A Generalized Transformation and a New Algorithm for Computing Infinite-Range Integrals High Performance Scientific Computing

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Abstract: In [1], the S transformation for spherical Bessel integral functions was introduced. S is based on a formalized integration by parts by $x\,dx$ and transforms spherical Bessel integrals into sine integrals. The S transformation, which requires the boundary terms to vanish at both limits, solves the difficulty arising from the strong oscillations of spherical Bessel functions and increases the efficiency of the transformations $\bar{D}$ [2] and G [3] in that the zeros of the new integrands are the zeros of $\sin(v\,x)$, which are equidistant.

In [1], the $\bar{D}$ transformation was used for the evaluation of the obtained sine integrals. This led to the $S\bar{D}$ method, which proved the most efficient approach compared to all previously used alternatives. Recurrence relations were developed for the computation of the approximations $S\bar{D}_n^{(2,j)}$ of the integrals, allowing for the control of the degree of accuracy. The $S\bar{D}$ method was successfully applied to molecular integrals and leading experts in the field showed a considerable interest in this method.

The main objective of this research work is the generalization of the S transformation, which will eliminate the boundary conditions and will expand applicability beyond spherical Bessel integrals. This generalization will require the development of new formulae for higher order derivatives, which will be obtained using the formulae for derivatives that we introduced in [4]. A recursive algorithm based on the generalized S is developed. The numerical results are obtained for challenging integrals clearly demonstrate showed the high accuracy of the developed method and algorithm.

References

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