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Note

Voigt lineshape function as a solution of the parabolic partial differential equation

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Abstract

The goal of this paper is to show that the Voigt function may be found as a solution of a parabolic partial differential equation, like the heat conduction equation or other diffusion equations. A square of the Gaussian half-width of the Voigt function plays the role of 'time' and initial conditions are determined by a Lorentz function. Some questions concerning the practical application of the numerical grid methods for the calculation of the Voigt function are discussed. It is shown, that in some cases the offered calculation algorithm can be both faster and more accurate than other known algorithms.

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Keywords: Voigt function; Voigt lineshape

1. Introduction

The convolution between a Gauss and a Lorentz function is known as a Voigt function (Voigt profile, Voigt lineshape, Voigt integral). Because this function arises in many different fields of physics, such as theory of neutron reactions, atmosphere transmittance, astrophysical spectroscopy, plasma physics, laser physics, Mössbauer spectroscopy, X-ray diffraction, etc., there has been much interest to rapidly and accurately computing it, e.g. [1–23].

The expression for the Voigt profile normalized to unity is given by

$$V(x,y,g)=\frac{y}{\pi\sqrt{2\pi g}}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-t^2/(2g)}}{(x-t)^2+y^2}\,\mathrm{d}t, \tag{1}$$

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