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Diffraction of non-relativistic electron waves by a cylindrical capacitor

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Abstract. The diffraction of non-relativistic electron waves by a cylindrical capacitor is considered for an electric voltage at the capacitor small compared with the energy of the incident electrons. On the basis of the exact general solution of the Schrödinger equation for an electron in an attractive logarithmic potential, asymptotic solutions inside the capacitor which are similar to JWKB-type solutions, but with a significant modification, are derived. Application of appropriate boundary conditions to our asymptotic solutions yields an angular momentum expansion of the scattered wave which is further evaluated by means of the Sommerfeld-Watson transformation. The change of various well known diffraction phenomena with increasing electric voltage at the capacitor is calculated explicitly and discussed in detail; in particular, the convergence of electron interference fringes towards the optical axis is one of the main results of our investigation.

1. Introduction

In highly specialised electron optics laboratories, electron interference experiments offer the possibility of a simple demonstration of the wave behaviour of electrons which does not require any assumptions about the interactions between electrons and atoms and the distribution of atoms in crystalline lattices, as is necessary for the analysis of electron diffraction experiments in crystalline materials.

An electrostatic convergent biprisma, which enables one to observe electron interference phenomena, may be constructed from a capacitor consisting of a hollow cylinder and a central straight wire (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976). The electrostatic potential inside the cylinder is of logarithmic type,

$$V(r) = \epsilon \ln(r/b) \quad a \leq r \leq b \quad \epsilon > 0, \quad (1.1)$$

where a and b denote the radii of the wire and hollow cylinder respectively. This electric field attracts incident electrons towards the central wire; consequently the Fresnel zones due to diffraction by the wire converge towards the optical axis so that a large number of these zones can be observed with increasing electric field strength.

These interference phenomena can be calculated via an evaluation of the well established diffraction integral (Sommerfeld 1964, Glaser 1952, Glaser and Schiske 1953, Komrska 1971). The electron wavefunction at any observation point is derived from its experimentally prescribed boundary values on the diffraction plane (the plane perpendicular to the direction of the incident electrons and containing the axis of the

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central wire) by means of the Green function belonging to this plane. The boundary values of the wavefunction are obtained from an appropriate solution of the Schrödinger equation for an electron in the electrostatic field defined above by multiplication with the so called transmission function of the wire, which equals zero inside and one outside the wire, because the wire is considered as an impenetrable obstacle. The required solution of the Schrödinger equation is obtained using the quasiclassical approximation method (Olver 1974). In the case under consideration the diffraction integral can be simplified to an extent which allows the explanation of various significant properties of the interference pattern (Komska 1971). The geometrical shape of the central wire, i.e. its circular section, is not taken into account in this calculation, nor is the incident electron wave decomposed into partial waves in order to study the influence of the electrostatic field on geometrically reflected waves and creeping modes.

Here we start with the rigorous general solution of the Schrödinger equation for an electron in the logarithmic potential defined above, which may be expanded into partial waves in the usual manner; each partial wave can be represented by a uniformly convergent perturbation expansion (Gesztesy and Pittner 1978). If the electrostatic field inside the capacitor is sufficiently weak, dominant terms of this expansion can be summed up to Bessel-type functions. These approximations, which are similar to JWKB solutions (but with a significant modification), satisfy the Schrödinger equation asymptotically in the domain $a \leq r \leq b$, and their asymptotic behaviour for $r \rightarrow 0$ is just the expected one (Gesztesy and Pittner 1978, Olver 1974).

Inserting appropriate boundary conditions, which describe an impenetrable cylindrical wire of radius a , $V(a-0) = \infty$, and freely propagating electrons outside the hollow cylinder of radius b , one obtains the partial-wave expansion of the scattered wave, which differs significantly from the corresponding result for scattering off an impenetrable cylinder alone without an electrostatic field (Keller *et al* 1956, Franz 1957, Levy and Keller 1959).

As usual in high-frequency scattering, in analogy to the field-free case ($\epsilon = 0$), the Sommerfeld-Watson transformation may be applied, but the usual shifting of integration paths brings about two additional contributions to the scattered wave which arise from cuts in the complex angular momentum plane. These discontinuities can be estimated to be small compared with the main part of the scattered wave, which in turn may be obtained approximately from the corresponding expression in the field-free case by an analytic continuation in the scattering angle ϕ ,

$$\phi \rightarrow \phi + i \ln[E/(E - \epsilon \ln(a/b))], \quad (1.2)$$

where E denotes the energy of the incident electrons.

The decomposition of electron waves into eigenfunctions of angular momentum enables one to explain the influence of the logarithmic potential on each single partial wave, on geometrically reflected waves, on passing waves, and especially on the creeping modes.

The changes of various well known diffraction phenomena in the deep shadow region, the lit region, the Fraunhofer region, and especially the convergence of Fresnel zones to the optical axis with increasing electric field strength, are calculated explicitly and discussed in detail. As a result, the Fresnel zones reach this axis approximately at the point where the classical trajectory of an electron with angular momentum $l = a(2mE)^{1/2}$ crosses the axis (see figure 1).

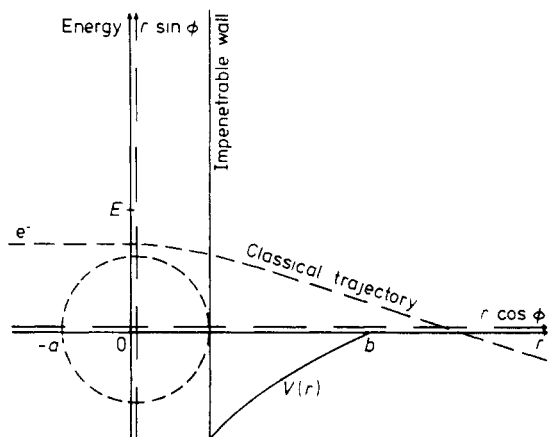


Figure 1. Solid lines, logarithmic potential $V(r)$, cut off at $r = b$, and impenetrable wall at $r = a$; broken lines, classical trajectory of an electron with energy E and angular momentum $l = a(2mE)^{1/2}$.

2. General solution

Under suitable boundary conditions, the Schrödinger equation with the logarithmic potential defined in the introduction,

$$(-\Delta/(2m) + V(r) - E)\Psi(r, \phi) = 0 \quad a \leq r \leq b \quad 0 \leq \phi \leq 2\pi, \tag{2.1}$$

can be solved uniquely (Gesztesy and Pittner 1978). By separation of variables,

$$\Psi(r, \phi) = r^{-1/2} g_l(r) \exp(\pm il\phi) \quad l = 0, 1, 2, \dots, \tag{2.2}$$

one obtains the radial equations

$$[-d^2/dr^2 + (l^2 - 1/4)r^{-2} + 2mV(r) - 2mE]g_l(r) = 0 \tag{2.3}$$

which may be transformed via

$$g_l(r) = e^{x/2} y_l(x) \quad x = \ln(r/b) - E/\epsilon \tag{2.4}$$

to the linear differential equations

$$(d^2/dx^2 - l^2 - \mu x e^{2x})y_l(x) = 0 \quad \mu = 2mb^2 \epsilon e^{2E/\epsilon}, \tag{2.5}$$

the general solutions of which are entire functions of x .

The infinite series

$$y_l^{(\pm)}(x) = e^{\pm lx} \sum_{n=0}^{\infty} \mu^n e^{2nx} p_{n,l}^{(\pm)}(x) \quad x \text{ complex} . \tag{2.6}$$

with the polynomials $p_{n,l}^{(\pm)}$ defined by the recursion scheme

$$[4n(n \pm l) + 2(2n \pm l) d/dx + d^2/dx^2]p_{n,l}^{(\pm)}(x) = xp_{n-1,l}^{(\pm)}(x), \tag{2.7}$$

$$n = 1, 2, 3, \dots \quad p_{0,l}^{(\pm)}(x) = 1 \quad l = 0, 1, 2, \dots$$

converge uniformly on each compact subset of the complex plane, and uniformly on the

negative real line; they solve the differential equations (2.5), and obviously have the limits (Gesztesy and Pittner 1978).

$$\lim_{x \rightarrow -\infty} y_l^{(\pm)}(x) e^{\mp lx} = 1 \quad l = 0, 1, 2, \dots \tag{2.8}$$

3. Approximation by Bessel functions

For our further calculations we shall try to single out the dominant terms from these expansions (for each $l = 0, 1, 2, \dots$), such that physically relevant boundary conditions can most easily be imposed on the resulting approximations to the exact solutions (2.6). For the moment, we restrict our investigation to the solutions $y_l^{(+)}$. The polynomials read explicitly

$$p_{n,l}^{(+)}(x) = \sum_{\nu=0}^n c_{n,l}^{(\nu)} x^\nu \quad c_{n,l}^{(n)} = \frac{l!}{4^n n!(n+l)!} \quad n, l = 0, 1, 2, \dots \tag{3.1}$$

The coefficient estimate (Gesztesy and Pittner 1978)

$$|c_{n,l}^{(n-k)}| \leq 2^{k-1} \frac{n!}{(n-k)!} c_{n,l}^{(n)} \quad k = 1, 2, \dots, n \tag{3.2}$$

enables one to majorise the expansions $\sum_{n=0}^\infty \mu^n e^{2nx} p_{n,l}^{(+)}(x)$ by the series

$$\sum_{n=0}^\infty \frac{(\mu|x|e^{2x})^n}{4^n (n!)^2} \sum_{k=0}^n \left(\frac{2}{|x|}\right)^k \frac{n!}{(n-k)!} \leq \sum_{n=0}^\infty \frac{(\frac{1}{2}\mu|x|e^{2x+2})^n}{n^{2n+1}} \frac{1 - (n/|x|)^{n+1}}{1 - (n/|x|)}, \tag{3.3}$$

the terms of which (rather their absolute values) decrease exponentially for $n > N \geq b(mE)^{1/2}$ in the interval $\ln(a/b) \leq x + E/\epsilon \leq 0$, if the condition $\epsilon b \ll (E/m)^{1/2}$ is assumed to be valid. Then $N \ll E/\epsilon \leq |x|$, which in turn implies dominance of the highest powers $c_{n,l}^{(n)} x^n$ of the polynomials $p_{n,l}^{(+)}(x)$. These dominant terms may be summed up easily to the asymptotic solutions

$$y_l^{(+)}(x) \approx |x|^{-l/2} J_l(\xi) \quad \xi = (\mu|x|)^{1/2} e^x \tag{3.4}$$

$x \rightarrow -\infty, \quad l = 0, 1, 2, \dots$

where J_l denote Bessel functions (Abramowitz and Stegun 1972); note here that the restriction $a \leq r \leq b$ implies the variable x to be located near $-\infty$ in the sense of the asymptotic approximation.

Conversely, for $\epsilon/E \ll 1$, by careful investigation one can show that the functions on the right-hand side of (3.4) solve the differential equations (2.5) asymptotically for $x \rightarrow -\infty$, and the asymptotic behaviour (for $x \rightarrow -\infty$) of the solutions (3.4) also agrees with the limit relation (2.8).

The experimental values of E and ϵ are of the order of 10^4 eV and a few eV respectively (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976); thus we may assume $\epsilon/E \ll 1$.

An analogous treatment of the solutions $y_l^{(-)}$ —via an analytic continuation of l to non-integer values to avoid the singularity at $n = l$ during the polynomial recursion, replacing the Bessel functions J_{-l} by Hankel functions $H_l^{(1)}$, and then returning to integer values of l —finally leads to the general asymptotic solutions

$$y_l(x) \approx c_l |x|^{-l/2} J_l(\xi) + d_l |x|^{l/2} H_l^{(1)}(\xi) \quad x \rightarrow -\infty, l = 0, 1, 2, \dots \tag{3.5}$$

with arbitrary complex constants c_l and d_l to be determined by suitable boundary conditions.

In terms of cylinder coordinates r and ϕ , the general asymptotic solution of the Schrödinger equation (2.1) reads

$$\Psi(r, \phi) = \sum_{l=0}^{\infty} \cos(l\phi) [c_l(k(r))^{-l} J_l(k(r)r) + d_l(k(r))^l H_l^{(1)}(k(r)r)]$$

$$k(r) = [2m(E - V(r))]^{1/2} \quad a \leq r \leq b, \quad 0 \leq \phi \leq 2\pi. \tag{3.6}$$

This asymptotic solution differs from the exact solution of the free Schrödinger equation in cylinder coordinates by the radial dependence of the momentum $k(r)$ and the factors $(k(r))^{\pm l}$ in front of the cylinder functions.

4. Boundary conditions

To impose appropriate boundary conditions on the general solution (3.6), we introduce the incident electron wave

$$\Phi(r, \phi) = \exp(i\rho \cos \phi) = J_0(\rho) + 2 \sum_{l=1}^{\infty} i^l J_l(\rho) \cos(l\phi) \tag{4.1}$$

$$\rho = r(2mE)^{1/2}$$

and the scattered electron wave

$$\chi(r, \phi) = \sum_{l=0}^{\infty} i^l S_l H_l^{(1)}(\rho) \cos(l\phi) \xrightarrow{r \rightarrow \infty} r^{-1/2} e^{i\rho} A(\phi) \tag{4.2}$$

with the scattering amplitude

$$A(\phi) = (2/\pi)^{1/2} (2mE)^{-1/4} e^{-i\pi/4} \sum_{l=0}^{\infty} S_l \cos(l\phi) \tag{4.3}$$

which determine the total cross section

$$\Sigma = \int_0^{2\pi} d\phi |A(\phi)|^2 = 2(2mE)^{-1/2} \left(2|S_0|^2 + \sum_{l=1}^{\infty} |S_l|^2 \right). \tag{4.4}$$

The boundary conditions for scattering off an impenetrable cylindrical wire of radius a under the influence of an electrostatic field inside the hollow cylinder of radius b then read

$$\Psi(a, \phi) = 0 \quad (\Psi - \Phi - \chi)(b, \phi) = 0 \quad \frac{\partial}{\partial r} (\Psi - \Phi - \chi)(r, \phi)|_{r=b} = 0. \tag{4.5}$$

By straightforward insertion of the general solution (3.6) these conditions yield rather complicated expressions for the scattering coefficients S_l , but for $\epsilon/E \ll 1$ these expressions can be approximated by the simple ratios

$$S_0 = -J_0(\alpha)/H_0^{(1)}(\alpha) \quad S_l = -2\nu^l J_l(\alpha)/H_l^{(1)}(\alpha) \quad l = 1, 2, 3, \dots$$

$$\alpha = a[2m(E - V(a))]^{1/2} \quad \nu = E/(E - V(a)). \tag{4.6}$$

Therefore the scattered electron wave

$$\chi(r, \phi) = -\frac{J_0(\alpha)}{H_0^{(1)}(\alpha)} H_0^{(1)}(\rho) - 2 \sum_{l=1}^{\infty} \nu^l i^l \frac{J_l(\alpha)}{H_l^{(1)}(\alpha)} H_l^{(1)}(\rho) \cos(l\phi) \tag{4.7}$$

differs from the corresponding expression in the absence of an electrostatic field ($\epsilon = 0$) by the argument $\alpha = ak(a)$ of the cylinder functions (where the radial-dependent momentum $k(r)$ is taken on the surface of the charged wire ($r = a$)) and by the factors ν^l . Although $1 - \nu \ll 1$ for $\epsilon/E \ll 1$, our following investigations will show that these factors ν^l play an important role in the explicit calculation of the scattered wave (4.7), because the summation over partial waves must be performed at least up to values of the angular momentum l which are somewhat larger than α .

5. Integral representation of the scattered wave

Here we perform the usual analytic continuation in the angular momentum l in order to obtain an integral representation of the wavefunction of the outgoing electrons. This method enables one to calculate explicitly the series (4.7) in the case of high-frequency scattering. It brings about two discontinuities due to the factors ν^l in the partial-wave expansion (4.7). We write this expansion as a contour integral in the complex angular momentum plane and then shift the path of integration appropriately.

For this purpose we start with the notations

$$\check{\Phi}(r, \phi) = J_0(\rho) + 2 \sum_{l=1}^{\infty} \nu^l i^l J_l(\rho) \cos(l\phi) \tag{5.1}$$

and

$$\check{\Psi}(r, \phi) = \check{\Phi}(r, \phi) + \chi(r, \phi) \quad r \geq b, \quad 0 \leq \phi \leq \pi \tag{5.2}$$

such that the wavefunction of the outgoing electrons reads

$$\Psi(r, \phi) = \Phi(r, \phi) + \chi(r, \phi) = \check{\Psi}(r, \phi) + \Phi(r, \phi) - \check{\Phi}(r, \phi). \tag{5.3}$$

At first we concentrate on the evaluation of $\check{\Psi}$; the difference $\Phi - \check{\Phi}$ will be considered later.

The well known Sommerfeld–Watson transformation, based on the residues

$$\begin{aligned} & (1/2\pi i) \oint_{(\text{around } l)} d\lambda / \sin(\pi\lambda) \\ &= \text{res} \left(\frac{1}{\sin(\pi\lambda)}; \lambda = l \right) = \lim_{\lambda \rightarrow l} \frac{\lambda - l}{\sin(\pi\lambda)} = \frac{(-1)^l}{\pi} \quad l \text{ integer,} \end{aligned} \tag{5.4}$$

then leads to the integral representation

$$\begin{aligned} \check{\Psi}(r, \phi) &= \frac{1}{2} h_0(\rho) + \sum_{l=1}^{\infty} \nu^l i^l h_l(\rho) \cos(l\phi) \\ &= \frac{1}{2} i \left(\oint_{\text{T}} + \frac{1}{2} \oint_{(\text{around } 0)} \right) d\lambda \frac{e^{-i\pi\lambda/2}}{\sin(\pi\lambda)} \cos(\lambda\phi) h_\lambda(\rho) \nu^\lambda \\ &= \lim_{\epsilon \rightarrow 0} \frac{1}{2} i \int_{\text{R}} d\lambda \frac{e^{-i\pi\lambda/2}}{\sin(\pi\lambda + i\epsilon)} \cos(\lambda\phi) h_\lambda(\rho) \nu^{|\lambda|} \end{aligned} \tag{5.5}$$

with the integrand

$$h_\lambda(\rho) = (H_\lambda^{(2)}(\rho)H_\lambda^{(1)}(\alpha) - H_\lambda^{(1)}(\rho)H_\lambda^{(2)}(\alpha))/H_\lambda^{(1)}(\alpha), \tag{5.6}$$

λ complex, where the real axis is denoted by R .

These manipulations can be performed because the Hankel functions $H_\lambda^{(1,2)}$ depend holomorphically on their order λ , and the zeros of $H_\lambda^{(1)}(\alpha)$ with respect to λ are non-real (see figure 2). The zeros of the Hankel functions $H_\lambda^{(1,2)}$, as functions of their order λ , and their asymptotic behaviour for $|\lambda| \rightarrow \infty$ have been investigated in detail (Keller *et al* 1963, Cochran 1965, Nussenzveig 1965). The path of integration can be shifted from T to R due to well known relations between Hankel functions (Abramowitz and Stegun 1972).

Using the above-mentioned asymptotic behaviour of Hankel functions, with the restriction $0 \leq \phi < \frac{1}{2}\pi$, we may close the path of integration R along the half-circle $\lambda = |\lambda|e^{i\gamma}$, $0 \leq \gamma \leq \pi$, with $|\lambda| \rightarrow \infty$, thus including all the zeros of $H_\lambda^{(1)}(\alpha)$ and the cut of $\nu^{|\lambda|}$ along the positive imaginary axis I_+ , and obtain the integral representation

$$\begin{aligned} \tilde{\Psi}(r, \phi) &= \Psi_1(r, \phi) + \Psi_{\text{cut}}(r, \phi) \\ \Psi_1(r, \phi) &= \frac{1}{2i} \oint_H d\lambda \frac{e^{-i\pi\lambda/2}}{\sin(\pi\lambda)} \cos(\lambda\phi) h_\lambda(\rho) \nu^\lambda \\ \Psi_{\text{cut}}(r, \phi) &= \frac{1}{2i} \int_{I_+} d\lambda \frac{e^{-i\pi\lambda/2}}{\sin(\pi\lambda)} \cos(\lambda\phi) h_\lambda(\rho) (\nu^\lambda - \nu^{-\lambda}) \end{aligned} \tag{5.7}$$

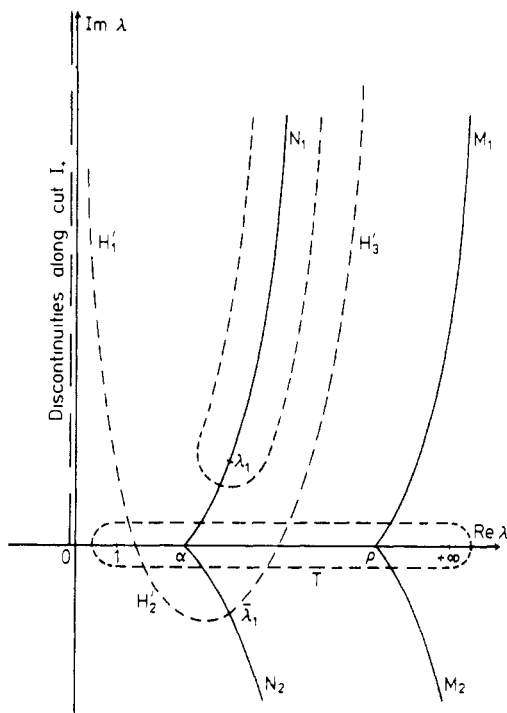


Figure 2. Paths of integration in the complex angular momentum plane; the zeros of $H_\lambda^{(i)}(\alpha)$ and $H_\lambda^{(i)}(\rho)$ lie on the curves N_i and M_i , respectively, $i = 1, 2$; the first zero of $H_\lambda^{(1)}(\alpha)$ is denoted by λ_1 .

where the closed path H includes the zeros of $H_\lambda^{(1)}(\alpha)$ in the upper half-plane (see figure 2).

Before calculating explicitly the loop integral Ψ_1 , we now derive an approximation to the cut contribution Ψ_{cut} , which may be written as

$$\Psi_{\text{cut}}(r, \phi) = - \int_0^{+\infty} d\tau \frac{e^{\pi\tau/2}}{e^{\pi\tau} - e^{-\pi\tau}} (e^{\phi\tau} + e^{-\phi\tau}) h_{i\tau}(\rho) \sin(\tau \ln \nu). \tag{5.8}$$

Since only the section $0 \leq \tau \ll \alpha$ essentially contributes to this integral, the asymptotic representation of Hankel functions of large arguments may be used,

$$h_{i\tau}(\rho) \approx d(\rho) e^{-\pi\tau/2} \quad d(\rho) = \left(\frac{2}{\pi\rho}\right)^{1/2} e^{i\pi/4} (e^{-i\rho} - e^{i(\rho-2\alpha)}), \tag{5.9}$$

yielding

$$\begin{aligned} \Psi_{\text{cut}}(r, \phi) &\approx \frac{d(\rho)}{4\pi i} \int_0^{+\infty} \frac{d\tau}{1 - e^{-\tau}} (\exp[-\frac{1}{2}\tau(1 - \phi\pi^{-1} - i\delta\pi^{-1})] \\ &\quad - \exp[-\frac{1}{2}\tau(1 - \phi\pi^{-1} + i\delta\pi^{-1})] \\ &\quad + \exp[-\frac{1}{2}\tau(1 + \phi\pi^{-1} - i\delta\pi^{-1})] - \exp[-\frac{1}{2}\tau(1 + \phi\pi^{-1} + i\delta\pi^{-1})]) \\ &= \frac{d(\rho)}{4i} (\tan \frac{1}{2}(\phi + i\delta) - \tan \frac{1}{2}\phi - i\delta) \approx \frac{1}{4}\delta d(\rho) (\cos \frac{1}{2}\phi)^{-2} \end{aligned} \tag{5.10}$$

with the abbreviation $\delta = |\ln \nu|$.

The second discontinuity arises from the function $\tilde{\Phi}$ defined by (5.1). We decompose

$$\tilde{\Phi}(r, \phi) = \exp[i\rho \cos(\phi - i\delta)] + \Phi_{\text{cut}}(r, \phi) \tag{5.11}$$

$$\Phi_{\text{cut}}(r, \phi) = \sum_{l=1}^{\infty} J_l(\rho) e^{il(\pi/2+\phi)} (\nu^l - \nu^{-l}) = \frac{1}{2i} \oint_{\Gamma} d\lambda \frac{e^{-i\pi\lambda/2}}{\sin(\pi\lambda)} e^{i\lambda\phi} J_\lambda(\rho) (\nu^\lambda - \nu^{-\lambda})$$

by means of the Sommerfeld–Watson transformation. Due to the asymptotic behaviour of the integrand as $|\lambda| \rightarrow \infty$ for $0 < \phi < \pi$, the path of integration can be shifted to the imaginary axis,

$$\Phi_{\text{cut}}(r, \phi) = 2 \int_{-\infty}^{+\infty} d\tau \frac{e^{\tau(\pi/2-\phi)}}{e^{\pi\tau} - e^{-\pi\tau}} J_{i\tau}(\rho) \sin(\tau\delta). \tag{5.12}$$

By means of the asymptotic representation of Bessel functions of large arguments, in a similar manner to that above, one obtains the approximation

$$\Phi_{\text{cut}}(r, \phi) \approx \frac{\frac{1}{2}\delta}{(2\pi\rho)^{1/2}} \left(\frac{e^{i(\rho-\pi/4)}}{(\sin \frac{1}{2}\phi)^2} + \frac{e^{-i(\rho-\pi/4)}}{(\cos \frac{1}{2}\phi)^2} \right), \tag{5.13}$$

which is valid only for values of ϕ lying neither near 0 nor π .

6. Residue series

Here we are going to evaluate explicitly the loop integral Ψ_1 by means of the residue theorem. The zeros of Hankel functions with respect to their order are of first order.

Therefore we may expand

$$\Psi_1(r, \phi) = \pi \sum_{n=1}^{\infty} \frac{e^{-i\pi\lambda_n/2}}{\sin(\pi\lambda_n)} \cos(\lambda_n\phi) \nu^{\lambda_n} H_{\lambda_n}^{(1)}(\rho) R_n$$

$$R_n = H_{\lambda_n}^{(2)}(\alpha) (\partial H_{\lambda}^{(1)}(\alpha) / \partial \lambda |_{\lambda=\lambda_n})^{-1} \tag{6.1}$$

with the sequence $\{\lambda_n; n = 1, 2, 3, \dots\}$ of zeros of $H_{\lambda}^{(1)}(\alpha)$ in the upper half-plane (see figure 2) (Keller *et al* 1963, Cochran 1965). Insertion of the asymptotic behaviour of the Hankel functions $H_{\lambda}^{(1,2)}$ as $|\lambda| \rightarrow \infty$ enables one to prove the convergence of this residue series for $0 \leq \phi < \frac{1}{2}\pi$.

This expansion is of practical use only if the first few terms dominate. Using the asymptotic representation of $H_{\lambda}^{(1,2)}(\alpha)$ by Airy functions, and the Debye asymptotic expansion of $H_{\lambda_n}^{(1)}(\rho)$, in a manner similar to the field-free case ($\epsilon = 0$; compare with the case of an impenetrable sphere (Nussenzveig 1965)), we get $\Psi_1 = \Psi_1^{(+)} + \Psi_1^{(-)}$:

$$\Psi_1^{(\pm)}(r, \phi) \approx (2\pi)^{-1/2} e^{i\pi/4} \alpha^{1/3} e^{-i\pi/6(\rho^2 - \alpha^2)^{-1/4}}$$

$$\times \exp[i(\rho^2 - \alpha^2)^{1/2}] \sum_{\substack{n=1,2,3,\dots \\ \{n \text{ small}\}}} (\text{Ai}'(-c_n))^{-2} \exp[(i\alpha + \frac{1}{2}ic_n)(\frac{1}{2}\alpha)^{1/3}$$

$$- c_n \frac{1}{2}\sqrt{3}(\frac{1}{2}\alpha)^{1/3})(\pm\phi + \sigma + i\delta)] + \text{higher residue terms} \tag{6.2}$$

with the geometrical shadow boundary $\sigma = \sin^{-1}(\alpha/\rho) \approx \alpha/\rho, \rho - \alpha \gg \alpha^{1/3} \gg 1$, and the negative zeros c_n of Airy functions, $\text{Ai}(-c_n) = 0, n = 1, 2, 3, \dots$; obviously $\Psi_1^{(-)}$ dominates over $\Psi_1^{(+)}$ for $\phi \gg \alpha^{-1/3}$.

Thus we recognise that the residue series (6.2) is rapidly decreasing if $\sigma - \phi + \delta/\sqrt{3} \gg \alpha^{-1/3}$. In this region of the scattering angle ϕ , which in the field-free case ($\epsilon = 0, \delta = 0$) is called the deep shadow region, only the first few surface waves (creeping modes; Franz 1957) associated with the first few zeros $\lambda_n, n = 1, 2, 3, \dots$, contribute significantly. With increasing electric field strength, i.e. increasing δ , these creeping modes suffer some loss of intensity described by the factor ν^α due to the expansion (6.2), but on the other hand the difference $\Phi - \check{\Phi}$ in the decomposition (5.3) of Ψ then tends towards Φ and therefore Ψ tends towards $\Psi_1^{(-)} + \Phi$. The physical meaning of this formal result lies in the fact that with increasing electric field strength incident electrons with angular momentum $l > \alpha$ are deflected into the region $\sigma - \phi + \delta/\sqrt{3} \gg \alpha^{-1/3}$, thus confining the deep shadow region.

7. Lit region

Here we try to evaluate explicitly the integral representation (5.7) of the wavefunction Ψ_1 in the region $\sigma - \phi + \delta/\sqrt{3} \leq \alpha^{-1/3}$ by the method of steepest descent.

For this purpose we decompose (Franz 1957)

$$\cos(\lambda\phi) = e^{i\pi\lambda} \cos(\lambda\psi) - i e^{i\lambda\psi} \sin(\pi\lambda) \quad \psi = \pi - \phi. \tag{7.1}$$

Then for $\phi + \sigma + \delta/\sqrt{3} \gg \alpha^{-1/3}$, the first term is of negligible order, as may be seen from its contribution to the residue series; thus we are left with

$$\Psi_1(r, \phi) = \oint_{\text{H}} \frac{1}{2} d\lambda e^{i\lambda(\pi/2 - \phi)} h_{\lambda}(\rho) \nu^{\lambda}. \tag{7.2}$$

Now the path H may be shifted to another path H' consisting of three parts H'_i , $i = 1, 2, 3$ (see figure 2). Since $H_\lambda^{(2)}(\rho) \rightarrow 0$ exponentially as $|\lambda| \rightarrow \infty$ along H'_1 or H'_3 , we get

$$\oint_{H'} d\lambda e^{i\lambda(\pi/2-\phi)} H_\lambda^{(2)}(\rho) \nu^\lambda = 0 \tag{7.3}$$

because the path H' does not include any singularity of the integrand. Therefore

$$\Psi_1(r, \phi) = -\oint_{H'} \frac{1}{2} d\lambda e^{i\lambda(\pi/2-\phi)} H_\lambda^{(1)}(\rho) g(\lambda) \nu^\lambda \tag{7.4}$$

$$g(\lambda) = H_\lambda^{(2)}(\alpha) / H_\lambda^{(1)}(\alpha) \rightarrow -1 \quad \text{as } |\lambda| \rightarrow \infty \text{ along } H'_3.$$

We denote

$$\Psi_{1,i}(r, \phi) = -\int_{H'_i} \frac{1}{2} d\lambda e^{i\lambda(\pi/2-\phi)} H_\lambda^{(1)}(\rho) g(\lambda) \nu^\lambda \quad i = 1, 2, 3. \tag{7.5}$$

Along H'_3 we may use the Debye asymptotic expansion of $H_\lambda^{(1)}(\rho)$, which leads to

$$\begin{aligned} \Psi_{1,3}(r, \phi) &= \int_{H'_3} d\lambda A_3(\lambda) e^{iE_3(\lambda)} & A_3(\lambda) &= (2\pi)^{-1/2} (\rho^2 - \lambda^2)^{-1/4} \\ E_3(\lambda) &= \lambda(\pi/2 - \phi + i\delta) + (\rho^2 - \lambda^2)^{1/2} - \lambda \cos^{-1}(\lambda/\rho) - \frac{1}{4}\pi, \end{aligned} \tag{7.6}$$

and by the method of steepest descent we obtain

$$\Psi_{1,3}(r, \phi) \approx \exp[i\rho \cos(\phi - i\delta)]. \tag{7.7}$$

Along H'_1 all three Hankel functions may be approximated asymptotically by their Debye expansions, leading to

$$\begin{aligned} \Psi_{1,1}(r, \phi) &= \int_{H'_1} d\lambda A_1(\lambda) e^{iE_1(\lambda)} & A_1(\lambda) &= -A_3(\lambda) \\ E_1(\lambda) &= \lambda(\pi/2 - \phi + i\delta) + (\rho^2 - \lambda^2)^{1/2} - 2(\alpha^2 - \lambda^2)^{1/2} \\ &\quad - \lambda \cos^{-1}(\lambda/\rho) + 2\lambda \cos^{-1}(\lambda/\alpha) + \frac{1}{4}\pi, \end{aligned} \tag{7.8}$$

and again by the method of steepest descent, for $\alpha \ll \rho$, we get the result

$$\Psi_{1,1}(r, \phi) \approx -\left(\frac{2\rho}{\alpha \sin \frac{1}{2}(\phi - i\delta)} - 1\right)^{-1/2} \exp[i(\rho - 2\alpha \sin \frac{1}{2}\phi) - \alpha\delta \cos \frac{1}{2}\phi]. \tag{7.9}$$

The contribution from H'_2 is small because this path passes through the zero $\bar{\lambda}_1$ of $H_\lambda^{(2)}(\alpha)$ (see figure 2). Thus the wavefunction of outgoing electrons, neglecting the discontinuities (5.10) and (5.13),

$$\Psi(r, \phi) \approx \Phi(r, \phi) + \Psi_{1,1}(r, \phi) \tag{7.10}$$

represents freely passing electrons and geometrically reflected electrons respectively.

The contribution from the first term in the decomposition (7.1) to the residue series for Ψ_1 represents the continuation to the lit region of the surface waves which we have described in the preceding section.

8. Fresnel pattern

We are interested mainly in the Fresnel pattern which arises in the region $\alpha \ll \rho \ll \alpha^{4/3}$ near the shadow boundary, i.e. $|\phi - \sigma| \leq \alpha^{-1/2}$. Here $\phi + \sigma + \delta/\sqrt{3} \gg \alpha^{-1/3}$, such that we may start with expression (7.4). But the corresponding two saddle points on the paths H_1' and H_3' both tend towards α as $\phi \rightarrow \sigma$ and $\delta \rightarrow 0$, such that the Debye asymptotic expansions of $H_\lambda^{(1,2)}(\alpha)$ fail to yield any reasonable result. In this case we decompose

$$\begin{aligned} \Psi_1 &= \Psi_1^{(1)} + \Psi_1^{(2)} + \Psi_1^{(3)} \\ \Psi_1^{(1)}(r, \phi) &= - \int_{H_1'} \frac{1}{2} d\lambda e^{i\lambda(\pi/2-\phi)} \nu^\lambda H_\lambda^{(1)}(\rho) g(\lambda) \\ \Psi_1^{(2)}(r, \phi) &= - \int_{H_3'} d\lambda e^{i\lambda(\pi/2-\phi)} \nu^\lambda H_\lambda^{(1)}(\rho) J_\lambda(\alpha) / H_\lambda^{(1)}(\alpha) \\ \Psi_1^{(3)}(r, \phi) &= \int_{H_3'} \frac{1}{2} d\lambda e^{i\lambda(\pi/2-\phi)} \nu^\lambda H_\lambda^{(1)}(\rho) = \int_{H_3'} d\lambda A_3(\lambda) e^{iE_3(\lambda)}. \end{aligned} \tag{8.1}$$

Since the main contribution to $\Psi_1^{(3)}$ stems from the neighbourhood of α ,

$$\Psi_1^{(3)}(r, \phi) \approx A_3(t) e^{iE_3(t)} \int_{D_3} d\lambda \exp[\frac{1}{2}iE_3'(t)(\lambda - t)^2]$$

along

$$\begin{aligned} D_3 &= \{\lambda = t + \tau\pi^{1/2}(\rho^2 - t^2)^{1/4}; \tau \geq \tau_0\} \\ \tau_0 &= \rho(\sigma - \phi + i\delta)\pi^{-1/2}(\rho^2 - t^2)^{-1/4} \quad t = \rho \sin(\phi - i\delta), \end{aligned} \tag{8.2}$$

where again the method of steepest descent from the saddle point t has been used. Hence we obtain

$$\Psi_1^{(3)}(r, \phi) \approx 2^{-1/2} e^{-i\pi/4} \exp[i\rho \cos(\phi - i\delta)](F(+\infty) - F(\tau_0)) \tag{8.3}$$

with the Fresnel integral (Abramowitz and Stegun 1972)

$$F(z) = \int_0^z d\zeta \exp(\frac{1}{2}i\pi\zeta^2) \quad z \text{ complex, } F(+\infty) = 2^{-1/2} e^{i\pi/4}. \tag{8.4}$$

For $|\phi - \sigma| \geq \alpha^{-1/2}$, we have $|\tau_0| \gg 1$, such that we may employ the approximation

$$F(+\infty) - F(\tau_0) \approx \frac{i}{\pi\tau_0} \exp(\frac{1}{2}i\pi\tau_0^2), \tag{8.5}$$

which leads to the result

$$\Psi_1^{(3)}(r, \phi) \approx (2\pi\rho)^{-1/2} (\sigma - \phi + i\delta)^{-1} \exp[i\pi/4 + i\rho \cos \phi - \alpha\delta + \frac{1}{2}i\rho((\phi - \sigma)^2 - \delta^2)], \tag{8.6}$$

exhibiting some loss of intensity due to the factor ν^α , and some shift of the Fresnel pattern towards the axis to be discussed below.

For $|\tau_0| \ll 1$, on the geometrical shadow boundary, $F(\tau_0) \approx \tau_0$ and therefore

$$\Psi_1^{(3)}(r, \phi) \approx 2^{-1/2} e^{-i\pi/4} \exp[i\rho \cos(\phi - i\delta)][2^{-1/2} e^{i\pi/4} - (\rho/\pi)^{1/2}(\sigma - \phi + i\delta)]; \tag{8.7}$$

for $\phi = \sigma$ and $\delta = 0$, $\Psi_1^{(3)}$ represents just one half of the incident electron wave.

The contributions from $\Psi_1^{(1)}$ and $\Psi_1^{(2)}$ are only corrections of order $O[\alpha^{1/3}(\phi - \sigma)]$ (Rubinow and Wu 1956). Since the discontinuities (5.10) and (5.13) are negligible in the region defined above, especially $|\Phi_{\text{cut}}(r, \phi)| \ll \delta$ for $\rho \ll \alpha^{4/3}$ and $\phi \approx \sigma$, the wavefunction of outgoing electrons in the Fresnel region consists mainly of three terms,

$$\Psi(r, \phi) \approx \exp(i\rho \cos \phi) - \exp[i\rho \cos(\phi - i\delta)] + \Psi_1^{(3)}(r, \phi). \tag{8.8}$$

Expression (8.3) provides the well known diffraction maxima, i.e. maxima of $|\Psi(r, \phi)|$; the distance on the screen between two consecutive maxima is approximately equal to $\{\rho[2m(E - V(a))]\}^{1/2}$.

With increasing electric field strength the Fresnel zones converge to the optical axis which is reached as soon as $\alpha/\rho = \delta$ or, equivalently,

$$a/r = (\epsilon/E) \ln(b/a). \tag{8.9}$$

More precisely, the ‘centre’ of the Fresnel pattern, in the field-free case defined by the geometrical shadow boundary, $\phi_{\text{centre}} = a/r$ for $\epsilon = 0$, tends towards the axis according to the law

$$\phi_{\text{centre}} \approx \sigma - \delta^2/\sigma \quad \sigma \approx a/r \quad \delta \approx (\epsilon/E) \ln(b/a), \tag{8.10}$$

as can be deduced easily from the result (8.3) and its approximation (8.6). Condition (8.9) relates values of ϵ/E and a/r such that the classical trajectory of an incident electron with kinetic energy E and angular momentum $l = a(2mE)^{1/2}$ approximately crosses the axis.

For sufficiently strong electric fields the second term of approximation (8.8) vanishes such that the first term dominates, representing the deflection of incident electrons with angular momentum $l > \alpha$ towards the axis.

9. Fraunhofer region

In the region $\alpha^{4/3} \leq \rho \ll \alpha^2$, $\phi \leq \sigma$, where the condition $\phi + \sigma + \delta/\sqrt{3} \gg \alpha^{-1/3}$ is violated, we start with the integral representation (5.7) and insert the Poisson summation formula

$$e^{-i\pi\lambda/2}(\sin(\pi\lambda))^{-1} = -2i e^{i\pi\lambda/2} \sum_{n=0}^{\infty} e^{2\pi i\lambda n}, \tag{9.1}$$

which converges uniformly in the upper half-plane. By means of the residue series along the zeros of $H_\lambda^{(1)}(\alpha)$ we find that only the first term ($n = 0$) of the series (9.1) essentially contributes to Ψ_1 , such that

$$\Psi_1 = \Psi_1^{(+)} + \Psi_1^{(-)} \quad \Psi_1^{(\pm)}(r, \phi) = -\oint_{\mathcal{H}'} \frac{1}{2} d\lambda e^{i\lambda(\pi/2 \pm \phi)} H_\lambda^{(1)}(\rho) g(\lambda) \nu^\lambda. \tag{9.2}$$

Insertion of the Debye asymptotic expansion of $H_\lambda^{(1)}(\rho)$ and partial integration then yields

$$\Psi_1^{(+)}(r, \phi) \approx (2\pi\rho)^{-1/2} (\sigma + \phi + i\delta)^{-1} \exp[i(\pi/4 + \rho + \alpha\phi) - \alpha\delta]. \tag{9.3}$$

In the lit region $\phi \gg \alpha^{-1/3}$, the term $\Psi_1^{(+)}$ is dominated by

$$\Psi_1^{(-)}(r, \phi) \approx \exp[i\rho \cos(\phi - i\delta)] + \Psi_{1,1}(r, \phi), \tag{9.4}$$

as evaluated in § 7, such that the differential cross section becomes

$$|A(\phi)|^2 \approx \frac{1}{2}\alpha |\sin \frac{1}{2}(\phi - i\delta)| \exp(-2\alpha\delta \cos \frac{1}{2}\phi). \quad (9.5)$$

Near the geometrical shadow boundary, for $|\phi - \sigma| \geq \alpha^{-1/2}$, we have

$$\Psi_1(r, \phi) \approx (2\pi\rho)^{-1/2} \exp[i(\pi/4 + \rho) - \alpha\delta] \\ \times [(\sigma - \phi + i\delta)^{-1} \exp\{\frac{1}{2}i\rho[(\sigma - \phi)^2 - \delta^2]\} + (\sigma + \phi + i\delta)^{-1} \exp(i\alpha\phi)],$$

similar to our result (8.6) in the Fresnel region.

In the Fraunhofer region $\rho \gg \alpha^2$, for $|\phi - \sigma| \geq \alpha^{-1/2}$, we finally obtain

$$\Psi_1(r, \phi) \approx (\frac{1}{2}\pi\rho)^{-1/2} \exp[i(3\pi/4 + \rho) - \alpha\delta] \sin(\alpha\phi)/\phi, \quad (9.7)$$

exhibiting the familiar diffraction peak in the forward direction.

10. Conclusion

Apart from suitable asymptotic approximation methods, our calculations are based on two simplifications of the actual situation in the electron interference experiments quoted in the introduction. Firstly, the electrostatic biprisma was represented by a capacitor consisting of a central wire and a hollow cylinder. Secondly, we represent the incident electrons by a plane wave, whereas in the experiments (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976) the electrons are emitted from a linear source. If, however, this last simplification were not made, one would have to resort to purely numerical methods.

In this context we should note that reducing the distance between the linear source and the biprisma, with fixed distance between biprisma and screen, enlarges the distances between the Fresnel zones, thus facilitating their experimental observation.

Nevertheless the problem of diffraction of an electron wave by a cylindrical capacitor has in principle been solved here; in particular, the convergence of Fresnel fringes to the optical axis is described by the simple laws (8.9) and (8.10), which follow from our rigorous solution of the Schrödinger equation (Gesztesy and Pittner 1978).

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