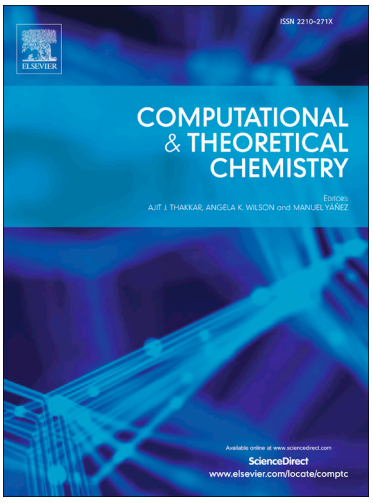

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PII: S2210-271X(18)30374-8
DOI: https://doi.org/10.1016/j.comptc.2018.09.007
Reference: COMPTC 12345

To appear in: *Computational & Theoretical Chemistry*

Received Date: 1 August 2018
Accepted Date: 19 September 2018

Please cite this article as: S.J.C. Salazar, R.P. Sagar, Numerical calculation of the Spherical Bessel Transform from Gaussian quadrature in the complex-plane, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.09.007

Numerical calculation of the Spherical Bessel Transform from Gaussian quadrature in the complex-plane.

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Abstract

A numerical method for the calculation of spherical Bessel transforms via Gaussian quadrature in the complex plane is presented. The method is evaluated by transforming Slater and Gaussian-type spherical coordinate basis functions, used in electronic structure calculations, from position space to momentum space. The feasibility and efficiency of the method is explored for different regions of momenta and different orders of the spherical Bessel transform. The results illustrate that in general the method performs very well in the large p regions when applied to the Slater-type functions. On the other hand, a parameter has to be introduced for the application to Gaussian-type functions in order to avoid cancellation. In this case, the method performs well but accuracy is lost at larger p. Use of the parameter in application to Slater functions yields accurate results for all regions of p.

Keywords: Spherical Bessel Transform, reverse Bessel polynomials, Slater-type basis function, Gaussian-type basis function, complex-plane Gaussian quadrature
PACS: 02.30.Uu, 02.60.Jh

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