Fourier transform of a two-center product of exponential-type orbitals. Application to one- and two-electron multicenter integrals

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A new formula for the Fourier transform (FT) of a two-center RBF (reduced Bessel function) charge distribution permitting partial-wave analysis is derived with the use of Feynman's identity. This formula is valid for all quantum numbers. It is also independent of the orientation of the coordinate axes. A new representation for the two-center overlap integral (to which the kinetic energy, two-center attraction and Coulomb repulsion integrals can be readily reduced) and for the three-center attraction integral is obtained with the help of the FT. It is stable for all values of the orbital exponents. The method developed by Graovac *et al.* for computing repulsion integrals for *s* states is generalized to include all states. Numerical test values of several one- and two-electron integrals are also reported. A strategy which should enhance the efficiency of computation by making maximal use of the FT's already computed is suggested.

I. INTRODUCTION

Reduced Bessel functions (RBF's), proposed by Shavitt[1] with a view to facilitate the evaluation of molecular multicenter integrals over exponential-type function (ETF) bases, have been investigated by Filter and Steinborn[2–4] and by Weniger.[5] Application to H_2^+ and HeH^{2+} systems were carried out by Steinborn and Weniger.[6,7] Numerical aspects were also studied by Antolović and Delhalle[8] and Weniger and Steinborn.[9] The two-center overlap integral was found to be the basic building block appearing in the kinetic energy, the two-center nuclear attraction, and the Coulomb repulsion integrals.

In this paper we apply the Fourier transform theory to the RBF's. The Fourier transform of a product of two ETF's with centers separated by $\vec{R}$ is of interest in its own right in fields such as x-ray crystallography and electron diffraction off molecules. It also forms the basic building block of the multicenter electron repulsion integrals. Further, it provides a framework which is readily extended to accommodate the treatment of three-center nuclear attraction integrals. The two-center overlap integral, itself of considerable importance as just mentioned, immediately follows as a special case of the two-center Fourier transform with zero momentum transfer. For all these reasons, Sec. II is devoted to the two-center Fourier transform with RBF's. The RBF's also happen to be the ETF basis with probably the simplest structure under Fourier transformations.[5] In Sec. III we consider the two-center overlap integral. A new formula is presented along with some numerical aspects and results. The three-center nuclear attraction integral is treated in Sec. IV while the general two-electron multicenter integral is considered in Sec. V. We conclude with a summary and discussion in Sec. VI.

II. TWO-CENTER FOURIER TRANSFORM WITH REDUCED BESSEL FUNCTIONS

For two-center charge distributions described by the product of two ETF's, Fourier transforms have been difficult to compute until recently. Junker[10] was able to formulate a compact explicit expression (requiring a one-dimensional numerical integration) for Slater-type orbitals (STO's) by using elliptical coordinates. He has also programmed his expression.[11] Unfortunately, this expression is unsuitable for a partial-wave analysis of the Fourier transform.

Bonham *et al.*[12,13] derived an explicit expression (also requiring a one-dimensional numerical integration) using the so-called Feynman identity. Their expression lends itself readily to partial-wave decomposition but is restricted to combinations of *s*-type orbitals only. Guidotti *et al.*[14] were able to generalize this expression to states of higher angular momentum but only on a case by case basis by repeated differentiation with respect to the Cartesian components of the momentum-transfer vector. Predictably, this results in a rapidly lengthening list of formulas, one for each combination of the two STO's. The list also grows in complexity quite rapidly with higher quantum numbers of the STO's. Finally, the momentum-transfer vector appears in

this formulation in terms of products of its Cartesian components which must be regrouped to perform angular momentum analysis.

Here we derive a compact, general expression along the lines of Bonham *et al.*[12,13] which is capable of angular momentum decomposition and is valid for all quantum numbers and orbital scaling parameters of the participating orbitals. Like all other expressions mentioned above, it also involves a one-dimensional numerical integration.

A. Definitions

The ETF's used here are the B functions of Filter and Steinborn[3] with an RBF describing the radial dependence

$$B^m_{n,l}(\rho\vec{r})=[2^{n+l}(n+l)!]^{-1}\mathscr{Y}^m_l(\rho\vec{r})\hat{k}_{n-1/2}(\rho r) . \tag{2.1}$$

Here the *solid* harmonic

$$\mathscr{Y}^m_l(\rho\vec{r})=(\rho r)^l Y^m_l(\hat{r}) , \tag{2.2}$$

where $Y^m_l(\hat{r})$ is the usual spherical harmonic with the phase convention of Condon and Shortley.[15] Also, the RBF

$$\hat{k}_\nu(x)=(2/\pi)^{1/2}x^\nu K_\nu(x) , \tag{2.3}$$

where $K_\nu(x)$ is the modified Bessel function of the second kind.[16] The following representation and recurrence relation are also known[3]:

$$\hat{k}_{-1/2}(x)=e^{-x}/x , \tag{2.4}$$

$$\hat{k}_{n-1/2}(x)=(e^{-x}/x)\sum_{j=1}^{n}\frac{(2n-j-1)!}{(j-1)!(n-j)!}\,2^{j-n}x^j , \tag{2.5}$$

$$x^2\hat{k}_{\nu-1/2}(x)+(2\nu+1)\hat{k}_{\nu+1/2}(x)-\hat{k}_{\nu+3/2}(x)=0 . \tag{2.6}$$

The symmetric Fourier transform of $B^m_{n,l}(\rho r)$, which we shall denote by $\bar{B}^m_{n,l}(\rho,\vec{k})$, is given by[5,9]

$$\bar{B}^m_{n,l}(\rho,\vec{k})\equiv(2\pi)^{-3/2}\int d\vec{r}\,e^{-i\vec{k}\cdot\vec{r}}B^m_{n,l}(\rho\vec{r})$$

$$=(2\pi)^{1/2}\frac{\rho^{2n-1}}{(\rho^2+k^2)^{n+l+1}}\mathscr{Y}^m_l(-i\rho\vec{k}) . \tag{2.7}$$

Consideration of other types of ETF's[5,17] generally yields a function of the type above multiplied by a hypergeometric function characteristic of the polynomial part of the radial function describing the chosen ETF.

For a pair of mutual Fourier transforms $u(\rho\vec{r})$ and $\bar{u}(\rho,\vec{k})$ related to each other by the relations

$$\bar{u}(\rho,\vec{k})=(2\pi)^{-3/2}\int d\vec{r}\,e^{-i\vec{k}\cdot\vec{r}}u(\rho\vec{r}) ,$$

$$u(\rho\vec{r})=(2\pi)^{-3/2}\int d\vec{k}\,e^{i\vec{k}\cdot\vec{r}}\bar{u}(\rho,\vec{k}) , \tag{2.8}$$

it can be shown that

$$\langle u_1(\rho_1\vec{r})\,|\,e^{-i\vec{k}\cdot\vec{r}}\,|\,u_2(\rho_2(\vec{r}-\vec{R}))\rangle_{\vec{r}}=e^{-i\vec{k}\cdot\vec{R}}\langle\bar{u}_1(\rho_1,\vec{q})\,|\,e^{-i\vec{q}\cdot\vec{R}}\,|\,\bar{u}_2(\rho_2,\vec{q}+\vec{k})\rangle_{\vec{q}} . \tag{2.9}$$

(The vector subscript denotes the variable of integration.) The pairs $u_1,\bar{u}_1$ and $u_2,\bar{u}_2$ are related as in Eq. (2.8). The first matrix element is, apart from the missing factor $(2\pi)^{-3/2}$, the Fourier transform of a two-center charge distribution defined as the product of $u_1(\rho_1\vec{r})$ centered at the origin and $u_2(\rho_2(\vec{r}-\vec{R}))$ centered at $\vec{R}$.

B. Application to B functions

In the above section, specializing $u_1(\rho_1\vec{r})$ to $B^{m_1}_{n_1l_1}(\rho_1\vec{r})$ and $u_2(\rho_2(\vec{r}-\vec{R}))$ to $B^{m_2}_{n_2l_2}(\rho_2(\vec{r}-\vec{R}))$, we get from Eqs. (2.2) and (2.7)–(2.9) that

$$\langle B^{m_1}_{n_1l_1}(\rho_1\vec{r})\,|\,e^{-i\vec{k}\cdot\vec{r}}\,|\,B^{m_2}_{n_2l_2}(\rho_2(\vec{r}-\vec{R}))\rangle_{\vec{r}}=(2/\pi)\rho_1^{2n_1-1}\rho_2^{2n_2-1}(+i\rho_1)^{l_1}(-i\rho_2)^{l_2}$$

$$\times e^{-i\vec{k}\cdot\vec{R}}I_{n_1+l_1+1,n_2+l_2+1}(\vec{k},\vec{R}) , \tag{2.10}$$

where

$$I_{j_1,j_2}(\vec{k},\vec{R})=\int d\vec{q}\,\frac{\mathscr{Y}^{m_1*}_{l_1}(\vec{q})\mathscr{Y}^{m_2}_{l_2}(\vec{q}+\vec{k})e^{-i\vec{q}\cdot\vec{R}}}{(\rho_1^2+\vec{q}^{\,2})^{j_1}[\rho_2^2+(\vec{q}+\vec{k})^2]^{j_2}} , \tag{2.11}$$

the subscripts j_1 and j_2 on the left-hand side of Eq. (2.11) being the powers of $(\rho_1^2+\vec{q}^{\,2})$ and $[\rho_2^2+(\vec{q}+\vec{k})^2]$, respectively, in the denominator of the integrand on the right-hand side. We note that the integral $I_{j_1,j_2}(\vec{k},\vec{R})$

is a function of l_1, m_1, ρ_1, l_2, m_2, and ρ_2, in addition to the explicitly indicated indices and variables. It is obvious that

$$I_{j_1,j_2}(\vec{k},\vec{R})=\frac{(-1)^{j_1+j_2}}{(j_1-1)!(j_2-1)!}\left[\frac{\partial}{\partial\rho_1^2}\right]^{j_1-1}\left[\frac{\partial}{\partial\rho_2^2}\right]^{j_2-1}I_{1,1}(\vec{k},\vec{R})\ . \tag{2.12}$$

It turns out that one can find an expression for $I_{1,1}(\vec{k},\vec{R})$ and differentiate it with respect to ρ_1^2 and ρ_2^2 repeatedly.

Following Bonham *et al.*,[12,13] we make use of the so-called Feynman's identity[18]

$$(ab)^{-1}=\int_0^1 d\alpha[a+(b-a)\alpha]^{-2}\ . \tag{2.13}$$

Applying it to the integrand of $I_{1,1}(\vec{k},\vec{R})$ and translating the momentum space origin so that $\vec{q}\to\vec{q}-\alpha\vec{k}$, we obtain, by setting $a=\vec{q}^2+\rho_1^2$ and $b=(\vec{q}+\vec{k})^2+\rho_2^2$,

$$I_{1,1}(\vec{k},\vec{R})=\int_0^1 d\alpha\, e^{i\alpha\vec{k}\cdot\vec{R}}\left[\int d\vec{q}\frac{e^{-i\vec{q}\cdot\vec{R}}\mathscr{Y}_{l_1}^{m_1*}(\vec{q}-\alpha\vec{k})\mathscr{Y}_{l_2}^{m_2}[\vec{q}+(1-\alpha)\vec{k}]}{[\vec{q}^2+\beta^2(\alpha)]^2}\right]$$

$$=-\int_0^1 d\alpha\, e^{i\alpha\vec{k}\cdot\vec{R}}\left[\frac{\partial}{\partial\beta^2}\mathscr{I}(\beta)\right]\ , \tag{2.14}$$

where

$$\beta^2(\alpha)=k^2\alpha(1-\alpha)+\rho_1^2(1-\alpha)+\rho_2^2\alpha \tag{2.15}$$

and

$$\mathscr{I}(\beta)=\int d\vec{q}\frac{e^{-i\vec{q}\cdot\vec{R}}\mathscr{Y}_{l_1}^{m_1*}(\vec{q}-\alpha\vec{k})\mathscr{Y}_{l_2}^{m_2}[\vec{q}+(1-\alpha)\vec{k}]}{\vec{q}^2+\beta^2}\ . \tag{2.16}$$

Noting that

$$\left[\frac{\partial}{\partial\rho_1^2}\right]^{j_1-1}=\left[\frac{\partial\beta^2}{\partial\rho_1^2}\frac{\partial}{\partial\beta^2}\right]^{j_1-1}=(1-\alpha)^{j_1-1}\left[\frac{\partial}{\partial\beta^2}\right]^{j_1-1},$$

$$\left[\frac{\partial}{\partial\rho_2^2}\right]^{j_2-1}=\left[\frac{\partial\beta^2}{\partial\rho_2^2}\frac{\partial}{\partial\beta^2}\right]^{j_2-1}=\alpha^{j_2-1}\left[\frac{\partial}{\partial\beta^2}\right]^{j_2-1}, \tag{2.17}$$

and combining Eqs. (2.12), (2.14), (2.16), and (2.17), we get

$$I_{j_1,j_2}(\vec{k},\vec{R})=\frac{(-1)^{j_1+j_2+1}}{(j_1-1)!(j_2-1)!}\int_0^1 d\alpha(1-\alpha)^{j_1-1}\alpha^{j_2-1}e^{i\alpha\vec{k}\cdot\vec{R}}\left[\frac{\partial}{\partial\beta^2}\right]^{j_1+j_2-1}\mathscr{I}(\beta)\ . \tag{2.18}$$

Now it is necessary to separate out the angular dependence on $\vec{k}$ from the integrand of Eq. (2.16) so that the $\vec{q}$ integration may be explicitly carried out to evaluate $\mathscr{I}(\beta)$. We use the addition theorem of the solid spherical harmonic[19,20]

$$\mathscr{Y}_l^m(\vec{r}_1+\vec{r}_2)=4\pi(2l+1)!!\sum_{l'=0}^{l}\sum_{m'=-l'}^{l'}\frac{\langle lm\,|\,l'm'\,|\,l-l'm-m'\rangle\mathscr{Y}_{l'}^{m'}(\vec{r}_1)\mathscr{Y}_{l-l'}^{m-m'}(\vec{r}_2)}{(2l'+1)!![2(l-l')+1)]!!}\ , \tag{2.19}$$

where the Gaunt coefficient

$$\langle l_1m_1\,|\,l_2m_2\,|\,l_3m_3\rangle=\int Y_{l_1}^{m_1*}(\hat{r})Y_{l_2}^{m_2}(\hat{r})Y_{l_3}^{m_3}(\hat{r})d\Omega\ . \tag{2.20}$$

Additionally, we use the easily derived recombination result[21]

$$\mathscr{Y}_{l_1}^{m_1*}(\vec{r})\mathscr{Y}_{l_2}^{m_2}(\vec{r})=\sum_l\langle l_2m_2\,|\,l_1m_1\,|\,lm_2-m_1\rangle\mathscr{Y}_l^{m_2-m_1}(\vec{r})r^{l_1+l_2-l} \tag{2.21}$$

and arrive at

$$\mathscr{I}(\beta)=(4\pi)^2(2l_1+1)!!(2l_2+1)!!$$
$$\times\sum_{l_1'=0}^{l_1}\sum_{m_1'=-l_1'}^{l_1'}\frac{\langle l_1m_1\,|\,l_1'm_1'\,|\,l_1-l_1'm_1-m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!}\mathscr{Y}_{l_1-l_1'}^{m_1-m_1'*}(-\alpha\vec{\mathbf{k}})$$
$$\times\sum_{l_2'=0}^{l_2}\sum_{m_2'=-l_2'}^{l_2'}\frac{\langle l_2m_2\,|\,l_2'm_2'\,|\,l_2-l_2'm_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!}\mathscr{Y}_{l_2-l_2'}^{m_2-m_2'}((1-\alpha)\vec{\mathbf{k}})$$
$$\times\sum_{l}\langle l_2'm_2'\,|\,l_1'm_l'\,|\,lm_2'-m_1'\rangle G(l;m_1'l_1',m_2'l_2';\beta,\vec{\mathbf{R}})\,. \tag{2.22}$$

Here

$$G(l;m_1'l_1',m_2'l_2';\beta,\vec{\mathbf{R}})=\int d\vec{\mathbf{q}}\,\frac{e^{-i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}}\mathscr{Y}_l^{m_2'-m_1'}(\vec{\mathbf{q}})q^{l_1'+l_2'-l}}{\vec{\mathbf{q}}^2+\beta^2}\,. \tag{2.23}$$

By expanding $e^{-i\vec{\mathbf{q}}\cdot\vec{\mathbf{R}}}$ in spherical waves[22] and using the relation[23]

$$\int_0^\infty dq\,q^2\frac{q^{l+2m}j_l(qR)}{\vec{\mathbf{q}}^2+\rho^2}=(-1)^m\frac{\pi}{2}R^{-l-1}\rho^{2m}\hat{k}_{l+1/2}(\rho R),\quad m=0,1,2,\ldots \tag{2.24}$$

it can be shown that

$$G(l;m_1'l_1';m_2'l_2';\beta,\vec{\mathbf{R}})=2\pi^2i^l(-1)^{(l_1'+l_2'+l)/2}R^{-l-1}Y_l^{m_2'-m_1'}(\hat{R})(\beta^2)^{\Delta l}\hat{k}_{l+1/2}(\beta R)\,, \tag{2.25a}$$

$$\Delta l=(l_1'+l_2'-l)/2,\quad 0\le\Delta l\le\min(l_1',l_2')\,. \tag{2.25b}$$

Noting that the differential operator in Eq. (2.18) operates on $G(l;m_1'l_1',m_2'l_2';\beta,\vec{\mathbf{R}})$ only, we consider

$$\left[\frac{\partial}{\partial\beta^2}\right]^n[(\beta^2)^{\Delta l}\hat{k}_{l+1/2}(\beta R)]=\sum_{j=0}^n\begin{bmatrix}n\\j\end{bmatrix}\left[\left[\frac{\partial}{\partial\beta^2}\right]^j(\beta^2)^{\Delta l}\right]\left[\left[\frac{\partial}{\partial\beta^2}\right]^{n-j}\hat{k}_{l+1/2}(\beta R)\right] \tag{2.26}$$

by Leibniz's formula. Making use of[3]

$$\left[\frac{\partial}{\partial\beta^2}\right]^n\hat{k}_\nu(\beta R)=(-R^2/2)^n\hat{k}_{\nu-n}(\beta R)\,, \tag{2.27}$$

$$\hat{k}_{-(l+1/2)}(x)=(x^2)^{-(l+1/2)}\hat{k}_{l+1/2}(x)\,, \tag{2.28}$$

and

$$\left[\frac{\partial}{\partial\beta^2}\right]^j(\beta^2)^{\Delta l}=\frac{(\Delta l)!}{(\Delta l-j)!}(\beta^2)^{\Delta l-j}\,, \tag{2.29}$$

and defining $\Delta n=n-(l_1'+l_2'+3)$, Eq. (2.26) simplifies to

$$\left[\frac{\partial}{\partial\beta^2}\right]^n[(\beta^2)^{\Delta l}\hat{k}_{l+1/2}(\beta R)]=\frac{(\Delta l)!(R^2)^{n-\Delta l}}{(\beta R)^{5+2(\Delta l+\Delta n)}}\sum_{j=0}^{\Delta l}\begin{bmatrix}n\\j\end{bmatrix}\frac{(-1/2)^{n-j}}{(\Delta l-j)!}\hat{k}_{\Delta n+2\Delta l-j+5/2}(\beta R)\,. \tag{2.30}$$

Identifying n in Eq. (2.30) with j_1+j_2-1 in Eq. (2.18) and further identifying j_1 and j_2 with n_1+l_1+1 and n_2+l_2+1 in Eq. (2.10), the complete expression for the Fourier transform of a two-center product wave function emerges. After minor algebra, the result is most concisely expressed as

$$\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \mid e^{-i\vec{k}\cdot\vec{r}} \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\rangle_{\vec{r}}$$
$$=(-1)^{l_2}(4\pi)^3(2l_1+1)!!(2l_2+1)!!\frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\rho_1^{2n_1+l_1-1}\rho_2^{2n_2+l_2-1}$$
$$\times\sum_{l_1'=0}^{l_1}\sum_{m_1'=-l_1'}^{l_1'}\frac{\langle l_1 m_1 \mid l_1' m_1' \mid l_1-l_1' m_1-m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!}\mathscr{Y}^{m_1-m_1'*}_{l_1-l_1'}(\vec{k})\cdot(-1)^{l_1-l_1'}$$
$$\times\sum_{l_2'=0}^{l_2}\sum_{m_2'=-l_2'}^{l_2'}\frac{\langle l_2 m_2 \mid l_2' m_2' \mid l_2-l_2' m_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!}\mathscr{Y}^{m_2-m_2'}_{l_2-l_2'}(\vec{k})$$
$$\times\sum_{l}\langle l_2' m_2' \mid l_1' m_1' \mid l m_2'-m_1'\rangle i^{l+l_1+l_2}(-1)^{(l_1'+l_2'+l)/2}$$
$$\times\int_0^1 d\alpha\, e^{-i(1-\alpha)\vec{k}\cdot\vec{R}}\frac{\alpha^{n_2+l_2+l_1-l_1'}(1-\alpha)^{n_1+l_1+l_2-l_2'}}{[\beta(\alpha)]^{2(n_1+l_1+n_2+l_2)-(l_1'+l_2')+1}}$$
$$\times\left[\sum_{j=0}^{\Delta l}(-1)^j\binom{\Delta l}{j}B^{m_2'-m_1'}_{n_1+n_2+2\Delta l_0+1-j,l}(\beta(\alpha)\vec{R})\right] \tag{2.31a}$$

with

$$\beta^2(\alpha)=k^2\alpha(1-\alpha)+(1-\alpha)\rho_1^2+\alpha\rho_2^2\,, \tag{2.31b}$$
$$\Delta l=(l_1'+l_2'-l)/2\,, \tag{2.31c}$$

and

$$\Delta l_0=(l_1+l_2-l)/2\,. \tag{2.31d}$$

Evaluation of the integral in Eq. (2.31a) has been elaborately discussed by Guidotti *et al.*[14] and by Monkhorst and Harris.[24] The sum within the square brackets persits in all formulas and merits attention. This is discussed in Sec. III.

Integral (2.31a) is readily decomposed into constituent angular momentum partial waves. This property will be especially helpful for the multicenter repulsion integrals (Sec. V).

Expanding the imaginary exponential in the α integral in Eq. (2.31a) and combining all the angular momentum functions in $\vec{k}$, Eq. (2.31a) can be written in terms of its partial-wave components

$$\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \mid e^{-i\vec{k}\cdot\vec{r}} \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\rangle_{\vec{r}}\equiv\sum_{LM}\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \mid e^{-i\vec{k}\cdot\vec{r}} \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\rangle_{LM}Y_L^M(\hat{k})\,, \tag{2.32}$$

where

$$\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \mid e^{-i\vec{k}\cdot\vec{r}} \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\rangle_{LM}$$
$$=N\sum_{l_1'=0}^{l_1}\sum_{m_1'=-l_1'}^{l_1'}\frac{\langle l_1 m_1 \mid l_1' m_1' \mid l_1-l_1' m_1-m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!}(-k)^{l_1-l_1'}$$
$$\times\sum_{l_2'=0}^{l_2}\sum_{m_2'=-l_2'}^{l_2'}\frac{\langle l_2 m_2 \mid l_2' m_2' \mid l_2-l_2' m_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!}k^{l_2-l_2'}$$
$$\times\sum_{l}\langle l_2' m_2' \mid l_1' m_1' \mid l m_2'-m_1'\rangle i^{l+l_1+l_2}(-1)^{(l_1'+l_2'+l)/2}$$
$$\times\sum_{l_{12}}\langle l_2-l_2' m_2-m_2' \mid l_1-l_1' m_1-m_1' \mid l_{12} m_{12}\rangle$$
$$\times\sum_{l_{123}}(-i)^{l_{123}}\langle l_{12} m_{12} \mid LM \mid l_{123} m_{123}\rangle Y^{m_{123}}_{l_{123}}(\hat{R})$$
$$\times\int_0^1 d\alpha\, j_{l_{123}}((1-\alpha)kR)\frac{\alpha^{n_2+l_2+l_1-l_1'}(1-\alpha)^{n_1+l_1+l_2-l_2'}}{[\beta(\alpha)]^{2(n_1+l_1+n_2+l_2)-(l_1'+l_2')+1}}$$
$$\times\left[\sum_{j=0}^{\Delta l}(-1)^j\binom{\Delta l}{j}B^{m_2'-m_1'}_{n_1+n_2+2\Delta l_0+1-j,l}(\beta(\alpha)\vec{R})\right], \tag{2.33}$$

where

$$m_{12}=m_2-m_2'-(m_1-m_1'),\quad m_{123}=m_{12}-M\ ,$$

and

$$N=(-1)^{l_2}(4\pi)^4(2l_1+1)!!(2l_2+1)!!\frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\rho_1^{2n_1+l_1-1}\rho_2^{2n_2+l_2-1}\ . \tag{2.34}$$

III. TWO-CENTER OVERLAP INTEGRAL

The two-center overlap integral appears as a building block in the kinetic energy, two-center nuclear attraction, and Coulomb integrals. Filter and Steinborn[3] derived several formulas to evaluate it; each formula being the most suitable according to whether $\rho_1/\rho_2\approx 1$ or $\rho_1/\rho_2\gg$ or $\ll 1$. Antolović and Delhalle[8] as well as Weniger and Steinborn[9] have considered the numerical performance of these formulas.

Here we derive yet another representation for the two-center overlap integral over B functions. This results from simply letting $\vec{k}\to 0$ in the two-center Fourier transform expression Eq. (2.31a). We get

$$\begin{aligned}\langle B^{m_1}_{n_1l_1}(\rho_1\vec{r})\,|\,B^{m_2}_{n_2l_2}(\rho_2(\vec{r}-\vec{R}))\rangle_{\vec{r}}&\\ =(-1)^{l_2}4\pi\frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}\rho_1^{2n_1+l_1-1}\rho_2^{2n_2+l_2-1}&\\ \times\sum_l\langle l_2m_2\,|\,l_1m_1\,|\,lm_2-m_1\rangle\int_0^1 d\alpha\frac{\alpha^{n_2+l_2}(1-\alpha)^{n_1+l_1}}{[\beta_0(\alpha)]^{2n_1+2n_2+l_1+l_2+1}}&\\ \times\left[\sum_{j=0}^{\Delta l_0}(-1)^j\binom{\Delta l_0}{j}B^{m_2-m_1}_{n_1+n_2+2\Delta l_0+1-j,l}(\beta_0(\alpha)\vec{R})\right]&\end{aligned} \tag{3.1}$$

with now

$$\beta_0^2(\alpha)=(1-\alpha)\rho_1^2+\alpha\rho_2^2 \tag{3.2}$$

and

$$\Delta l_0=(l_1+l_2-l)/2\ . \tag{3.3}$$

For $\rho_1=\rho_2$ this reduces to the known result[25]

$$\begin{aligned}\langle B^{m_1}_{n_1l_1}(\rho\vec{r})\,|\,B^{m_2}_{n_2l_2}(\rho(\vec{r}-\vec{R}))\rangle=(-1)^{l_2}4\pi\rho^{-3}\sum_l\langle l_2m_2\,|\,l_1m_1\,|\,lm_2-m_1\rangle&\\ \times\left[\sum_{j=0}^{\Delta l_0}(-1)^j\binom{\Delta l_0}{j}B^{m_2-m_1}_{n_1+n_2+2\Delta l_0+1-j,l}(\rho\vec{R})\right]\ .&\end{aligned} \tag{3.4}$$

The sum in the square bracket [Eqs. (2.31a), (3.1), and (3.4)] appears repeatedly and deserves consideration. The alternating sign with the combinatorial indicates possible loss of significant digits. This is indeed borne out by experimenting with n_1+n_2, l_1, l_2, and ρR values. It turns out that the number of significant digits lost increases as Δl_0 increases to $(\Delta l_0)_{\max}$ $[=\min(l_1,l_2)]$ but is insensitive to the value of the argument ρR and to n_1+n_2. For $l_1=l_2=4$ and $\Delta l_0=4$, one loses four significant digits. For $l_1=l_2=20$ and $\Delta l_0=20$, one loses 18 digits. Unfortunately, the contribution of the sum increases as Δl_0 approaches $(\Delta l_0)_{\max}$. The difficulty therefore cannot be ignored. In practice, we have skirted around this problem by evaluating the quantity in the square bracket of Eq. (3.1) in higher precision.

Using single precision (which is greater than 10 but less than 11 decimal digits on our machine) for the rest of the calculation, we were easily able to compute the overlap integral (3.1) to relative accuracy of one part in 10^8 (see Table I). The integration was performed with the help of the subroutine DCADRE of the IMSL package.[26] The definite integral had to be computed numerically, but this presented no problems. [In contrast, the same integration in Eq. (2.31) requires care[14,24] as $\vec{k}$ is nonzero.] Equation (3.1) is stable for all values—except zero—of orbital scaling parameters ρ_1 and ρ_2, and the time taken to evaluate the integral is insensitive to the ratio $\rho_1:\rho_2$.

TABLE I. Overlap integral $\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\rangle$ with $n_1=l_1=m_1=n_2=l_2=m_2=5$, $(R,\theta,\phi)=(2,45°,0°)$, and fixed $\rho_1=1.5$ for various ρ_2 values between 1.5 and 9.0. Average time 3 sec/integral.[a]

ρ_2	This paper	Exact[b]
1.5	$9.867\,702\,185\times10^{-8}$	$9.867\,702\,185\times10^{-8}$
1.6	$8.502\,669\,245\times10^{-8}$	$8.502\,669\,244\times10^{-8}$
1.7	$7.255\,486\,069\times10^{-8}$	$7.255\,486\,068\times10^{-8}$
1.8	$6.144\,525\,625\times10^{-8}$	$6.144\,525\,629\times10^{-8}$
1.9	$5.173\,375\,779\times10^{-8}$	$5.173\,375\,778\times10^{-8}$
2.0	$4.336\,429\,110\times10^{-8}$	$4.336\,429\,110\times10^{-8}$
3.0	$6.919\,278\,951\times10^{-9}$	$6.919\,278\,951\times10^{-9}$
4.5	$5.467\,156\,782\times10^{-10}$	$5.467\,156\,782\times10^{-10}$
6.0	$6.472\,563\,755\times10^{-11}$	$6.472\,563\,755\times10^{-11}$
7.0	$1.901\,023\,397\times10^{-11}$	$1.901\,023\,397\times10^{-11}$
8.0	$6.364\,670\,749\times10^{-12}$	$6.364\,670\,749\times10^{-12}$
9.0	$2.380\,365\,441\times10^{-12}$	$2.380\,365\,441\times10^{-12}$

[a]As a guide to the speed of our Telefunken TR 440 computer, a square-root evaluation takes 0.43 msec.
[b]Exact results (to ten digits) from Ref. 5, Table 6.8.

IV. THREE-CENTER NUCLEAR ATTRACTION INTEGRAL

The two-center Fourier transform [Eq. (2.32)] provides the starting ground this time. The three-center nuclear attraction integral with the center of attraction at $\vec{R}_c$ is written as

$$\left\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \left| \frac{1}{|\vec{r}-\vec{R}_c|} \right| B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\right\rangle = \frac{1}{2\pi^2}\int \frac{d\vec{k}}{k^2}\cdot\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \mid e^{-i\vec{k}\cdot(\vec{r}-\vec{R}_c)} \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\rangle \tag{4.1}$$

using the formal identity

$$\frac{1}{r}=\frac{1}{2\pi^2}\int d\vec{k}\frac{e^{-i\vec{k}\cdot\vec{r}}}{k^2}\,. \tag{4.2}$$

Substituting for the Fourier transform from Eqs. (2.32) and (2.33) we eventually arrive at the result that

$$\begin{aligned}
&\left\langle B^{m_1}_{n_1 l_1}(\rho_1\vec{r}) \left| \frac{1}{|\vec{r}-\vec{R}_c|} \right| B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}-\vec{R}))\right\rangle \\
&= (-1)^{l_2} 8(4\pi)^2 \frac{(n_1+l_1+n_2+l_2+1)!}{(n_1+l_1)!(n_2+l_2)!}(2l_1+1)!!(2l_2+1)!!\rho_1^{2n_1+l_1-1}\rho_2^{2n_2+l_2-1} \\
&\times \sum_{l_1'=0}^{l_1}\sum_{m_1'=-l_1'}^{l_1'} \frac{\langle l_1 m_1 \mid l_1' m_1' \mid l_1-l_1' m_1-m_1'\rangle}{(2l_1'+1)!![2(l_1-l_1')+1]!!}(-1)^{l_1-l_1'} \\
&\times \sum_{l_2'=0}^{l_2}\sum_{m_2'=-l_2'}^{l_2'} \frac{\langle l_2 m_2 \mid l_2' m_2' \mid l_2-l_2' m_2-m_2'\rangle}{(2l_2'+1)!![2(l_2-l_2')+1]!!} \\
&\times \sum_{l} i^{l_1+l_2+1}(-1)^{(l_1'+l_2'+l)/2}\langle l_2' m_2' \mid l_1' m_1' \mid l m_2'-m_1'\rangle \\
&\times \sum_{l_{12}}(-i)^{l_{12}}\langle l_2-l_2' m_2-m_2' \mid l_1-l_1' m_1-m_1' \mid l_{12} m_2-m_2'-m_1+m_1'\rangle \\
&\times \int_0^1 d\alpha\, \alpha^{n_2+l_2+l_1-l_1'}(1-\alpha)^{n_1+l_1+l_2-l_2'} \\
&\times Y_{l_{12}}^{m_2-m_2'-m_1+m_1'}\left(\frac{(1-\alpha)\vec{R}-\vec{R}_c}{|(1-\alpha)\vec{R}-\vec{R}_c|}\right) \\
&\times \int_0^\infty dk \frac{k^{l_1-l_1'+l_2-l_2'} j_{l_{12}}(k\,|(1-\alpha)\vec{R}-\vec{R}_c|)}{[\beta(\alpha)]^{2(n_1+l_1+n_2+l_2)-(l_1'+l_2')+1}} \\
&\times \left[\sum_{j=0}^{\Delta l}(-1)^j\binom{\Delta l}{j} B^{m_2'-m_1'}_{n_1+n_2+2\Delta l_0+1-j,l}(\beta(\alpha)\vec{R})\right]\,.
\end{aligned} \tag{4.3}$$

We recall from Eqs. (2.31b)–(2.31d) repeated below, respectively, that

$$\beta^2(\alpha)=k^2\alpha(1-\alpha)+(1-\alpha)\rho_1^2+\alpha\rho_2^2$$

and

$$\Delta l=(l_1'+l_2'-l)/2,\quad \Delta l_0=(l_1+l_2-l)/2\ .$$

Here $j_{l_{12}}(x)$ is the spherical Bessel function of the first kind[27] of order l_{12}.

Performing the k integration first has distinct advantages, for the two-center Fourier transform is a very complicated function of $\vec{k}$.[28,29] We know that the (single-center) Fourier transform of a $1s$ orbital decreases as k^{-4} for large $|\vec{k}|$ [Eq. (2.7)] and as $k^{-2(n+1)-l}$ in general for an nl state. A two-center transform is roughly similar but has local modulations of complicated structure superposed on it, which often bring about sign changes as k increases. Numerical integration of such a function over the semi-infinite interval $(0,\infty)$, taken together with its slow decay rate as k^{-4}, poses immense problems. In contrast, carrying out the k integration first has the advantages that (i) the term in the square bracket decreases *exponentially* as k increases, and (ii) the structure of the integrand is sufficiently well understood for convergence acceleration techniques[30,31] to be employed with reasonable confidence.

We present some numerical results for the three-center nuclear attraction integral computed using Eq. (4.3) in Table II. We had no difficulty obtaining values correct to eight places despite the double integration. The use of Shank's acceleration techniques[31,32] was made with great profit.

V. MULTICENTER REPULSION INTEGRAL

The application to a multicenter repulsion integral is straightforward:

$$\left\langle B_{n_1l_1}^{m_1}(\rho_1(\vec{r}_a-\vec{R}_1))B_{n_3l_3}^{m_3}(\rho_3(\vec{r}_b-\vec{R}_3))\left|\frac{1}{r_{ab}}\right|B_{n_2l_2}^{m_2}(\rho_2(\vec{r}_a-\vec{R}_2))B_{n_4l_4}^{m_4}(\rho_4(\vec{r}_b-\vec{R}_4))\right\rangle$$

$$=\frac{1}{2\pi^2}\int\frac{d\vec{k}}{k^2}e^{-i\vec{k}\cdot(\vec{R}_1-\vec{R}_4)}\langle B_{n_1l_1}^{m_1}(\rho_1(\vec{r}_a-\vec{R}_1))\,|\,e^{-i\vec{k}\cdot(\vec{r}_a-\vec{R}_1)}\,|\,B_{n_2l_2}^{m_2}(\rho_2(\vec{r}_a-\vec{R}_2))\rangle_{\vec{r}_a}$$

$$\times\langle B_{n_4l_4}^{m_4}(\rho_4(\vec{r}_b-\vec{R}_4))\,|\,e^{-i\vec{k}\cdot(\vec{r}_b-\vec{R}_4)}\,|\,B_{n_3l_3}^{m_3}(\rho_3(\vec{r}_b-\vec{R}_3))\rangle_{\vec{r}_b}^{*}$$

$$=\frac{1}{2\pi^2}\int\frac{d\vec{k}}{k^2}e^{-i\vec{k}\cdot\vec{R}_{14}}\langle B_{n_1l_1}^{m_1}(\rho_1\vec{r}_a)\,|\,e^{-i\vec{k}\cdot\vec{r}_a}\,|\,B_{n_2l_2}^{m_2}(\rho_2(\vec{r}_a-\vec{R}_{21}))\rangle_{r_{\vec{a}}}$$

$$\times\langle B_{n_4l_4}^{m_4}(\rho_4\vec{r}_b)\,|\,e^{-i\vec{k}\cdot\vec{r}_b}\,|\,B_{n_3l_3}^{m_3}(\rho_3(\vec{r}_b-\vec{R}_{34}))\rangle_{\vec{r}_b}^{*}\qquad(5.1)$$

with

$$\vec{R}_{ij}=\vec{R}_i-\vec{R}_j\ .\qquad(5.2)$$

Substituting from Eq. (2.31a) for the two-center Fourier transform yields the desired expression for the multicenter repulsion integral.

We note that the problem is separated into two one-electron problems (a property of Fourier transform). This means that in a large molecular calculation one can "assemble" multicenter integrals

TABLE II. Three-center nuclear attraction integral

$$\langle B_{n_1l_1}^{m_1}(\rho_1\vec{r})\,|\,(\,|\,\vec{r}-\vec{R}_c\,|\,)^{-1}\,|\,B_{n_2l_2}^{m_2}(\rho_2\,|\,\vec{r}-\vec{R}\,|\,)\rangle$$

for s states ($l_1=m_1=l_2=m_2=0$). Estimated relative error 10^{-8}. Average time 65 sec/integral.

ρ_1	n_1	ρ_2	n_2	$\vec{R}_c(R_c,\theta_c,\phi_c)$	$\vec{R}(R,\theta,\phi)$	Integral
0.2	1	0.2	1	(2.0,90°,0°)	(2.0,90°,60°)	$1.810\,1838\times10^{-1}$
		10.0				$7.574\,2801\times10^{-3}$
		0.2		(5.0,90°,0°)	(5.0,90°,60°)	$1.275\,4128\times10^{-1}$
1.0	1	5.0	1	(0.5,90°,0°)	(2.0,90°,0°)	$7.173\,2965\times10^{-2}$
		1.0				$3.410\,2136\times10^{-1}$
		5.0		(0.5,90°,180°)		$4.116\,6529\times10^{-2}$
		1.0				$4.499\,5538\times10^{-1}$

out of two-center Fourier transforms, which implies that the latter can be computed and stored as "intermediate information" which can be repeatedly drawn upon as and when needed.

One approach is to break down the exponential factor and the two Fourier transforms in the integrand of Eq. (4.1) into partial waves whereupon the angular integration is readily performed, leaving behind two infinite sums over radial integrals in the most general case. This problem along with the attendant numerical considerations is treated at great length by Graovac *et al.*[28,29] and will not be discussed here.

Another approach, which we have investigated in a preliminary fashion as a possible alternative, is to move the k integration within the integrals over Feynman's dummy variables—one each for both Fourier transforms—i.e., α in Eq. (2.31a). The k integration is carried out first and has good convergence properties as noted in Sec. IV. The two dummy integration variables are now parameters of the k integral. The remaining double integral is the price to be paid for avoiding partial-wave expansions in infinite series.

The k integration was performed with the help of the subroutine D01AAF (Clenshaw-Curtis method) of the NAG[33] library. Accelerated convergence techniques were again profitably implemented. The double integral (over dummy variables) was evaluated with the help of subroutine DBLINT.[26] For homonuclear molecules this approach works satisfactorily as seen in Table III where we present some two-, three-, and four-center results. As in the case of three-center attraction integral, the time taken depends on the accuracy desired as well as on the geometry. For significant deviation from the homonuclearity constraint, however, problems with the accuracy of the double-integral soon arise. A detailed investigation is necessary to determine how this difficulty can be economically overcome.

VI. DISCUSSION AND SUMMARY

We have derived a compact, general expression for the Fourier transform of a charge distribution described by the product of two B functions with their centers separated by R. The final expression holds for all quantum numbers and orbital scaling parameters and involves a one-dimensional numerical integration. We also point out that the expression (2.31a) remains valid not only for all nonnegative values of n_1 and n_2 but also for

$$n_1 = -1, -2, \ldots, -l_1$$

and

$$n_2 = -1, -2, \ldots, -l_2 \ .$$

The result, Eq. (2.31a), is a systematic generalization of the Bonham, Peacher, and Cox result.[12,13] This new formula is then applied to one- and two-electron multicenter integrals. A useful strategy for the evaluation of the multicenter repulsion integral along the lines advocated by Graovac *et al.* is also indicated. Numerical test results are also reported.

TABLE III. Some special cases of the general two-electron integral

$$\langle B^{m_1}_{n_1 l_1}(\rho_1(\vec{r}_a - \vec{R}_1)) B^{m_3}_{n_3 l_3}(\rho_3(\vec{r}_b - \vec{R}_3)) \mid r_{ab}^{-1} \mid B^{m_2}_{n_2 l_2}(\rho_2(\vec{r}_a - \vec{R}_2)) B^{m_4}_{n_4 l_4}(\rho_4(\vec{r}_b - \vec{R}_4)) \rangle \ ,$$

k integration performed first. All states are 1s and $\rho_1 = \rho_2 = \rho_3 = \rho_4 = \rho$.

ρ	$\vec{R}_1$[a]	$\vec{R}_2$[a]	$\vec{R}_3$[a]	$\vec{R}_4$[a]	Integral	Type
1.0	(0,0,0)	(1.5,0,0)	(0,0,0)	(1.5,0,0)	0.296 835[b]	Two-center exch.
1.2	(0,0,0)	(2.0,0,0)	(0,0,0)	(1.0,1.0,0)	0.194 469[b]	Three-center exch.
1.0	(0,0,0)	(1.0,0,0)	(0,1.0,0)	(0,0,1.0)	0.3455	Four-center integral
1.0				(1.0,1.0,0)	0.3927	(time decreasing
2.0					0.2738	from
3.0					0.1091	27 to
						6 sec)
4.0					0.0335	
5.0					0.0089	
6.0					0.0021	

[a] $\vec{R} = (R_x, R_y, R_z)$.

[b] Comparison Ref. 28; average time 65 sec.

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