



The refractive index in electron microscopy and the errors of its approximations



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ABSTRACT

In numerical calculations for electron diffraction often a simplified form of the electron-optical refractive index, linear in the electric potential, is used. In recent years improved calculation schemes have been proposed, aiming at higher accuracy by including higher-order terms of the electric potential. These schemes start from the relativistically corrected Schrödinger equation, and use a second simplified form, now for the refractive index squared, being linear in the electric potential. The second and higher-order corrections thus determined have, however, a large error, compared to those derived from the relativistically correct refractive index. The impact of the two simplifications on electron diffraction calculations is assessed through numerical comparison of the refractive index at high-angle Coulomb scattering and of cross-sections for a wide range of scattering angles, kinetic energies, and atomic numbers.

1. Introduction

In 1933 Walter Glaser specified the correct relativistic form of the refractive index for the propagation of an electron wave through electric and magnetic fields [1]. On the theory of high-energy electron diffraction employed in transmission electron microscopy the fields are commonly assumed to be weak, and thus often a simplified form of the refractive index, expanded to first order of the field components, is used for diffraction calculations [2]. In recent years there has been a growing attention to the effect of the second and higher-order terms, partly stimulated by the improved spatial resolution of modern low-voltage transmission electron microscopy, and a couple of calculation schemes have been devised to improve the accuracy of electron diffraction simulations [3–7].

These improved calculation schemes all start, to the best of our knowledge, from the so-called relativistically corrected Schrödinger equation, which is linear in the electric potential, to develop the higher order terms to electron scattering. If, however, the correct relativistic energy-momentum relation were used, an additional term quadratic in the electric potential would appear already in the wave equation [4], so that the quadratic and higher order terms to electron scattering would be distinctly modified, compared to the standard approach on the relativistically corrected Schrödinger equation.

In order to investigate the relative importance of the quadratic electrical-potential term ignored so far, first the standard approach to electron scattering is reviewed including the relevant approximations and neglecting the effects of electron spin and magnetic field. Then the approximations are assessed through numerical comparison of the refractive index at high-angle scattering and of cross-sections for a

wide range of scattering angles, energies, and atomic numbers. Finally the impact of the approximations on diffraction calculations is discussed.

2. Theory

2.1. Approximations of the refractive index

The refractive index due to an electrical field [1] can be written in the form (see Appendix A)

$$n = \sqrt{1 + \frac{V}{E^*} + \frac{1}{4}\beta^2 \left(\frac{V}{E^*}\right)^2}, \quad (1)$$

with $V = e\Phi$, the positive elementary charge e , electrical potential Φ , $\beta = v/c$, electron speed in vacuum v , speed of light c ,

$$E^* = \frac{1}{2}m^*v^2, \quad (2)$$

$m^* = m_0/\sqrt{1-\beta^2}$, and rest mass m_0 . Further

$$\gamma = \frac{1}{\sqrt{1-\beta^2}} = 1 + \frac{E}{E_0}, \quad (3)$$

for kinetic energy E , and rest energy $E_0 = m_0c^2$. We follow the convention that V is positive for an electron in the electric field of a positive charge; thus V denotes the negative potential energy, see Appendix A. The form (1) reflects the relativistic energy-momentum relation underlying the Klein-Gordon equation, see e. g. [4] and Appendix A.

The phase difference between points P_1 and P_2 on an electron

trajectory S , measured relative to the phase difference in vacuum along the same trajectory, is given by the line integral [8]

$$\phi = \frac{2\pi}{\lambda_0} \int_{p_1}^{p_2} (n-1) ds, \quad (4)$$

with ds a line element on the trajectory, vacuum wavelength λ_0 from the de Broglie relation for the momentum in vacuum,

$$p_0 = m^*v = \frac{h}{\lambda_0}, \quad (5)$$

and Planck constant h .

The standard theory of high-energy electron diffraction comprises the following approximations [8]. First, the refractive index is simplified by neglecting the term quadratic in V relative to the linear term,

$$n \approx n_1 = \sqrt{1 + \frac{V}{E^*}}. \quad (6)$$

This form is compatible with the so-called relativistically corrected Schrödinger equation. Second, the square root is expanded to first order in V ,

$$n_1 \approx n_2 = 1 + \frac{V}{2E^*}, \quad (7)$$

which is a convenient choice, as the line integral (4) for the phase extends directly over the potential. Third, in the phase-grating approximation for the electron wave function ψ ,

$$\psi(\mathbf{R}, z_2) \approx \psi(\mathbf{R}, z_1) \exp\left(\frac{2\pi i}{\lambda_0} \int_{z_1}^{z_2} (n(\mathbf{R}, z) - 1) dz\right) \quad (8)$$

the trajectories are assumed to be straight, along a coordinate z , which involves the small-angle approximation of high-energy electron scattering, and \mathbf{R} denotes a coordinate vector perpendicular to the trajectory direction \hat{z} .

In improved calculation schemes, starting from the relativistically corrected Schrödinger equation and aiming at higher accuracy, n_1 is expanded to higher orders,

$$n_1 = 1 + \frac{V}{2E^*} - \frac{1}{8} \left(\frac{V}{E^*}\right)^2 + \frac{1}{16} \left(\frac{V}{E^*}\right)^3 + O\left(\left(\frac{V}{E^*}\right)^4\right); \quad (9)$$

the expansion for n yields, however,

$$n = 1 + \frac{V}{2E^*} - \frac{1}{8}(1 - \beta^2) \left(\frac{V}{E^*}\right)^2 + \frac{1}{16}(1 - \beta^2) \left(\frac{V}{E^*}\right)^3 + O\left(\left(\frac{V}{E^*}\right)^4\right). \quad (10)$$

In the correct expansion there appears a factor $1 - \beta^2$ in the second-order and third-order terms, and thus the respective terms in n_1 are in error by β^2 .

Further, in the limit $E \rightarrow 0$, $\beta \rightarrow 0$, $v \rightarrow 0$ the refractive index tends to

$$n \rightarrow n_1 = \sqrt{1 + \frac{V}{E^*}}, \quad (11)$$

and thus n_1 is a reasonable approximation for low energies. In the limit $E \rightarrow \infty$, $\beta \rightarrow 1$, $v \rightarrow c$ the refractive index tends to

$$n \rightarrow n_2 = 1 + \frac{V}{2E^*}, \quad (12)$$

and thus the apparently inferior approximation n_2 is reasonable for high energies, as second and higher orders vanish. For medium energies neither limit applies, and the full expression for n should be used.

2.2. Scattering from a Coulomb potential

In the above considerations on the second-order and higher-order terms the relative influence of the magnitude of V/E^* has been left aside. It may vary over a wide range, as can be seen for the Coulomb potential energy

$$V = \frac{ZE_0 r_e}{r}, \quad (13)$$

with atomic number Z , and classical electron radius r_e . Then

$$\frac{V}{E^*} = \frac{ZR_e}{\gamma\beta^2 r}, \quad (14)$$

becomes large near the origin. The closest distance to the origin on the hyperbolic trajectory of Rutherford scattering is [9]

$$r_{\min} = \sqrt{a^2 + b^2} - a, \quad (15)$$

with impact parameter b , and

$$a = \frac{ZR_e}{\gamma\beta^2}. \quad (16)$$

The scattering angle θ of Rutherford scattering fulfills

$$\tan \frac{\theta}{2} = \frac{a}{b}, \quad (17)$$

and thus

$$\frac{V_{\max}}{E^*} = \frac{2a}{\sqrt{a^2 + b^2} - a} = \frac{2\sin \frac{\theta}{2}}{1 - \sin \frac{\theta}{2}} = \frac{\lambda_0 g}{1 - \frac{1}{2}\lambda_0 g} \quad (18)$$

depends only on the scattering angle, which may be substituted by the wavelength and the magnitude of the scattering vector g .

A value for the largest scattering vector relevant in numerical simulations can be derived from the reasonable assumption that thermal atomic vibration poses a limit. In this work we have chosen the radius at $e^{-\pi} = 0.0432\dots$ of the atomic vibration envelope $\exp(-Bg^2/4)$,

$$g_{\max} = \sqrt{\frac{4\pi}{B}}, \quad (19)$$

with the Debye-Waller parameter $B = 8\pi^2 \langle u^2 \rangle$, and $\langle u^2 \rangle$ the mean squared atom displacement. We further assume isotropic atom vibrations, and then: $\langle u_x^2 \rangle = \langle u_y^2 \rangle = \langle u_z^2 \rangle = \langle u^2 \rangle/3$.

2.3. Scattering cross-sections for a screened Coulomb potential

The second-order and higher-order terms in the expansion of n , which are wrong in n_1 and neglected in n_2 , affect the high-angle scattering of a Coulomb potential, and it is thus instructive to compare scattering cross-sections σ for n , n_1 , and n_2 . In the numerical simulation of cross-sections for the scattering into the solid angle Ω limited by scattering angles θ_1 and θ_2 , considering the azimuthal symmetry of the Coulomb potential,

$$\sigma = \iint_{\Omega} |f|^2 d\Omega = 2\pi \int_{\theta_1}^{\theta_2} |f|^2 \sin \theta d\theta. \quad (20)$$

The phase grating approximation (8) is used for the calculation of the scattering factor [8]

$$f(\mathbf{g}) = -\frac{i}{\lambda_0} \iint_{\Sigma} (\exp(i\phi_p(\mathbf{R})) - 1) \exp(-2\pi i \mathbf{g} \cdot \mathbf{R}) d\Sigma, \quad (21)$$

with scattering vector \mathbf{g} , a coordinate vector \mathbf{R} in a plane Σ perpendicular to the trajectory direction \hat{z} , and the projected phase

$$\phi_p(\mathbf{R}) = \frac{2\pi}{\lambda_0} \int_{-\infty}^{\infty} (n(\mathbf{R}, z) - 1) dz. \quad (22)$$

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