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Diffraction of relativistic electron waves by a cylindrical capacitor

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Abstract. The diffraction of relativistic electron waves by a cylindrical capacitor is investigated, starting from the exact general solution of the Dirac equation for an electron in a logarithmic potential in two dimensions. Suitable asymptotic approximations to these solutions are derived, which allow the convenient insertion of appropriate boundary conditions. The partial wave expansion of the scattered electron wave is evaluated by means of the Sommerfeld–Watson transformation. The influence of the electrostatic field inside the capacitor on various diffraction phenomena is calculated analytically, in particular the convergence of Fresnel fringes towards the optical axis with increasing voltage at the capacitor. The effect of electron spin–orbit coupling is described explicitly.

1. Introduction

The diffraction of electron waves by a cylindrical capacitor permits the observation of electron interference fringes without the use of any intermediate crystal (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976). The capacitor consists of a hollow cylinder with radius b and a central wire with radius a, such that the electrostatic potential inside the capacitor depends logarithmically on the radius r:

$$V(r)=\epsilon \ln(r/b), \qquad a\leqslant r\leqslant b, \quad \epsilon>0. \tag{1.1}$$

Since this electrostatic field deflects the incident electrons towards the central wire, the capacitor serves as an analogue to the Fresnel biprism in classical optics. Due to the attraction of electrons towards the wire, the Fresnel fringes converge towards the optical axis, so that a large number of these fringes can be observed for sufficiently high voltages at the capacitor.

In the experiments (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976), the incident electrons are accelerated to kinetic energies of about 10^4 eV, so that relativistic kinematics should be used. The voltages at the capacitor amount to a few eV; thus $\epsilon \ll E-m$, where E denotes the relativistic energy of incident electrons.

Within the framework of non-relativistic electron diffraction theory, interference phenomena are calculated through the evaluation of the diffraction integral (Glaser 1952, Komrska 1971), which is constructed from the boundary values of the electron wavefunction on the diffraction plane and the Green function of the Schrödinger equation. This method does not take into account the circular section of the wire, and the influence of the electrostatic field on each single partial wave, in particular the

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creeping modes, cannot be investigated. Nevertheless, it would be interesting to establish the diffraction integral in relativistic electron optics and to evaluate this integral in experimental situations.

In a similar manner to our treatment of the Schrödinger equation for electrons in the logarithmic potential defined above (Gesztesy and Pittner 1978a), the exact general solution of the Dirac equation for electrons in this potential may be expanded into partial waves, each of which can be represented by a uniformly convergent perturbation expansion (Gesztesy and Pittner 1978b). For sufficiently weak electric voltages at the capacitor, dominant terms of this series may be summed up to a JWKB-type solution, which satisfies the corresponding radial Dirac equation approximately inside the capacitor ($a \leqslant r \leqslant b$), and in particular exhibits the expected asymptotic behaviour near the origin ($r \to 0$) (Gesztesy and Pittner 1978b, Coppel 1965).

Inserting boundary conditions which describe the impenetrable wire and the electric field cut-off at the hollow cylinder, one obtains the partial wave expansion of the diffracted relativistic electron wave propagating towards the screen.

In a similar manner to our calculation of high-frequency scattering of spinless non-relativistic electrons (Gesztesy and Pittner 1979), the scattered electron wave can be evaluated explicitly by means of the Sommerfeld–Watson transformation. Roughly stated, our results may be obtained from the corresponding expressions for diffraction by an impenetrable cylinder of radius a by means of an analytic continuation in the scattering angle ϕ,

$$\phi \to \phi + \mathrm{i} \ln [\![(E^2 - m^2)/\{[E - \epsilon \ln(a/b)]^2 - m^2\}]\!]. \tag{1.2}$$

The changes in the diffraction phenomena with an increasing electric voltage at the capacitor, and in particular the convergence of the Fresnel fringes towards the optical axis, will be calculated explicitly. The effects of relativistic kinematics and electron spin are discussed in comparison with our non-relativistic treatment for spinless particles (Gesztesy and Pittner 1979).

2. Exact solution

The formal matrix differential operator

$$T = \boldsymbol{\alpha} \cdot \nabla/\mathrm{i} + \beta m + V(r), \tag{2.1}$$

with the usual Dirac matrices $\boldsymbol{\alpha}$, β (for our notation see Bjorken and Drell 1964) and the logarithmic potential V defined in the Introduction, may be written in terms of cylindrical coordinates r, ϕ, x^3 as

$$T = \alpha^+ D_- + \alpha^- D_+ + \alpha^3(\partial/\mathrm{i}\,\partial x^3) + \beta m + V(r), \tag{2.2}$$

$$\sqrt{2}\alpha^\pm = \alpha^1 \pm \mathrm{i}\,\alpha^2, \qquad \sqrt{2}D_\pm = \partial/\mathrm{i}\,\partial x^1 \pm \partial/\partial x^2 = \mathrm{e}^{\pm \mathrm{i}\phi}(\partial/\mathrm{i}\,\partial r \pm \partial/r\partial\phi).$$

On the Dirac spinors

$$\Psi_l^{(+)}(r,\phi) = r^{-1/2}\begin{pmatrix} \mathrm{e}^{\mathrm{i}l\phi} g_{0,l}^{(+)}(r) \\ 0 \\ 0 \\ \mathrm{i}\mathrm{e}^{\mathrm{i}(l+1)\phi} g_{1,l}^{(+)}(r) \end{pmatrix}, \qquad \Psi_l^{(-)}(r,\phi) = r^{-1/2}\begin{pmatrix} 0 \\ \mathrm{i}\mathrm{e}^{\mathrm{i}(l+1)\phi} g_{1,l}^{(-)}(r) \\ \mathrm{e}^{\mathrm{i}l\phi} g_{0,l}^{(-)}(r) \\ 0 \end{pmatrix},$$

$$l = 0, \pm 1, \pm 2, \ldots \tag{2.3}$$

the formal matrix differential operators representing the projections of total angular momentum and spin perpendicular to the scattering plane ($x^3=0$) act in the following way:

$$\begin{aligned} &J^3\Psi_l^{(\pm)}(r,\phi)=j^3\Psi_l^{(\pm)}(r,\phi),\\ &\beta\sigma^3J^3\Psi_l^{(\pm)}(r,\phi)=\pm j^3\Psi_l^{(\pm)}(r,\phi),\\ &J^3=\partial/\mathrm{i}\,\partial\phi+\tfrac12\sigma^3, \qquad j^3=l+\tfrac12=\pm\tfrac12,\ \pm\tfrac32,\ \pm\tfrac52,\ldots. \end{aligned} \tag{2.4}$$

The formal energy eigenvalue equation

$$T\Psi_l^{(\pm)}(r,\phi)=E\Psi_l^{(\pm)}(r,\phi) \tag{2.5}$$

then decomposes into the radial equations

$$\begin{aligned} &\mathrm{d}\,G_l^{(\pm)}(r)/\mathrm{d}r=W_l^{(\pm)}(r)G_l^{(\pm)}(r),\\ &G_l^{(+)}(r)=\begin{pmatrix} g_{0,l}^{(+)}(r)\\ g_{1,l}^{(+)}(r)\end{pmatrix}, \qquad G_l^{(-)}(r)=\begin{pmatrix} g_{1,l}^{(-)}(r)\\ g_{0,l}^{(-)}(r)\end{pmatrix},\\ &W_l^{(\pm)}(r)=\pm\begin{pmatrix} j^3/r & V(r)-E-m\\ E-m-V(r) & -j^3/r\end{pmatrix}. \end{aligned} \tag{2.6}$$

These radial equations may be transformed to the regular differential equations

$$\begin{aligned} &\mathrm{d}Y_l^{(\pm)}(x)/\mathrm{d}x=(C_l^{(\pm)}+B^{(\pm)}(x))Y_l^{(\pm)}(x),\\ &C_l^{(\pm)}=\pm j^3\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \qquad B^{(\pm)}(x)=\pm\begin{pmatrix}0 & (\beta x-\lambda)\,\mathrm{e}^x\\ (\mu-\beta x)\,\mathrm{e}^x & 0\end{pmatrix},\\ &G_l^{(\pm)}(r)=Y_l^{(\pm)}(x)=\begin{pmatrix} y_l^{(\pm)}(x)\\ z_l^{(\pm)}(x)\end{pmatrix}, \end{aligned} \tag{2.7}$$

in which $x=\ln(r/b)$, $\beta=b\epsilon$, $\lambda=b(E+m)$, $\mu=b(E-m)$, and the solutions of which are all entire functions of x. The general solutions of these two systems of linear differential equations can be expanded in terms of exponential polynomials,

$$y_l^{(\pm)}(x)=\mathrm{e}^{\pm j^3x}\sum_{n=0}^{\infty}\mathrm{e}^{2nx}p_{n,l}^{(\pm)}(x), \qquad z_l^{(\pm)}(x)=\mathrm{e}^{\mp j^3x}\sum_{n=0}^{\infty}\mathrm{e}^{2nx}q_{n,l}^{(\pm)}(x), \tag{2.8}$$

with polynomials $p_{n,l}^{(\pm)}$ and $q_{n,l}^{(\pm)}$ determined by rather complicated recursion formulae (Gesztesy and Pittner 1978b); with respect to x, these series converge uniformly on each compact subset of the complex plane and uniformly on the negative real line, which is of interest because $x\to-\infty$ means $r\to0$.

3. Approximation by Bessel functions

Aiming at the insertion of suitable boundary conditions, we now try to single out and sum the dominant terms of the expansions (2.8). In analogy to our non-relativistic treatment (Gesztesy and Pittner 1979), for $\epsilon b\ll p/E$ with $p=(E^2-m^2)^{1/2}$, estimates for the coefficients of the polynomials $p_{n,l}^{(\pm)}$ and $q_{n,l}^{(\pm)}$ (inequalities (4.14) and (4.15) in Gesztesy and Pittner (1978b)) allow us to take as an asymptotic approximation, in the interval $\ln(a/b) \leqslant x \leqslant 0$, the highest powers in $[(\lambda-\beta x)(\mu-\beta x)]^{1/2}$ of these polynomials. Then one obtains the following JWKB-type solutions:

for $l = 0, 1, 2, \ldots,$

$$\begin{aligned}
y_l^{(+)}(x) &= e^{x/2}(c_l^{(+)}s^{-l}J_l(t) + d_l^{(+)}s^l H_l^{(1)}(t)),\\
z_l^{(+)}(x) &= e^{x/2}(c_l^{(+)}s^{-l}J_{l+1}(t) + d_l^{(+)}s^l H_{l+1}^{(1)}(t))[(\mu-\beta x)/(\lambda-\beta x)]^{1/2},\\
y_l^{(-)}(x) &= e^{x/2}(c_l^{(-)}s^{-l}J_{l+1}(t) + d_l^{(-)}s^l H_{l+1}^{(1)}(t))[(\lambda-\beta x)/(\mu-\beta x)]^{1/2},\\
z_l^{(-)}(x) &= e^{x/2}(c_l^{(-)}s^{-l}J_l(t) + d_l^{(-)}s^l H_l^{(1)}(t));
\end{aligned} \tag{3.1}$$

for $l = -1, -2, -3, \ldots,$

$$\begin{aligned}
y_l^{(+)}(x) &= e^{x/2}(c_l^{(+)}s^{l}J_l(t) + d_l^{(+)}s^{-l} H_l^{(1)}(t))(\lambda-\beta x),\\
z_l^{(+)}(x) &= e^{x/2}(c_l^{(+)}s^{l}J_{l+1}(t) + d_l^{(+)}s^{-l} H_{l+1}^{(1)}(t))[(\lambda-\beta x)(\mu-\beta x)]^{1/2},\\
y_l^{(-)}(x) &= e^{x/2}(c_l^{(-)}s^{l}J_{l+1}(t) + d_l^{(-)}s^{-l} H_{l+1}^{(1)}(t))[(\lambda-\beta x)(\mu-\beta x)]^{1/2},\\
z_l^{(-)}(x) &= e^{x/2}(c_l^{(-)}s^{l}J_l(t) + d_l^{(-)}s^{-l} H_l^{(1)}(t))(\mu-\beta x);
\end{aligned}$$

in which $t = se^x$, $s = [(\lambda-\beta x)(\mu-\beta x)]^{1/2}$, with arbitrary complex numbers $c_l^{(\pm)}$ and $d_l^{(\pm)}$.

These approximations to the exact general solutions of the matrix differential equations (2.7) behave asymptotically for $x \to -\infty$ in the expected manner (Gesztesy and Pittner 1978b). Careful insertion of the functions (3.1) into the equations (2.7) shows that they fulfil these equations asymptotically for $\ln(a/b) \leqslant x \leqslant 0$ and $\epsilon E \ll E^2 - m^2$, or equivalently for $a \leqslant r \leqslant b$ and $\epsilon \ll E - m$.

Rewritten in terms of cylindrical coordinates, these partial waves may be summed up to the general asymptotic solution

$$\Psi(r,\phi) = \sum_{l=0}^{\infty} \cos(l\phi)\left[\begin{pmatrix} c_l^{(1)} \\ c_l^{(2)} \\ c_l^{(3)} \\ c_l^{(4)} \end{pmatrix}(bk(r))^{-l}J_l(rk(r)) + \begin{pmatrix} d_l^{(1)} \\ d_l^{(2)}(bk(r))^2 \\ d_l^{(3)} \\ d_l^{(4)}(bk(r))^2 \end{pmatrix}(bk(r))^l H_l^{(1)}(rk(r))\right], \tag{3.2}$$

in which $k(r) = [(E - V(r))^2 - m^2]^{1/2}$, $a \leqslant r \leqslant b$, with arbitrary complex numbers $c_l^{(i)}$ and $d_l^{(i)}$, $i = 1, \ldots, 4$. This asymptotic solution differs from the exact general solution of the Dirac equation for free electrons by the radial dependence of the relativistic momentum $k(r)$.

4. Boundary conditions

The incident electrons are described by the plane wave

$$\Phi(r,\phi) = u \exp(\mathrm{i}\rho\cos\phi), \tag{4.1}$$

where

$$u = \begin{pmatrix} u^{(1)} \\ u^{(2)} \\ u^{(3)} \\ u^{(4)} \end{pmatrix} = \left(\frac{E+m}{2E}\right)^{1/2}\begin{pmatrix} w \\ [\boldsymbol{p}\cdot\boldsymbol{\sigma}/(E+m)]w \end{pmatrix},$$

$$\rho = pr, \qquad w = \begin{pmatrix} c \\ d \end{pmatrix}, \qquad u^\dagger u = w^\dagger w = |c|^2 + |d|^2 = 1.$$

The scattered electron wave is expanded in the usual manner,

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

with $A(\phi)$ the scattering amplitude.

The diffraction of electron waves by an impenetrable wire of radius a under the influence of an electrostatic field in the region $a \leq r \leq b$ is then described by the insertion of our general solution into the boundary conditions

$$\Psi(a, \phi) = 0, \qquad (\Psi - \Phi - \chi)(b, \phi) = 0, \qquad (\partial/\partial r)(\Psi - \Phi - \chi)(r, \phi)|_{r=b} = 0. \tag{4.3}$$

The resulting expressions for the scattering coefficients S_l are rather complicated, but for $\epsilon \ll E - m$ they may be approximated by

$$S_0 = -vJ_0(\alpha)/H_0^{(1)}(\alpha),$$

where

$$v = \begin{pmatrix} u^{(1)} \\ u^{(2)}\nu \\ u^{(3)} \\ u^{(4)}\nu \end{pmatrix},$$

and

$$S_l = -2v\nu^l J_l(\alpha)/H_l^{(1)}(\alpha), \qquad l = 1, 2, 3, \ldots, \tag{4.4}$$

where

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

This approximate result for the relativistic scattered electron wave can be obtained from the corresponding spinless non-relativistic expressions (equations (4.6) and (4.7) in Gesztesy and Pittner (1979)) by the use of relativistic kinematics in the expressions for α and ν, and the insertion of the Dirac spinor v. The second and fourth components of this spinor v contain a factor ν which describes the relativistic electron spin–orbit coupling in an electrostatic field. The resulting spin effect, which will be evaluated in the next section, is very small in the range of validity of our asymptotic approximation by means of Bessel functions, because $1 - \nu \ll 1$ for $\epsilon \ll E - m$.

As in the spinless non-relativistic case, the factors ν^l in the partial wave expansion of the scattered wave are decisive for an explicit calculation of the changes of various diffraction phenomena with increasing electric voltage at the capacitor, because only the partial waves with $l \geq \alpha \gg 1$ give rise to electron interference.

5. Fresnel pattern

For an explicit evaluation of the outgoing electron wave and the interference phenomena on the screen due to diffraction by the cylindrical capacitor, we may perform the Sommerfeld–Watson transformation and shift the path of integration in the complex angular momentum plane, in analogy to the spinless non-relativistic case. The two discontinuities along the positive imaginary axis (equations (5.10) and (5.13) in Gesztesy and Pittner (1979)), the residue series, the path integrals in the lit region, the Fresnel region and the Fraunhofer region may be treated in the same way as in our previous work (Gesztesy and Pittner 1979).

As an example which exhibits the influence of an external electrostatic field on the diffraction of charged matter waves, and in particular the effects of relativistic kinematics and spin, we present here our relativistic result for the convergence of Fresnel fringes towards the optical axis with increasing electric field strength. The wavefunction of outgoing electrons in the region $\alpha \ll \rho \ll \alpha^{4/3}$ near the shadow boundary, i.e. $|\phi-\sigma| \leqslant \alpha^{-1/2}$, $\sigma = \sin^{-1}(\alpha/\rho)$, can be approximated by

$$\Psi(r,\phi) \approx u \exp(\mathrm{i}\rho\cos\phi) - v\exp[\mathrm{i}\rho\cos(\phi-\mathrm{i}\delta)] + v 2^{-1/2}\,\mathrm{e}^{-\mathrm{i}\pi/4}\exp[\mathrm{i}\rho\cos(\phi-\mathrm{i}\delta)](F(+\infty)-F(\tau_0)), \tag{5.1}$$

where

$$\delta = |\ln \nu|, \qquad \tau_0 = \rho(\sigma-\phi+\mathrm{i}\delta)\pi^{-1/2}(\rho^2-t^2)^{-1/4}, \qquad t = \rho\sin(\phi-\mathrm{i}\delta),$$

with the Fresnel integral

$$F(z) = \int_0^z \mathrm{d}\zeta \exp\left(\mathrm{i}\frac{\pi}{2}\zeta^2\right) \qquad (z \text{ complex}), \qquad F(+\infty) = 2^{-1/2}\,\mathrm{e}^{\mathrm{i}\pi/4}, \tag{5.2}$$

in analogy to our non-relativistic results (Gesztesy and Pittner 1979).

Due to well-known properties of the Fresnel integral (Abramowitz and Stegun 1972), the maxima of $|\Psi(r,\phi)|$ tend towards the axis according to the law

$$\phi_{\text{centre}} \approx \sigma - \delta^2/\sigma, \tag{5.3}$$

where ϕ_{centre} denotes the scattering angle which belongs to the centre of the Fresnel pattern, i.e. $\phi_{\text{centre}} = \sigma$ for $\epsilon = 0$. The Fresnel fringes reach the optical axis as soon as $\sigma = \delta$, i.e.

$$a/r \approx [2E/(E^2-m^2)]\epsilon \ln(b/a). \tag{5.4}$$

According to this relation, the Fresnel zones reach the axis approximately at the point where the classical trajectory of an electron with energy E and angular momentum $l = ap$ crosses the axis.

These results differ from the corresponding non-relativistic expressions only by the use of relativistic kinematics. For an explicit evaluation of the effect of relativistic electron spin–orbit coupling we define helicity states

$$w_{\pm} = 2^{-1/2}\begin{pmatrix}\pm 1\\ 1\end{pmatrix}, \qquad (\boldsymbol{\sigma}\cdot\boldsymbol{p}/|\boldsymbol{p}|)w_{\pm} = \sigma^1 w_{\pm} = \pm w_{\pm}, \tag{5.5}$$

with the usual Pauli spin matrix σ^1 and $|\boldsymbol{p}| = p^1$, $p^2 = p^3 = 0$. We denote by $u_{\pm}$ and $v_{\pm}$ the corresponding Dirac spinors, where the Pauli spinors $w_{\pm}$ are inserted for w in the definition (4.1). Then by means of the spin flip matrix

$$\tau = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}, \qquad \tau w_{\pm} = w_{\mp}, \tag{5.6}$$

the probability for an electron spin flip in the electrostatic potential $V(r)$ amounts to

$$\frac{\chi_\pm^\dagger(r,\phi)\tau\chi_\pm(r,\phi)}{\chi_\pm^\dagger(r,\phi)\chi_\pm(r,\phi)}=\frac{v_\pm^\dagger\tau v_\pm}{v_\pm^\dagger v_\pm}=-\frac{1-\nu^2}{1+\nu^2}\approx\frac{2E\epsilon}{E^2-m^2}\ln\frac{a}{b}. \tag{5.7}$$

According to these matrix elements, the electron spin is not flipped during diffraction by an impenetrable cylinder without any external electromagnetic field.

The polarisation of electrons by an electrostatic field inside the capacitor may be calculated in the following way. Starting with unpolarised incident electrons, namely with the Pauli spinor

$$\bar{w}=2^{-3/2}\begin{pmatrix}3^{1/2}-1\\3^{1/2}+1\end{pmatrix},\qquad \bar{w}^\dagger\bar{w}=1,\qquad \bar{w}^\dagger\sigma^1 w=\tfrac{1}{2}, \tag{5.8}$$

inserted for w in the definition (4.1), and the corresponding Dirac spinors $\bar{u}$ and $\bar{v}$ respectively, we obtain the final helicity mean value

$$\frac{\bar{v}^\dagger\sigma^1\bar{v}}{\bar{v}^\dagger\bar{v}}\approx\frac{1}{2}\left(1-\frac{3^{1/2}}{2}\,\frac{2E\epsilon}{E^2-m^2}\ln\frac{a}{b}\right), \tag{5.9}$$

which indicates a small polarisation of the order $\epsilon/(E-m)$.

Looking at the scalar product

$$\bar{v}^\dagger\bar{v}\approx 1+\left(1+\frac{3^{1/2}}{2}\right)\frac{2E\epsilon}{E^2-m^2}\ln\frac{a}{b}, \tag{5.10}$$

we see that the intensity loss of the scattered electron wave, which is described by the factor ν^α in the approximate result (5.1), is slightly enhanced by the electron spin–orbit coupling.

6. Conclusions

For the sake of simplicity, as in our previous work on the diffraction of non-relativistic electrons without spin (Gesztesy and Pittner 1979), we have represented the electrostatic biprism by a cylindrical capacitor and the incident electrons by a plane wave, so that the influence of an external electrostatic field on the diffraction of relativistic electron waves can be evaluated analytically. The effect of electron spin was shown to be small, of the order $\epsilon/(E-m)$.

The diffraction of an incident cylindrical wave by a cylindrical capacitor, since it is emitted from a linear electron source in the actual experiments (Möllenstedt and Düker 1956, Donati *et al* 1973, Merli *et al* 1976), can presumably be treated only with the aid of numerical methods. For this purpose one should also modify the boundary conditions appropriately in order to describe the electrostatic field cut-off as realised experimentally.

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