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The Fourier Transform of a Two-center Product of Exponential-type Functions and Its Efficient Evaluation

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We analyze the analytical and numerical properties of the hitherto known formulas of the Fourier transform of a two-center product of exponentially declining functions (exponential-type functions, ETFs) which are derived with the help of the Fourier convolution theorem and Feynman's identity. In detail, we consider B functions which are a special class of ETFs having advantageous properties under Fourier transformation. Other ETFs (orbitals) can be expressed in terms of B functions by linear combinations. In our derivations we use the properties of the differential operator $\mathcal{Y}_l^m(\mathbf{V})$ specifying a solid harmonic whose argument is the nabla operator $\partial/\partial\mathbf{r}$ instead of the vector $\mathbf{r}$ in order to generate multicenter integrals over nonscalar functions from integrals over scalar functions. Applying the generating differential operator $\mathcal{Y}_l^m(\mathbf{V})$ we obtain a recently derived new formula for the Fourier transform of a two-center product of B functions in a much more straightforward manner. Furthermore, we present an efficient procedure to compute this new formula which is valid for arbitrary quantum numbers and exponential parameters and report various numerical test values.

I. INTRODUCTION

A matrix element which has the form of a Fourier transform of a product of two basis functions separated by a distance vector $\mathbf{R}$ plays an important role in various quantum-mechanical approximations. Integrals of this type occur in the theory of electron and x-ray scattering from molecules in the first Born approximation. For example, the coherent and incoherent intensities for scattered x-rays and electrons depend on integrals of the type [1–3]

$$I = \int d\mathbf{r}\, \Phi_1^*(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}} \Phi_2(\mathbf{r}-\mathbf{R}), \tag{1.1}$$

if the many-electron wave function for the molecule is taken as an antisymmetric product of one-electron functions. Φ_1 and Φ_2 are centered at two different nuclei, separated by $\mathbf{R}$. Depending on the choice of $\mathbf{R}$, Φ_1 and Φ_2 can be centered at the various nuclei of the molecule. The integral (1.1) also plays an important role in the

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theory of molecular multicenter integrals which occur inevitably in calculations of the electronic structure of molecules using the LCAO-MO method. It forms the basic building block of multicenter electron repulsion integrals if one evaluates these matrix elements with the help of the Fourier transformation method [4, 5]. The evaluation of the three-center nuclear attraction integrals can be treated in a similar way using the Fourier convolution theorem [5]. The two-center overlap integral follows as a special case of the Fourier transform of a two-center product with zero transformation vector **k**.

Several expressions have been given in the literature for the Fourier transform of a two-center charge distribution in the most common bases, i.e., exponential-type orbitals (ETOs), usually Slater-type orbitals (STOs), and Gaussian-type orbitals (GTOs). For ETOs, surely the more difficult case, there exist two main methods to evaluate the two-center integral (1.1): (i) the application of special coordinate systems and (ii) the application of the Fourier convolution theorem in connection with the so-called Feynman identity [6]. Bentley and Stuart [7] employed the prolate spheroidal coordinate system [8] and expanded the plane-wave factor $e^{-i\mathbf{k}\cdot\mathbf{r}}$ in terms of spheroidal wavefunctions. They obtained an analytical expression which holds for Slater-type orbitals with arbitrary quantum numbers and exponential (scaling) parameters. However, their expression contains five infinite sums and requires a number of recursion relations for the evaluation of various integrals and coefficients. Therefore, it is not clear how useful this method is with regard to rapid convergence of the summations and stability of the recursion relations. Another general expression for the integral (1.1) with STOs as basis functions Φ_1 and Φ_2 was derived recently by Junker [9, 10] using elliptical coordinates. Junker's expression (involving a 1-dimensional semi-infinite integration) is a generalization of McCarroll's approach [11] to non-spherical orbitals. It depends upon the orientation of the coordinate system and is not suited for a partial-wave decomposition, a fact which is important for an application of the Fourier transforms of a two-center charge distribution in the evaluation of one- and two-electron multicenter integrals [5]. For *s*-type orbitals Bonham *et al.* [4, 12] derived an expression involving a 1-dimensional finite integration which does not depend on the orientation of the coordinate axes in space using the Fourier convolution theorem in connection with the Feynman identity. Monkhorst and Harris [13] developed a computational scheme for the accurate calculation of this expression. Later, on the basis of the formula of Bonham *et al.*, Guidotti *et al.* [14] derived expressions which are applicable to states of higher angular momentum. They gave one special formula for each combination of two STOs. Their formulas are obtained by differentiation with respect to the Cartesian components of the transformation vector **k**. Their derivation is based upon a special coordinate system, whose z axis coincides with the vector **R**. Recently Trivedi and Steinborn [5] derived a single general expression along the lines of Bonham *et al.*, for another basis set of ETOs, the so-called B functions [15], which is capable of angular momentum decomposition and is independent of the orientation of the coordinate axes. B functions can be expressed as linear combinations of STOs [16]. Therefore, Trivedi and Steinborn's

result is a generalization of the formulas discussed so far. Although B functions have a much more complicated analytical structure than STOs they seem to have much more appealing properties than STOs in multicenter problems. B functions have extremely compact convolution integrals [15, 17] as well as Coulomb integrals [15]. These advantageous properties can all be explained in terms of their simple Fourier transform [18].

In this article we give a new and simpler derivation of Trivedi and Steinborn's formula for the Fourier transform of a two-center product of B functions. For this purpose, we use a differentiation technique which is able to generate multicenter integrals over nonscalar B functions from integrals over scalar B functions. With this method analytical results for nonscalar functions with arbitrary integer quantum numbers can be derived much more easily. Furthermore, we present an efficient numerical method to calculate the Fourier transform of a two-center charge distribution described by the product of two B functions and report various numerical test values. Because of the fact that Slater-type orbitals are given by a linear combination of B functions, these results facilitate the applicability of the Fourier transform of a two-center charge density substantially.

II. Definitions and Basic Formulas

The ETOs used in this article are the B functions of Filter and Steinborn which are defined as follows [15]:

$$B_{n,l}^{m}(\alpha, \mathbf{r}) = [2^{n+l}(n+l)!]^{-1} \mathscr{Y}_l^m(\alpha \mathbf{r})\, \hat{k}_{n-1/2}(\alpha r) \tag{2.1a}$$

$$n \in \mathbb{Z}, \qquad -l \leqslant n < \infty. \tag{2.1b}$$

Here, $\mathscr{Y}_l^m(\mathbf{r})$ stands for the regular solid harmonic

$$\mathscr{Y}_l^m(\mathbf{r}) = r^l Y_l^m(\theta, \phi). \tag{2.2}$$

The spherical harmonics $Y_l^m(\theta, \phi)$ are defined with the use of the phase conventions of Condon and Shortley [19], i.e., they are given by the expression [20]

$$Y_l^m(\theta, \phi) = i^{m+|m|} \left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{1/2} P_l^{|m|}(\cos\theta)\, e^{im\phi}. \tag{2.3}$$

Here, $P_l^{|m|}(\cos\theta)$ is an associated Legendre polynomial [21]

$$P_l^m(x) = (1-x^2) \frac{d^{l+m}}{dx^{l+m}} \frac{(x^2-1)^l}{2^l l!}. \tag{2.4}$$

The radial part of the B function is described by a reduced Bessel function (RBF) [22, 23] which is defined by

$$\hat{k}_\nu(z) = (2/\pi)^{1/2} z^\nu K_\nu(z), \tag{2.5}$$

where $K_\nu(z)$ is the modified Bessel function of the second kind [24]. The RBFs satisfy the following three-term recurrence relation [25]:

$$\hat{k}_{\nu+1}(z) = 2\nu\hat{k}_\nu(z) + z^2\hat{k}_{\nu-1}(z) \tag{2.6}$$

As the RBFs are the dominant solution of this difference equation, the recurrence formula (2.6) may safely be used in the upward direction. In the case of half-integral orders, $\nu = n + \frac{1}{2}$, $n \in \mathbb{N}_0$, the RBFs can be represented by an exponential multiplied by a terminating confluent hypergeometric function ${}_1F_1$ [26]:

$$\hat{k}_{n+1/2}(z) = 2^n(1/2)_n e^{-z}\,{}_1F_1(-n; -2n; 2z) \tag{2.7}$$

Here, $(a)_n$ stands for the Pochhammer symbol [27] which may be defined in terms of the gamma function $\Gamma(z)$ according to

$$(a)_n = \Gamma(a+n)/\Gamma(a) = a\cdot(a+1)\cdots(a+n-1), \qquad (a)_0 = 1. \tag{2.8}$$

The normalized STOs are written as

$$\chi^m_{n,l}(\alpha, \mathbf{r}) = N(n, \alpha)\, e^{-\alpha r}(\alpha r)^{n-1} Y^m_l(\theta, \phi) \tag{2.9a}$$

with

$$N(n, \alpha) = \alpha^{-n+1}[(2\alpha)^{2n+1}/(2n)!]^{1/2}, \tag{2.9b}$$

$\alpha > 0$ and integer n, l, and m.

In the following text we shall use the symmetric version of the Fourier transformation, i.e., a given absolutely integrable function $f \in L^1(\mathbb{R}^3)$ and its Fourier transform $\bar{f}(\mathbf{p}) \in L^1(\mathbb{R}^3)$ are connected by the relationships [28]:

$$\bar{f}(\mathbf{p}) = (2\pi)^{-3/2} \int \exp(-i\mathbf{p}\cdot\mathbf{r})\, f(\mathbf{r})\, d\mathbf{r}, \tag{2.10}$$

$$f(\mathbf{r}) = (2\pi)^{-3/2} \int \exp(i\mathbf{r}\cdot\mathbf{p})\, \bar{f}(\mathbf{p})\, d\mathbf{p}. \tag{2.11}$$

The two-centric convolution integral of two functions f, $g \in L^1(\mathbb{R}^3)$ can be transformed into the one-centric Fourier integral [29]:

$$\int d\mathbf{r}\, f(\mathbf{R}-\mathbf{r})\, g(\mathbf{r}) = \int d\mathbf{p}\, e^{i\mathbf{R}\cdot\mathbf{p}} \bar{f}(\mathbf{p})\, \bar{g}(\mathbf{p}), \tag{2.12}$$

where $\bar{f}$ and $\bar{g}$ are the Fourier transforms of f and g according to Eq. (2.10). The integral transformation Eq. (2.12) is called the Fourier convolution theorem and is closely related to the following integral transformation for the overlap integral of f and g:

$$\int d\mathbf{r}\, f^*(\mathbf{r})\, g(\mathbf{r}-\mathbf{R}) = \int d\mathbf{p}\, e^{-i\mathbf{R}\cdot\mathbf{p}} \bar{f}^*(\mathbf{p})\, \bar{g}(\mathbf{p}). \tag{2.13}$$

For the integral of three spherical harmonics, the so-called Gaunt coefficient [30], we write

$$\langle l_3 m_3 \mid l_2 m_2 \mid l_1 m_1 \rangle = \int Y_{l_3}^{m_3*}(\Omega)\, Y_{l_2}^{m_2}(\Omega)\, Y_{l_1}^{m_1}(\Omega)\, d\Omega. \tag{2.14}$$

The double factorial function is defined by

$$(2n)!! = 2 \times 4 \times \cdots \times (2n) = 2^n n!, \tag{2.15}$$

$$(2n-1)!! = 1 \times 3 \times \cdots \times (2n+1) = (1/2)_n 2^n, \tag{2.16}$$

$$0!! = 1!! = 1. \tag{2.17}$$

We want to mention that an STO can be expressed by B functions according to the following formula [31]

$$\chi_{n,l}^m(\alpha, \mathbf{r}) = N(n, \alpha) \sum_{p=\min p}^{n-l} \frac{(-1)^{n-l-p}(n-l)!2^{l+p}(l+p)!}{(2p-n+l)!(2n-2l-2p)!!} B_{p,l}^m(\alpha, \mathbf{r}), \tag{2.18}$$

$$\begin{aligned} \min p &= (n-l)/2, && \text{for} \quad n-l \text{ even}, \\ &= (n-l+1)/2, && \text{for} \quad n-l \text{ odd}. \end{aligned} \tag{2.19}$$

The complex conjugate of $f: \mathbb{R}^3 \to \mathbb{C}$ is denoted by f^*. In the special case of spherical harmonics, we also use the notation

$$Y_l^{m*}(\theta, \phi) = [Y_l^m(\theta, \phi)]^*. \tag{2.20}$$

In Condon–Shortley's phase convention, it is

$$Y_l^{m*}(\theta, \phi) = (-1)^m Y_l^{-m}(\theta, \phi). \tag{2.21}$$

III. The Fourier Transform of a Two-Center Product of B Functions

We consider the integral representing the Fourier transform of a product of two B functions with centers separated by a distance $\mathbf{R}$:

$$S_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\alpha, \beta, \mathbf{R}, \mathbf{k}) = \int d\mathbf{r}\, e^{-i\mathbf{r}\cdot\mathbf{k}} B_{n_1 l_1}^{m_1*}(\alpha, \mathbf{r})\, B_{n_2 l_2}^{m_2}(\beta, \mathbf{r}-\mathbf{R}). \tag{3.1}$$

It should be noted that in the case $\mathbf{k} = 0$ the Fourier integral (3.1) simplifies to the overlap integral of two B functions which is usually written as $S_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\alpha, \beta, \mathbf{R})$ [16, 25].

One of the most important methods for the evaluation of two-center integrals, such as the two-center Fourier integral (3.1), has been the application of the

Fourier convolution theorem. The usefulness of this theorem for the evaluation of two-center integrals in quantum mechanics was first noticed by Prosser and Blanchard [32]. The convolution theorem itself can be found much earlier in the mathematical literature in a book by Bochner [33]. Let f and g be two absolutely integrable functions of $L^1(\mathbb{R}^3)$. Then, the Fourier transform of the two-center product $f^*(\mathbf{r})\, g(\mathbf{r}-\mathbf{R})$ can be represented with the help of the integral transformation, Eq. (2.13), in the following way:

$$\int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}} f^*(\mathbf{r})\, g(\mathbf{r}-\mathbf{R}) = \int d\mathbf{p}\, e^{-i(\mathbf{k}+\mathbf{p})\cdot\mathbf{R}} \bar{f}^*(\mathbf{p})\, \bar{g}(\mathbf{p}+\mathbf{k}) \tag{3.2}$$

Here, $\bar{f}$ and $\bar{g}$ are the Fourier transforms of f and g as defined in Eq. (2.10). For $\mathbf{k}=0$ we obtain Eq. (2.13) from Eq. (3.2). Obviously, the difficulty of evaluating the momentum space integral in Eq. (3.2) depends crucially upon the functional form of the Fourier transform of the functions involved. For B functions the Fourier transform has the following simple analytic structure [18]:

$$\bar{B}^m_{n,l}(\alpha, \mathbf{p}) = (2/\pi)^{1/2} \frac{\alpha^{2n+l-1}}{[\alpha^2+p^2]^{n+l+1}} \mathscr{Y}^m_l(-i\mathbf{p}). \tag{3.3}$$

In momentum space B functions may be considered as kind of basic ETOs. In fact, the Fourier transform of other ETOs like STOs or A functions [34] may be expressed as linear combinations of Fourier transforms of B functions [35]. For $n \geqslant 1$ we have $B^m_{n,l}(\alpha, \mathbf{r}) \in L^1(\mathbb{R}^3)$, and we obtain with the help of Eqs. (3.2) and (3.3):

$$S^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\alpha, \beta, \mathbf{R}, \mathbf{k}) = (2/\pi)\, \alpha^{2n_1+l_1-1} \beta^{2n_2+l_2-1} \times \int d\mathbf{p}\, \frac{\mathscr{Y}^{m_1}_{l_1}(-i\mathbf{p})\, \mathscr{Y}^{m_2}_{l_2}[-i(\mathbf{p}+\mathbf{k})]\, e^{-i(\mathbf{p}+\mathbf{k})\cdot\mathbf{R}}}{[\alpha^2+p^2]^{n_1+l_1+1}[\beta^2+(\mathbf{p}+\mathbf{k})^2]^{n_2+l_2+1}}. \tag{3.4}$$

The regular solid harmonic $\mathscr{Y}^m_l(\mathbf{r})$ is a homogeneous polynomial of degree l in the Cartesian components x, y, and z of $\mathbf{r}$ [36]. We can replace these components of $\mathbf{r}$ by the corresponding Cartesian components of the gradient ∇—$\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$—to obtain the operator $\mathscr{Y}^m_l(\nabla)$. Application of this operator to a plane wave yields [37]

$$\mathscr{Y}^m_l(\nabla_{\mathbf{r}})\, e^{i\mathbf{r}\cdot\mathbf{p}} = \mathscr{Y}^m_l(i\mathbf{p})\, e^{i\mathbf{r}\cdot\mathbf{p}}. \tag{3.5}$$

If we apply Eq. (3.5) twice under the integral sign of the momentum integral in Eq. (3.4) we can take the differential operators in front of the integral sign and obtain

$$\begin{aligned} &S^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\alpha, \beta, \mathbf{R}, \mathbf{k}) \\ &\quad = (2/\pi)\, \alpha^{2n_1+l_1-1} \beta^{2n_2+l_2-1}\, e^{-i\mathbf{k}\cdot\mathbf{R}} (-1)^{l_1} \\ &\qquad \times \mathscr{Y}^{m_1^*}_{l_1}(\nabla_{\mathbf{R}})\, e^{i\mathbf{k}\cdot\mathbf{R}}\, \mathscr{Y}^{m_2}_{l_2}(\nabla_{\mathbf{R}})\, I_{n_1+l_1+1, n_2+l_2+1}(\alpha, \beta, \mathbf{k}, \mathbf{R}), \end{aligned} \tag{3.6a}$$

where

$$I_{j_1,j_2}(\alpha, \beta, \mathbf{k}, \mathbf{R}) = \int d\mathbf{p} \frac{e^{-i(\mathbf{p}+\mathbf{k})\cdot\mathbf{R}}}{[\alpha^2+p^2]^{j_1}[\beta^2+(\mathbf{p}+\mathbf{k})^2]^{j_2}} \tag{3.6b}$$

with

$$j_1 = n_1 + l_1 + 1 \tag{3.7a}$$

and

$$j_2 = n_2 + l_2 + 1. \tag{3.7b}$$

For the evaluation of integral (3.6b) we use the following relationship [38]:

$$\frac{1}{a^{j_1}b^{j_2}} = \int_0^1 dt \frac{(j_1+j_2-1)!(1-t)^{j_1-1}t^{j_2-1}}{(j_1-1)!(j_2-1)![bt+(1-t)a]^{j_1+j_2}}, \tag{3.8}$$

which is a generalization of the so-called Feynman's identity

$$\frac{1}{ab} = \int_0^1 dt \frac{1}{[bt+(1-t)a]^2}, \tag{3.9}$$

and can be obtained easily from this identity by repeated differentiation with respect to a and b. Applying Eq. (3.8) to the integrand of $I_{j_1,j_2}(\alpha, \beta, \mathbf{k}, \mathbf{R})$, followed by a change of variables $\mathbf{p} \to \mathbf{p} - t\mathbf{k}$, we obtain by setting $a = p^2 + \alpha^2$, $b = (\mathbf{p}+\mathbf{k})^2 + \beta^2$ and by interchanging the order of integrations,

$$I_{j_1,j_2}(\alpha, \beta, \mathbf{k}, \mathbf{R}) = \frac{(j_1+j_2-1)!}{(j_1-1)!(j_2-1)!} \int_0^1 dt(1-t)^{j_1-1}t^{j_2-1}e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}} \times \int d\mathbf{p} \frac{e^{-i\mathbf{p}\cdot\mathbf{R}}}{\{p^2+[\gamma(t)]^2\}^{j_1+j_2}}, \tag{3.10a}$$

where

$$[\gamma(t)]^2 = k^2t(1-t) + \alpha^2(1-t) + \beta^2 t. \tag{3.10b}$$

From Eqs. (3.3) and (2.10) we see that, apart from an unimportant factor, the $\mathbf{p}$ integral in Eq. (3.10a) is simply the representation of a scalar B function in terms of a Fourier integral. Therefore, we have

$$I_{j_1,j_2}(\alpha, \beta, \mathbf{k}, \mathbf{R}) = 4\pi^{5/2} \frac{(j_1+j_2-1)!}{(j_1-1)!(j_2-1)!} \times \int_0^1 dt \frac{(1-t)^{j_1-1}t^{j_2-1}}{[\gamma(t)]^{2(j_1+j_2)-3}} e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}} B^0_{j_1+j_2-1,0}[\gamma(t), \mathbf{R}]. \tag{3.11}$$

According to our experience it seems that there is no closed-form analytical expression for the remaining t integral in Eq. (3.11) containing only a finite number of terms. But we can get an analytic expression by expanding the integrand of the t integral in a Taylor series, followed by term-by-term integration. For instance, we can expand the B function $B^0_{j_1+j_2-1,0}[\gamma(t), \mathbf{R}]$ in a Taylor series using the multiplication theorem of B functions [15]:

$$B^m_{n,l}(\lambda, \mathbf{r}) = (\lambda/\delta)^{2n+l-1} \sum_{p=0}^{\infty} \frac{(n+l+1)_p}{p!} \left[1 - \frac{\lambda^2}{\delta^2}\right]^p B^m_{n+p,l}(\delta, \mathbf{r}). \tag{3.12}$$

Here, the infinite series converges only if $|1-\lambda^2/\delta^2| < 1$ holds. If we choose $\lambda^2 = \gamma^2(t)$ and $\delta^2 = \gamma^2(\frac{1}{2})$, we obtain

$$\left|1 - \frac{\gamma^2(t)}{\gamma^2(1/2)}\right| \leqslant \frac{k^2/4 + (\beta^2 - \alpha^2)/2}{k^2/4 + (\beta^2 + \alpha^2)/2} < 1 \tag{3.13}$$

for all $0 \leqslant t \leqslant 1$ ($\alpha, \beta > 0$). Thus, the infinite series in Eq. (3.12) converges uniformly on the integration interval [0, 1], i.e., we can interchange integration and summation. The resulting infinite series representation of the two-center Fourier transform of B functions which is rather complicated, is derived in Appendix B. A similar approach for $1s$ Slater-type orbitals only has already been studied by Monkhorst and Harris [13]. They inserted the Lommel expansion for the spherical modified Bessel functions [39],

$$\frac{k_n[z(s^2-t^2)^{1/2}]}{(s^2-t^2)^{n/2}} = \sum_{m=0}^{\infty} \frac{(zt^2/2)^m}{s^{m+n}} \frac{k_{m+n}(z \cdot s)}{m!}, \tag{3.14a}$$

$$k_n(z) = (\pi/2z)^{1/2} K_{n+1/2}(z), \tag{3.14b}$$

into the integrand of an integral similar to $I_{j_1,j_2}(\alpha, \beta, \mathbf{k}, \mathbf{R})$. But Lommel's series expansion of the spherical modified Bessel functions is equivalent to the multiplication theorem of RBFs [40]

$$\hat{k}_\nu(\lambda z) = \lambda^{2\nu} \sum_{n=0}^{\infty} [1-\lambda^2]^n \frac{\hat{k}_{\nu+n}(z)}{2^n n!}, \tag{3.15}$$

as can be seen immediately by the substitutions $t^2 = 1 - \lambda^2$ and $s = 1$ and a few simple series manipulations. From Eq. (3.15) the multiplication theorem of B functions, Eq. (3.12), can be derived quite easily. The rate of convergence of the infinite series in Eq. (3.12) is determined by the factor

$$1 - \lambda^2/\delta^2, \tag{3.16}$$

i.e., the infinite series converges more rapidly if the convergence factor (3.16)

approaches zero, or equivalently, if λ approaches δ. Now we insert the representation of integral $I_{j_1,j_2}(\alpha, \beta, \mathbf{R}, \mathbf{k})$, Eq. (3.11), in Eq. (3.6a) and obtain

$$
\begin{aligned}
&S^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\alpha, \beta, \mathbf{R}, \mathbf{k}) \\
&\quad = (-1)^{l_1}(4\pi)^{3/2}\alpha^{2n_1+l_1-1}\beta^{2n_2+l_2-1} \\
&\qquad \times \frac{(n_1+n_2+l_1+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, \mathscr{Y}^{m_1^*}_{l_1}(\nabla_{\mathbf{R}})\, e^{i\mathbf{k}\cdot\mathbf{R}}\, \mathscr{Y}^{m_2}_{l_2}(\nabla_{\mathbf{R}}) \\
&\qquad \times \int_0^1 dt\, \frac{t^{n_2+l_2}(1-t)^{n_1+l_1}}{[\gamma(t)]^{2(n_1+n_2+l_1+l_2)+1}}\, e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}}\, B^0_{n_1+n_2+l_1+l_2+1,0}[\gamma(t), \mathbf{R}].
\end{aligned}
\tag{3.17}
$$

We still have to apply the differential operator $\mathscr{Y}^{m_1^*}_{l_1}(\nabla_{\mathbf{R}})\, e^{i\mathbf{k}\cdot\mathbf{R}}\mathscr{Y}^{m_2}_{l_2}(\nabla_{\mathbf{R}})$ to the product function $e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}}B^0_{n_1+n_2+l_1+l_2+1,0}[\gamma(t), \mathbf{R}]$ consisting of a plane-wave and a scalar B function. The differentiation can be performed quite easily using some special differentiation properties of the solid harmonic and the B functions in connection with the Fourier transformation method. This is shown explicitly in Appendix A. We eventually arrive at the remarkable expression for the Fourier transform of the two-center charge distribution $B^{m_1^*}_{n_1,l_1}(\alpha, \mathbf{r})\, B^{m_2}_{n_2,l_2}(\beta, \mathbf{r}-\mathbf{R})$ derived by Trivedi and Steinborn [41]

$$
\begin{aligned}
&S^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\alpha, \beta, \mathbf{R}, \mathbf{k}) \\
&\quad = (4\pi)^3(2l_1+1)!!\,(2l_2+1)!!\,\frac{(n_1+n_2+l_1+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!} \\
&\qquad \times \alpha^{2n_1+l_1-1}\beta^{2n_2+l_2-1}\sum_{l_1'=0}^{l_1}\sum_{m_1'}\frac{\langle l_1 m_1 \mid l_1' m_1' \mid l_1 - l_1' m_1 - m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!} \\
&\qquad \times [\mathscr{Y}^{m_1-m_1'}_{l_1-l_1'}(\mathbf{k})]^* \\
&\qquad \times \sum_{l_2'=0}^{l_2}\sum_{m_2'}\frac{\langle l_2 m_2 \mid l_2' m_2' \mid l_2 - l_2' m_2 - m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!}\, \mathscr{Y}^{m_2-m_2'}_{l_2-l_2'}(\mathbf{k}) \\
&\qquad \times \sum_{l=l_{\min}}^{l_1'+l_2'} {}^{(2)}\langle l_2' m_2' \mid l_1' m_1' \mid l m_2' - m_1'\rangle\, i^{l_1+l_2+l_1'+l_2'}(-1)^{l_1+l_2+l_2'} \\
&\qquad \times \int_0^1 dt\, e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}}\,\frac{t^{n_2+l_2+l_1-l_1'}(1-t)^{n_1+l_1+l_2-l_2'}}{[\gamma(t)]^{2(n_1+n_2+l_1+l_2)-(l_1'+l_2')+1}} \\
&\qquad \times \left[\sum_{j=0}^{\Delta l}(-1)^j\binom{\Delta l}{j}B^{m_2'-m_1'}_{n_1+n_2+2\Delta l_0+1-j,l}[\gamma(t), \mathbf{R}]\right],
\end{aligned}
\tag{3.18a}
$$

where

$$
\Delta l = (l_1' + l_2' - l)/2 \tag{3.18b}
$$

and

$$\Delta l_0 = (l_1 + l_2 - l)/2. \tag{3.18c}$$

The symbol $\sum^{(2)}$ indicates that the summation is to be performed in steps of two. The summation limits of m_1', m_2', and $l_{\min}$ follow directly from the selection rules for the Gaunt coefficients [42]. Another consequence of these selection rules is that $(l_1' + l_2' - l)/2$ is always a positive integer or zero.

Monkhorst and Harris [13] have replaced their t-integral for 1s-Slater-type functions by a sum of integrals over subintervals $I_i = [u_i, u_{i-1}]$ and expanded the spherical modified Bessel functions belonging to I_i in Taylor series around the points $\bar{u}_i = (u_i + u_{i-1})/2$ using Lommel's series expansion with the intention of accelerating the convergence of the infinite series by decreasing the convergence factor for each subinterval. Guidotti *et al.* noted that the numerical procedure of Monkhorst and Harris does not prove to be practically convenient for STOs of higher principal and angular momentum quantum numbers, since the convergence of the Taylor series around the points $\bar{u}_i$ slows down. In the next section we shall show that it is computationally more efficient to use an automatic and adaptive integration procedure for the evaluation of the remaining t-integration instead of series expansions where the computational problems due to the slow convergence seem to be insurmountable.

IV. An Efficient Method for the Numerical Evaluation of the Two-Center Fourier Transform of B Functions

First we rewrite the formula for the two-center Fourier transform of B functions, Eqs. (3.18a)–(3.18c), in a way which is advantageous for computational purposes. In Eq. (3.18a), there occur Gaunt coefficients of the special form

$$\langle lm \mid l'm' \mid l - l' m - m' \rangle. \tag{4.1}$$

These Gaunt coefficients can be expressed in closed form. This fact becomes obvious if the representation of Gaunt coefficients in terms in 3jm symbols is considered [43]:

$$\langle lm \mid l'm' \mid l - l' m - m' \rangle = (-1)^m \left[\frac{(2l+1)(2l'+1)[2(l-l')+1]}{4\pi} \right]^{1/2} \times \begin{pmatrix} l-l' & l' & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l-l' & l' & l \\ m-m' & m' & -m \end{pmatrix}. \tag{4.2}$$

These special 3jm symbols can be expressed by relatively simple closed form expressions containing only factorials [44]:

$$\begin{pmatrix} l-l' & l' & l \\ 0 & 0 & 0 \end{pmatrix}$$

$$= (-1)^l \left[\frac{(2l')!(2l-2l')!}{(2l+1)!} \right]^{1/2} \frac{l!}{l'!(l-l')!} \tag{4.3}$$

$$\begin{pmatrix} l-l' & l' & l \\ m-m' & m' & -m \end{pmatrix}$$

$$= (-1)^{m+l} \left[\frac{(2l-2l')!(2l')!(l+m)!(l-m)!}{(2l+1)!(l-l'+m-m')!(l-l'-m+m')!} \times \frac{1}{(l'+m')!(l'-m')!} \right]^{1/2}. \tag{4.4}$$

If we insert these expressions into Eq. (4.2), we obtain

$$\langle lm \mid l'm' \mid l-l'm-m' \rangle = \frac{(2l'+1)!!\,[2(l-l')+1]!!}{(2l+1)!!} \times \left[\frac{(2l+1)(l+m)!(l-m)!}{4\pi(2l'+1)[2(l-l')+1](l-l'+m-m')!(l-l'-m+m')!(l'+m')!(l'-m')!} \right]^{1/2}. \tag{4.5}$$

The first two Gaunt coefficients in Eq. (3.18a) are replaced by the expression on the r.h.s. of Eq. (4.5). In Eq. (3.18a) we introduce the new integration variable $s = 1 - t$ and rearrange the order of the m_1' and l_2' summations. This yields the following expression which is quite convenient for computational purposes:

$$S^{n_1 l_1 m_1}_{n_2 l_2 m_2}(\alpha, \beta, \mathbf{R}, \mathbf{k}) = C \cdot \int_0^1 ds \frac{g(s)\, e^{-is\mathbf{k}\cdot\mathbf{R}}}{[\gamma(s)]^{2(n_1+n_2+l_1+l_2)+1}}, \tag{4.6a}$$

where

$$g(s) = \sum_{l_1'=0}^{l_1} \frac{k^{l_1-l_1'}(1-s)^{n_2+l_2+l_1-l_1'}[\gamma(s)]^{l_1'}}{[(2l_1'+1)(2l_1-2l_1'+1)]^{1/2}} \times \sum_{l_2'=0}^{l_2} \frac{k^{l_2-l_2'} s^{n_1+l_1+l_2-l_2'}[\gamma(s)]^{l_2'}}{[(2l_2'+1)(2l_2-2l_2'+1)]^{1/2}} (-1)^{l_1+l_2+l_2'} i^{l_1+l_2+l_1'+l_2'} \times \sum_{m_1'=\max(-l_1', m_1-l_1+l_1')}^{\min(l_1', m_1+l_1-l_1')}$$

$$\times \frac{[Y_{l_1-l_1'}^{m_1-m_1'}(\mathbf{k}/k)]^*}{[(l_1'-m_1')!\,(l_1'+m_1')!\,(l_1-l_1'-m_1+m_1')!\,(l_1-l_1'+m_1-m_1')!]^{1/2}}$$

$$\times \sum_{m_2'=\max(-l_2',m_2-l_2+l_2')}^{\min(l_2',m_2+l_2-l_2')}$$

$$\times \frac{Y_{l_2-l_2'}^{m_2-m_2'}(\mathbf{k}/k)}{[(l_2'-m_2')!(l_2'+m_2')!\,(l_2-l_2'-m_2+m_2')!\,(l_2-l_2'+m_2-m_2')!]^{1/2}}$$

$$\times \sum_{l=l_{\min}}^{l_1'+l_2'} {}^{(2)}\langle l_2'm_2' |\, l_1'\, m_1' \,|\, lm_2'-m_1'\rangle [R\gamma(s)]^l\, Y_l^{m_2'-m_1'}(\mathbf{R}/R) \tag{4.6b}$$

$$\times \sum_{j=0}^{\Delta l} \frac{(\Delta l-j+1)_j}{j!}(-2)^j(n_1+n_2+l_1+l_2-j+2)_j$$

$$\times \hat{k}_{n_1+n_2+l_1+l_2-l-j+1/2}[\gamma(s)R],$$

$$C=(4\pi)^2 \frac{\alpha^{2n_1+l_1-1}\beta^{2n_2+l_2-1}}{(n_1+l_1)!(n_2+l_2)!\,2^{n_1+n_2+l_1+l_2+1}}$$

$$\times [(2l_1+1)(2l_2+1)(l_1-m_1)!\,(l_1+m_1)!\,(l_2-m_2)!\,(l_2+m_2)!]^{1/2}, \tag{4.6c}$$

and

$$\gamma^2(s)=k^2s(1-s)+\alpha^2s+(1-s)\,\beta^2. \tag{4.6d}$$

In order to obtain a reliable and economical procedure for the numerical integration of the 1-dimensional integral (4.6a) we have to examine the integrand. It is particularly important to find out whether singularities occur and if they do, where, and in which region the contribution to the value of the integral is negligible. The function $g(s)$, which occurs in the integrand and which consists of six partly nested finite sums is well behaved and vanishes at the endpoints of the integration interval $[0, 1]$. For larger values of $\Delta l=(l_1'+l_2'-l)/2$, the inner j sum of the function $g(s)$ will lead inevitably to a loss of some significant digits as has been noted by Trivedi and Steinborn [5]. Fortunately, extremely large values of Δl do not occur and for all practical applications, the evaluation of $g(s)$ should yield a satisfactory accuracy. The behavior of the integrand is dominated by the following parts:

$$w(s)=e^{-is\mathbf{k}\cdot\mathbf{R}} \tag{4.7}$$

and

$$h(s)=1/[\gamma(s)]^{2(n_1+n_2+l_1+l_2)+1}. \tag{4.8}$$

For larger values of $\mathbf{k}\cdot\mathbf{R}$ the function $w(s)$ oscillates heavily, and for larger $k=|\mathbf{k}|$ the function $g(s)\cdot h(s)$ exhibits high peaks in the vicinity of 0 and/or 1, the

endpoints of the integration interval. The sharpness of these peaks depends upon the magnitude of the quantum numbers n_1, n_2, l_1, l_2, and the exponential parameters α, β as well as on the ratio α/β. This may be seen easily from Eqs. (4.8) and (4.6d). As a result of the special behavior of $w(s)$ and $h(s)$, a direct application of one of the standard quadrature rules, such as Gauss–Legendre or Gauss–Jacobi

number of abscissae to be used, is chosen with respect to the complexity of the integrand. This may lead to an unnecessarily large number of function evaluations in order to obtain a certain given accuracy for the integral approximation. This is an annoying fact, especially when the integrand contains such a complicated function as $g(s)$, the evaluation of which is the most time-consuming step in the integration procedure. Therefore it is advisable to replace the integral (4.6a) by a sum of integrals over suitable subintervals—depending upon the local behavior of $w(s)$ and $g(s)$—in order to obtain a better integral approximation. This method was used by Guidotti *et al.* [14] using the Gauss formulas to approximate the subintegrals. A disadvantage of this approach is, that, given a certain relative accuracy, one has to find experimentally not only the optimal subdivision of the integration interval, but also the optimal number of integration points for each subinterval. Another shortcoming is the fact that for larger values of $\mathbf{k} \cdot \mathbf{R}$ the integrand $f(s) = g(s)\, h(s)\, e^{-is\mathbf{k} \cdot \mathbf{R}}$ oscillates rapidly, and the application of the Gauss quadrature formulas turns out to be inconvenient. Therefore, it is advantageous to use an automatic, adaptive integration method which takes into account the oscillatory nature of the exponential $e^{-is\mathbf{k} \cdot \mathbf{R}}$. A quadrature routine is automatic if it provides an approximation of specified tolerance. It is called adaptive if for calculating a sequence of integral approximations the location of the integration points of the nth iterate depends on information gathered from iterates $1,\ldots, n-1$. This is usually achieved by a successive partitioning of the integration interval, in such a way that many points are located in the neighborhood of a difficult region of the integrand, causing there a high density of quadrature points. Currently, various automatic, adaptive integrators for the approximation of the sine transform

$$S(\omega) = \int_a^b \sin(\omega x)\, f(x)\, dx \tag{4.9}$$

and the cosine transform

$$C(\omega) = \int_a^b \cos(\omega x)\, f(x)\, dx \tag{4.10}$$

are available [45–46]. Especially for strongly peaked functions $f(x)$ the algorithm AINOS of Piessens and Branders [45] seems to be very efficient for the evaluation of integrals with the oscillatory weight functions $\sin(\omega x)$ or $\cos(\omega x)$. After extensive numerical experimentation we came to the conclusion that the subroutine

DØ1ANF of the NAG library [47], which is based upon the algorithm AINOS, is the most efficient adaptive integrator for the evaluation of the 1-dimensional integral representation of the two-center Fourier integral over B functions (4.6a). DØ1ANF is a QUADPACK [48] routine and has the following main components: Assume that a subinterval has length $L = |a-b|\, 2^{-l}$. If $L\omega > 4$ and $l \leqslant 20$, the integration over the subinterval is performed by mean of a modified 25–point Clenshaw–Curtis procedure, and the error estimate is computed from this approximation together with the result of the 13–point formula. If the above conditions do not hold, Gauss' 7-point and Kronrod's 15-point rules [49] are used. The application of the Clenshaw–Curtis and Gauss–Kronrod quadrature rules has the great advantage that the order of quadrature may be doubled without losing function evaluations. Thus error estimates require no additional function evaluations. The algorithm, described in [48], incorporates a global interval partitioning strategy (as defined by Malcolm and Simpson [50]) together with the ε algorithm [51] to perform extrapolation.

We have written a computer program based on Eqs. (4.6a)–(4.6d). As mentioned above, the evaluation of the complex-valued function $g(s)$ is the most time-consuming step. Since the integration procedure requires repeated evaluation of the integrand function at the various abscissae, we precomputed all s-independent coefficients of $g(s)$, such as Gaunt coefficients, spherical harmonics, etc., and stored them in appropriate arrays in order to save CPU time. As a further element for optimizing the integration procedure it is convenient to consider special cases of the transformation vector $\mathbf{k}$. If $\mathbf{k}$ lies along the z axis of the coordinate system we have $\theta_{\mathbf{k}} = 0$ or 180°, respectively, which yields

$$P_l^{|m|}(\pm 1) = 0 \tag{4.11}$$

for $m \neq 0$. Thus $Y_l^{|m|}(\mathbf{k}|k) = 0$ for $m \neq 0$, and the inner m_1'- and m_2'-sums of $g(s)$ vanish. For $\mathbf{k} = 0$ the l_1'- and l_2'-sums of $g(s)$ also vanish and we obtain the 1-dimensional integral representation for the two-center overlap integral over B functions of Trivedi and Steinborn [5]. In Eq. (4.6b), where $g(s)$ is defined, there occur products of Gaunt coefficients and spherical harmonics,

$$\langle l_2' m_2' |\, l_1' m_1' \,|\, l m_2' - m_1' \rangle\, Y_l^{m_2'-m_1'}(\mathbf{R}/R), \tag{4.12}$$

where l is a summation index whose limits are determined by the selection rules of the Gaunt coefficient. The computation of these coefficients was performed recursively in l with the help of the subroutines GAUNT and RECYLM of Weniger and Steinborn [42]. Considering that $G(s) = g(s)\, h(s)$ is a complex-valued function on [0, 1], the evaluation of the integral

$$S_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\alpha, \beta, \mathbf{R}, \mathbf{k}) = C \cdot \int_0^1 ds\, G(s)\, e^{-is\mathbf{k}\cdot\mathbf{R}} \tag{4.13}$$

requires the computation of two finite sine transforms of type (4.9) and two finite

TABLE I

Some Special Values for Integral (4.13)

n_1	l_1	m_1	α	n_2	l_2	m_2	β	k	ACCREL	Real part of the integral	Imaginary part of the integral	N	ABSRE	ABSIM
1	0	0	1.2	1	0	0	5.7	5.0	1.0*E*–03	0.6987757224*E*–04	−0.3711105336*E*–04	145	0.6*E*–08	0.9*E*–08
1	0	0	1.2	1	0	0	5.7	5.0	1.0*E*–07	0.6987757224*E*–04	−0.3711105336*E*–04	175	0.2*E*–11	0.2*E*–11
1	0	0	1.2	1	0	0	5.7	10.0	1.0*E*–03	0.3755937242*E*–05	−0.1433026600*E*–04	195	0.1*E*–08	0.9*E*–08
1	0	0	1.2	1	0	0	5.7	10.0	1.0*E*–07	0.3755937242*E*–05	−0.1433026600*E*–04	255	0.6*E*–14	0.2*E*–13
5	5	5	1.5	5	5	5	1.5	2.0	1.0*E*–03	−0.1632035536*E*–09	0.1033750757*E*–08	165	0.7*E*–14	0.4*E*–12
5	5	5	1.5	5	5	5	1.5	2.0	1.0*E*–07	−0.1632035536*E*–09	0.1033750756*E*–08	405	0.3*E*–17	0.2*E*–17
5	5	5	1.5	5	5	5	1.5	6.0	1.0*E*–03	0.7786217593*E*–15	−0.1533779614*E*–14	315	0.5*E*–18	0.1*E*–17
5	5	5	1.5	5	5	5	1.5	6.0	1.0*E*–07	0.7786219304*E*–15	−0.1533779238*E*–14	195	0.8*E*–23	0.6*E*–23
1	1	1	1.0	5	5	−5	10.0	2.0	1.0*E*–03	−0.4816787625*E*–08	−0.1215319721*E*–08	165	0.1*E*–12	0.1*E*–12
1	1	1	1.0	5	5	−5	10.0	2.0	1.0*E*–07	−0.4816787625*E*–08	−0.1215319720*E*–08	225	0.2*E*–15	0.7*E*–16
1	1	1	1.0	5	5	−5	10.0	10.0	1.0*E*–03	0.2820440383*E*–07	−0.7213698244*E*–08	255	0.7*E*–12	0.3*E*–11
1	1	1	1.0	5	5	−5	10.0	10.0	1.0*E*–07	0.2820440382*E*–07	−0.7213698220*E*–08	285	0.1*E*–14	0.5*E*–15
5	5	−5	1.0	1	1	1	10.0	2.0	1.0*E*–03	−0.6609158900*E*–11	−0.4098249446*E*–10	225	0.2*E*–15	0.2*E*–15
5	5	−5	1.0	1	1	1	10.0	2.0	1.0*E*–07	−0.6609158901*E*–11	−0.4098249446*E*–10	255	0.5*E*–19	0.6*E*–19
5	5	−5	1.0	1	1	1	10.0	10.0	1.0*E*–03	0.1455019954*E*–10	−0.2565665972*E*–10	285	0.4*E*–16	0.2*E*–15
5	5	−5	1.0	1	1	1	10.0	10.0	1.0*E*–07	0.1455019955*E*–10	−0.2565665973*E*–10	315	0.2*E*–19	0.4*E*–19
5	0	0	1.5	5	0	0	9.9	0.0	1.0*E*–03	0.1528918286*E*–04	0.0	165	0.5*E*–09	0.0
5	0	0	1.5	5	0	0	9.9	0.0	1.0*E*–07	0.1528918287*E*–04	0.0	225	0.3*E*–13	0.0

Note. We always have: $R = 2.00$, THETAR = 45.00°, PHIR = 60.00°, THETAK = 90.00°, and PHIK = 60.00°.

cosine transforms of type (4.10). In Table I we have summarized some typical test values for integral (4.13). ACCREL denotes the required relative accuracy, N the number of evaluations of the function $G(s)$, and ABSRE and ABSIM the estimated absolute error of the real part and imaginary part of integral (4.13), respectively. The various integrals are computed with a relative accuracy of 10^{-3} and 10^{-7} using single precision which corresponds to approximately 10 decimal digits on our machine. A comparison of the integral approximations with the corresponding absolute error estimates of Table I shows that the required relative accuracy is satisfied in all cases. However, the most integral approximations have a much better relative accuracy by far. This can be seen by comparing the values with a required relative error of 10^{-3} with those of a relative error of 10^{-7}. As may be expected, the convergence of the integration procedure is slower if the integrand function possesses high peaks. This becomes immediately evident if we compare the results given in Table I for the integrals S_{555}^{555} with $\alpha = \beta = 1.5$ and either $k = 2.0$ or $k = 6.0$. In the case of ACCREL $= 10^{-3}$ and $k = 2.0$, 165 function evaluations are needed compared to 315 function evaluations for $k = 6.0$. The relatively slow convergence in the case $k = 6.0$ is due to the fact that for this symmetric overlap distribution with large values of n and l—the exponent $q = 2(n_1 + n_2 + l_1 + l_2) + 1$ in the function $h(s) = 1/[\gamma(s)]^q$ is 41—the integrand $f(s)$ is strongly peaked in the vicinity of the endpoints of the integration interval $[0, 1]$ if k is much larger than α and β. Apart from an unimportant numerical factor, a 1s STO is equal to $B_{1,0}^0$. We have explicitly

$$\chi_{1,0}^0(\alpha, \mathbf{r}) = 4\alpha^{3/2} B_{1,0}^0(\alpha, \mathbf{r}). \tag{4.14}$$

Hence, we can compare the first four integral approximations in Table I with those in Table 1 of Guidotti *et al.* [14] for the Fourier transform of a two-center product of 1s Slater functions. If we multiply our values by $16(\alpha \cdot \beta)^{3/2}$ and take into account that Guidotti *et al.* used the transformation vector $-\mathbf{k}$ instead of $\mathbf{k}$, we obtain an excellent agreement between our results for the function $B_{1,0}^0$ and the results of Guidotti *et al.* for the 1s Slater function $\chi_{1,0}^1$. In the limiting case $\mathbf{k} = 0$ we obtain the two-center overlap integral over B functions. Recently these integrals have been computed by Weniger and Steinborn [26] close to machine accuracy, which corresponds approximately to 24 decimal digits in double precision, by using the convolution theorems of B functions. A comparison between the results for the two-center overlap integral in Table I and the corresponding results in Table II of Weniger and Steinborn [26] provides further support for our claims concerning the reliability of the numerical procedure which is presented in this article.

Summary

In this article we analyzed the analytical and numerical properties of the Fourier transform of a two-center product of B functions. Other exponential-type functions, like Slater-type orbitals, can be expanded in terms of B functions. Therefore, these

investigations facilitate an application of the Fourier transform of a two-center product of exponential-type functions of various different specific forms as they are needed in many quantum-mechanical calculations and interpretations of experiments, for instance, in the field of scattering theory [1–3]. We give a new and simpler derivation of a known general formula [5] for the Fourier transform of a two-center product of B functions. Our method utilizes a differentiation technique which makes it possible to generate multicenter integrals over nonscalar B functions from integrals over scalar functions. With this method analytical results for nonscalar functions can be derived much more easily than it was possible so far. We exploited the properties of the differential operator $\mathscr{Y}_l^m(\nabla)$ which is an irreducible spherical tensor of rank l. It is obtained from the regular solid harmonic $\mathscr{Y}_l^m(\mathbf{r})$ by replacing the Cartesian components of $\mathbf{r}$ by the Cartesian components of $\nabla_{\mathbf{r}}$. We then analyzed the numerical properties of the expression for the Fourier transform of a two-center product of B functions which requires a 1-dimensional numerical quadrature over a finite integration interval. According to our experience the application of a special automatic, adaptive quadrature which takes into account the peaked nature and oscillatory behavior of the integrand, appears to be the most efficient and economical numerical tool for evaluating this integral. We used a QUADPACK [45] routine whose main components are: the global interval partitioning strategy of Malcolm and Simpson, the application of a modified Clenshaw–Curtis procedure, and the Gauss–Kronrod quadrature rules. Various numerical test results are also reported.

APPENDIX A

We want to compute the action of the differential operator

$$P_{l_1 m_1}^{l_2 m_2}(\mathbf{k}, \nabla_{\mathbf{R}}) = \mathscr{Y}_{l_1}^{m_1 *}(\nabla_{\mathbf{R}})\, e^{i\mathbf{k}\cdot\mathbf{R}} \mathscr{Y}_{l_2}^{m_2}(\nabla_{\mathbf{R}}) \tag{A1}$$

upon the product

$$f(\mathbf{R}) = e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}} B_{n,0}^0(\gamma, \mathbf{R}). \tag{A2}$$

Here, we use the abbreviations $\gamma = \gamma(t)$ (see Eq. (3.10b)) and $n = n_1 + n_2 + l_1 + l_2 + 1$. First we use Eq. (2.11) to represent the scalar B function $B_{n,0}^0$ as a Fourier integral,

$$B_{n,0}^0(\gamma, \mathbf{R}) = (2\pi)^{-3/2} \int d\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{R}} \bar{B}_{n,0}^0(\gamma, \mathbf{p}). \tag{A3}$$

Now we insert Eq. (A3) into (A2) and use the relationship (3.5) twice under the

integral sign of (A3). The application of the differential operator (A1) onto the product (A2) then yields:

$$P^{l_2 m_2}_{l_1 m_1}(\mathbf{k}, \nabla_{\mathbf{R}})\, f(\mathbf{R}) = (2\pi)^{-3/2}(-1)^{l_1} \int d\mathbf{p}\, \mathscr{Y}^{m_1^*}_{l_1}[i(\mathbf{p}+t\mathbf{k})] \times \mathscr{Y}^{m_2}_{l_2}[i\mathbf{p}-(1-t)\mathbf{k}]\, e^{i(\mathbf{p}+t\mathbf{k})\cdot\mathbf{R}} \bar{B}^0_{n,0}(\gamma, \mathbf{p}) \tag{A4}$$

The separation of $\mathbf{p}$ and $\mathbf{k}$ variables in the solid spherical harmonics occurring in the momentum space integral (A4) is accomplished by the addition theorem of the solid spherical harmonic [52]:

$$\mathscr{Y}^m_l(\mathbf{r}_1+\mathbf{r}_2) = 4\pi(2l+1)!! \sum_{l'=0}^{l} \sum_{m'} \frac{\langle lm \mid l'm' \mid l-l'm-m' \rangle}{(2l'+1)!![2(l-l')+1]!!} \times \mathscr{Y}^{m'}_{l'}(\mathbf{r}_1)\, \mathscr{Y}^{m-m'}_{l-l'}(\mathbf{r}_2). \tag{A5}$$

Again applying the differentiation rule (3.5) twice and using Eq. (2.12) we arrive at

$$\begin{aligned} &P^{l_2 m_2}_{l_1 m_1}(\mathbf{k}, \nabla_R)\, f(\mathbf{R}) \\ &\quad = (4\pi)^2 (2l_1+1)!!\,(2l_2+1)!!\,(-1)^{l_1+l_1'} \\ &\quad\quad \times \sum_{l_1'=0}^{l_1} \sum_{m_1'} \frac{\langle l_1 m_1 \mid l_1' m_1' \mid l_1 - l_1' m_1 - m_1' \rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!} [\mathscr{Y}^{m_1-m_1'}_{l_1-l_1'}(it\mathbf{k})]^* \\ &\quad\quad \times \sum_{l_2'=0}^{l_2} \sum_{m_2'} \frac{\langle l_2 m_2 \mid l_2' m_2' \mid l_2 - l_2' m_2 - m_2' \rangle}{(2l_2'+1)!!\,[2(l_2-l_2')+1]!!} \mathscr{Y}^{m_2-m_2'}_{l_2-l_2'}[-i(1-t)\mathbf{k}] \\ &\quad\quad \times e^{it\mathbf{k}\cdot\mathbf{R}} \mathscr{Y}^{m_1'^*}_{l_1'}(\nabla_{\mathbf{R}})\, \mathscr{Y}^{m_2'}_{l_2'}(\nabla_{\mathbf{R}})\, B^0_{n,0}(\gamma, \mathbf{R}). \end{aligned} \tag{A6}$$

The operators $\mathscr{Y}^{m'}_{l'}(\nabla)$ are irreducible spherical tensors. Therefore they can be coupled in exactly the same manner as ordinary solid harmonics, i.e., we have [18]

$$\mathscr{Y}^{m_1'^*}_{l_1'}(\nabla)\mathscr{Y}^{m_2'}_{l_2'}(\nabla) = \sum_{l=l_{\min}}^{l_1'+l_2'} {}^{(2)}\Delta^{(l_1'+l_2'-l)/2} \langle l_2' m_2' \mid l_1' m_1' \mid l m_2' - m_1' \rangle \mathscr{Y}^{m_2'-m_1'}_{l}(\nabla) \tag{A7}$$

Applying the special differentiation properties of B functions [18],

$$\mathscr{Y}^m_l(\nabla)\, B^0_{n+l,0}(\gamma, \mathbf{R}) = (-\gamma)^l (4\pi)^{-1/2} B^m_{n,l}(\gamma, \mathbf{R}) \tag{A8}$$

and

$$\gamma^{-2\nu} \Delta^\nu B^m_{n,l}(\gamma, \mathbf{R}) = \sum_{t=0}^{\nu} (-1)^t \binom{\nu}{t} B^m_{n-t,l}(\gamma, \mathbf{R}), \tag{A9}$$

we eventually obtain the final result

$$P^{l_2m_2}_{l_1m_1}(\mathbf{k}, \nabla_R)\, f(\mathbf{R})$$
$$= (4\pi)^{3/2}(2l_1+1)!!\,(2l_2+1)!!\,(-1)^{l_1}$$
$$\times \sum_{l_1'=0}^{l_1} \sum_{m_1'} \frac{\langle l_1 m_1 \,|\, l_1' m_1' \,|\, l_1 - l_1' m_1' \rangle}{(2l_1'+1)!!\,[2(l_1-l_1')+1]!!}\, [\mathscr{Y}^{m_1-m_1'}_{l_1-l_1'}(it\mathbf{k})]^*\, \gamma^{l_1'}$$
$$\times \sum_{l_2'=0}^{l_2} \sum_{m_2'} \frac{\langle l_2 m_2 \,|\, l_2' m_2' \,|\, l_2 - l_2' m_2 - m_2' \rangle}{(2l_2'+1)!!\,[2(l_2-l_2')+1]!!}\, \mathscr{Y}^{m_2-m_2'}_{l_2-l_2'}[-i(1-t)\mathbf{k}](-\gamma)^{l_2'}$$
$$\times e^{it\mathbf{k}\cdot\mathbf{R}} \sum_{l=l_{\min}}^{l_1'+l_2'} {}^{(2)}\langle l_2' m_2' \,|\, l_1' m_1' \,|\, l m_2' - m_1' \rangle \sum_{t=0}^{\Delta l} (-1)^t \binom{\Delta l}{t} B^{m_2'-m_1'}_{n-l-t,l}(\gamma, \mathbf{R}),$$
$$\Delta t = (l_1' + l_2' - l)/2. \tag{A10}$$

Appendix B

The starting point for deriving a series representation of the Fourier transform of a two-center product of B functions is Eq. (3.11). Expanding the t-dependent scalar B function in the integrand of the t integral in Eq. (3.11) in an infinite series with the help of the multiplication theorem of B functions, Eq. (3.12), by choosing the parameters $\lambda = \gamma(t)$ and $\delta = \gamma(\frac{1}{2})$, we obtain

$$I_{j_1,j_2}(\alpha, \beta, \mathbf{k}, \mathbf{R}) = \frac{4\pi^{5/2}(j_1+j_2-1)!}{\delta^{2(j_1+j_2-1)-1}(j_1-1)!(j_2-1)!}$$
$$\times \sum_{p=0}^{\infty} \frac{(j_1+j_2)_p}{p!}\, B^0_{j_1+j_2+p-1,0}(\delta, \mathbf{R})$$
$$\times \int_0^1 dt \left[1 - \frac{\gamma^2(t)}{\delta^2}\right]^p (1-t)^{j_1-1} t^{j_2-1}\, e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}}. \tag{B1}$$

Here, we used the fact that the infinite series expansion converges uniformly in t on $[0, 1]$ as has been shown by the inequality (3.13) so that we may integrate term-by-term. Identifying j_1 and j_2 with $n_1 + l_1 + 1$ and $n_2 + l_2 + 1$ and inserting Eq. (B1) into Eq. (3.6a) yields

$$S^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\alpha, \beta, \mathbf{R}, \mathbf{k})$$
$$= \frac{8\pi^{3/2}(n_1+n_2+l_1+l_2+1)!\,\alpha^{2n_1+l_1-1}\beta^{2n_2+l_2-1}e^{-i\mathbf{k}\cdot\mathbf{R}}}{\delta^{2(n_1+n_2+l_1+l_2)+1}(n_1+l_1)!\,(n_2+l_2)!}$$
$$\times \sum_{p=0}^{\infty} \frac{(n_1+n_2+l_1+l_2+2)_p}{p!}\, \mathscr{Y}^{m_1^*}_{l_1}(\nabla_{\mathbf{R}})\, e^{i\mathbf{k}\cdot\mathbf{R}}\, \mathscr{Y}^{m_2}_{l_2}(\nabla_{\mathbf{R}})$$
$$\times B^0_{n_1+n_2+l_1+l_2+p+1,0}(\delta, \mathbf{R})$$
$$\times \int_0^1 dt\, e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}} (1-t)^{n_1+l_1} t^{n_2+l_2} \left[1 - \frac{\gamma^2(t)}{\delta^2}\right]^p \tag{B2}$$

Before evaluating the t integral in Eq. (B2) we apply the differential operator $\mathscr{Y}^{m_1^*}_{l_1}(\nabla_{\mathbf{R}})\, e^{i\mathbf{k}\cdot\mathbf{R}}\mathscr{Y}^{m_2}_{l_2}(\nabla_{\mathbf{R}})$ to the product function $B^0_{n_1+n_2+l_1+l_2+p+1,0}(\delta, \mathbf{R})\, e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}}$ Using the result (A10) we arrive at

$$
\begin{aligned}
&S^{n_2 l_2 m_2}_{n_1 l_1 m_1}(\alpha, \beta, \mathbf{R}, \mathbf{k}) \\
&\quad = (4\pi)^2 (2l_1+1)!!(2l_2+1)!! \frac{\alpha^{2n_1+l_1-1}\beta^{2n_2+l_2-1}}{\delta^{2(n_1+n_2+l_1+l_2)-2}} (-1)^{l_1} \\
&\quad \times \frac{(n_1+n_2+l_1+l_2+2)!}{(n_1+l_1)!\,(n_2+l_2)!} \sum_{p=0}^{\infty} \frac{(n_1+n_2+l_1+l_2+2)_p}{p!} \\
&\quad \times \sum_{l_1'=0}^{l_1} \sum_{m_1'} \frac{\langle l_1 m_1 \mid l_1' m_1' \mid l_1 - l_1' m_1 - m_1' \rangle}{(2l_1'+1)!!\,[2(l_1-l_1')+1]!!} [\mathscr{Y}^{m_1-m_1'}_{l_1-l_1'}(i\mathbf{k})]^* \\
&\quad \times \sum_{l_2'=0}^{l_2} \sum_{m_2'} \frac{\langle l_2 m_2 \mid l_2' m_2' \mid l_2 - l_2' m_2 - m_2' \rangle}{(2l_2'+1)!!\,[2(l_2-l_2')+1]!!} \mathscr{Y}^{m_2-m_2'}_{l_2-l_2'}(-i\mathbf{k}) \\
&\quad \times \delta^{l_1'+l_2'} S^{n_2+l_2-l_2', l_2', m_2'}_{n_1+l_1-l_1'+p, l_1', m_1'}(\delta, \delta, \mathbf{R}, 0) \\
&\quad \times \int_0^1 dt\, e^{-i(1-t)\mathbf{k}\cdot\mathbf{R}} (1-t)^{n_1+l_1+l_2-l_2'} t^{n_2+l_2+l_1-l_1'} \left[1 - \frac{\gamma^2(t)}{\delta^2}\right]^p .
\end{aligned}
\tag{B3}
$$

In Eq. (B3) we used the fact that the two-center overlap integral over B functions with equal scaling parameters is given by a simple linear combination of B functions [15]:

$$
\begin{aligned}
&S^{n_2+l_2-l_2', l_2', m_2'}_{n_1+l_1-l_1'+p, l_1', m_1'}(\delta, \delta, \mathbf{R}, 0) \\
&\quad = (4\pi)\,\delta^{-3}(-1)^{l_2'} \sum_{l=l_{\min}}^{l_1'+l_2'} {}^{(2)}\langle l_2' m_2' \mid l_1' m_1' \mid l m_2' - m_1' \rangle \\
&\quad \times \sum_{j=0}^{\Delta l} (-1)^j \binom{\Delta l}{j} B^{m_2'-m_1'}_{n_1+n_2+l_1+l_2+p-l-j+1, l}(\delta, \mathbf{R}).
\end{aligned}
\tag{B4}
$$

The remaining t integral in Eq. (B3) can best be evaluated by factorizing $[1-(\gamma(t)/\delta)^2]^p$ in the following way:

$$
\left[1 - \left(\frac{\gamma(t)}{\delta}\right)^2\right]^p = (1-2t)^p \left[1 - \frac{2k^2}{k^2+2(\alpha^2-\beta^2)}\, t\right]^p \left[\frac{k^2+2(\alpha^2-\beta^2)}{k^2+2(\alpha^2+\beta^2)}\right]^p . \tag{B5}
$$

Integrals such as

$$
\begin{aligned}
&I(n_1, l_1, l_1', n_2, l_2, l_2', p, \alpha, \beta, \mathbf{k}, \mathbf{R}) \\
&\quad = \int_0^1 dt\, e^{it\mathbf{k}\cdot\mathbf{R}} (1-t)^{n_1+l_1+l_2-l_2'} t^{n_2+l_2+l_1-l_1'} (1-2t)^p \left[1 - \frac{2k^2}{k^2+2(\alpha^2+\beta^2)}\, t\right]^p
\end{aligned}
\tag{B6}
$$

occur in statistics in connection with the generalized beta distribution and may be calculated in terms of the confluent hypergeometric function $\Phi_D^{(3)}$ with three variables. We have [53]

$$I(n_1, l_1, l_1', n_2, l_2, l_2', p, \alpha, \beta, \mathbf{k}, \mathbf{R})$$
$$= \frac{(n_1+l_1+l_2-l_2')!\,(n_2+l_2+l_1-l_1')!}{(n_1+n_2+l_1+l_2+l_2-l_2'+l_1-l_1'+1)!}$$
$$\times \Phi_D^{(3)}(n_2+l_2+l_1-l_1'+1, -p, -p; n_1+n_2+l_1+l_2+l_2-l_2'+l_1-l_1'+2;$$
$$2, \frac{2k^2}{k^2+2(\alpha^2-\beta^2)}, i\mathbf{k}\cdot\mathbf{R}\Big), \tag{B7}$$

where $\Phi_D^{(3)}$ is defined by

$$\Phi_D^{(3)}(a, b_1, b_2; c; x_1, x_2, x_3)$$
$$= \sum_{m_1,m_2,m_3=0}^{\infty} \frac{(a)_{m_1+m_2+m_3}(b_1)_{m_1}(b_2)_{m_2}}{(c)_{m_1+m_2+m_3} m_1!\, m_2!\, m_3!} x_1^{m_1} x_2^{m_2} x_3^{m_3}. \tag{B8}$$

It should be noted that two of the three infinite sums in the confluent hypergeometric function (B7) terminate because of the negative argument of two Pochhammer symbols. Inserting Eq. (B7) in (B3) yields the final result:

$$S_{n_1 l_1 m_1}^{n_2 l_2 m_2}(\alpha, \beta, \mathbf{R}, \mathbf{k})$$
$$= (4\pi)^2 (2l_1+1)!!\,(2l_2+1)!!\,\frac{\alpha^{2n_1+l_1-1}\beta^{2n_2+l_2-1}}{\delta^{2(n_1+n_2+l_1+l_2)-2}} e^{-i\mathbf{k}\cdot\mathbf{R}}(-1)^{l_1}$$
$$\times \sum_{l_1'=0}^{l_1} \sum_{m_1'} \frac{\langle l_1 m_1 \,|\, l_1' m_1' \,|\, l_1 - l_1' m_1 - m_1' \rangle}{(2l_1'+1)!!\,[2(l_1-l_1')+1]!!} [\mathscr{Y}_{l_1-l_1'}^{m_1-m_1'}(\mathbf{k})]^* (n_2+l_2+1)_{l_1-l_1'}$$
$$\times \sum_{l_2'=0}^{l_2} \sum_{m_2'} \frac{\langle l_2 m_2 \,|\, l_2' m_2' \,|\, l_2 - l_2' m_2 - m_2' \rangle}{(2l_2'+1)!!\,[2(l_2-l_2')+1]!!} \mathscr{Y}_{l_2-l_2'}^{m_2-m_2'}(\mathbf{k})(n_1+l_1+1)_{l_2-l_2'}$$
$$\times \frac{(-i)^{l_1+l_2}(i\delta)^{l_1'+l_2'}}{(n_1+n_2+l_1+l_2+2)_{l_1-l_1'+l_2-l_2'}}$$
$$\times \sum_{p=0}^{\infty} \frac{(n_1+n_2+l_1+l_2+2)_p}{p!} \left[\frac{k^2+2(\alpha^2-\beta^2)}{k^2+2(\alpha^2+\beta^2)}\right]^p$$
$$\times \Phi_D^{(3)}\Big(n_2+l_2+l_1-l_1'+1, -p, -p; n_1+n_2+l_1+l_2+l_2-l_2'$$
$$+ l_1-l_1'+2; 2, \frac{2k^2}{k^2+2(\alpha^2-\beta^2)}, i\mathbf{k}\cdot\mathbf{R}\Big)$$
$$\times S_{n_1+l_1-l_1'+p, l_1', m_1'}^{n_2+l_2-l_2', l_2', m_2'}(\delta, \delta, \mathbf{R}, 0). \tag{B9}$$

Numerical test calculations have shown that the infinite series (B3) converges extremely slowly if k and the difference between α and β become larger. This becomes immediately evident if the convergence factor

$$\left[\frac{k^2+2(\alpha^2-\beta^2)}{k^2+2(\alpha^2+\beta^2)}\right]^p \tag{B10}$$

in Eq. (B9) is considered. A further delicate procedure in the evaluation of the infinite series representation of the Fourier transform of a two-center product of B functions is the computation of the hypergeometric function $\Phi_D^{(3)}$ with imaginary argument $i\mathbf{k}\cdot\mathbf{R}$ which is not only time-consuming but also quite susceptible to rounding errors.

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REFERENCES

1. C. TAVARD, M. ROUAULT, M. ROUX, AND M. CORNILLE, *J. Chem. Phys.* **61** (1961), 1324.
2. I. WALLER AND D. R. HARTREE, *Proc. R. Soc. London* **124** (1929), 119.
3. L. S. BARTELL AND R. M. GAVIN, JR., *J. Amer. Chem. Soc.* **86** (1964), 3493.
4. R. A. BONHAM, J. L. PEACHER, AND H. L. COX, JR., *J. Chem. Phys.* **40** (1964), 3083.
5. H. P. TRIVEDI AND E. O. STEINBORN, *Phys. Rev. A* **27** (1983), 670.
6. R. P. FEYNMAN, *Phys. Rev.* **76** (1949), 769, Eq. (14a).
7. J. BENTLEY AND F. STUART, *J. Comput. Phys.* **11** (1973), 127.
8. G. ARFKEN, "Mathematical Methods for Physicists," p. 103, Academic Press, New York, 1970.
9. R. B. JUNKER, *J. Phys. B* **13** (1980), 1049.
10. R. B. JUNKER, *Comput. Phys. Commun.* **23** (1981), 377.
11. R. MCCARROLL, *Proc. R. Soc. London* **264** (1961), 547.
12. R. A. BONHAM, *J. Phys. Soc. Japan* **20** (1965), 2260.
13. H. J. MONKHORST AND F. E. HARRIS, *Int. J. Quantum Chem.* **6** (1972), 601.
14. G. GUIDOTTI, G. P. ARRIGHINI, AND F. MARINELLI, *Theor. Chim. Acta* **53** (1979), 165.
15. E. FILTER AND E. O. STEINBORN, *Phys. Rev. A.* **18** (1978), 1.
16. E. FILTER AND E. O. STEINBORN, *J. Math. Phys.* **21** (1980), 2725.
17. E. FILTER AND E. O. STEINBORN, *J. Math. Phys.* **19** (1978), 79.
18. E. J. WENIGER AND E. O. STEINBORN, *J. Chem. Phys.* **78** (1983), 6121.
19. E. U. CONDON AND G. H. SHORTLEY, "The Theory of Atomic Spectra," p. 48, Cambridge Univ. Press, Cambridge, England, 1970.
20. M. WEISSBLUTH, "Atoms and Molecules," p. 3, Academic Press, New York, 1978.
21. M. MESSIAH, "Quantum Mechanics," Appendix B4, North-Holland, Amsterdam, 1961.
22. I. SHAVITT, *in* "Methods in Computational Physics" (B. Adler, S. Fernbach, and M. Rotenberg, Eds.), Vol. 2, p. 15, Academic Press, New York, 1963.
23. E. O. STEINBORN AND E. FILTER, *Theor. Chim. Acta* **38** (1975), 273.

24. W. MAGNUS, F. OBERHETTINGER, AND R. P. SONI, "Formulas and Theorems for the Special Functions of Mathematical Physics," p. 66, Springer-Verlag, Berlin, 1966.
25. See [15, p. 2, Eq. (2.12)].
26. E. J. WENIGER AND E. O. STEINBORN, *Phys. Rev. A* **28** (1983), 2026.
27. See [24, p. 2].
28. B. R. JUDD, "Angular Momentum Theory for Diatomic Molecules," p. 51, Academic Press, New York, 1975.
29. I. N. SNEDDON, 'The Use of Integral Transforms," p. 79, Eq. (2-13-19), McGraw–Hill, New York, 1972.
30. J. A. GAUNT, *Philos. Trans. R. Soc. London A* **228** (1929), 192, Appendix.
31. See [15, p. 3, Eqs. (2.3), (2.4)].
32. F. P. PROSSER AND C. H. BLANCHARD, *J. Chem. Phys.* **36** (1962), 1112.
33. S. BOCHNER, "Vorlesungen über Fouriersche Integrale," p. 189, Chelsea, New York, 1948.
34. See [16, p. 2728, Eq. (3.4)].
35. See [18, p. 6124–6125, Eqs. (3.22)–(3.24)].
36. L. C. BIEDENHARN AND J. D. LOUCK, "Angular Momentum Theory in Quantum Physics," p. 71. Eq. (3.153), Addison–Wesley, Reading, Mass., 1981.
37. B. F. BAYMAN, *J. Math. Phys.* **19** (1978), 2558.
38. C. J. JOACHAIN, "Quantum Collision Theory," p. 678, Appendix D, Eq. (D.3), North–Holland, Amsterdam, 1975.
39. G. N. WATSON, "A Treatise on the Theory of Bessel Functions," p. 140, Cambridge Univ. Press, Cambridge, 1966.
40. See [26, p. 2028, Eq. (3.11)].
41. See [5, p. 674, Eqs. (2.31a)–(2.31d)].
42. E. J. WENIGER AND E. O. STEINBORN, *Comput. Phys. Commun.***25** (1982), 189.
43. See [20, p. 11, Eq. (1.2–29)].
44. I. I. SOBEL'MAN, "Introduction to the Theory of Atomic Spectra," p. 73, Eqs. (13.20), (13.22), Pergamon, Oxford, 1972.
45. R. PIESSENS AND M. BRANDERS, *J. Comp. Appl. Math.* **1** (1975), 153.
46. (a) B. EINARSSON, *BIT* **8** (1968), 279; (b) B. EINARSSON, *Comm. ACM* **15** (1972), 47; (c) P. LINZ, *Comm. ACM* **15** (1972), 358; (d) E. A. FLINN, *J. Assoc. Comput. Mach.* **7** (1960), 181.
47. Numerical Algorithms Group, Mark 9, February, 1982, unpublished.
48. R. PIESSENS, E. DE DONCKER-KAPENGA, C. W. ÜBERHUBER, AND D. K. KAHANER, "QUADPACK, A Subroutine Package for Automatic Integration," p. 66, Springer-Verlag, Berlin, 1983.
49. A. S. KRONROD, "Nodes and Weights of Quadrature Formulas," p. 12, Consultants Bureau, New York, 1965.
50. M. A. MALCOLM AND R. B. SIMPSON, *ACM Trans. Math. Software* 1 (1976), 129.
51. P. WYNN, *MTAC* **10** (1956), 91.
52. E. O. STEINBORN AND K. RUEDENBERG, *Adv. Quantum Chem.* **7** (1973), 1.
53. H. EXTON, "Multiple Hypergeometric Functions and Applications," p. 230, Eq. (4.7.1.1), Wiley, New York, 1976.[1]

[1] In Eq. (7.4.1.1) the factor $\Gamma[{}^{\nu_1+\nu_2}_{\nu_1,\nu_2}] = \Gamma(\nu_1+\nu_2)/[\Gamma(\nu_1)\,\Gamma(\nu_2)]$ should read $\Gamma[{}^{\nu_1,\nu_2}_{\nu_1+\nu_2}]$.