Orthogonality of Hermite Polynomials

The orthogonality relation of the Hermite polynomials is (here regarded as postulated)

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} H_n(x) H_m(x) = \delta_{m,n}\, 2^n \sqrt{\pi}\, n! \ , \tag{1}$$

where we know that $H_n(x)$ is a polynomial of n^{th} order ($n \geq 0$).

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0. We begin with H_0, the first in the collection. As a polynomial of 0^{th} order, this is a constant, $H_0(x) = a_0$, and there is only the normalization condition to determine a_0. From Eq. (1), we read off ($n = m = 0$) that

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \big[H_0(x)\big]^2 = \sqrt{\pi} \ . \tag{2}$$

On the other hand, we calculate:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \big[H_0(x)\big]^2 \ = \ \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} [a_0]^2 \ = \ {a_0}^2 \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \ . \tag{3}$$

So, we need to evaluate the integral on the far right. The substitution $u = x^2$ (should!) recommend itself, so as to simplify the exponential function. Then we have

$$x = \sqrt{u} \ , \qquad \mathrm{d}x = \frac{1}{2} \frac{\mathrm{d}u}{\sqrt{u}} \ . \tag{4}$$

However, note that the variable x is being integrated over both negative and positive values in Eq. (3). Since the substitution $x = \sqrt{u}$ by default implies a positive value for the square-root, this would only be appropriate for the part of integration where $x \geq 0$. Therefore, we *must* divide the integration in two parts:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \ = \ \int_{-\infty}^{0} \mathrm{d}x\, e^{-x^2} + \int_{0}^{+\infty} \mathrm{d}x\, e^{-x^2} \ . \tag{5}$$

In the first integral, x takes negative values, so we must substitute $x = -\sqrt{u}$ there (and thus $\mathrm{d}x = -\frac{1}{2}\frac{\mathrm{d}u}{\sqrt{u}}$), while in the second integral $x \geq 0$ and so $x = +\sqrt{u}$ (and so $\mathrm{d}x = +\frac{1}{2}\frac{\mathrm{d}u}{\sqrt{u}}$) is alright.

With these substitutions, the integral (5) becomes (note limits!)

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \ = \ -\frac{1}{2} \int_{+\infty}^{0} \mathrm{d}u\, u^{-\frac{1}{2}}\, e^{-u} + \frac{1}{2} \int_{0}^{+\infty} \mathrm{d}u\, u^{-\frac{1}{2}}\, e^{-u} \ . \tag{6}$$

Swapping the limits on the first integral changes its sign from negative to positive, and the value of the fiirst integral is seen to be equal to that of the second, whence

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \ = \ \int_{0}^{+\infty} \mathrm{d}u\, u^{-\frac{1}{2}}\, e^{-u} \ = \ \int_{0}^{+\infty} \mathrm{d}u\, u^{\frac{1}{2}-1}\, e^{-u} \ = \ \Gamma(\tfrac{1}{2}) \ = \ \sqrt{\pi} \ . \tag{7}$$

So, $\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} [H_0(x)]^2 = {a_0}^2 \sqrt{\pi}$, and which should equal to $\sqrt{\pi}$ by Eq. (2). Therefore, ${a_0}^2 = 1$ and $H_0 = a_0 = \pm 1$.

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As a seemingly idle side-remark, note that the change of variables (4) was by no means necessary to determine that

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \;=\; 2\int_{0}^{+\infty} \mathrm{d}x\, e^{-x^2} \;. \tag{8}$$

This result, by itself, is easier to obtain by splitting the integration into two parts, as in (5), and than maneuvering the first integral into the form of the second one. To this end, simply substitute $x = -y$ in (note limits!)

$$\begin{aligned}\int_{-\infty}^{0} \mathrm{d}x\, e^{-x^2} \;&=\; \int_{-\infty}^{0} \mathrm{d}(-y)\, e^{-(-y)^2} \;=\; -\int_{+\infty}^{0} \mathrm{d}y\, e^{-y^2} \;,\\ &=\; +\int_{0}^{+\infty} \mathrm{d}y\, e^{-y^2} \;=\; +\int_{0}^{+\infty} \mathrm{d}x\, e^{-x^2} \;,\end{aligned} \tag{9}$$

where the third equlity follows upon swapping the limits of integration and the fourth equality simple states that it does not mater what letter we use for the integration variable in a definite integral [1)]. This proves that

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \;=\; 2\int_{0}^{+\infty} \mathrm{d}x\, e^{-x^2} \;, \tag{10}$$

and we may now proceed with the substitution $x = \sqrt{u}$, as above.

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1. We continue with $H_1(x)$, the next Hermite polynomial. Being a polynomial of 1^{st} order, $H_0(x) = b_0 + b_1 x$, and we need two conditions for the two coefficients: orthogonality with the only preceding polynomial, H_0, and the normalization.

Start with the orthogonality:

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} H_0(x) H_1(x) \;&=\; \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} a_0 (b_0 + b_1 x) \;,\\ &=\; b_0 \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} + b_1 \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x \;,\\ &=\; b_0\sqrt{\pi} \;+\; b_1 \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x \;,\end{aligned} \tag{11}$$

where we've used that $a_0 = 1$, and also the result (7). We remain with the calculation of the latter integral above. We may again use the substitution (4), and just as before, we *must* split the interal into two parts, one over negative x (where $x = -\sqrt{u}$), and the other over positive x (where $x = +\sqrt{u}$). Following this through, we obtain (note limits!)

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x \;&=\; \int_{+\infty}^{0} (-\tfrac{1}{2}\mathrm{d}u\, u^{-\frac{1}{2}})\, e^{-u} (-u^{+\frac{1}{2}}) \;+\; \int_{0}^{+\infty} (\tfrac{1}{2}\mathrm{d}u\, u^{-\frac{1}{2}})\, e^{-u} (+u^{+\frac{1}{2}}) \;.\\ &=\; \tfrac{1}{2}\int_{+\infty}^{0} \mathrm{d}u\, u^{-\frac{1}{2}+\frac{1}{2}}\, e^{-u} \;+\; \tfrac{1}{2}\int_{0}^{+\infty} \mathrm{d}u\, u^{-\frac{1}{2}+\frac{1}{2}}\, e^{-u} \;.\end{aligned} \tag{12}$$

1) …as long as it does not conflict with something else in the same expression!

Swapping the limits on the first integral changes its sign from positive to negative, and the value of the fiirst integral is seen to be equal in magnitude to that of the second—but opposite in sign, whence

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x \;=\; -\tfrac{1}{2}\int_{0}^{+\infty} \mathrm{d}u\, e^{-u} + \tfrac{1}{2}\int_{0}^{+\infty} \mathrm{d}u\, e^{-u} \;=\; 0\;. \tag{13}$$

So [since $H_0(x) \perp H_1(x)$], we have on one hand from (1) and on the other hand by the preceding direct calculation that

$$0 \;\stackrel{!}{=}\; \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} H_0(x) H_1(x) \;=\; b_0\sqrt{\pi} \;+\; b_1{\cdot}0\;, \tag{14}$$

which forces $b_0 = 0$, but says nothing about b_1. And only rightly so, since we still have to use the normalization condition, again read off (1). We calculate:

$$2^1\sqrt{\pi}\,1! \;\stackrel{!}{=}\; \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \big[H_1(x)\big]^2 \;=\; \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \big[b_1 x\big]^2 \;=\; {b_1}^2 \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x^2\;. \tag{15}$$

Now again, we split the integral at $x = 0$ and substitute $x = -\sqrt{u}$ for the $x \le 0$ part, and $x = \sqrt{u}$ for the $x \ge 0$ part. Now

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x^2 \;&=\; \int_{+\infty}^{0} (-\tfrac{1}{2}\mathrm{d}u\, u^{-\frac{1}{2}})\, e^{-u}(-\sqrt{u})^2 \;+\; \int_{0}^{+\infty} (\tfrac{1}{2}\mathrm{d}u\, u^{-\frac{1}{2}})\, e^{-u}(+\sqrt{u})^2\;.\\ &=\; -\tfrac{1}{2}\int_{+\infty}^{0} \mathrm{d}u\, u^{-\frac{1}{2}+1}\, e^{-u} \;+\; \tfrac{1}{2}\int_{0}^{+\infty} \mathrm{d}u\, u^{-\frac{1}{2}+1}\, e^{-u}\;.\end{aligned} \tag{16}$$

Swapping again the limits on the first integral changes its sign and

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} x^2 \;=\; \int_{0}^{+\infty} \mathrm{d}u\, u^{\frac{1}{2}}\, e^{-u} \;=\; \int_{0}^{+\infty} \mathrm{d}u\, u^{\frac{3}{2}-1}\, e^{-u} \;=\; \Gamma(\tfrac{3}{2})\;. \tag{17}$$

Using now that $\Gamma(z{+}1) = z\Gamma(z)$, we have $\Gamma(\frac{3}{2}) = \frac{1}{2}\Gamma(\frac{1}{2}) = \frac{1}{2}\sqrt{\pi}$. Therefore,

$$2\sqrt{\pi} \;\stackrel{!}{=}\; \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-x^2} \big[H_1(x)\big]^2 \;=\; {b_1}^2\, \tfrac{1}{2}\sqrt{\pi}\;, \tag{18}$$

or, ${b_1}^2 = 4$, so that $b_1 = \pm 2$ and $H_1(x) = \pm 2x$.

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The maneuver of splitting the integral (with symmetric limits at the mid-point) in Eq. (16) was again similar to the maneuvers done previously and one can easily prove the general results [see *Know Thy Math*]:

$$\int_{-L}^{+L} \mathrm{d}x\, f(x) \;=2\int_{0}^{+L} \mathrm{d}x\, f(x)\;, \qquad \text{if} \quad f(-x) \;= +f(x)\;, \tag{19\,\textit{even}}$$

$$\int_{-L}^{+L} \mathrm{d}x\, g(x) \;=0\;, \qquad \text{if} \quad g(-x) \;= -g(x)\;. \tag{19\,\textit{odd}}$$