Various Cases of Two-Electron Integrals

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April 11, 2023

Abstract Two-electron integrals are important for quantum chemistry, and in particular for Hartree-Fock methods. Because of this, there are many ways to compute these. Unfortunately, some methods only work when the four orbitals being integrated have different centers. Therefore, different formulae need to be derived for the cases when multiple orbitals share centers.

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1 Introduction

1.1 Notation

In the equations below, the following notations are used. $\mathbf{r}$ represents a position vector. Its components are $\mathbf{r} = (x, y, z)$, and its magnitude may be represented normally as $||\mathbf{r}||$ or $|\mathbf{r}|$. The square of its magnitude may be represented as $\mathbf{r}^2$ or simply r^2. Any subscript on the r will be transferred to its components, so $\mathbf{r}_1 = (x_1, y_1, z_1)$. Also, the term $\mathrm{d}\mathbf{r} = \mathrm{d}x\mathrm{d}y\mathrm{d}z$. Letters a, b, c, d will represents Cartesian orbitals, while letters p, q, r, s will represent Hermite orbitals. To avoid confusion, Hermite orbital indices will also be shown with an overbar when in vector form. Capital letters like $\mathbf{A}$ represent orbital centers and have components $\mathbf{A} = (A_x, A_y, A_z)$. Lower case letters represent angular momentum components. When bold, they represent a vector, such as $\mathbf{a} = (a_x, a_y, a_z)$, but when Roman they represent the sum of these components, $a = a_x + a_y + a_z$. When in equations, the letters a, A, α go together; b, B, β go together; $c, C\gamma$ go together; and d, D, δ go together. The vector $\mathbf{1}_i$ represents a unit vector along either the x, y, or z axis, where $i = x, y, z$.

2 Hermite Polynomials

For most of the integrals, the kernels can be reduced to a form involving Hermite polynomials. Hermite polynomials are defined using the following equation [1].

$$H_n(x)e^{-x^2} = (-1)^n \frac{d^n}{dx^n} e^{-x^2} \tag{2.1}$$

This definition can be used to show the following.

$$a^{\frac{n}{2}} H_n\left(x\sqrt{a}\right) e^{-ax^2} = (-1)^n \frac{d^n}{dx^n} e^{-ax^2} \tag{2.2}$$

This can be rewritten as a sum [1],

$$H_n(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} (-1)^k 2^{n-2k} x^{n-2k} \tag{2.3}$$

as well as a recurrence relation [1].

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{2.4}$$

From these, a multiple-argument formula can be derived [1].

$$H_n(\alpha t) = \alpha^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(1 - \frac{1}{\alpha^2}\right)^k H_{n-2k}(t) \tag{2.5}$$

2.1 Hermite Integrals

For the two-electron integrals, the following integral becomes useful.

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n\left(\alpha t\right) dt \tag{2.6}$$

To solve for equation 2.6, note the following, from [1].

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n\left(t\right) dt = 2^n \sqrt{\pi} a^n \tag{2.7}$$

Then, use equation 2.5 to expand.

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n(\alpha t) dt = \int_{-\infty}^{\infty} \alpha^n e^{-(a-t)^2} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(1 - \frac{1}{\alpha^2}\right)^k H_{n-2k}(t) dt \tag{2.8}$$

Manipulating this equation gives

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n(\alpha t) dt = \alpha^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(1 - \frac{1}{\alpha^2}\right)^k \int_{-\infty}^{\infty} e^{-(a-t)^2} H_{n-2k}(t) dt \tag{2.9}$$

Using equation 2.7 gives the following.

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n(\alpha t) dt = \alpha^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(1 - \frac{1}{\alpha^2}\right)^k 2^{n-2k} \sqrt{\pi} a^{n-2k} \tag{2.10}$$

Then, rewrite equation 2.10 to look more like eqation 2.3. We need to assume that $|\alpha| < 1$.

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n(\alpha t) dt = \sqrt{\pi} \alpha^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(\frac{1}{\alpha^2} - 1\right)^k (-1)^k 2^{n-k} a^{n-2k} \tag{2.11}$$

$$= \sqrt{\pi} \alpha^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(\frac{\alpha^2}{1-\alpha^2}\right)^{-k} (-1)^k 2^{n-2k} a^{n-2k} \tag{2.12}$$

$$= \sqrt{\pi} \alpha^n \left(\sqrt{\frac{1}{\alpha^2} - 1}\right)^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{k!(n-2k)!} \left(\sqrt{\frac{\alpha^2}{1-\alpha^2}}\right)^{n-2k} (-1)^k 2^{n-2k} a^{n-2k} \tag{2.13}$$

Finally, using equation 2.3 gives the final value of

$$\int_{-\infty}^{\infty} e^{-(a-t)^2} H_n(\alpha t) dt = \sqrt{\pi} \left(\sqrt{1-\alpha^2}\right)^n H_n\left(a \sqrt{\frac{\alpha^2}{1-\alpha^2}}\right) \tag{2.14}$$

2.2 Hermite Orbital Recurrence Relation

Suppose a Cartesian orbital has the following form.

$$\psi_{\mathbf{a}} = (x - A_x)^{a_x} \left(y - A_y\right)^{a_y} (z - A_z)^{a_z} \, e^{-\alpha(\mathbf{r}-\mathbf{A})^2} \tag{2.15}$$

Also suppose a Hermite orbital has the following form.

$$\overline{\psi_{\mathbf{p}}} = \zeta^{\frac{p}{2}} H_{p_x} \left(\sqrt{\zeta}\,(x - P_x)\right) H_{p_y} \left(\sqrt{\zeta}\,(y - P_y)\right) H_{p_z} \left(\sqrt{\zeta}\,(x - P_z)\right) e^{-\zeta(\mathbf{r}-\mathbf{P})^2} \tag{2.16}$$

Using equation 2.4 gives the following recurrence relation for Hermite orbitals. In all equations after this, i can be x, y, or z.

$$\overline{\psi_{\mathbf{p}+\mathbf{1}_i}} = 2\zeta\,(i - P_i)\,\overline{\psi_{\mathbf{p}}} - 2\zeta p_i \overline{\psi_{\mathbf{p}-\mathbf{1}_i}} \tag{2.17}$$

If $\mathbf{A} = \mathbf{P}$, then multiplying by $\psi_{\mathbf{a}-\mathbf{1}_i}/(2\zeta)$ gives the following.

$$\frac{1}{2\zeta}\psi_{\mathbf{a}-\mathbf{1}_i}\overline{\psi_{\mathbf{p}+\mathbf{1}_i}} = \psi_{\mathbf{a}}\overline{\psi_{\mathbf{p}}} - p_i\psi_{\mathbf{a}-\mathbf{1}_i}\overline{\psi_{\mathbf{p}-\mathbf{1}_i}} \tag{2.18}$$

If $[a\overline{p}|_{u,v} = \frac{(2\beta)^u}{(2\zeta)^v}[a\overline{p}|$, then equation 2.18 gives

$$[\mathbf{a}\overline{\mathbf{p}}|_{u,v} = p_i \left[(\mathbf{a}-\mathbf{1}_i)\,\overline{(\mathbf{p}-\mathbf{1}_i)}\right|_{u,v} + \left[(\mathbf{a}-\mathbf{1}_i)\,\overline{(\mathbf{p}+\mathbf{1}_i)}\right|_{u,v+1} \tag{2.19}$$

However, if $\mathbf{P} = \frac{\alpha\mathbf{A}+\beta\mathbf{B}}{\zeta}$, then the recurrence relation in equation 2.17 needs to be rewritten as

$$\overline{\psi_{\mathbf{p}+\mathbf{1}_i}} = 2\zeta\left(i - \frac{\alpha}{\zeta}A_i - \frac{\beta}{\zeta}A_i\right)\overline{\psi_{\mathbf{p}}} + 2\zeta\left(\frac{\beta}{\zeta}A_i - \frac{\beta}{\zeta}B_i\right)\overline{\psi_{\mathbf{p}}} - 2\zeta p_i\overline{\psi_{\mathbf{p}-\mathbf{1}_i}} \tag{2.20}$$

$$= 2\zeta\,(i - A_i)\,\overline{\psi_{\mathbf{p}}} + 2\beta\,(A_i - B_i)\,\overline{\psi_{\mathbf{p}}} - 2\zeta p_i\overline{\psi_{\mathbf{p}-\mathbf{1}_i}} \tag{2.21}$$

Then, multiplying equation 2.21 by $\psi_{\mathbf{a}-\mathbf{1}_i}/(2\zeta)$ gives the following.

$$\frac{1}{2\zeta}\psi_{\mathbf{a}-\mathbf{1}_i}\overline{\psi_{\mathbf{p}+\mathbf{1}_i}} = \psi_{\mathbf{a}}\overline{\psi_{\mathbf{p}}} + \frac{2\beta}{2\zeta}\,(A_i - B_i)\,\psi_{\mathbf{a}-\mathbf{1}_i}\overline{\psi_{\mathbf{p}}} - p_i\psi_{\mathbf{a}-\mathbf{1}_i}\overline{\psi_{\mathbf{p}-\mathbf{1}_i}} \tag{2.22}$$

By letting $[a\overline{p}|_{u,v} = \frac{(2\beta)^u}{(2\zeta)^v}[a\overline{p}|$, equation 2.22 can be rearranged to the following.

$$[\mathbf{a}\overline{\mathbf{p}}|_{u,v} = \left[(\mathbf{a}-\mathbf{1}_i)\,\overline{(\mathbf{p}+\mathbf{1}_i)}\right|_{u,v+1} - (A_i - B_i)\,[(\mathbf{a}-\mathbf{1}_i)\,\overline{\mathbf{p}}|_{u+1,v+1} + p_i\left[(\mathbf{a}-\mathbf{1}_i)\,\overline{(\mathbf{p}-\mathbf{1}_i)}\right|_{u,v} \tag{2.23}$$

3 Two-electron Integrals

For the derivations that follow, it is useful to write the forms of the orbitals being used. A Gaussian orbital centered around the origin has the form

$$G_{\mathbf{a}}(\mathbf{r}) = \sum_{k=1}^{K} D_k x^{a_x} y^{a_y} z^{a_z} e^{-\alpha_k r^2} \tag{3.24}$$

A Hermite orbital has a different form.

$$G_{\overline{\mathbf{p}}}(\mathbf{r}) = \sum_{k=1}^{K} D_k \alpha_k^{\frac{p}{2}} H_{p_x}\left(x\sqrt{\alpha_k}\right) H_{p_y}\left(y\sqrt{\alpha_k}\right) H_{p_z}\left(z\sqrt{\alpha_k}\right) e^{-\alpha_k r^2} \tag{3.25}$$

3.1 Four-Centered Integrals

As a first look at the integrals, consider the full case of four centers. This is the integral that follows.

$$(\mathbf{ab}|\mathbf{cd}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G_{\mathbf{a}}\left(\mathbf{r}_1 - \mathbf{A}\right) G_{\mathbf{b}}\left(\mathbf{r}_1 - \mathbf{B}\right) G_{\mathbf{c}}\left(\mathbf{r}_2 - \mathbf{C}\right) G_{\mathbf{d}}\left(\mathbf{r}_2 - \mathbf{D}\right) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \tag{3.26}$$

Using the definition of the Cartesian orbital in equation 3.24, it is possible to derive the following recurrence relation by multiplying the integral by $\frac{x_1 - A_x}{x_1 - B_x} + \frac{A_x - B_x}{x_1 - B_x} = 1$. This can be done for any coordinate.

$$(\mathbf{ab}|\mathbf{cd}) = \left(\left(\mathbf{a} + \mathbf{1}_i\right)\left(\mathbf{b} - \mathbf{1}_i\right)|\mathbf{cd}\right) + \left(A_i - B_i\right)\left(\mathbf{a}\left(\mathbf{b} - \mathbf{1}_i\right)|\mathbf{cd}\right) \tag{3.27}$$

Similarly, by multiplying the integral by $\frac{x_2 - C_x}{x_2 - D_x} + \frac{C_x - D_x}{x_2 - D_x}$, the other recurrence relation can be derived.

$$(\mathbf{ab}|\mathbf{cd}) = \left(\mathbf{ab}|\left(\mathbf{c} + \mathbf{1}_i\right)\left(\mathbf{d} - \mathbf{1}_i\right)\right) + \left(C_i - D_i\right)\left(\mathbf{ab}|\mathbf{c}\left(\mathbf{d} - \mathbf{1}_i\right)\right) \tag{3.28}$$

These recurrence relations also work termwise. Since this integral is over contracted basis functions, is should be rewritten in terms of uncontracted integrals to more easily manipulate the terms.

$$(\mathbf{ab}|\mathbf{cd}) = \sum_{k_A=1}^{K_A}\sum_{k_B=1}^{K_B}\sum_{k_C=1}^{K_C}\sum_{k_D=1}^{K_D} D_A D_B D_C D_D \left[\mathbf{ab}|\mathbf{cd}\right] \tag{3.29}$$

Note that while the uncontracted integral is not subscripted, it is assumed that its parameters change to the correpsonding values in each of the basis functions that make it up. This uncontracted integral obeys equations 3.27 and 3.28 as well. The integral of the uncontracted functions has the following form.

$$\begin{aligned}\left[\mathbf{ab}|\mathbf{cd}\right] = D_A D_B D_C D_D \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} & \left(x_1 - A_x\right)^{a_x}\left(y_1 - A_y\right)^{a_y}\left(z_1 - A_z\right)^{a_z} \\ & \left(x_1 - B_x\right)^{b_x}\left(y_1 - B_y\right)^{b_y}\left(z_1 - B_z\right)^{b_z} \\ & \left(x_2 - C_x\right)^{c_x}\left(y_2 - C_y\right)^{c_y}\left(z_2 - C_z\right)^{c_z} \\ & \left(x_2 - D_x\right)^{d_x}\left(y_2 - D_y\right)^{d_y}\left(z_2 - D_z\right)^{d_z} \\ & e^{-\alpha(\mathbf{r}_1 - \mathbf{A})^2} e^{-\beta(\mathbf{r}_1 - \mathbf{B})^2} e^{-\gamma(\mathbf{r}_2 - \mathbf{C})^2} e^{-\delta(\mathbf{r}_2 - \mathbf{D})^2} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2\end{aligned} \tag{3.30}$$

To make this easier to solve, combine the exponents.

$$\alpha r_1^2 - 2\alpha \mathbf{r}_1 \cdot \mathbf{A} + \alpha A^2 + \beta r_1^2 - 2\beta \mathbf{r}_1 \cdot \mathbf{B} + \beta B^2 \tag{3.31}$$

$$= (\alpha + \beta) r_1^2 - 2\mathbf{r}_1 \cdot (\alpha \mathbf{A} + \beta \mathbf{B}) + \alpha A^2 + \beta B^2 \tag{3.32}$$

Complete the square.

$$= (\alpha + \beta) r_1^2 - 2\mathbf{r}_1 \cdot (\alpha \mathbf{A} + \beta \mathbf{B}) + \alpha A^2 + \beta B^2 + \frac{\alpha^2 A^2 + \beta^2 B^2 + 2\alpha\beta \mathbf{A}\cdot\mathbf{B}}{\alpha + \beta} - \frac{\alpha^2 A^2 + \beta^2 B^2 + 2\alpha\beta \mathbf{A}\cdot\mathbf{B}}{\alpha + \beta} \tag{3.33}$$

$$= (\alpha + \beta)\left(\mathbf{r}_1 - \frac{\alpha \mathbf{A} + \beta \mathbf{B}}{\alpha + \beta}\right)^2 + \frac{\alpha^2 A^2 + \alpha\beta A^2 + \alpha\beta B^2 + \beta^2 B^2 - \alpha^2 A^2 - \beta^2 B^2 - 2\alpha\beta \mathbf{A}\cdot\mathbf{B}}{\alpha + \beta} \tag{3.34}$$

$$= (\alpha + \beta)\left(\mathbf{r}_1 - \frac{\alpha \mathbf{A} + \beta \mathbf{B}}{\alpha + \beta}\right)^2 + \frac{\alpha\beta}{\alpha + \beta}\left(\mathbf{A} - \mathbf{B}\right)^2 \tag{3.35}$$

Let $\zeta = \alpha + \beta$ and $\mathbf{P} = \frac{\alpha\mathbf{A}+\beta\mathbf{B}}{\zeta}$. Then the equation becomes the following.

$$= \zeta \left(\mathbf{r}_1 - \mathbf{P}\right)^2 + \frac{\alpha\beta}{\zeta}\left(\mathbf{A}-\mathbf{B}\right)^2 \tag{3.36}$$

A similar process can be done for the other two Gaussians. Plugging these in to the integral gives a new integral. For these, let $\eta = \gamma + \delta$ and $\mathbf{Q} = \frac{\gamma\mathbf{C}+\delta\mathbf{D}}{\eta}$.

$$\begin{aligned}[\mathbf{ab}|\mathbf{cd}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ (x_1-A_x)^{a_x}(y_1-A_y)^{a_y}(z_1-A_z)^{a_z}(x_1-B_x)^{b_x}(y_1-B_y)^{b_y}(z_1-B_z)^{b_z} \\ (x_2-C_x)^{c_x}(y_2-C_y)^{c_y}(z_2-C_z)^{c_z}(x_2-D_x)^{d_x}(y_2-D_y)^{d_y}(z_2-D_z)^{d_z} \\ e^{-\zeta(\mathbf{r}_1-\mathbf{P})^2} e^{-\eta(\mathbf{r}_2-\mathbf{Q})^2} \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2\end{aligned} \tag{3.37}$$

Using the recurrence relations in equations 3.27 and 3.28, it is possible to take these integrals down to the form $[\mathbf{e0}|\mathbf{f0}]$. Then, using the recurrence relation in equation 2.23, which can be applied to both sides, gives an integral of the following form.

$$\begin{aligned}[\mathbf{0}\overline{\mathbf{p}}|\mathbf{0}\overline{\mathbf{q}}] = [\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \zeta^{\frac{p}{2}}\eta^{\frac{q}{2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ H_{p_x}\left((x_1-P_x)\sqrt{\zeta}\right) H_{p_y}\left((y_1-P_y)\sqrt{\zeta}\right) H_{p_z}\left((z_1-P_z)\sqrt{\zeta}\right) \\ H_{q_x}\left((x_2-Q_x)\sqrt{\eta}\right) H_{q_y}\left((y_2-Q_y)\sqrt{\eta}\right) H_{q_z}\left((z_2-Q_z)\sqrt{\eta}\right) \\ e^{-\zeta(\mathbf{r}_1-\mathbf{P})^2} e^{-\eta(\mathbf{r}_2-\mathbf{Q})^2} \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2\end{aligned} \tag{3.38}$$

Note that for the recurrence relation in equation 2.23 to work, the u, v scaled integral needs to be defined as $|\mathbf{c}\overline{\mathbf{q}}]_{u,v} = \frac{(2\delta)^u}{(2\eta)^v}|\mathbf{c}\overline{\mathbf{q}}]$. Then use the following substitution.

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-t^2(\mathbf{r}_1-\mathbf{r}_2)^2}\mathrm{d}t \tag{3.39}$$

The integral then becomes the following.

$$\begin{aligned}[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \frac{\zeta^{\frac{p}{2}}\eta^{\frac{q}{2}}}{\sqrt{\pi}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ H_{p_x}\left((x_1-P_x)\sqrt{\zeta}\right) H_{p_y}\left((y_1-P_y)\sqrt{\zeta}\right) H_{p_z}\left((z_1-P_z)\sqrt{\zeta}\right) \\ H_{q_x}\left((x_2-Q_x)\sqrt{\eta}\right) H_{q_y}\left((y_2-Q_y)\sqrt{\eta}\right) H_{q_z}\left((z_2-Q_z)\sqrt{\eta}\right) \\ e^{-\zeta(\mathbf{r}_1-\mathbf{P})^2} e^{-\eta(\mathbf{r}_2-\mathbf{Q})^2} e^{-t^2(\mathbf{r}_1-\mathbf{r}_2)^2} \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \mathrm{d}t\end{aligned} \tag{3.40}$$

Let $\mathbf{r}_1' = \mathbf{r}_1 - \mathbf{P}$ and $\mathbf{r}_2' = \mathbf{r}_2 - \mathbf{Q}$. The integral then becomes the following.

$$\begin{aligned}[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \frac{\zeta^{\frac{p}{2}}\eta^{\frac{q}{2}}}{\sqrt{\pi}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ H_{p_x}\left(x_1'\sqrt{\zeta}\right) H_{p_y}\left(y_1'\sqrt{\zeta}\right) H_{p_z}\left(z_1'\sqrt{\zeta}\right) H_{q_x}\left(x_2'\sqrt{\eta}\right) H_{q_y}\left(y_2'\sqrt{\eta}\right) H_{q_z}\left(z_2'\sqrt{\eta}\right) \\ e^{-\zeta(\mathbf{r}_1')^2} e^{-\eta(\mathbf{r}_2')^2} e^{-t^2(\mathbf{r}_1'-\mathbf{r}_2'+\mathbf{P}-\mathbf{Q})^2} \mathrm{d}\mathbf{r}_1' \mathrm{d}\mathbf{r}_2' \mathrm{d}t\end{aligned} \tag{3.41}$$

Let $\mathbf{R} = \mathbf{Q} - \mathbf{P}$ and combine the Gaussians.

$$\zeta\left(\mathbf{r}_1'\right)^2 + \eta\left(\mathbf{r}_2'\right)^2 + t^2\left(\mathbf{r}_1'\right)^2 + t^2\left(\mathbf{r}_2'\right)^2 + t^2R^2 - 2t^2\mathbf{r}_1'\cdot\mathbf{R} + 2t^2\mathbf{r}_2'\cdot\mathbf{R} - 2t^2\mathbf{r}_1'\cdot\mathbf{r}_2' \tag{3.42}$$

$$= \left(\zeta+t^2\right)\left(\mathbf{r}_1'\right)^2 - 2t^2\mathbf{r}_1'\cdot\left(\mathbf{R}+\mathbf{r}_2'\right) + t^2R^2 + \left(\eta+t^2\right)\left(\mathbf{r}_2'\right)^2 + 2t^2\mathbf{r}_2'\cdot\mathbf{R} \tag{3.43}$$

$$= \left(\zeta+t^2\right)\left(\mathbf{r}_1' - t^2\frac{\mathbf{R}+\mathbf{r}_2'}{\zeta+t^2}\right)^2 + t^2R^2 + \left(\eta+t^2\right)\left(\mathbf{r}_2'\right)^2 + 2t^2\mathbf{r}_2'\cdot\mathbf{R} - t^4\frac{R^2 + 2\mathbf{R}\cdot\mathbf{r}_2' + \left(\mathbf{r}_2'\right)^2}{\zeta+t^2} \tag{3.44}$$

$$\begin{aligned}= \left(\zeta+t^2\right)&\left(\mathbf{r}_1' - t^2\frac{\mathbf{R}+\mathbf{r}_2'}{\zeta+t^2}\right)^2 \\ &+ \frac{\zeta t^2R^2 + t^4R^2 + \eta\zeta\left(\mathbf{r}_2'\right)^2 + \eta t^2\left(\mathbf{r}_2'\right)^2 + \zeta t^2\left(\mathbf{r}_2'\right)^2 + t^4\left(\mathbf{r}_2'\right)^2 + 2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R} + 2t^4\mathbf{r}_2'\cdot\mathbf{R}}{\zeta+t^2} \\ &- \frac{t^4R^2 + 2t^4\mathbf{r}_2'\cdot\mathbf{R} + t^4\left(\mathbf{r}_2'\right)^2}{\zeta+t^2}\end{aligned} \tag{3.45}$$

$$= \left(\zeta+t^2\right)\left(\mathbf{r}_1' - t^2\frac{\mathbf{R}+\mathbf{r}_2'}{\zeta+t^2}\right)^2 + \frac{\zeta t^2R^2 + \eta\zeta\left(\mathbf{r}_2'\right)^2 + \eta t^2\left(\mathbf{r}_2'\right)^2 + \zeta t^2\left(\mathbf{r}_2'\right)^2 + 2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R}}{\zeta+t^2} \tag{3.46}$$

$$= \left(\zeta+t^2\right)\left(\mathbf{r}_1' - t^2\frac{\mathbf{R}+\mathbf{r}_2'}{\zeta+t^2}\right)^2 + \frac{\left(\eta\zeta + \eta t^2 + \zeta t^2\right)\left(\mathbf{r}_2'\right)^2 + 2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R} + \zeta t^2R^2}{\zeta+t^2} \tag{3.47}$$

This means that the integral is now the following.

$$\begin{aligned}[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_AD_BD_CD_De^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2}e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\frac{\zeta^{\frac{p}{2}}\eta^{\frac{q}{2}}}{\sqrt{\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ H_{q_x}\left(x_2'\sqrt{\eta}\right)H_{q_y}\left(y_2'\sqrt{\eta}\right)H_{q_z}\left(z_2'\sqrt{\eta}\right)e^{-\frac{\left(\eta\zeta+\eta t^2+\zeta t^2\right)\left(\mathbf{r}_2'\right)^2+2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R}+\zeta t^2R^2}{\zeta+t^2}} \\ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}H_{p_x}\left(x_1'\sqrt{\zeta}\right)H_{p_y}\left(y_1'\sqrt{\zeta}\right)H_{p_z}\left(z_1'\sqrt{\zeta}\right)e^{-\left(\zeta+t^2\right)\left(\mathbf{r}_1'-t^2\frac{\mathbf{R}+\mathbf{r}_2'}{\zeta+t^2}\right)^2}\mathrm{d}\mathbf{r}_1'\mathrm{d}\mathbf{r}_2'\mathrm{d}t\end{aligned} \tag{3.48}$$

Using equation 2.14 on the $\mathbf{r}_1'$ component gives the following. Let $\mathbf{u} = \sqrt{\zeta+t^2}\mathbf{r}_1'$, with $\mathrm{d}\mathbf{r}_1' = \frac{\mathrm{d}\mathbf{u}}{\sqrt{\zeta+t^2}}$. Note that $1 - \frac{\zeta}{\zeta+t^2} = \frac{t^2}{\zeta+t^2}$ and $\frac{\zeta(\zeta+t^2)}{t^2(\zeta+t^2)} = \frac{\zeta}{t^2}$.

$$\begin{aligned}[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_AD_BD_CD_De^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2}e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\frac{\zeta^{\frac{p}{2}}\eta^{\frac{q}{2}}}{\sqrt{\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ H_{q_x}\left(x_2'\sqrt{\eta}\right)H_{q_y}\left(y_2'\sqrt{\eta}\right)H_{q_z}\left(z_2'\sqrt{\eta}\right)e^{-\frac{\left(\eta\zeta+\eta t^2+\zeta t^2\right)\left(\mathbf{r}_2'\right)^2+2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R}+\zeta t^2R^2}{\zeta+t^2}} \\ \frac{\pi^{\frac{3}{2}}}{\left(\zeta+t^2\right)^{\frac{3}{2}}}\left(\frac{t^2}{\zeta+t^2}\right)^{\frac{p}{2}}H_{p_x}\left(t^2\frac{R_x+x_2'}{\sqrt{\zeta+t^2}}\sqrt{\frac{\zeta}{t^2}}\right)H_{p_y}\left(t^2\frac{R_y+y_2'}{\sqrt{\zeta+t^2}}\sqrt{\frac{\zeta}{t^2}}\right)H_{p_z}\left(t^2\frac{R_z+z_2'}{\sqrt{\zeta+t^2}}\sqrt{\frac{\zeta}{t^2}}\right)\mathrm{d}\mathbf{r}_2'\mathrm{d}t\end{aligned} \tag{3.49}$$

$$\begin{aligned}[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_AD_BD_CD_De^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2}e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\zeta^{\frac{p}{2}}\eta^{\frac{q}{2}}\pi\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \\ H_{q_x}\left(x_2'\sqrt{\eta}\right)H_{q_y}\left(y_2'\sqrt{\eta}\right)H_{q_z}\left(z_2'\sqrt{\eta}\right)e^{-\frac{\left(\eta\zeta+\eta t^2+\zeta t^2\right)\left(\mathbf{r}_2'\right)^2+2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R}+\zeta t^2R^2}{\zeta+t^2}} \\ \frac{t^p}{\left(\zeta+t^2\right)^{\frac{p+3}{2}}}H_{p_x}\left(\left(R_x+x_2'\right)\sqrt{\frac{\zeta t^2}{\zeta+t^2}}\right)H_{p_y}\left(\left(R_y+y_2'\right)\sqrt{\frac{\zeta t^2}{\zeta+t^2}}\right)H_{p_z}\left(\left(R_z+z_2'\right)\sqrt{\frac{\zeta t^2}{\zeta+t^2}}\right)\mathrm{d}\mathbf{r}_2'\mathrm{d}t\end{aligned} \tag{3.50}$$

Now, try to separate the exponent.

$$\frac{\left(\eta\zeta+\eta t^2+\zeta t^2\right)\left(\mathbf{r}_2'\right)^2+2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R}+\zeta t^2R^2}{\zeta+t^2}=\frac{\zeta t^2}{\zeta+t^2}\left(\mathbf{r}_2'+\mathbf{R}\right)^2+\eta\left(\mathbf{r}_2'\right)^2 \tag{3.51}$$

This means that the integral can be rewritten using equation 2.2.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}]=D_AD_BD_CD_De^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2}e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\pi(-1)^{p+q}\int_{-\infty}^{\infty}\frac{1}{\left(\zeta+t^2\right)^{\frac{3}{2}}}$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{\partial^p}{\partial x_2'^{p_x}\partial y_2'^{p_y}\partial z_2'^{p_z}}e^{-\frac{\zeta t^2}{\zeta+t^2}\left(\mathbf{r}_2'+\mathbf{R}\right)^2}\right)\left(\frac{\partial^q}{\partial x_2'^{q_x}\partial y_2'^{q_y}\partial z_2'^{q_z}}e^{-\eta\left(\mathbf{r}_2'\right)^2}\right)\mathrm{d}\mathbf{r}_2'\mathrm{d}t \tag{3.52}$$

Then, solve the following equation using integration by parts.

$$(-1)^{n+m}\int_{-\infty}^{\infty}\left(\frac{\partial^n}{\partial x^n}e^{-ax^2}\right)\left(\frac{\partial^m}{\partial x^m}e^{-bx^2}\right)\mathrm{d}x \tag{3.53}$$

$$=(-1)^{n+m}\left(\frac{\partial^n}{\partial x^n}e^{-ax^2}\right)\left(\frac{\partial^{m+1}}{\partial x^{m+1}}e^{-bx^2}\right)\Bigg|_{-\infty}^{\infty}-(-1)^{n+m}\int_{-\infty}^{\infty}\left(\frac{\partial^{n-1}}{\partial x^{n-1}}e^{-ax^2}\right)\left(\frac{\partial^{m+1}}{\partial x^{m+1}}e^{-bx^2}\right)\mathrm{d}x \tag{3.54}$$

$$=(-1)^{n-1+m}\int_{-\infty}^{\infty}\left(\frac{\partial^{n-1}}{\partial x^{n-1}}e^{-ax^2}\right)\left(\frac{\partial^{m+1}}{\partial x^{m+1}}e^{-bx^2}\right)\mathrm{d}x \tag{3.55}$$

This means that ultimately,

$$(-1)^{m+n}\int_{-\infty}^{\infty}\left(\frac{\partial^n}{\partial x^n}e^{-ax^2}\right)\left(\frac{\partial^m}{\partial x^m}e^{-bx^2}\right)\mathrm{d}x=(-1)^m\int_{-\infty}^{\infty}e^{-ax^2}\left(\frac{\partial^{m+n}}{\partial x^{m+n}}e^{-bx^2}\right)\mathrm{d}x \tag{3.56}$$

$$a^{\frac{n}{2}}b^{\frac{m}{2}}\int_{-\infty}^{\infty}\left(H_n\left(\sqrt{a}x\right)e^{-ax^2}\right)\left(H_m\left(\sqrt{b}x\right)e^{-bx^2}\right)\mathrm{d}x=b^{\frac{m+n}{2}}(-1)^n\int_{-\infty}^{\infty}H_{n+m}\left(\sqrt{b}x\right)e^{-ax^2}e^{-bx^2}\mathrm{d}x \tag{3.57}$$

Using this makes equation 3.52 into the following.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}]=D_AD_BD_CD_De^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2}e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\pi(-1)^{q}\int_{-\infty}^{\infty}\frac{\left(\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\zeta+t^2\right)^{\frac{p+q+3}{2}}}$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\frac{\zeta t^2}{\zeta+t^2}\left(\mathbf{r}_2'+\mathbf{R}\right)^2}H_{p_x+q_x}\left(\left(x_2'+R_x\right)\sqrt{\frac{\zeta t^2}{\zeta+t^2}}\right)H_{p_y+q_y}\left(\left(y_2'+R_y\right)\sqrt{\frac{\zeta t^2}{\zeta+t^2}}\right)$$
$$H_{p_z+q_z}\left(\left(z_2'+R_z\right)\sqrt{\frac{\zeta t^2}{\zeta+t^2}}\right)e^{-\eta\left(\mathbf{r}_2'\right)^2}\mathrm{d}\mathbf{r}_2'\mathrm{d}t \tag{3.58}$$

Now, combine the exponents.

$$\frac{\left(\eta\zeta+\eta t^2+\zeta t^2\right)\left(\mathbf{r}_2'\right)^2+2\zeta t^2\mathbf{r}_2'\cdot\mathbf{R}+\zeta t^2R^2}{\zeta+t^2}=\frac{\eta\zeta+\eta t^2+\zeta t^2}{\zeta+t^2}\left(\mathbf{r}_2'\right)^2+2\frac{\zeta t^2}{\zeta+t^2}\mathbf{r}_2'\cdot\mathbf{R}+\frac{\zeta t^2}{\zeta+t^2}R^2 \tag{3.59}$$

$$=\frac{\eta\zeta+\eta t^2+\zeta t^2}{\zeta+t^2}\left(\mathbf{r}_2'+\frac{\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}\mathbf{R}\right)^2+\frac{\zeta t^2}{\zeta+t^2}R^2-\frac{\zeta^2t^4R^2}{\left(\zeta+t^2\right)\left(\eta\zeta+\eta t^2+\zeta t^2\right)} \tag{3.60}$$

$$=\frac{\eta\zeta+\eta t^2+\zeta t^2}{\zeta+t^2}\left(\mathbf{r}_2'+\frac{\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}\mathbf{R}\right)^2+\frac{\eta\zeta^2t^2R^2+\eta\zeta t^4R^2+\zeta^2t^4R^2-\zeta^2t^4R^2}{\left(\zeta+t^2\right)\left(\eta\zeta+\eta t^2+\zeta t^2\right)} \tag{3.61}$$

$$= \frac{\eta\zeta + \eta t^2 + \zeta t^2}{\zeta + t^2}\left(\mathbf{r}_2' + \frac{\zeta t^2}{\eta\zeta + \eta t^2 + \zeta t^2}\mathbf{R}\right)^2 + \frac{\eta\zeta t^2 R^2}{\eta\zeta + \eta t^2 + \zeta t^2} \tag{3.62}$$

This means that the integral becomes the following.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi(-1)^q \int_{-\infty}^{\infty} \frac{\left(\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\zeta + t^2\right)^{\frac{p+q+3}{2}}} e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta + \eta t^2 + \zeta t^2}}$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_{p_x+q_x}\left((x_2' + R_x)\sqrt{\frac{\zeta t^2}{\zeta + t^2}}\right) H_{p_y+q_y}\left((y_2' + R_y)\sqrt{\frac{\zeta t^2}{\zeta + t^2}}\right)$$
$$H_{p_z+q_z}\left((z_2' + R_z)\sqrt{\frac{\zeta t^2}{\zeta + t^2}}\right) e^{-\frac{\eta\zeta + \eta t^2 + \zeta t^2}{\zeta + t^2}\left(\mathbf{r}_2' + \frac{\zeta t^2}{\eta\zeta + \eta t^2 + \zeta t^2}\mathbf{R}\right)^2} \mathrm{d}\mathbf{r}_2'\mathrm{d}t \tag{3.63}$$

Let $\mathbf{u} = \sqrt{\frac{\eta\zeta + \eta t^2 + \zeta t^2}{\zeta + t^2}}\mathbf{r}_2'$. The integral becomes the following.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi(-1)^q \int_{-\infty}^{\infty} \frac{\left(\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\zeta + t^2\right)^{\frac{p+q}{2}}} \frac{1}{\left(\eta\zeta + \eta t^2 + \zeta t^2\right)^{\frac{3}{2}}} e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta + \eta t^2 + \zeta t^2}}$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_{p_x+q_x}\left(u_x\sqrt{\frac{\zeta t^2}{\eta\zeta + \zeta t^2 + \eta t^2}} + R_x\sqrt{\frac{\zeta t^2}{\zeta + t^2}}\right) H_{p_y+q_y}\left(u_y\sqrt{\frac{\zeta t^2}{\eta\zeta + \zeta t^2 + \eta t^2}} + R_y\sqrt{\frac{\zeta t^2}{\zeta + t^2}}\right)$$
$$H_{p_z+q_z}\left(u_z\sqrt{\frac{\zeta t^2}{\eta\zeta + \zeta t^2 + \eta t^2}} + R_z\sqrt{\frac{\zeta t^2}{\zeta + t^2}}\right) e^{-\left(\mathbf{u} + \frac{\zeta t^2}{\sqrt{\zeta + t^2}}\frac{\mathbf{R}}{\sqrt{\eta\zeta + \eta t^2 + \zeta t^2}}\right)^2} \mathrm{d}\mathbf{u}\mathrm{d}t \tag{3.64}$$

Let $\mathbf{v} = \mathbf{u} + \mathbf{R}\sqrt{\frac{\eta\zeta + \zeta t^2 + \eta t^2}{\zeta + t^2}}$. The integral then becomes the following.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi(-1)^q \int_{-\infty}^{\infty} \frac{\left(\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\zeta + t^2\right)^{\frac{p+q}{2}}} \frac{1}{\left(\eta\zeta + \eta t^2 + \zeta t^2\right)^{\frac{3}{2}}} e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta + \eta t^2 + \zeta t^2}}$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_{p_x+q_x}\left(v_x\sqrt{\frac{\zeta t^2}{\eta\zeta + \zeta t^2 + \eta t^2}}\right) H_{p_y+q_y}\left(v_y\sqrt{\frac{\zeta t^2}{\eta\zeta + \zeta t^2 + \eta t^2}}\right) H_{p_z+q_z}\left(v_z\sqrt{\frac{\zeta t^2}{\eta\zeta + \zeta t^2 + \eta t^2}}\right)$$
$$e^{-\left(\mathbf{v} - \sqrt{\frac{\eta\zeta + \zeta t^2 + \eta t^2}{\zeta + t^2}}\mathbf{R} + \frac{\zeta t^2}{\sqrt{\zeta + t^2}}\frac{\mathbf{R}}{\sqrt{\eta\zeta + \eta t^2 + \zeta t^2}}\right)^2} \mathrm{d}\mathbf{v}\mathrm{d}t \tag{3.65}$$

The exponent can be rewritten.

$$\sqrt{\frac{\eta\zeta + \zeta t^2 + \eta t^2}{\zeta + t^2}}\mathbf{R} - \frac{\zeta t^2}{\sqrt{\zeta + t^2}}\frac{\mathbf{R}}{\sqrt{\eta\zeta + \eta t^2 + \zeta t^2}} = \frac{\eta\zeta + \zeta t^2 + \eta t^2 - \zeta t^2}{\sqrt{\left(\zeta + t^2\right)\left(\eta\zeta + \eta t^2 + \zeta t^2\right)}}\mathbf{R} \tag{3.66}$$

$$= \eta\sqrt{\frac{\zeta + t^2}{\eta\zeta + \eta t^2 + \zeta t^2}}\mathbf{R} \tag{3.67}$$

Now, use equation 2.14 to transform the integral.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi(-1)^q \int_{-\infty}^{\infty} \frac{\left(\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\zeta+t^2\right)^{\frac{p+q}{2}}} \frac{1}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^{\frac{3}{2}}} e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta+\eta t^2+\zeta t^2}}$$
$$\pi^{\frac{3}{2}} \left(\frac{\eta\zeta+\zeta t^2+\eta t^2-\zeta t^2}{\eta\zeta+\zeta t^2+\eta t^2}\right)^{\frac{p+q}{2}} H_{p_x+q_x}\left(\sqrt{\frac{\left(\eta\zeta+\zeta t^2+\eta t^2\right)\left(\zeta t^2\right)}{\left(\eta\zeta+\eta t^2+\zeta t^2-\zeta t^2\right)\left(\eta\zeta+\eta t^2+\zeta t^2\right)}}\eta\sqrt{\frac{\zeta+t^2}{\eta\zeta+\eta t^2+\zeta t^2}}R_x\right)$$
$$H_{p_y+q_y}\left(\sqrt{\frac{\left(\eta\zeta+\zeta t^2+\eta t^2\right)\left(\zeta t^2\right)}{\left(\eta\zeta+\eta t^2+\zeta t^2-\zeta t^2\right)\left(\eta\zeta+\eta t^2+\zeta t^2\right)}}\eta\sqrt{\frac{\zeta+t^2}{\eta\zeta+\eta t^2+\zeta t^2}}R_y\right)$$
$$H_{p_z+q_z}\left(\sqrt{\frac{\left(\eta\zeta+\zeta t^2+\eta t^2\right)\left(\zeta t^2\right)}{\left(\eta\zeta+\eta t^2+\zeta t^2-\zeta t^2\right)\left(\eta\zeta+\eta t^2+\zeta t^2\right)}}\eta\sqrt{\frac{\zeta+t^2}{\eta\zeta+\eta t^2+\zeta t^2}}R_z\right)\mathrm{d}t \quad (3.68)$$

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi^{\frac{5}{2}}(-1)^q \int_{-\infty}^{\infty} \frac{\left(\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\zeta+t^2\right)^{\frac{p+q}{2}}} \frac{1}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^{\frac{3}{2}}} e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta+\eta t^2+\zeta t^2}}$$
$$\left(\frac{\eta\zeta+\eta t^2}{\eta\zeta+\zeta t^2+\eta t^2}\right)^{\frac{p+q}{2}} H_{p_x+q_x}\left(\eta R_x\sqrt{\frac{\zeta t^2}{\eta\zeta+\eta t^2}}\sqrt{\frac{\zeta+t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right)$$
$$H_{p_y+q_y}\left(\eta R_y\sqrt{\frac{\zeta t^2}{\eta\zeta+\eta t^2}}\sqrt{\frac{\zeta+t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right) H_{p_z+q_z}\left(\eta R_z\sqrt{\frac{\zeta t^2}{\eta\zeta+\eta t^2}}\sqrt{\frac{\zeta+t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right)\mathrm{d}t \quad (3.69)$$

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi^{\frac{5}{2}}(-1)^q \int_{-\infty}^{\infty} \frac{\left(\eta\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\eta\zeta+\zeta t^2+\eta t^2\right)^{\frac{p+q}{2}}} \frac{1}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^{\frac{3}{2}}}$$
$$e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta+\eta t^2+\zeta t^2}} H_{p_x+q_x}\left(R_x\sqrt{\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right)$$
$$H_{p_y+q_y}\left(R_y\sqrt{\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right) H_{p_z+q_z}\left(R_z\sqrt{\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right)\mathrm{d}t \quad (3.70)$$

Note that the integrand is even with respect to t, so the integral can be rewritten to take this into account.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2} \pi^{\frac{5}{2}}(-1)^q 2 \int_{0}^{\infty} \frac{\left(\eta\zeta t^2\right)^{\frac{p+q}{2}}}{\left(\eta\zeta+\zeta t^2+\eta t^2\right)^{\frac{p+q}{2}}} \frac{1}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^{\frac{3}{2}}}$$
$$e^{-\frac{\eta\zeta t^2 R^2}{\eta\zeta+\eta t^2+\zeta t^2}} H_{p_x+q_x}\left(R_x\sqrt{\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right)$$
$$H_{p_y+q_y}\left(R_y\sqrt{\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right) H_{p_z+q_z}\left(R_z\sqrt{\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}}\right)\mathrm{d}t \quad (3.71)$$

Let $u^2 = \frac{\eta+\zeta}{\eta\zeta}\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2}$. The integral will now go from 0 to $\lim_{t\to\infty}\frac{\eta+\zeta}{\eta\zeta}\frac{\eta\zeta t^2}{\eta\zeta+\eta t^2+\zeta t^2} = 1$. Now, find the derivative of u.

$$2u\frac{\mathrm{d}u}{\mathrm{d}t} = \frac{\eta+\zeta}{\eta\zeta}\frac{2\eta\zeta t\left(\eta\zeta+\eta t^2+\zeta t^2\right)-\eta\zeta t^2\left(2\eta t+2\zeta t\right)}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^2} \quad (3.72)$$

$$= \frac{\eta+\zeta}{\eta\zeta}\frac{2\eta^2\zeta^2 t+2\eta^2\zeta t^3+2\eta\zeta^2 t^3-2\eta^2\zeta t^3-2\eta\zeta^2 t^3}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^2} \quad (3.73)$$

$$= 2\frac{\eta+\zeta}{\eta\zeta}\frac{\eta^2\zeta^2 t}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^2} \tag{3.74}$$

$$= 2u\sqrt{\frac{\eta+\zeta}{\eta\zeta}}\frac{\eta^{\frac{3}{2}}\zeta^{\frac{3}{2}}}{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^{\frac{3}{2}}} \tag{3.75}$$

$$\mathrm{d}t = \mathrm{d}u\frac{\left(\eta\zeta+\eta t^2+\zeta t^2\right)^{\frac{3}{2}}}{\eta\zeta}\sqrt{\frac{1}{\eta+\zeta}} \tag{3.76}$$

The integral is then transformed into the following.

$$[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\pi^{\frac{5}{2}}(-1)^q 2\int_0^1 \frac{1}{\eta\zeta\sqrt{\eta+\zeta}}\left(\frac{\eta\zeta}{\eta+\zeta}\right)^{\frac{p+q}{2}} u^{p+q} e^{-\frac{\eta\zeta}{\eta+\zeta}u^2R^2}$$
$$H_{p_x+q_x}\left(R_x\sqrt{\frac{\eta\zeta}{\eta+\zeta}}u\right) H_{p_y+q_y}\left(R_y\sqrt{\frac{\eta\zeta}{\eta+\zeta}}u\right) H_{p_z+q_z}\left(R_z\sqrt{\frac{\eta\zeta}{\eta+\zeta}}u\right)\mathrm{d}u \tag{3.77}$$

Now, let $\overline{\mathbf{r}} = \overline{\mathbf{p}+\mathbf{q}}$ and $\vartheta^2 = \frac{\eta\zeta}{\eta+\zeta}$, and use the notation $[\overline{\mathbf{p}}|\overline{\mathbf{q}}] = (-1)^q\left[\overline{\mathbf{p}+\mathbf{q}}\right]$.

$$[\overline{\mathbf{r}}] = 2D_A D_B D_C D_D e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2} e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}\frac{\pi^{\frac{5}{2}}}{\eta\zeta\sqrt{\eta+\zeta}}\int_0^1 (\vartheta u)^r e^{-\vartheta^2u^2R^2}$$
$$H_{r_x}(R_x\vartheta u) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u \tag{3.78}$$

Let $K_P = \frac{\sqrt{2}\pi^{\frac{5}{4}}e^{-\frac{\alpha\beta}{\zeta}(\mathbf{A}-\mathbf{B})^2}}{\zeta}$, $K_Q = \frac{\sqrt{2}\pi^{\frac{5}{4}}e^{-\frac{\gamma\delta}{\eta}(\mathbf{C}-\mathbf{D})^2}}{\eta}$, $D_P = D_A D_B$, $D_Q = D_C D_D$, and $\omega = \frac{K_P D_P K_Q D_Q}{\sqrt{\eta+\zeta}}$. Then use equation 2.4 to transform the integral.

$$[\overline{\mathbf{r}}] = \omega\int_0^1 (\vartheta u)^r e^{-\vartheta^2u^2R^2}\left(2R_x\vartheta u H_{r_x-1}(R_x\vartheta u) - 2(r_x-1)H_{r_x-2}(R_x\vartheta u)\right) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u \tag{3.79}$$

$$[\overline{\mathbf{r}}] = 2\omega R_x\int_0^1 (\vartheta u)^{r+1} e^{-\vartheta^2u^2R^2} H_{r_x-1}(R_x\vartheta u) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u$$
$$- 2\omega(r_x-1)\int_0^1 (\vartheta u)^r e^{-\vartheta^2u^2R^2} H_{r_x-2}(R_x\vartheta u) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u \tag{3.80}$$

$$[\overline{\mathbf{r}}] = 2\omega R_x\int_0^1 (\vartheta u)^{r-1+2} e^{-\vartheta^2u^2R^2} H_{r_x-1}(R_x\vartheta u) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u$$
$$- 2\omega(r_x-1)\int_0^1 (\vartheta u)^{r-2+2} e^{-\vartheta^2u^2R^2} H_{r_x-2}(R_x\vartheta u) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u \tag{3.81}$$

Define a new integral.

$$[\overline{\mathbf{r}}]^{(m)} = \omega 2^m\int_0^1 (\vartheta u)^{r+2m} e^{-\vartheta^2u^2R^2} H_{r_x}(R_x\vartheta u) H_{r_y}(R_y\vartheta u) H_{r_z}(R_z\vartheta u)\,\mathrm{d}u \tag{3.82}$$

Then using this integral, equation 3.81 gives the following recurrence relation.

$$[\overline{\mathbf{r}}]^{(m)} = R_i\left[\overline{\mathbf{r}-\mathbf{1}_i}\right]^{(m+1)} - (r_i-1)\left[\overline{\mathbf{r}-\mathbf{2}_i}\right]^{(m+1)} \tag{3.83}$$

This means that eventually, all of these integrals can be expressed in the form of the following.

$$[\overline{\mathbf{0}}]^{(m)} = \omega \left(2\vartheta^2\right)^m \int_0^1 u^{2m} e^{-\vartheta^2 u^2 R^2} \mathrm{d}u \tag{3.84}$$

3.2 When Centers Match

Consider equation 3.41 for the case of $\mathbf{P} = \mathbf{Q}$.

References

[1] Oleg Marichev, Michael Trott, and Steven Wolfram. Wolfram function site - hermite polynomials, 1998-2023.