Supplementary Material: Intracule functional models. V. Recurrence relations for two-electron integrals in position and momentum space

If $G_{l,m,n}$ is redefined, as per Equation 35, the fundamental integral about $\mathcal{W}(\boldsymbol{u},\boldsymbol{v})$ becomes

$$[\mathbf{0000}]_W^{(l,m,n)} = S_{ab} G_{l,m,n}(U^2, V^2, \boldsymbol{U}\cdot\boldsymbol{V}) \tag{1}$$

Applying the previous strategy (Equations 28 to 30) to this integral results in the alternative 18-term RR

$$\begin{aligned}
[(\boldsymbol{a}+\mathbf{1}_i)\boldsymbol{bcd}]_W^{(l,m,n)} &= \frac{\beta(B_i-A_i)}{\alpha+\beta}[\boldsymbol{abcd}]_W^{(l,m,n)} + \frac{U_i}{\alpha+\beta}[\boldsymbol{abcd}]_W^{(l+1,m,n)} \\
&\quad + \frac{2\beta V_i}{\alpha+\beta}[\boldsymbol{abcd}]_W^{(l,m+1,n)} + \frac{V_i+2\beta U_i}{2(\alpha+\beta)}[\boldsymbol{abcd}]_W^{(l,m,n+1)} \\
&\quad + \frac{a_i}{2(\alpha+\beta)}[(\boldsymbol{a}-\mathbf{1}_i)\boldsymbol{bcd}]_W^{(l,m,n)} + \frac{a_i}{2(\alpha+\beta)^2}[(\boldsymbol{a}-\mathbf{1}_i)\boldsymbol{bcd}]_W^{(l+1,m,n)} \\
&\quad + \frac{2a_i\beta^2}{(\alpha+\delta)^2}[(\boldsymbol{a}-\mathbf{1}_i)\boldsymbol{bcd}]_W^{(l,m+1,n)} + \frac{a_i\beta}{(\alpha+\beta)^2}[(\boldsymbol{a}-\mathbf{1}_i)\boldsymbol{bcd}]_W^{(l,m,n+1)} \\
&\quad + \frac{b_i}{2(\alpha+\beta)}[\boldsymbol{a}(\boldsymbol{b}-\mathbf{1}_i)\boldsymbol{cd}]_W^{(l,m,n)} + \frac{b_i}{2(\alpha+\beta)^2}[\boldsymbol{a}(\boldsymbol{b}-\mathbf{1}_i)\boldsymbol{cd}]_W^{(l+1,m,n)} \\
&\quad - \frac{2b_i\alpha\beta}{(\alpha+\beta)^2}[\boldsymbol{a}(\boldsymbol{b}-\mathbf{1}_i)\boldsymbol{cd}]_W^{(l,m+1,n)} + \frac{b_i(\beta-\alpha)}{2(\alpha+\beta)^2}[\boldsymbol{a}(\boldsymbol{b}-\mathbf{1}_i)\boldsymbol{cd}]_W^{(l,m,n+1)} \\
&\quad - \frac{c_i}{2(\alpha+\beta)(\gamma+\delta)}[\boldsymbol{ab}(\boldsymbol{c}-\mathbf{1}_i)\boldsymbol{d}]_W^{(l+1,m,n)} - \frac{2c_i\beta\delta}{(\alpha+\beta)(\gamma+\delta)}[\boldsymbol{ab}(\boldsymbol{c}-\mathbf{1}_i)\boldsymbol{d}]_W^{(l,m+1,n)} \\
&\quad - \frac{c_i(\beta+\delta)}{2(\alpha+\beta)(\gamma+\delta)}[\boldsymbol{ab}(\boldsymbol{c}-\mathbf{1}_i)\boldsymbol{d}]_W^{(l,m,n+1)} \\
&\quad - \frac{d_i}{2(\alpha+\beta)(\gamma+\delta)}[\boldsymbol{abc}(\boldsymbol{d}-\mathbf{1}_i)]_W^{(l+1,m,n)} + \frac{2d_i\beta\gamma}{(\alpha+\beta)(\gamma+\delta)}[\boldsymbol{abc}(\boldsymbol{d}-\mathbf{1}_i)]_W^{(l,m+1,n)} \\
&\quad + \frac{d_i(\gamma-\beta)}{2(\alpha+\beta)(\gamma+\delta)}[\boldsymbol{abc}(\boldsymbol{d}-\mathbf{1}_i)]_W^{(l,m,n+1)}
\end{aligned} \tag{2}$$

For the special cases of $\mathcal{Z}=\mathcal{U}(\boldsymbol{u})$ or $\mathcal{V}(\boldsymbol{v})$, the $G_{l,m,n}(U^2,V^2,\boldsymbol{U}\cdot\boldsymbol{V})$ simplify to

$$G_{l,m,n}(U^2,V^2,\boldsymbol{U}\cdot\boldsymbol{V}) = \frac{\pi^{3/2}\left(\frac{\partial}{\partial U^2}\right)^l\left(\frac{\partial}{\partial V^2}\right)^m\left(\frac{\partial}{\partial(\boldsymbol{U}\cdot\boldsymbol{V})}\right)^n}{(\alpha+\beta+\gamma+\delta)^{3/2}}\int e^{-\nu^2|\boldsymbol{u}+\boldsymbol{U}|^2}\mathcal{U}(\boldsymbol{u})d\boldsymbol{u} \tag{3a}$$

$$G_{l,m,n}(U^2,V^2,\boldsymbol{U}\cdot\boldsymbol{V}) = \frac{\pi^{3/2}\sigma^3\left(\frac{\partial}{\partial U^2}\right)^l\left(\frac{\partial}{\partial V^2}\right)^m\left(\frac{\partial}{\partial(\boldsymbol{U}\cdot\boldsymbol{V})}\right)^n}{(\alpha+\beta)^{3/2}(\gamma+\delta)^{3/2}}\int e^{-\sigma^2|\boldsymbol{v}+i\boldsymbol{V}|^2}\mathcal{V}(\boldsymbol{v})d\boldsymbol{v} \tag{3b}$$

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and one finds that

$$G_{l,m,n}(U^2, V^2, \boldsymbol{U} \cdot \boldsymbol{V}) = 0, \quad \text{if } m, n > 0 \text{ and } \mathcal{W}(\boldsymbol{u}, \boldsymbol{v}) = \mathcal{U}(\boldsymbol{u}) \tag{4a}$$

$$G_{l,m,n}(U^2, V^2, \boldsymbol{U} \cdot \boldsymbol{V}) = 0, \quad \text{if } l, n > 0 \text{ and } \mathcal{W}(\boldsymbol{u}, \boldsymbol{v}) = \mathcal{V}(\boldsymbol{v}) \tag{4b}$$