Incomplete Bessel Functions in Periodic-System Electronic Structure Computations

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When Ewald-type convergence-acceleration processes are applied to electronic-structure computations for periodic systems using a Gaussian-type-orbital basis, the partitioning of the resultant integrals between direct and reciprocal (Fourier) space causes the occurrence of functions that can be identified as "incomplete" versions of the Macdonald function ordinarily assigned the symbol K_n. These incomplete Bessel functions, therefore designated $K_n(x,y)$, are needed for the argument range $x>0$, $y\geq 0$. These functions also occur in hydrology problems, where they are known as *leaky aquifer functions*, and in addition they have been discussed under the name *generalized incomplete gamma functions*, notably by Temme and colleagues. Moreover, they have the reputation of being difficult to evaluate.

The $K_n(x,y)$ satisfy a variety of functional relations, and we and others have developed a number of expansions for the K_n useful in various ranges of x and y. When used for systems of one-dimensional periodicity, the needed range of the index n is from zero to four times the maximum value of l, the orbital angular momentum. Thus, for general use, one might expect to need n to values reaching, in worst cases, as high as $n=12$. The accuracy needed in electronic structure computations is normally absolute (rather than relative), and we have tentatively determined that an absolute accuracy of $\delta=10^{-10}$ would be acceptable in most problems. The functions $K_n(x,y)$ decay exponentially in x, and with the chosen δ value all K_n with $x>20$ can be approximated as zero. However, for small x a wider range of y becomes relevant.

Some of the evaluation methods require values of the exponential integral $E_1(z)$, and some involve values of the Macdonald functions $K_0(z)$ and $K_1(z)$. Since electronic structure computations typically involve extremely large number of integral evaluations, we deemed it necessary to develop highly efficient evaluation procedures for E_1, K_0, and K_1. Since these auxiliary functions are used in the context of recursive procedures that are not entirely stable, we determined that they were needed to an absolute accuracy of 10^{-15}. We obtained expansions for these functions that are not much more extensive than those presented, e.g., in the *Handbook of Mathematical Functions*, but are many orders of magnitude more accurate. Based on all these considerations, we have identified a collection of procedures that give $K_n(x,y)$ to the target accuracy over its entire range.

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