Accuracy of B-spline expansion of Slater-type function

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Abstract

The accuracy of B-spline expansion of Slater-type functions (STFs) is examined by computing atomic one-electron integrals. The one-electron integrals are calculated with the B-spline expansion of the STFs. The accuracy of the B-spline expansion of the STFs is measured on the basis of the relative errors of the calculated integrals against the exact values. Consequently, the optimal parameters of a B-spline set which can accurately approximate the STFs are determined.

1 Introduction

In quantum mechanical calculations for atomic systems, atomic orbitals are often expanded with some basis functions, e.g. Slater-, Gaussian-, Laguerre-type functions, B-splines, and so on. In particular, the Slater-type function (STF) is usually employed. However, the linear dependence of STFs sometimes disturbs the calculations. To avoid this problem, one must employ B-splines which are piecewise polynomials. B-splines are free from computational linear dependence and are very flexible. Atomic calculations with B-splines yield highly accurate energies and properties [1-3]. Therefore, B-splines are very useful for the calculation of atomic systems.

The development of Hylleraas-type calculation with B-splines is very interesting and important. However, there are several difficulties associated with this development. One of the difficulties is to formulate many-electron integrals over B-splines which appear in the calculations. It is possible to avoid this difficulty using an approximate computational method of many-electron integrals proposed by Kutzelnigg's group [4]. This method approximates a many-electron integral to sums of products of two-electron integrals by using an incomplete set, e.g.

$$\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \chi_a^*(\mathbf{r}_1)\chi_b^*(\mathbf{r}_2)\chi_c^*(\mathbf{r}_3)\, r_{12}^m\, r_{13}^n\, \chi_d(\mathbf{r}_1)\chi_e(\mathbf{r}_2)\chi_f(\mathbf{r}_3)$$

$$= \sum_i \left[\int d\mathbf{r}_1 d\mathbf{r}_2 \chi_a{}^*(\mathbf{r}_1)\chi_b{}^*(\mathbf{r}_2)\, r_{12}^m\ \psi_i(\mathbf{r}_1)\chi_e(\mathbf{r}_2) \right] \times \left[\int d\mathbf{r}_1 d\mathbf{r}_2\, \psi_i{}^*(\mathbf{r}_1)\chi_c{}^*(\mathbf{r}_2)\, r_{12}^n\ \chi_d(\mathbf{r}_1)\chi_f(\mathbf{r}_2) \right], \quad (1)$$

where χ are the B-spline-type orbitals, and $\{\psi_i\}$ is an incomplete set. If ψ_i are expanded with some flexible basis functions, Eq.(1) may yield highly accurate values. Hence, B-splines are suitable for Kutzelnigg's approximation method. We are developing this approximation method with B-splines.

There are many formulations and calculations of many-electron integrals that appear in the Hylleraas-type calculations. Most of them are works for the integrals over the STFs. It is impossible to check the accuracy of the above approximation by comparing with the literature values. For this purpose, it is essential to transform the B-spline many-electron integrals into the STF integrals by using the B-spline expansion coefficients of the STFs. Since B-splines are very flexible, the STFs should be accurately expanded with B-splines. Our purpose in this work is to check the accuracy of the B-spline expansion of the STFs and to determine optimal parameters of the B-splines. To this end, we measure the relative errors of the transformed one-electron integrals against the exact values.

Below, Section 2 provides a brief review of the B-splines and details on the computation. Section 3 summarizes and discusses the relative errors of the transformed one-electron integrals.

2 Theory and computation

The B-splines of order K, $\{B_{i,K}(r)\}$, are piecewise polynomials of degree K-1 on a knot sequence in a cavity of radius R [5,6]. The knot sequence $\{t_i\}$ is a set of points defined on an interval $0 \le r \le R$. Several methods that generate the knot sequence are proposed by Gilbert and Bertoncini [7]. The quality of the B-splines depends on not only their order and size, but also the knot sequence. In atomic calculations, the knot sequence that concentrates near the nucleus is required because the atomic orbitals rapidly change near the nucleus. Hence, an exponential [7] or a geometric [1] knot sequence is suitable for atomic calculations. B-splines can be constructed recursively by de Boor-Cox relation:

$$B_{i,1}(r) = \begin{cases} 1, & t_i \le r < t_{i+1}, \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

and

$$B_{i,K}(r) = \frac{r - t_i}{t_{i+K-1} - t_i}\ B_{i,K-1}(r) + \frac{t_{i+K} - r}{t_{i+K} - t_{i+1}} B_{i+1,K-1}(r). \quad (3)$$

$B_{i,K}$ is nonzero in the interval $t_i \le r < t_{i+K}$.

Let us apply the B-splines to the expansion of atomic orbitals. An atomic orbital with angular momentum l can be expressed as

$$\psi_{nlm}(r, \theta, \phi) = r^{-1} P_{nl}(r) Y_l^m(\theta, \phi). \tag{4}$$

The radial function $P_{nl}(r)$ is expanded with the B-splines and enforces the boundary conditions $P_{nl}(0)=0$ and $P_{nl}(R)=0$. Since the first and the last terms of the B-splines with K-fold multiple knots are nonzero at $r = 0$ and at $r = R$, respectively, they are removed from the basis function to satisfy the boundary conditions. P_{nl} is expanded with the N-term B-spline set $(B_{2,K}, \cdots, B_{N+1,K})$.

In this work, the STF $r^{n-1}e^{-\zeta r}$ is expanded with the B-spline set in the same manner as the atomic orbital as follows:

$$r^n e^{-\zeta r} \approx \sum_{i=2}^{N+1} C_i^{n,\zeta} B_{i,K}(r), \tag{5}$$

where $C_i^{n,\zeta}$ are the linear expansion coefficients. We employ 100-term B-spline sets constructed on the exponential knot sequences, with endpoints of K-fold multiplicity. The parameters K, R, and R_1 of the B-spline sets take all combinations of

$K = 9, 11, 13, 15,$

$R = 40, 60, 80, 100,$

$R_1 = 10^{-4},$

where R_1 is the initial interval of the knot sequence. We determine $C_i^{n,\zeta}$ by solving the system of linear equations

$$\sum_{j=2}^{N+1} \left[\int_0^R dr\, B_{i,K}(r)\, B_{j,K}(r) \right] C_j^{n,\zeta} = \int_0^R dr\, B_{i,K}(r)\, r^n\, e^{-\zeta r}, \quad (i=2, \cdots, N+1). \tag{6}$$

These integrals are evaluated by the Gauss integration procedure. $C_i^{n,\zeta}$ can also be determined by solving Schrödinger equation:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{n(n-1)}{2r^2} - \frac{n\zeta}{r} \right] C_i^{n,\zeta} B_{i,K}(r) = E\, C_i^{n,\zeta} B_{i,K}(r), \quad (i=2, \cdots, N+1), \tag{7}$$

where E is the energy of hydrogen-like atoms.

The transformed one-electron integrals are calculated using the B-spline expansion coefficients of STFs $C_i^{n,\zeta}$ as follows:

$$I^v(n, \zeta) = \sum_{ij} C_i^{n,\zeta} C_j^{n,\zeta} \int_0^R dr\, r^v\, B_{i,K}(r)\, B_{j,K}(r), \tag{8}$$

where ν is an integer. In this work, $I^{\nu}(n, \zeta)$ are calculated with $\nu = -1, 0, 1, 2, 3, 4, 5$. As a measure of accuracy of the integral, we use the relative error

$$\left| \frac{I^{\nu}(n, \zeta) - I^{\nu}_{\mathrm{STF}}(n, \zeta)}{I^{\nu}_{\mathrm{STF}}(n, \zeta)} \right|, \tag{9}$$

where I^{ν}_{STF} is the following exact integral value:

$$I^{\nu}_{\mathrm{STF}}(n, \zeta) = \int_0^{\infty} dr\, r^{2n+\nu} e^{-2\zeta} = \frac{(2n+\nu)!}{(2\zeta)^{2n+\nu+1}}. \tag{10}$$

We examine the B-spline expansion of 1s-, 2p-, and 3d-type STFs (i.e. STFs with $n = 1$, 2, and 3), and consider exponential parameters $\zeta = 0.5$, 1, 10, 50. All the calculations are performed at double precision.

3 Results and discussion

We determined the B-spline expansion coefficients of the STFs by solving Eq.(6), and we calculated one-electron integrals $I^{\nu}(n, \zeta)$ and $I^{\nu}_{\mathrm{STF}}(n, \zeta)$ for $n = 1, 2, 3$, $\zeta = 0.5$, 1, 10, 50, and $\nu = -1$, 0, 1, 2, 3, 4, 5 at double precision. We also attempted to calculate $I^{\nu}(n, \zeta)$ by variationally solving Eq.(7). The errors of the resulting $I^{\nu}(n, \zeta)$ were slightly larger than those of the integrals calculated with solutions of Eq.(6). Therefore, it is desirable to employ Eq.(6).

First, we discuss the accuracy of the B-spline expansion of 1s-STFs. Tables 1 and 2 list the relative errors for $I^{\nu}(1, \zeta)$ ($\zeta = 0.5$, 1, 10, 50). The expansion of 1s-STF with $\zeta = 0.5$ requires the B-spline set with large R owing to its diffuseness. Accordingly, the B-spline sets with $R = 40$ yield large errors for $I^{\nu}(1, 0.5)$ with $\nu \geq 1$, regardless of the values of K. Accurate $I^{\nu}(1, 0.5)$ for all the values of ν can be obtained by the B-spline sets with $K \geq 11$ and $R \geq 60$. All the values of $I^{\nu}(1, 1)$ and $I^{\nu}(1, 10)$ are independent of R within a range of R under consideration. The accurate integral values are given by the B-spline sets with $K \geq 11$. 1s-STF with $\zeta = 50$ localizes near the nucleus, and hence the B-spline sets with large R yield large errors for $I^{\nu}(1, 50)$. In particular, the relative errors for $I^{4}(1, 50)$ and $I^{5}(1, 50)$ are large. Consequently, it is desirable to use the B-spline sets with $R = 60$ and $K \geq 11$ in order to accurately expand 1s-STFs.

Table 1: Relative errors of transformed integrals $I^{\nu}(1, \zeta)$ for ζ= 0.5 and 1. $A(B)$ implies $A \times 10^{B}$.

	ζ = 0.5				ζ = 1			
ν	R=40	R=60	R=80	R=100	R=40	R=60	R=80	R=100
K = 9								
−1	5.6(−16)	2.2(−16)	8.9(−16)	2.2(−16)	8.9(−16)	2.2(−16)	1.1(−16)	0.0
0	4.3(−15)	6.7(−16)	0.0	4.4(−16)	4.4(−16)	6.7(−16)	4.4(−16)	0.0
1	5.6(−14)	7.4(−16)	5.9(−16)	3.0(−16)	7.4(−16)	8.9(−16)	1.5(−16)	3.0(−16)
2	5.7(−13)	0.0	1.0(−15)	8.9(−16)	3.0(−16)	3.0(−16)	8.9(−16)	3.0(−16)
3	4.6(−12)	2.4(−16)	1.8(−15)	2.0(−15)	8.3(−16)	9.5(−16)	1.1(−15)	2.5(−15)
4	3.2(−11)	3.0(−15)	4.9(−15)	6.6(−15)	2.2(−15)	3.2(−15)	6.0(−15)	7.1(−15)
5	1.9(−10)	1.2(−14)	1.8(−14)	2.5(−14)	7.4(−15)	1.1(−14)	1.8(−14)	2.3(−14)
Average	3.2(−11)	2.4(−15)	3.8(−15)	5.1(−15)	1.8(−15)	2.5(−15)	3.8(−15)	4.8(−15)
K = 11								
−1	7.8(−16)	4.4(−16)	0.0	0.0	0.0	6.7(−16)	4.4(−16)	8.9(−16)
0	4.8(−15)	4.4(−16)	3.3(−16)	2.2(−16)	8.9(−16)	6.7(−16)	1.1(−16)	3.3(−16)
1	5.3(−14)	5.9(−16)	8.9(−16)	1.5(−16)	1.3(−15)	7.4(−16)	5.9(−16)	0.0
2	5.5(−13)	3.0(−16)	5.9(−16)	4.4(−16)	7.4(−16)	7.4(−16)	8.9(−16)	3.0(−16)
3	4.5(−12)	5.9(−16)	2.4(−16)	1.2(−16)	3.6(−16)	2.4(−16)	4.7(−16)	1.2(−16)
4	3.1(−11)	3.2(−16)	3.2(−16)	1.6(−16)	9.5(−16)	1.6(−16)	1.6(−16)	3.2(−16)
5	1.8(−10)	1.8(−16)	7.2(−16)	5.4(−16)	3.6(−16)	3.6(−16)	3.6(−16)	9.0(−16)
Average	3.1(−11)	4.1(−16)	4.4(−16)	2.3(−16)	6.6(−16)	5.1(−16)	4.3(−16)	4.1(−16)
K = 13								
−1	4.4(−16)	4.4(−16)	2.2(−16)	1.1(−16)	1.1(−15)	4.4(−16)	0.0	2.2(−16)
0	3.7(−15)	7.8(−16)	4.4(−16)	4.4(−16)	2.2(−16)	4.4(−16)	2.2(−16)	8.9(−16)
1	5.2(−14)	3.0(−16)	5.9(−16)	4.4(−16)	4.4(−16)	1.2(−15)	4.4(−16)	5.9(−16)
2	5.4(−13)	3.0(−16)	1.5(−16)	3.0(−16)	3.0(−16)	4.4(−16)	1.5(−16)	4.4(−16)
3	4.4(−12)	4.7(−16)	1.1(−15)	5.9(−16)	3.6(−16)	5.9(−16)	1.2(−16)	4.7(−16)
4	3.0(−11)	9.5(−16)	4.7(−16)	3.2(−16)	1.1(−15)	9.5(−16)	1.1(−15)	1.6(−16)
5	1.8(−10)	1.8(−16)	1.1(−15)	5.4(−16)	3.6(−16)	1.6(−15)	1.6(−15)	1.8(−16)
Average	3.0(−11)	4.9(−16)	5.8(−16)	3.9(−16)	5.6(−16)	8.1(−16)	5.2(−16)	4.2(−16)
K = 15								
−1	2.2(−16)	8.9(−16)	4.4(−16)	4.4(−16)	1.1(−15)	8.9(−16)	2.2(−16)	2.2(−16)
0	2.7(−15)	3.3(−16)	6.7(−16)	4.4(−16)	1.1(−16)	4.4(−16)	8.9(−16)	3.3(−16)
1	5.3(−14)	1.5(−16)	4.4(−16)	4.4(−16)	3.0(−16)	3.0(−16)	3.0(−16)	1.5(−16)
2	5.3(−13)	3.0(−16)	1.3(−15)	1.0(−15)	0.0	1.5(−16)	7.4(−16)	1.0(−15)
3	4.4(−12)	9.5(−16)	4.7(−16)	2.4(−16)	7.1(−16)	0.0	4.7(−16)	0.0
4	3.0(−11)	1.6(−15)	9.5(−16)	3.2(−16)	4.7(−16)	4.7(−16)	6.3(−16)	6.3(−16)
5	1.8(−10)	1.4(−15)	7.2(−16)	1.6(−15)	1.3(−15)	1.8(−16)	7.2(−16)	3.6(−16)
Average	3.0(−11)	8.1(−16)	7.2(−16)	6.5(−16)	5.7(−16)	3.5(−16)	5.7(−16)	3.9(−16)

Table 2: Relative errors of transformed integrals $I^{\nu}(1, \zeta)$ for ζ= 10 and 50. $A(B)$ implies $A \times 10^{B}$.

	ζ = 10				ζ = 50			
ν	R=40	R=60	R=80	R=100	R=40	R=60	R=80	R=100
K = 9								
−1	1.7(−16)	1.7(−16)	1.2(−15)	1.7(−16)	9.5(−16)	1.4(−16)	4.1(−16)	1.5(−15)
0	0.0	2.2(−16)	8.7(−16)	4.3(−16)	0.0	1.3(−15)	4.2(−16)	1.5(−15)
1	1.3(−15)	3.6(−16)	1.8(−16)	5.4(−16)	0.0	2.2(−16)	4.4(−16)	4.4(−16)
2	6.8(−16)	6.8(−16)	0.0	3.4(−16)	3.4(−16)	5.2(−16)	1.7(−16)	3.4(−16)
3	1.4(−15)	7.9(−16)	1.1(−15)	2.1(−15)	4.3(−16)	1.7(−15)	6.5(−16)	1.5(−15)
4	2.3(−15)	2.8(−15)	5.6(−15)	7.5(−15)	1.9(−15)	3.0(−15)	4.8(−15)	7.4(−15)
5	7.5(−15)	1.2(−14)	1.8(−14)	2.4(−14)	5.8(−15)	1.2(−14)	1.8(−14)	2.4(−14)
Average	1.9(−15)	2.4(−15)	3.8(−15)	5.1(−15)	1.3(−15)	2.7(−15)	3.6(−15)	5.3(−15)
K = 11								
−1	8.7(−16)	3.5(−16)	3.5(−16)	3.5(−16)	8.1(−16)	2.7(−16)	2.7(−16)	2.7(−16)
0	8.7(−16)	4.3(−16)	6.5(−16)	1.1(−15)	1.1(−15)	1.3(−15)	4.2(−16)	2.1(−16)
1	1.8(−16)	3.6(−16)	7.2(−16)	1.8(−16)	2.2(−16)	6.6(−16)	2.2(−16)	2.2(−16)
2	1.8(−15)	1.1(−16)	1.1(−16)	3.4(−16)	6.9(−16)	1.2(−15)	5.2(−16)	3.4(−16)
3	1.8(−15)	9.0(−16)	5.6(−16)	4.5(−16)	2.2(−16)	6.5(−16)	4.3(−16)	1.1(−15)
4	5.6(−16)	3.8(−16)	0.0	7.5(−16)	2.2(−16)	2.2(−16)	3.4(−16)	6.7(−16)
5	8.1(−16)	1.3(−16)	1.3(−16)	5.4(−16)	4.0(−16)	2.0(−16)	1.6(−15)	1.2(−15)
Average	9.9(−16)	3.8(−16)	3.6(−16)	5.3(−16)	5.2(−16)	6.4(−16)	5.4(−16)	5.7(−16)
K = 13								
−1	5.2(−16)	3.5(−16)	1.7(−16)	5.2(−16)	5.4(−16)	1.4(−16)	2.7(−16)	2.7(−16)
0	4.3(−16)	2.2(−16)	1.7(−15)	4.3(−16)	2.1(−16)	2.1(−16)	4.2(−16)	4.2(−16)
1	5.4(−16)	3.6(−16)	1.1(−15)	7.2(−16)	4.4(−16)	8.8(−16)	6.6(−16)	0.0
2	5.6(−16)	3.4(−16)	6.8(−16)	1.1(−16)	8.6(−16)	5.2(−16)	6.9(−16)	1.9(−15)
3	5.6(−16)	5.6(−16)	0.0	7.9(−16)	6.5(−16)	0.0	6.5(−16)	1.1(−15)
4	1.1(−15)	3.8(−16)	1.1(−15)	3.8(−16)	1.2(−15)	5.6(−16)	6.7(−16)	4.5(−16)
5	1.3(−16)	2.7(−16)	6.7(−16)	1.3(−15)	1.4(−15)	1.4(−15)	8.0(−16)	1.1(−14)
Average	5.6(−16)	3.5(−16)	7.8(−16)	6.1(−16)	7.6(−16)	5.3(−16)	6.0(−16)	2.1(−15)
K = 15								
−1	5.2(−16)	1.7(−16)	1.2(−15)	8.7(−16)	5.4(−16)	2.7(−16)	1.8(−15)	5.4(−16)
0	4.3(−16)	0.0	1.5(−15)	1.1(−15)	8.5(−16)	1.3(−15)	2.1(−16)	2.1(−16)
1	5.4(−16)	1.1(−15)	0.0	0.0	2.2(−16)	2.2(−16)	4.4(−16)	4.4(−16)
2	2.3(−16)	6.8(−16)	6.8(−16)	2.3(−16)	6.9(−16)	6.9(−16)	0.0	3.4(−16)
3	1.0(−15)	5.6(−16)	4.5(−16)	6.8(−16)	6.5(−16)	6.5(−16)	1.5(−15)	1.3(−15)
4	5.6(−16)	0.0	5.6(−16)	1.9(−16)	2.2(−16)	4.5(−16)	1.1(−16)	7.9(−16)
5	4.0(−16)	1.3(−16)	6.7(−16)	5.2(−15)	1.6(−15)	1.1(−14)	8.9(−14)	5.0(−13)
Average	5.3(−16)	3.8(−16)	7.3(−16)	1.2(−15)	6.8(−16)	2.1(−15)	1.3(−14)	7.1(−14)

Next, we discuss the accuracy of the B-spline expansion of $2p$- and $3d$-STFs. The relative errors of $I^{\nu}(2, \zeta)$ and $I^{\nu}(3, \zeta)$ are summarized in Tables 3-4 and Tables 5-6, respectively. The B-spline sets with K=9 and 11 yield large relative errors for $I^{\nu}(2, \zeta)$ and $I^{\nu}(3, \zeta)$ with ν = 4 and 5, regardless with ζ. Accurate calculations of $I^{\nu}(2, \zeta)$ and $I^{\nu}(3, \zeta)$ require the B-spline sets with $K \geq 13$ and $K \geq 15$, respectively. The relative errors of $I^{\nu}(2, \zeta)$ and $I^{\nu}(3, \zeta)$ also depend on the values of R as $I^{\nu}(1, \zeta)$. B-spline sets with R = 60 are suitable for the expansion of $2p$- and $3d$-STFs.

Table 3: Relative errors of transformed integrals $I^{\nu}(2, \zeta)$ for ζ= 0.5 and 1. $A(B)$ implies $A \times 10^{B}$.

	ζ = 0.5				ζ = 1			
ν	R=40	R=60	R=80	R=100	R=40	R=60	R=80	R=100
K = 9								
−1	5.5(−14)	1.5(−16)	8.9(−16)	4.4(−16)	5.9(−16)	1.5(−16)	5.9(−16)	5.9(−16)
0	5.6(−13)	5.9(−16)	5.9(−16)	5.9(−16)	4.4(−16)	3.0(−16)	7.4(−16)	3.0(−16)
1	4.6(−12)	1.2(−16)	5.9(−16)	2.4(−16)	2.4(−16)	5.9(−16)	7.1(−16)	3.6(−16)
2	3.2(−11)	1.3(−15)	6.3(−16)	1.9(−15)	0.0	1.4(−15)	3.0(−15)	2.2(−15)
3	1.9(−10)	3.4(−15)	5.1(−15)	8.5(−15)	1.4(−15)	4.3(−15)	6.7(−15)	6.7(−15)
4	6.0(−03)	6.9(−05)	3.3(−06)	6.1(−07)	5.8(−05)	3.8(−06)	9.0(−07)	3.1(−07)
5	3.7(−02)	3.3(−04)	9.9(−06)	1.2(−06)	3.2(−04)	1.0(−05)	1.7(−06)	4.8(−07)
Average	6.1(−03)	5.6(−05)	1.9(−06)	2.6(−07)	5.3(−05)	2.0(−06)	3.8(−07)	1.1(−07)
K = 11								
−1	5.3(−14)	5.9(−16)	4.4(−16)	8.9(−16)	7.4(−16)	5.9(−16)	8.9(−16)	1.5(−16)
0	5.5(−13)	1.5(−16)	0.0	1.5(−16)	3.0(−16)	7.4(−16)	8.9(−16)	1.5(−15)
1	4.5(−12)	5.9(−16)	3.6(−16)	4.7(−16)	1.2(−16)	5.9(−16)	9.5(−16)	7.1(−16)
2	3.1(−11)	7.9(−16)	0.0	3.2(−16)	6.3(−16)	2.1(−15)	6.3(−16)	6.3(−16)
3	1.8(−10)	9.0(−16)	1.8(−16)	1.3(−15)	3.6(−16)	1.1(−15)	1.4(−15)	1.1(−15)
4	2.5(−06)	1.5(−09)	5.5(−11)	1.3(−11)	1.1(−09)	1.0(−10)	2.4(−11)	8.4(−12)
5	1.8(−05)	7.0(−09)	9.7(−11)	1.4(−11)	3.7(−09)	1.8(−10)	3.2(−11)	9.0(−12)
Average	2.9(−06)	1.2(−09)	2.2(−11)	3.8(−12)	6.9(−10)	4.0(−11)	8.1(−12)	2.5(−12)
K = 13								
−1	5.1(−14)	8.9(−16)	3.0(−16)	1.5(−16)	8.9(−16)	5.9(−16)	0.0	1.0(−15)
0	5.4(−13)	1.2(−15)	3.0(−16)	5.9(−16)	4.4(−16)	5.9(−16)	7.4(−16)	5.9(−16)
1	4.4(−12)	4.7(−16)	3.6(−16)	1.2(−16)	4.7(−16)	1.2(−15)	0.0	4.7(−16)
2	3.0(−11)	0.0	9.5(−16)	0.0	3.2(−16)	0.0	7.9(−16)	6.3(−16)
3	1.8(−10)	9.0(−16)	0.0	0.0	3.6(−16)	1.8(−16)	3.6(−16)	5.4(−16)
4	1.0(−09)	3.4(−13)	2.1(−14)	1.6(−15)	6.8(−14)	2.7(−15)	3.6(−16)	1.3(−15)
5	1.1(−08)	2.5(−12)	1.5(−13)	9.8(−15)	1.0(−12)	2.9(−14)	0.0	1.6(−16)
Average	1.7(−09)	4.1(−13)	2.5(−14)	1.8(−15)	1.6(−13)	4.9(−15)	3.2(−16)	6.7(−16)
K = 15								
−1	5.2(−14)	5.9(−16)	1.5(−16)	7.4(−16)	5.9(−16)	1.5(−16)	3.0(−16)	1.6(−15)
0	5.3(−13)	5.9(−16)	8.9(−16)	4.4(−16)	5.9(−16)	7.4(−16)	3.0(−16)	4.4(−16)
1	4.4(−12)	8.3(−16)	1.3(−15)	2.4(−16)	4.7(−16)	1.2(−16)	5.9(−16)	0.0
2	3.0(−11)	7.9(−16)	1.6(−16)	0.0	4.7(−16)	1.3(−15)	1.6(−16)	1.1(−15)
3	1.8(−10)	1.3(−15)	5.4(−16)	0.0	5.4(−16)	1.8(−16)	5.4(−16)	7.2(−16)
4	9.0(−10)	9.0(−16)	5.4(−16)	7.2(−16)	1.8(−16)	1.8(−16)	2.0(−15)	1.3(−15)
5	4.1(−09)	8.0(−16)	9.6(−16)	9.6(−16)	1.3(−15)	3.2(−16)	3.2(−16)	9.6(−16)
Average	7.5(−10)	8.2(−16)	6.5(−16)	4.4(−16)	5.9(−16)	4.2(−16)	6.0(−16)	8.8(−16)

Table 4: Relative errors of transformed integrals $I^{\nu}(2, \zeta)$ for ζ= 10 and 50. $A(B)$ implies $A \times 10^{B}$.

	ζ = 10				ζ = 50			
ν	R=40	R=60	R=80	R=100	R=40	R=60	R=80	R=100
K = 9								
−1	1.1(−15)	5.4(−16)	1.3(−15)	7.2(−16)	6.6(−16)	4.4(−16)	2.2(−16)	0.0
0	2.3(−16)	2.3(−16)	3.4(−16)	0.0	5.2(−16)	1.7(−16)	1.7(−16)	5.2(−16)
1	7.9(−16)	1.1(−16)	2.3(−16)	5.6(−16)	1.1(−15)	0.0	4.3(−16)	6.5(−16)
2	1.1(−15)	1.7(−15)	1.5(−15)	3.2(−15)	1.3(−15)	1.3(−15)	1.7(−15)	2.7(−15)
3	3.0(−15)	4.0(−15)	5.8(−15)	8.3(−15)	2.4(−15)	3.6(−15)	6.2(−15)	8.2(−15)
4	3.0(−06)	5.6(−07)	1.8(−07)	7.8(−08)	5.9(−07)	1.5(−07)	5.9(−08)	3.0(−08)
5	7.4(−06)	9.9(−07)	2.5(−07)	9.2(−08)	1.1(−06)	2.0(−07)	6.6(−08)	2.9(−08)
Average	1.5(−06)	2.2(−07)	6.2(−08)	2.4(−08)	2.4(−07)	5.1(−08)	1.8(−08)	8.3(−09)
K = 11								
−1	3.6(−16)	7.2(−16)	1.8(−16)	1.8(−16)	4.4(−16)	0.0	0.0	6.6(−16)
0	1.1(−16)	2.3(−16)	6.8(−16)	4.5(−16)	5.2(−16)	1.0(−15)	5.2(−16)	5.2(−16)
1	6.8(−16)	4.5(−16)	3.4(−16)	2.3(−16)	2.2(−16)	2.2(−16)	4.3(−16)	2.2(−16)
2	1.9(−16)	5.6(−16)	3.8(−16)	0.0	4.5(−16)	0.0	1.1(−16)	1.1(−16)
3	4.0(−16)	1.3(−16)	1.3(−16)	4.0(−16)	1.0(−15)	0.0	2.0(−16)	4.0(−16)
4	1.1(−10)	2.0(−11)	6.4(−12)	2.8(−12)	2.6(−11)	6.6(−12)	2.6(−12)	1.3(−12)
5	1.9(−10)	2.6(−11)	6.6(−12)	2.4(−12)	3.6(−11)	6.7(−12)	2.2(−12)	9.5(−13)
Average	4.3(−11)	6.5(−12)	1.9(−12)	7.3(−13)	8.9(−12)	1.9(−12)	6.8(−13)	3.2(−13)
K = 13								
−1	3.6(−16)	2.2(−15)	3.6(−16)	7.2(−16)	8.8(−16)	2.2(−16)	0.0	1.3(−15)
0	1.1(−15)	2.3(−16)	1.1(−16)	2.3(−16)	1.0(−15)	6.9(−16)	3.4(−16)	5.2(−16)
1	2.3(−16)	9.0(−16)	0.0	0.0	1.5(−15)	2.2(−16)	2.2(−16)	1.1(−15)
2	5.6(−16)	1.9(−16)	1.5(−15)	7.5(−16)	9.0(−16)	2.2(−16)	3.4(−16)	1.1(−16)
3	2.7(−16)	1.3(−15)	0.0	0.0	1.6(−15)	6.0(−16)	3.4(−15)	2.0(−16)
4	1.7(−16)	8.4(−16)	1.0(−15)	1.7(−15)	1.3(−15)	1.7(−15)	6.3(−16)	9.4(−16)
5	1.5(−15)	1.3(−15)	7.5(−16)	3.7(−16)	1.7(−15)	6.1(−15)	1.2(−13)	4.9(−13)
Average	6.0(−16)	1.0(−15)	5.3(−16)	5.4(−16)	1.3(−15)	1.4(−15)	1.8(−14)	7.0(−14)
K = 15								
−1	3.6(−16)	1.8(−16)	9.0(−16)	1.8(−16)	4.4(−16)	1.5(−15)	8.8(−16)	0.0
0	7.9(−16)	7.9(−16)	4.5(−16)	3.4(−16)	3.4(−16)	1.7(−16)	1.7(−16)	6.9(−16)
1	1.1(−16)	6.8(−16)	3.4(−16)	4.5(−16)	2.2(−16)	1.7(−15)	6.5(−16)	8.6(−16)
2	2.4(−15)	1.1(−15)	0.0	5.6(−16)	1.1(−15)	1.5(−15)	1.1(−15)	5.6(−16)
3	4.0(−16)	1.1(−15)	1.3(−16)	2.3(−15)	0.0	1.4(−15)	8.0(−16)	1.8(−15)
4	1.7(−16)	1.3(−15)	1.7(−16)	1.7(−16)	1.3(−15)	1.7(−15)	1.9(−15)	1.6(−16)
5	7.5(−16)	3.5(−15)	9.3(−15)	1.9(−14)	3.5(−15)	7.8(−15)	3.8(−13)	7.3(−14)
Average	7.2(−16)	1.2(−15)	1.6(−15)	3.3(−15)	9.8(−16)	2.3(−15)	5.5(−14)	1.1(−14)

Table 5: Relative errors of transformed integrals $I^{\nu}(3, \zeta)$ for ζ= 0.5 and 1. $A(B)$ implies $A \times 10^{B}$.

	ζ = 0.5				ζ = 1			
ν	R=40	R=60	R=80	R=100	R=40	R=60	R=80	R=100
K = 9								
−1	4.6(−12)	1.2(−16)	7.1(−16)	5.9(−16)	8.3(−16)	1.2(−16)	7.1(−16)	1.1(−15)
0	3.2(−11)	4.7(−16)	1.6(−16)	3.2(−16)	4.7(−16)	0.0	0.0	1.6(−16)
1	1.9(−10)	3.6(−16)	0.0	1.3(−15)	7.2(−16)	1.8(−16)	7.2(−16)	5.4(−16)
2	9.5(−10)	4.2(−15)	6.0(−15)	8.5(−15)	1.1(−15)	3.6(−15)	7.2(−15)	8.8(−15)
3	4.4(−09)	1.3(−14)	2.0(−14)	2.9(−14)	6.9(−15)	1.3(−14)	2.1(−14)	2.9(−14)
4	8.9(−03)	1.4(−04)	4.9(−06)	6.1(−07)	8.9(−05)	3.2(−06)	6.6(−07)	2.2(−07)
5	4.7(−02)	6.0(−04)	1.5(−05)	1.3(−06)	5.2(−04)	9.1(−06)	1.3(−06)	3.4(−07)
Average	7.9(−03)	1.0(−04)	2.9(−06)	2.7(−07)	8.7(−05)	1.8(−06)	2.8(−07)	8.0(−08)
K = 11								
−1	4.5(−12)	8.3(−16)	4.7(−16)	5.9(−16)	8.3(−16)	2.4(−16)	4.7(−16)	4.7(−16)
0	3.1(−11)	0.0	1.6(−16)	1.3(−15)	3.2(−16)	0.0	6.3(−16)	1.6(−16)
1	1.8(−10)	9.0(−16)	1.8(−16)	9.0(−16)	7.2(−16)	9.0(−16)	3.6(−16)	5.4(−16)
2	9.3(−10)	3.6(−16)	1.8(−16)	1.1(−15)	3.6(−16)	9.0(−16)	9.0(−16)	5.4(−16)
3	4.3(−09)	8.0(−16)	1.8(−15)	1.9(−15)	4.8(−16)	1.6(−16)	1.9(−15)	2.2(−15)
4	6.7(−06)	4.8(−09)	4.5(−11)	8.6(−12)	1.1(−09)	6.4(−11)	1.4(−11)	4.4(−12)
5	4.0(−05)	2.4(−08)	7.2(−11)	1.2(−11)	3.8(−09)	1.5(−10)	2.0(−11)	4.4(−12)
Average	6.6(−06)	4.1(−09)	1.7(−11)	3.0(−12)	6.9(−10)	3.0(−11)	4.7(−12)	1.3(−12)
K = 13								
−1	4.4(−12)	8.3(−16)	0.0	1.2(−16)	1.8(−15)	1.2(−16)	7.1(−16)	0.0
0	3.0(−11)	4.7(−16)	3.2(−16)	6.3(−16)	6.3(−16)	3.2(−16)	1.3(−15)	3.2(−16)
1	1.8(−10)	5.4(−16)	9.0(−16)	1.8(−16)	3.6(−16)	7.2(−16)	9.0(−16)	0.0
2	9.1(−10)	5.4(−16)	1.8(−16)	1.6(−15)	1.4(−15)	1.1(−15)	7.2(−16)	3.6(−16)
3	4.2(−09)	1.6(−16)	0.0	0.0	1.4(−15)	4.8(−16)	1.3(−15)	2.4(−15)
4	1.1(−08)	1.4(−12)	1.6(−13)	4.3(−14)	1.1(−12)	2.8(−14)	0.0	1.2(−15)
5	2.4(−08)	8.5(−12)	9.7(−13)	2.7(−13)	1.3(−11)	3.5(−13)	1.4(−14)	2.8(−15)
Average	5.7(−09)	1.4(−12)	1.6(−13)	4.5(−14)	2.1(−12)	5.4(−14)	2.7(−15)	1.0(−15)
K = 15								
−1	4.4(−12)	7.1(−16)	1.2(−16)	4.7(−16)	5.9(−16)	8.3(−16)	5.9(−16)	5.9(−16)
0	3.0(−11)	3.2(−16)	0.0	7.9(−16)	1.3(−15)	4.7(−16)	1.7(−15)	3.2(−16)
1	1.8(−10)	3.6(−16)	5.4(−16)	3.6(−16)	1.3(−15)	9.0(−16)	1.6(−15)	3.6(−16)
2	9.0(−10)	1.1(−15)	7.2(−16)	1.1(−15)	3.6(−16)	3.6(−16)	7.2(−16)	7.2(−16)
3	4.1(−09)	6.4(−16)	4.8(−16)	6.4(−16)	1.6(−16)	8.0(−16)	1.6(−16)	3.2(−16)
4	1.7(−08)	3.8(−16)	1.3(−15)	1.3(−16)	3.8(−16)	0.0	0.0	2.6(−16)
5	6.4(−08)	8.6(−15)	1.9(−16)	7.5(−16)	2.1(−15)	1.7(−15)	9.3(−16)	1.3(−15)
Average	1.2(−08)	1.7(−15)	4.8(−16)	6.0(−16)	8.7(−16)	7.2(−16)	8.2(−16)	5.5(−16)

Table 6: Relative errors of transformed integrals $I^{\nu}(3, \zeta)$ for ζ= 10 and 50. $A(B)$ implies $A \times 10^{B}$.

	ζ = 10				ζ = 50			
ν	R=40	R=60	R=80	R=100	R=40	R=60	R=80	R=100
K = 9								
−1	4.5(−16)	3.4(−16)	3.4(−16)	1.1(−16)	0.0	4.3(−16)	4.3(−16)	4.3(−16)
0	0.0	5.6(−16)	1.5(−15)	7.5(−16)	1.3(−15)	9.0(−16)	0.0	5.6(−16)
1	6.7(−16)	2.7(−16)	0.0	8.1(−16)	2.0(−16)	6.0(−16)	6.0(−16)	8.0(−16)
2	1.8(−15)	4.0(−15)	5.5(−15)	8.9(−15)	3.1(−15)	4.9(−15)	6.1(−15)	8.6(−15)
3	7.5(−15)	1.3(−14)	2.0(−14)	3.0(−14)	6.3(−15)	1.3(−14)	2.1(−14)	2.8(−14)
4	2.4(−06)	4.3(−07)	1.3(−07)	5.5(−08)	4.8(−07)	1.1(−07)	4.3(−08)	2.1(−08)
5	6.0(−06)	7.5(−07)	1.9(−07)	6.5(−08)	8.8(−07)	1.6(−07)	4.8(−08)	2.0(−08)
Average	1.2(−06)	1.7(−07)	4.5(−08)	1.7(−08)	1.9(−07)	3.9(−08)	1.3(−08)	5.9(−09)
K = 11								
−1	4.5(−16)	1.1(−16)	9.0(−16)	5.6(−16)	6.5(−16)	8.6(−16)	2.2(−16)	0.0
0	1.9(−16)	3.8(−16)	2.1(−15)	1.9(−16)	0.0	3.4(−16)	9.0(−16)	3.4(−16)
1	0.0	4.0(−16)	6.7(−16)	1.3(−16)	2.0(−16)	2.0(−16)	2.0(−16)	4.0(−16)
2	1.7(−16)	1.0(−15)	1.3(−15)	6.7(−16)	3.1(−16)	6.3(−16)	1.1(−15)	9.4(−16)
3	0.0	7.5(−16)	1.5(−15)	1.5(−15)	0.0	4.3(−16)	1.3(−15)	3.0(−15)
4	6.8(−11)	1.2(−11)	3.6(−12)	1.5(−12)	1.7(−11)	3.8(−12)	1.4(−12)	6.8(−13)
5	1.2(−10)	1.5(−11)	3.7(−12)	1.3(−12)	2.3(−11)	4.0(−12)	1.2(−12)	6.3(−13)
Average	2.7(−11)	3.8(−12)	1.0(−12)	3.9(−13)	5.6(−12)	1.1(−12)	3.8(−13)	1.9(−13)
K = 13								
−1	6.8(−16)	2.3(−16)	1.1(−16)	1.1(−16)	1.5(−15)	6.5(−16)	1.1(−15)	4.3(−16)
0	5.6(−16)	1.9(−16)	3.8(−16)	1.9(−16)	1.1(−16)	9.0(−16)	2.2(−16)	2.2(−16)
1	5.4(−16)	8.1(−16)	1.2(−15)	5.4(−16)	2.0(−16)	4.0(−16)	2.0(−16)	6.0(−16)
2	8.4(−16)	5.0(−16)	1.8(−15)	6.7(−16)	3.1(−16)	1.6(−16)	6.3(−16)	4.7(−16)
3	1.9(−15)	5.6(−16)	0.0	1.9(−16)	4.3(−16)	8.7(−16)	1.1(−15)	4.3(−16)
4	5.6(−16)	1.9(−16)	1.9(−15)	2.4(−15)	0.0	4.1(−16)	1.1(−15)	3.0(−15)
5	5.1(−16)	5.1(−16)	5.9(−14)	2.7(−13)	1.7(−15)	1.2(−13)	5.6(−15)	1.1(−12)
Average	7.9(−16)	4.3(−16)	9.2(−15)	3.9(−14)	6.1(−16)	1.7(−14)	1.4(−15)	1.6(−13)
K = 15								
−1	4.5(−16)	7.9(−16)	1.1(−16)	0.0	4.3(−16)	6.5(−16)	2.2(−16)	4.3(−16)
0	7.5(−16)	5.6(−16)	3.8(−16)	1.9(−16)	7.9(−16)	0.0	2.2(−16)	6.7(−16)
1	9.4(−16)	8.1(−16)	1.2(−15)	8.1(−16)	6.0(−16)	8.0(−16)	2.0(−16)	0.0
2	5.0(−16)	0.0	1.7(−16)	3.4(−16)	3.1(−16)	9.4(−16)	0.0	1.9(−15)
3	3.7(−16)	3.7(−16)	0.0	1.9(−16)	3.0(−15)	1.7(−15)	1.1(−15)	8.7(−16)
4	9.3(−16)	1.9(−16)	4.9(−15)	1.9(−14)	8.2(−16)	1.0(−14)	4.3(−14)	2.4(−13)
5	1.0(−15)	1.0(−15)	4.9(−13)	2.5(−12)	1.1(−13)	4.1(−12)	2.2(−11)	1.5(−10)
Average	7.1(−16)	5.3(−16)	7.1(−14)	3.6(−13)	1.7(−14)	5.9(−13)	3.1(−12)	2.2(−11)

From the above discussion, we conclude that the B-spline set with K = 15 and R = 60 can accurately expand 1s-, 2p-, and 3d-STFs with $0.5 \le \zeta \le 50$, and can yield accurate $I^{\nu}(n, \zeta)$ values. Tables 7-9 summarize $I^{\nu}(n, \zeta)$ over the B-spline set with K = 15 and R = 60, along with the exact values. Most of the $I^{\nu}(n, \zeta)$ values are in agreement to 14-15 digits of the exact values. Therefore, the B-spline set with these parameters enable accurate calculation of the transformed many-electron integrals. Work for many-electron integrals over the B-spline set is in progress.

Table 7: Transformed integrals $I^{\nu}(1, \zeta)$ and exact integrals $I^{\nu}_{\mathrm{STF}}(1, \zeta)$ obtained using the 100-term B-spline set with K=15 and R=60.

ν	$I^{\nu}(1, \zeta)$	$I^{\nu}_{\mathrm{STF}}(1, \zeta)$
ζ=0.5		
−1	0.1000 0000 0000 0001E+01	0.1000 0000 0000 0000E+01
0	0.1999 9999 9999 9999E+01	0.2000 0000 0000 0000E+01
1	0.5999 9999 9999 9999E+01	0.6000 0000 0000 0000E+01
2	0.2399 9999 9999 9999E+02	0.2400 0000 0000 0000E+02
3	0.1200 0000 0000 0001E+03	0.1200 0000 0000 0000E+03
4	0.7200 0000 0000 0011E+03	0.7200 0000 0000 0000E+03
5	0.5040 0000 0000 0007E+04	0.5040 0000 0000 0000E+04
ζ=1		
−1	0.2500 0000 0000 0002E+00	0.2500 0000 0000 0000E+00
0	0.2500 0000 0000 0001E+00	0.2500 0000 0000 0000E+00
1	0.3750 0000 0000 0001E+00	0.3750 0000 0000 0000E+00
2	0.7499 9999 9999 9999E+00	0.7500 0000 0000 0000E+00
3	0.1875 0000 0000 0000E+01	0.1875 0000 0000 0000E+01
4	0.5624 9999 9999 9997E+01	0.5625 0000 0000 0000E+01
5	0.1968 7500 0000 0000E+02	0.1968 7500 0000 0000E+02
ζ=10		
−1	0.2500 0000 0000 0000E−02	0.2500 0000 0000 0000E−02
0	0.2500 0000 0000 0000E−03	0.2500 0000 0000 0000E−03
1	0.3750 0000 0000 0004E−04	0.3750 0000 0000 0000E−04
2	0.7499 9999 9999 9995E−05	0.7500 0000 0000 0000E−05
3	0.1875 0000 0000 0001E−05	0.1875 0000 0000 0000E−05
4	0.5625 0000 0000 0000E−06	0.5625 0000 0000 0000E−06
5	0.1968 7500 0000 0000E−06	0.1968 7500 0000 0000E−06
ζ=50		
−1	0.1000 0000 0000 0000E−03	0.1000 0000 0000 0000E−03
0	0.2000 0000 0000 0002E−05	0.2000 0000 0000 0000E−05
1	0.5999 9999 9999 9998E−07	0.5999 9999 9999 9999E−07
2	0.2400 0000 0000 0002E−08	0.2400 0000 0000 0000E−08
3	0.1200 0000 0000 0001E−09	0.1200 0000 0000 0000E−09
4	0.7200 0000 0000 0003E−11	0.7200 0000 0000 0000E−11
5	0.5040 0000 0000 0056E−12	0.5040 0000 0000 0000E−12

Table 8: Transformed integrals $I^{\nu}(2, \zeta)$ and exact integrals $I^{\nu}_{\mathrm{STF}}(2, \zeta)$ obtained using the 100-term *B*-spline set with K=15 and R=60.

ν	$I^{\nu}(2,\zeta)$	$I^{\nu}_{\mathrm{STF}}(2,\zeta)$
ζ=0.5		
−1	0.6000 0000 0000 0004E+01	0.6000 0000 0000 0000E+01
0	0.2400 0000 0000 0001E+02	0.2400 0000 0000 0000E+02
1	0.1200 0000 0000 0001E+03	0.1200 0000 0000 0000E+03
2	0.7200 0000 0000 0006E+03	0.7200 0000 0000 0000E+03
3	0.5039 9999 9999 9994E+04	0.5040 0000 0000 0000E+04
4	0.4032 0000 0000 0004E+05	0.4032 0000 0000 0000E+05
5	0.3628 8000 0000 0003E+06	0.3628 8000 0000 0000E+06
ζ=1		
−1	0.3750 0000 0000 0001E+00	0.3750 0000 0000 0000E+00
0	0.7499 9999 9999 9994E+00	0.7500 0000 0000 0000E+00
1	0.1875 0000 0000 0000E+01	0.1875 0000 0000 0000E+01
2	0.5625 0000 0000 0007E+01	0.5625 0000 0000 0000E+01
3	0.1968 7500 0000 0000E+02	0.1968 7500 0000 0000E+02
4	0.7874 9999 9999 9999E+02	0.7875 0000 0000 0000E+02
5	0.3543 7500 0000 0001E+03	0.3543 7500 0000 0000E+03
ζ=10		
−1	0.3750 0000 0000 0000E−04	0.3750 0000 0000 0000E−04
0	0.7500 0000 0000 0006E−05	0.7500 0000 0000 0000E−05
1	0.1875 0000 0000 0001E−05	0.1875 0000 0000 0000E−05
2	0.5625 0000 0000 0006E−06	0.5625 0000 0000 0000E−06
3	0.1968 7500 0000 0002E−06	0.1968 7500 0000 0000E−06
4	0.7875 0000 0000 0011E−07	0.7875 0000 0000 0000E−07
5	0.3543 7500 0000 0013E−07	0.3543 7500 0000 0000E−07
ζ=50		
−1	0.6000 0000 0000 0009E−07	0.5999 9999 9999 9999E−07
0	0.2400 0000 0000 0000E−08	0.2400 0000 0000 0000E−08
1	0.1200 0000 0000 0002E−09	0.1200 0000 0000 0000E−09
2	0.7200 0000 0000 0011E−11	0.7200 0000 0000 0000E−11
3	0.5040 0000 0000 0007E−12	0.5040 0000 0000 0000E−12
4	0.4032 0000 0000 0007E−13	0.4032 0000 0000 0000E−13
5	0.3628 8000 0000 0029E−14	0.3628 8000 0000 0000E−14

Table 9: Transformed integrals $I^{\nu}(3, \zeta)$ and exact integrals $I^{\nu}_{\mathrm{STF}}(3, \zeta)$ obtained using the 100-term B-spline set with K=15 and R=60.

ν	$I^{\nu}(3,\zeta)$	$I^{\nu}_{\mathrm{STF}}(3,\zeta)$
ζ=0.5		
−1	0.1200 0000 0000 0001E+03	0.1200 0000 0000 0000E+03
0	0.7199 9999 9999 9998E+03	0.7200 0000 0000 0000E+03
1	0.5039 9999 9999 9998E+04	0.5040 0000 0000 0000E+04
2	0.4032 0000 0000 0004E+05	0.4032 0000 0000 0000E+05
3	0.3628 8000 0000 0002E+06	0.3628 8000 0000 0000E+06
4	0.3628 7999 9999 9999E+07	0.3628 8000 0000 0000E+07
5	0.3991 6799 9999 9966E+08	0.3991 6800 0000 0000E+08
ζ=1		
−1	0.1875 0000 0000 0002E+01	0.1875 0000 0000 0000E+01
0	0.5625 0000 0000 0003E+01	0.5625 0000 0000 0000E+01
1	0.1968 7499 9999 9998E+02	0.1968 7500 0000 0000E+02
2	0.7874 9999 9999 9997E+02	0.7875 0000 0000 0000E+02
3	0.3543 7499 9999 9997E+03	0.3543 7500 0000 0000E+03
4	0.1771 8750 0000 0000E+04	0.1771 8750 0000 0000E+04
5	0.9745 3125 0000 0016E+04	0.9745 3125 0000 0000E+04
ζ=10		
−1	0.1875 0000 0000 0002E−05	0.1875 0000 0000 0000E−05
0	0.5625 0000 0000 0003E−06	0.5625 0000 0000 0000E−06
1	0.1968 7500 0000 0002E−06	0.1968 7500 0000 0000E−06
2	0.7875 0000 0000 0000E−07	0.7875 0000 0000 0000E−07
3	0.3543 7500 0000 0002E−07	0.3543 7500 0000 0000E−07
4	0.1771 8750 0000 0000E−07	0.1771 8750 0000 0000E−07
5	0.9745 3125 0000 0009E−08	0.9745 3124 9999 9999E−08
ζ=50		
−1	0.1199 9999 9999 9999E−09	0.1200 0000 0000 0000E−09
0	0.7200 0000 0000 0000E−11	0.7200 0000 0000 0000E−11
1	0.5039 9999 9999 9996E−12	0.5040 0000 0000 0000E−12
2	0.4031 9999 9999 9996E−13	0.4032 0000 0000 0000E−13
3	0.3628 8000 0000 0006E−14	0.3628 8000 0000 0000E−14
4	0.3628 8000 0000 0037E−15	0.3628 8000 0000 0000E−15
5	0.3991 6800 0001 6304E−16	0.3991 6800 0000 0000E−16

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