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Journal of Approximation Theory 228 (2018) 21–57

Journal of Approximation Theory

www.elsevier.com/locate/jat

Full Length Article

Gaussian integration formulas for logarithmic weights and application to 2-dimensional solid-state lattices

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Received 16 April 2015; received in revised form 18 November 2017; accepted 2 February 2018
Available online 8 February 2018

Communicated by Andrei Martinez-Finkelshtein

Abstract

The making of Gaussian numerical integration formulas is considered for weight functions with logarithmic singularities. Chebyshev modified moments are found most convenient here. The asymptotic behavior of the relevant recurrence coefficients is stated in two conjectures. The relation with the recursion method in solid-state physics is summarized, and more details are given for some two-dimensional lattices (square lattice and hexagonal (graphene) lattice).

MSC: 42A16; 42C05; 42C10; 47B36; 65D32; 65Q30; 81Q05

Keywords: Numerical analysis; Integration formulas; Logarithmic singularities; Solid-state physics; 2-dimensional lattices; Graphene

Contents

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https://doi.org/10.1016/j.jat.2018.02.001
0021-9045/

Nothing exists per se except atoms and the void
... however solid objects seem,

Lucretius, *On the Nature of Things*,
Translated by William Ellery Leonard

1. Orthogonal polynomials and Gaussian quadrature formulas

Let μ be a positive measure on a real interval $[a, b]$, and P_n the related monic orthogonal polynomial of degree n, i.e., such that

$$P_n(x) = x^n + \cdots \ , \quad \int_a^b P_n(t)P_m(t)d\mu(t) = 0, m \neq n, \qquad n = 0, 1, \dots . \tag{1}$$

An enormous amount of work has been spent since about 200 years on the theory and the applications of these functions. One of their most remarkable properties is the recurrence relation

$$P_{n+1}(x) = (x - b_n)P_n(x) - a_n^2 P_{n-1}(x), \qquad n = 1, 2, \dots, \tag{2}$$

with $P_0(x) \equiv 1$, $P_1(x) = x - b_0$. See, among numerous other sources, books by Chihara [16], Gautschi [39,41], Ismail [55], chap. 18 of NIST handbook [89], and other surveys [44,69,70].

Orthogonal polynomials are critically involved in the important class of Gaussian integration formulas. A classical integration formula $\int_a^b f(t)d\mu(t) \approx w_1 f(x_1) + \cdots + w_N f(x_N)$ (Newton–Cotes, Simpson, etc.) is the integral $\int_a^b p(t)\ d\mu(t)$ of the polynomial interpolant p of f at the