrons of the lattice

$$\hat{H}_{\text{int}} = -\frac{1}{c} \int d\vec{r} \cdot \hat{j}(\vec{r}) \cdot \hat{A}(\vec{r}) \quad (2)$$

where $\hat{A}(\vec{r})$ is the vector potential operator for the quantized electromagnetic free field

$$\hat{A}(\vec{r}) = \sum_{\vec{k}} \sqrt{\frac{2\pi c^2 k}{V \cdot \omega_{\vec{k}}}} \{ \vec{e}_{\vec{k}} \cdot \vec{a}_{\vec{k}} \cdot e^{i\vec{k}\vec{r}} + \vec{e}_{\vec{k}}^* \cdot \vec{a}_{\vec{k}}^+ \cdot e^{-i\vec{k}\vec{r}} \} \quad (3)$$

$\hat{j}(\vec{r})$ — is the density current operator for the electrons

$$\begin{aligned} \hat{j}(\vec{r}) = & \frac{e}{2m} \cdot \sum_{\alpha} \{ \hat{p}_{\alpha} \cdot \delta(\vec{r} - \vec{r}_{\alpha}) + \delta(\vec{r} - \vec{r}_{\alpha}) \cdot \hat{p}_{\alpha} \} - \\ & - \frac{e^2}{mc} \cdot \sum_{\alpha} \hat{A}(\vec{r}) \cdot \delta(\vec{r} - \vec{r}_{\alpha}) \end{aligned} \quad (4)$$

here α — is the index summation over all the electrons of crystal.

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The initial and final state vectors Φ_i and Φ_f are eigenvectors of the Hamiltonian of the free system "crystal plus field"

$$\hat{H}_0 \Phi_i = E_i \Phi_i \quad \hat{H}_0 \Phi_f = E_f \cdot \Phi_f. \quad (5)$$

where E_i and E_f are energy of the system "crystal plus field" at $t \rightarrow \pm \infty$, when $H_{\text{int}} \rightarrow 0$.

In the interaction picture the evolution of the initial state vector of system Φ_i for $t \rightarrow -\infty$ in the final state vector Φ_f for $t \rightarrow +\infty$ is described by the scattering S -matrix

$$\Phi_f = S \cdot \Phi_i. \quad (6)$$

The transition probability $i \rightarrow f$ is defined by the square of the matrix element

$$|\langle f | S | i \rangle|^2 \quad (7)$$

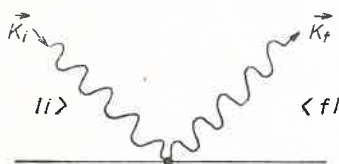


Fig. 1

where the scattering S -matrix is defined by the well known formula

$$S = \hat{P} \left\{ \exp \left(-\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \cdot \hat{H}_{\text{int}}(t) \right) \right\} \quad (8)$$

here: \hat{P} — is the chronological operator and

$\hat{H}_{\text{int}}(t)$ — is the interaction Hamiltonian in the interaction representation

$$\hat{H}_{\text{int}}(t) = \exp \left(\frac{i}{\hbar} \hat{H}' \cdot t \right) \cdot \hat{H}_{\text{int}} \cdot \exp \left(-\frac{i}{\hbar} \hat{H}'_0 t \right). \quad (9)$$

The use of the last term in (4)

$$-\frac{e^2}{mc^2} \cdot \sum_{\alpha} \hat{A}(\vec{r}) \cdot \delta(\vec{r} - \vec{r}_{\alpha}) \quad (10)$$

together with the first term of the expansion of the scattering S -matrix

$$S^{(1)} = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \cdot \hat{H}_{\text{int}}(t) \quad (11)$$

results in the so called direct scattering of the photons, which corresponds to the diagram in Fig. 1.

The inscription (7) is necessary to multiply with the density of final states of a scattered X-rays

$$\frac{k_f^2 \cdot dk_f \cdot d\Omega \cdot V}{(2\pi)^3} \quad (12)$$

averaging over the initial states and by summation over the final ones.

Thus, the final expression for the probability scattering $i \rightarrow f$ is given by

$$W_{i \rightarrow f} = \sum_f \overline{|\langle f | S^{(1)} | i \rangle|^2} \cdot \frac{\varepsilon_f^2 \cdot d\varepsilon_f \cdot d\Omega \cdot V}{(2\pi\hbar c)^3} \quad (13)$$

where the horizontal line signifies the average over the initial states of the system.

The standard quantum-mechanical calculation is the following. A δ -function $\delta(E_i - E_f)$ is obtained after the integration over t . One δ -function is replaced by the time of the interaction. The integration of the outgoing energy ε_f of the scattered X-quantum with the δ -function under the integral is carried out as usual. Dividing by the time of the interaction, $d\Omega$ and the density of the incident beams $\frac{C}{V}$, one obtains the following expression for the differential elastic scattering cross-section per unit solid angle (assuming that electronic and lattice wave functions are separated):

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2 \cdot \frac{1 + \cos\vartheta}{2} \cdot \sum_n \varrho_n \cdot \left| \left\langle n_{\vec{q},1}, \varphi \left| \sum_{\alpha} e^{i\vec{K}\vec{r}_{\alpha}} \right| n_{\vec{q},s}, \varphi \right\rangle \right|^2 \quad (14)$$

the term $\frac{1}{2}(1 + \cos\vartheta)$, where ϑ is the scattering angle is obtained by averaging over the initial polarization incident X-quantum and summing over the final polarization the scattered X-quantum in the expression $|\vec{e}_{\vec{k}_i} \cdot \vec{e}_{\vec{k}_f}|^2$, under the assumption that the incident beam is unpolarized. $\vec{K} = \vec{k}_i - \vec{k}_f$ where $\langle \varphi |$ is the wave function of the electronic subsystem, $\langle \eta_{\vec{q},s} |$ is the wave function of the lattice subsystem within the representation of the occupation numbers and $\eta_{\vec{q},s}$ is the number of the phonons with the wave vector for the s -th vibration branch.

For the lattice which is in the thermal equilibrium state at the temperature T , ϱ_n is defined with the help of Gibbs's distribution.

The further transformation of (14) is connected with the consideration of the thermal vibration of the lattice and of crystal structures.

1. "Frozen" primitive lattice

For "frozen" lattice $\varrho_n = 1$ and all $n_{\vec{q},s} = 0$. In the elementary cell of the primitive lattice one atom is contained, therefore the coordinate of the electron may be written as

$$\vec{r}_{\alpha} = n_j^0 + \vec{r}_v \quad (15)$$

n — is the vector of the lattice, and \vec{r}_v — is the coordinate of the v -th electron of the j -th

The square of the matrix element of the electron sum is transformed to the following form:

$$|\langle 0, \varphi | \sum_{\alpha} e^{i\vec{K}\vec{r}_{\alpha}} | 0, \varphi \rangle|^2 = \left| \sum_{j=1}^N e^{i\vec{K}\vec{n}_j} \right|^2 \cdot \left| \langle \varphi | \sum_{\nu=1}^Z e^{i\vec{K}\vec{r}_{\nu}} | \varphi \rangle \right|^2. \quad (16)$$

The first term is well known as the function interference, the second multiplier is the atomic scattering factor.

2. "Frozen" lattice with basis

For the lattice with the basis at the elementary cell of which there are σ atoms the equilibrium position of the β — atom at the j -th elementary cell may be represented as

$$\vec{R}_{j\beta}^0 = \vec{n}_j^0 + \vec{Q}_{\beta}^0, \quad \beta = 1, 2, \dots, \sigma \quad (17)$$

\vec{Q}_{β}^0 — is the vector, pointing at the equilibrium position of β -th atom in the j -th cell

$$\begin{aligned} & |\langle 0, \varphi | \sum_{\alpha} e^{i\vec{K}\cdot\vec{r}_{\alpha}} | 0, \varphi \rangle|^2 \\ &= \left| \sum_{j=1}^N e^{i\vec{K}\vec{n}_j} \right|^2 \cdot \left| \sum_{\beta=1}^{\sigma} e^{i\vec{K}\vec{Q}_{\beta}^0} \cdot \langle \varphi | \sum_{\nu=1}^{Z_{\beta}} e^{i\vec{K}\vec{r}_{\nu}} | \varphi \rangle \right|^2. \end{aligned} \quad (18)$$

The second term is the structure factor.

3. The considering of the thermal vibrations of the primitive lattice

$$\vec{r}_{\alpha} = \vec{n}_j + \delta\vec{n}_j + \vec{r}_{\nu} \quad (19)$$

where $\delta\vec{n}_j$ is the replacement of the j -th atom from the equilibrium position as the result of the thermal movement.

$$\begin{aligned} & \sum_n Q_n |n_{\vec{q},s}, \varphi | \sum_{\alpha} e^{i\vec{K}\vec{r}_{\alpha}} |n_{\vec{q},s}, \varphi \rangle|^2 \\ &= \left| \sum_{j=1}^N e^{i\vec{K}\vec{n}_j} \right|^2 \cdot \sum Q_n |\langle n_{\vec{q},s} | e^{i\vec{K}\delta\vec{n}_j} | n_{\vec{q},s} \rangle|^2 \cdot \left| \langle \varphi | \sum_{\nu=1}^Z e^{i\vec{K}\vec{r}_{\nu}} | \varphi \rangle \right|^2 \\ &= \left| \sum_{j=1}^N e^{i\vec{K}\vec{n}_j} \right|^2 \cdot e^{-2W} \cdot \left| \langle \varphi | \sum_{\nu=1}^Z e^{i\vec{K}\vec{r}_{\nu}} | \varphi \rangle \right|^2 \end{aligned} \quad (20)$$

where $\exp(-2W)$ is the Debye-Waller's thermal factor.

4. Considering the thermal vibrations in the lattice with the basis

$$\vec{r}_{\alpha} = \vec{n}_j + \vec{Q}_{\beta}^0 + \delta\vec{Q}_{\beta} + \vec{r}_{\nu} \quad (21)$$

$$\begin{aligned} & \sum Q_n |\langle n_{\vec{q},s}, \varphi | \sum_{\alpha} e^{i\vec{K}\vec{r}_{\alpha}} | n_{\vec{q},s}, \varphi \rangle|^2 \\ &= \sum_{j=1}^N e^{i\vec{K}\vec{n}_j} \cdot \sum_{\beta=1}^{\sigma} e^{i\vec{K}\vec{r}_{\beta}^0} \cdot e^{-W_{\beta}} \cdot \left| \langle \varphi | \sum_{\nu=1}^{Z_{\beta}} e^{i\vec{K}\vec{r}_{\nu}} | \varphi \rangle \right|^2. \end{aligned} \quad (22)$$