THE DIFFRACTION OF AN ELECTRON-WAVE AT A SINGLE LAYER OF ATOMS

By M. v. Laue*

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Abstract

This paper undertakes to estimate the influence of the gradual transition between the field exterior to, and in the interior of a crystal, on the diffraction of electrons. This gradual transition is required by electrostatics. The result is, that this influence may be neglected for electrons whose energy is two hundred volts or more. One can then treat the transition as discontinuous. In the case of slower electrons it seems doubtful, if such a treatment is permissible.

Introduction

THE theory of the diffraction of electrons by a space-lattice has been discussed by Bethe and later, under simplifying assumptions by Morse.[1] These authors integrate the Schrödinger-equation for the internal field in so complete a manner, that little more is to be said. Their treatment of the incidence and reflection at the surface cannot be considered as equally satisfactory. They treat the triply periodic internal field as though it ceases suddenly at a certain plane. This is in complete contradiction to electrostatics, as one may not consider this plane as charged without coming into conflict with the atomistic foundations of the whole theory. The field certainly dies off asymptotically as one proceeds outward. This is doubtless a lack in the theory which, as it seems to us,—might cast doubt on its applicability to the experiments. At least it should be examined to see if and under what circumstances this approximation is justifiable. As a matter of fact it will appear that this is not always the case.

Properly one should treat the atoms as having a finite extension but then the calculations based on the Schrödinger-equation would encounter a difficulty which is only too well known in optics, namely the reflection and refraction at a plane plate with continuously variable refractive index. Of necessity, then, we will treat the atoms as point charges. The order of magnitude of our results will probably not be influenced.

To obtain a comparison let us glance at the theory of Röntgen-interference which is similar to Bethe's in many points. In this treatment one considers the space-lattice of diffracting centers to be bounded by a definite lattice-plane; one can also object to this since the atoms in the boundary planes actually do not occupy exactly the position which they would have if the crystal were continued beyond the boundary. But since a single layer of atoms contributes very little to the resultant intensity of Röntgen-rays this

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[1] H. Bethe, Ann. d. Physik **87**, 55 (1928); P. M. Morse, Phys. Rev. **35**, 1910 (1930).

assumption can have little influence. In the case of electron-diffraction things are essentially different.

Let the primitive periods of the lattice-plane be the vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$; the reciprocal vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ which lie in the same plane are defined by the equations

$$(\boldsymbol{a}_1\boldsymbol{b}_1) = 1,\ (\boldsymbol{a}_1\boldsymbol{b}_2) = 0,\ (\boldsymbol{a}_2\boldsymbol{b}_1) = 0,\ (\boldsymbol{a}_2\boldsymbol{b}_2) = 1. \tag{1}$$

The surface-density of electricity in this plane will be

$$\rho = \sum_1 \rho_m e^{2\pi i(\boldsymbol{b}_m\boldsymbol{r})} \tag{2}$$

where $\boldsymbol{r}$ is the vector drawn from an arbitrary origin in the lattice-plane to the point of consideration, and

$$\boldsymbol{b}_m = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2. \tag{3}$$

The coefficient ρ_0 is zero, since the total charge must vanish. The other coefficients are given by the equation

$$\rho_m = \frac{1}{F}\int \rho e^{-2\pi i(\boldsymbol{b}_m\boldsymbol{r})} d\sigma,$$

in which F is the area of the parallelogram subtended by $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and the integration is to be extended over such a parallelogram. If a positive pole of charge Z lie at $\boldsymbol{r}_+ = \delta_1\boldsymbol{a}_1 + \delta_2\boldsymbol{a}_2$ a negative pole of the same strength at $\boldsymbol{r}_- = -(\delta_1\boldsymbol{a}_1 + \delta_2\boldsymbol{a}_2)$ then according to 1):

$$\rho_m = -\frac{2Z\epsilon}{F} i \sin 2\pi(m_1\delta_1 + m_2\delta_2). \tag{4}$$

We assume that the lattice plane has the equation $z=0$. Then these charges produce the potential

$$\phi = \sum \phi_m e^{2\pi i(\boldsymbol{b}_m\boldsymbol{r})} e^{-2\pi|\boldsymbol{b}_m||z|} \tag{5}$$

in which[2]

$$\phi_m = \frac{\rho_m}{|\boldsymbol{b}_m|}. \tag{6}$$

The coefficient ϕ_0 vanishes. It would have to be—because of $\Delta\phi = 0$—a linear function of z and this must vanish because of the boundary conditions at $z = \pm\infty$.

It would be otherwise if we had, e.g., two parallel planes of which the one had a net positive charge, the other an equal negative: then ϕ_0 would be different from zero between the two planes. Also if the atoms were not taken to be point-charges there would be regions in which ϕ_0 did not vanish.

[2] This series is naturally double. The index m represents the pair of indices m_1 and m_2 which occur in (3) explicitly.

The Schrödinger-equation of the free electron

$$\Delta\psi + \frac{8\pi^2\mu}{h^2}E\psi = 0$$

is integrated by the function

$$\psi = e^{2\pi i(\boldsymbol{K}_0\boldsymbol{R})}, \quad (\boldsymbol{K}_0) = \frac{1}{h}(2\mu E)^{1/2} \tag{7}$$

in which $\boldsymbol{R}$ is the three-dimensional vector to the point under consideration (Aufpunkt); $\boldsymbol{r}$ is the component of $\boldsymbol{R}$ parallel to the plane $z=0$, μ the mass of electron. We also resolve the vector $\boldsymbol{K}_0$ into a component $\boldsymbol{k}_0$ parallel to this plane and one parallel to the z axis—z the magnitude of the latter is $\kappa_0=(\boldsymbol{K}_0^2-\boldsymbol{k}_0^2)^{1/2}$. Then Eq. (7) becomes

$$\psi = \psi_0(z)e^{2\pi i(\boldsymbol{k}_0\boldsymbol{r})}, \quad \psi_0(z) = e^{2\pi i\kappa_0 z} \tag{8}$$

We assume that κ_0 is positive; the wave than proceeds from positive to negative z-values.

The Schrödinger-equation of the electron as perturbed by the lattice-plane

$$\Delta\psi + \frac{8\pi^2\mu}{r^2}(E - \epsilon\phi)\psi = 0$$

we attempt to resolve in the form

$$\psi = \sum\psi_m(z)e^{2\pi i(\boldsymbol{k}_0+\boldsymbol{b}_m,\boldsymbol{r})}.$$

It then reads

$$\Delta\psi = \sum\left(\frac{d^2\psi_m}{dz^2} - 4\pi^2(\boldsymbol{k}_0 + \boldsymbol{b}_m)^2\psi_m\right)e^{2\pi i(\boldsymbol{k}_0+\boldsymbol{b}m,\boldsymbol{r})} \tag{9}$$

from which we can cancel the factor $e^{2\pi i\boldsymbol{k}_0\boldsymbol{r}}$. The remaining equation is then:

$$\sum_m\left(\frac{d^2\psi_m}{dz^2} + 4\pi^2(\boldsymbol{K}_0^2 - (\boldsymbol{k}_0 + \boldsymbol{b}_m)^2)\psi_m\right)e^{2\pi i(\boldsymbol{b}_m\boldsymbol{r})}$$

$$= \frac{8\pi^2\epsilon\mu}{h^2}\sum_{p,q}\psi_p(z)\phi_q e^{-2\pi|b_q|[z]}e^{2\pi i(\boldsymbol{b}_q+\boldsymbol{b}_q,\boldsymbol{r})}$$

According to Eq. (3)

$$\boldsymbol{b}_p + \boldsymbol{b}_q = \boldsymbol{b}_{p+q}.$$

Since this equation must be true for every value of the vector $\boldsymbol{r}$, the separate terms on each side which have the same exponential factor must be identical, i.e.

$$\frac{d^2\psi_m}{dz^2} + 4\pi^2(\boldsymbol{K}_0^2 - (\boldsymbol{k}_0 + \boldsymbol{b}_m)^2)\psi_m = \frac{8\pi^2\epsilon\mu}{h^2}\sum_p\psi_p(z)\phi_{m-p}e^{-2\pi|\boldsymbol{b}_m-p||z|} \tag{10}$$

To solve this system of infinitely many differential-equations with infinitely many unknowns $\psi_m(z)$ we use a method of approximation. As first approximation one will substitute for ψ_0 the value (8) of the wave-function of the unperturbed incident wave, and retain only the term in ψ_0 on the right side of (10). The weaker the intensity of the diffracted waves comes out, the better will be this approximation. Since $\phi_0 = 0$ we then obtain the equation:

$$\frac{d^2\psi_m}{dz^2} + 4\pi^2(K_0^2 - (k_0 + b_m)^2)\psi_m = \frac{8\pi^2\epsilon\mu}{h^2}\psi_0(z)\phi_m e^{-2\pi|b_m||z|} \tag{11}$$

of which the solution satisfies the condition that it must represent *emergent* waves at $z = \pm\infty$ is

$$\begin{aligned}\psi_m(z) = 2\pi i\frac{\epsilon\mu}{h^2}\frac{\phi_m}{\epsilon_m}\Big\{ & e^{2\pi i\epsilon_m z}\int_z^\infty \psi_0(\zeta)e^{-2\pi|b_m||\zeta|}e^{-2\pi i\epsilon_m\zeta}d\zeta \\ & + e^{-2\pi i\epsilon_m z}\int_{-\infty}^z \psi_0(\zeta)e^{-2\pi|b_m||\zeta|}e^{+2\pi i\epsilon_m\zeta}d\zeta\Big\}.\end{aligned} \tag{12}$$

The abbreviation

$$\epsilon_m = (K_0^2 - (k_0 + b_m)^2)^{1/2} \tag{13}$$

has been used. That this is a solution of Eq. (11) will be seen on substitution. For $z = +\infty$ we obtain from (12):

$$\psi_m = 2\pi i\frac{\epsilon\mu}{h^2}\frac{\phi_m}{\epsilon_m}e^{-2\pi i\epsilon_m z}\int_{-\infty}^{+\infty}\psi_0(\zeta)e^{-2\pi|b_m||\zeta|}e^{+2\pi i\epsilon_m\zeta}d\zeta \tag{14}$$

At $z = -\infty$ correspondingly

$$\psi_m = 2\pi i\frac{\epsilon\mu}{h^2}\frac{\phi_m}{\epsilon_m}e^{+2\pi i\epsilon_m z}\int_{-\infty}^{+\infty}\psi_0(\zeta)e^{-2\pi|b_m||\zeta|}e^{-2\pi i\epsilon_m\zeta}d\zeta. \tag{15}$$

These are the emergent waves required by the boundary conditions, at least, if ϵ_m is real and positive.

The latter may always be assumed to be the case, as the sign is not defined by (13). The former is not always true according to (13). In addition to the diffracted homogeneous waves there are also inhomogeneous ones which are propagated along the lattice-plane and die off asymptotically in a direction perpendicular to this plane. For every pair with indices m with real ϵ_m there are always two emergent waves on each side of the lattice-plane.

It will be remarked that Eq. (12) is still valid for such index pairs, m, for which $i\epsilon_m$ is positive and real.[3] If one draws the factor $e^{\pm 2\pi i\epsilon_m z}$ under the integral sign, than the bracket in (13) has the value

$$\int_z^\infty \psi_0(\zeta)e^{-2\pi|b_m||\zeta|}e^{2\pi i\epsilon_m(z-\zeta)}d\zeta + \int_{-\infty}^z \psi_0(\zeta)e^{-2\pi|b_m||\zeta|}e^{-2\pi i\epsilon_m(z-\zeta)}d\zeta$$

[3] Negative real values may be left out of account since the sign of the root in (13) is arbitrary; they must be left out of account, because Eq. (12) is not longer valid when $i\epsilon_m < 0$.

in the first of these integrals $z-\zeta$ is negative, in the second positive. They both exist therefore. Only Eqs. (14) and (15) must be changed for this case; but our interest is only for the homogeneous waves, i.e., real values of ϵ_m.

For the justification of this calculation it is essential that Eq. (11) applied to the index pair 0,0 possesses the solution $\psi_0(z)$ as given in Eq. (8). This would not be the case, if ϕ_0 did not vanish. In that case we would encounter the problem of the plane parallel plate as remarked in the introduction and would have to use its solution in evaluating the other ψ_m.

The integrals in (14) and (15) are to be evaluated for real values of ϵ_m and ψ_0 as in (8). They are

$$\int_{-\infty}^{+\infty} e^{2\pi i(\kappa_0 \pm \epsilon_m)\zeta} e^{-2\pi|b_m||\zeta|} d\zeta$$

$$\int_0^{\infty} e^{2\pi i(\kappa_0 \pm \epsilon_m)\zeta} e^{-2\pi|b_m|\zeta} d\zeta + \int_{-\infty}^{0} e^{2\pi i(\kappa_0 \pm \epsilon_m)\zeta} e^{+2\pi|b_m|\zeta} d\zeta$$

$$= 2\int_0^{-\infty} \cos\,(2\pi(\kappa_0 \pm \epsilon_m)\zeta) e^{-2\pi|b_m|\zeta} d\zeta = \frac{1}{\pi} \frac{|b_m|}{(\kappa_0 + \epsilon_m)^2 + b_m^2}$$

If we now use the value of ϕ_m given by (6) and ρ_m given by (4), we obtain

$$\psi_m(z) = \frac{4Z\epsilon^2\mu}{h^2} \frac{\sin 2\pi(m_1\delta_1 + m_2\delta_2)}{F} \frac{e^{\mp 2\pi i \epsilon_m z}}{\epsilon_m[(\kappa_0 \pm \epsilon_m)^2 + b_m^2]} \quad \text{for } z = \pm\infty \tag{16}$$

in which the abbreviations

$$\kappa_0 = (K_0^2 - k_0^2)^{1/2} = |K_0| \cos\theta, \quad |K_0| = \frac{1}{h}(2\mu E)^{1/2}$$

$$\epsilon_m = (K_0^2 - (k_0 + b_m)^2)^{1/2} = (K_0^2 \cos^2\theta - 2(k_0 b_m) - b_m^2)^{1/2}$$

have been used. The angle θ is the angle of incidence of the original electron wave. Only the last of the three fractions in (16) depends on the energy of the electrons, and it diminishes with increasing E approximately as $E.^{-3/2}$ For sufficiently fast electrons the amplitude of every ψ_m-wave is so small, that the diffracting-power of the single atomic layer is insignificant. The neglect of the surface layers is then justified. To obtain an estimate of the lower limit above which this is true we will later evaluate Eq. (16) numerically.

One can best estimate the strength of an inhomogeneous wave if one determines its amplitude in the lattice-plane itself ($z=0$). We designate the real positive quantity $i\epsilon_m$ by η_m. From (12), (6) and (4) it then follows without difficulty that:

$$\psi_m(0) = \frac{4Z\epsilon^2\mu}{h^2} i \sin 2\pi(m_1\delta_1 + m_2\delta_2) \frac{|\boldsymbol{b}_m| + \eta_m}{|\boldsymbol{b}_m|(\eta_m)[(\boldsymbol{b}_m + \eta_m)^2 + \kappa_0^2]}.$$

One notices the diminution of the amplitude with increasing indices m_1, m_2.

For numerical purposes we suppose the vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ perpendicular the one to another and both of length 4×10^{-8} cm. Then the reciprocal vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ will also be perpendicular and of the magnitude 2.5×10^7 cm^{-1}. In each square formed by $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ we suppose one positive and one negative charge—each of $Z=1$, but we do not determine their positions more definitely, i.e., the numbers δ_1, δ_2 are thus undetermined. Then the first factor in (16) is

$$\frac{4\epsilon^2\mu}{h^2F} = 1.25\times 10^{22}\ \text{cm}^{-3}.$$

We suppose an electron beam of 150 volts energy to be incident normally on this lattice plane. The de Broglie wave-length is 10^{-8} cm, also $\kappa_0 = |k_0| = 10^8$ cm^{-1}. Then only those homogeneous waves can appear, for which the indices m_1, m_2 are any combination of the numbers ± 1 and 0. This results in 8 emergent beams from each side of the lattice plane. If one index is 0, the other ± 1 Eq. (16) gives

$$\frac{|\psi|^2_{z=+\infty}}{\sin^2(2\pi(m_1\delta_1 + m_2\delta_2))} = 10^{-5}, \quad \frac{|\psi|^2_{z=-\infty}}{\sin^2(2\pi(m_1\delta_1 + m_2\delta_2))} = 4\times 10^{-2}$$

If both indices are ± 1, then one finds

$$\frac{|\psi|^2_{z=+\infty}}{\sin^2(2\pi(m_1\delta_1 + m_2\delta_2))} = 1.5 \times 10^{-5}, \quad \frac{|\psi|^2_{z=-\infty}}{\sin^2(2\pi(m_1\delta_1 + m_2\delta_2))} = 3\times 10^{-3}$$

$\sin^2(\ )$ is the structure factor and obviously depends on the position of the two pointcharges in the elementary parallelogram. Since we set the intensity of the incident wave equal to 1, the foregoing numbers represent the relative intensity of the diffracted rays. As they are small compared with 1, one will conclude firstly, that the present approximation is sufficient, and secondly, that the diffracting-power of the single plane is so small that it is justified to neglect the surface fields as Bethe and Morse have done.

The result is quite different if we consider electrons of energy 37.5 volts, other things remaining the same (wave-length $\lambda = 2\times 10^{-8}$ cm). Then the only possible homogeneous waves are those for which one index is 0, the other ± 1. At $z=+\infty$ the fraction $|\psi|^2/\sin^2(\ )$ has a sufficiently small value, namely 10^{-3}; but for $z=-\infty$ it becomes even greater than 1, which naturally means that the present approximation is useless. In this case it seems that space lattice theories of Bethe and Morse require extension by considerations regarding the surface layers.

In summary we may safely say, despite the fact that the case here considered is far from the real one, that for electrons of 200 or more volts energy

the neglect of the surface action in the space lattice theory of electron diffraction is justified, but that this is not obviously true at smaller velocities.

In the experiments of Stern and his collaboraters on the diffraction of atoms and molecules by crystals, the plane-grating-action of the surface is the only thing observed, no space-lattice effects. The theory of these phenomena one must probably attempt to carry through in a similar manner to the above. The essential difference will be in a different value of the coefficients ϕ_m of the Fourier-series for the potential energy. The form (9) for the wave-function and the approximation introduced in (11) may probably be retained.