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Rational approximation to the Fermi-Dirac function with applications in density functional theory. (English) Zbl 1211.65026

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Summary: We are interested in computing the Fermi-Dirac matrix function in which the matrix argument is the Hamiltonian matrix arising from density functional theory (DFT) applications. More precisely, we are really interested in the diagonal of this matrix function. We discuss rational approximation methods to the problem, specifically the rational Chebyshev approximation and the continued fraction representation. These schemes are further decomposed into their partial fraction expansions, leading ultimately to computing the diagonal of the inverse of a shifted matrix over a series of shifts. We describe Lanczos and sparse direct methods to address these systems. Each approach has advantages and disadvantages that are illustrated with experiments.

MSC:

65D20 Computation of special functions and constants, construction of tables
81Q05 Closed and approximate solutions to the Schrödinger, Dirac, Klein-Gordon and other equations of quantum mechanics
65F05 Direct numerical methods for linear systems and matrix inversion
33E20 Other functions defined by series and integrals
33F05 Numerical approximation and evaluation of special functions

Keywords:

diagonal of matrix inverse; electronic structure calculations; density functional theory; continued fraction; numerical examples; Fermi-Dirac matrix function; Hamiltonian matrix; rational Chebyshev approximation; sparse direct methods

Software:

Expokit; ITSOL; PARSEC ; SPARSKIT

Full Text: DOI

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