Some New Closed Expressions for Integrals Involving Hermite Functions

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1. INTRODUCTION

The wave function $\psi_n(x)$ of an harmonic oscillator is given by [2, p. 273]

$$\psi_n(x) = \left( \frac{\alpha}{2^v! \pi^{1/2}} \right)^{1/2} H_v(\zeta) \exp\left(-\frac{\zeta^2}{2}\right)$$

(1)

$$\alpha = \frac{m \omega_0}{\hbar} \quad \zeta = \alpha^{1/4} x$$

$m$ mass of the particle

$\omega_0$ classical angular frequency of the oscillator

$h$ Planck's constant divided by $2\pi$

$H_v(\zeta)$ Hermite polynomials of order $v$ [7].

For the computation of the matrix elements of the inverse operator $\hat{O} = 1/x$ integrals of the form

$$I_{n,m} = \int_{-\infty}^{+\infty} e^{-x^2} H_n(x) \frac{1}{x} H_m(x) \, dx$$

(2)

must be solved. A closed expression for this integral seems to be unknown [5, 6, 8, 3, 4]. It will be derived in the next section. Some other integrals similar to $I_{n,m}$ will be considered in this paper. Their abbreviations are listed here for convenience.

$$J_n = I_{n,n+1}$$

(3)
INTEGRALS WITH HERMITE FUNCTIONS

\[ K_{n,m} = \int_{-\infty}^{+\infty} e^{-x^2} H_n(x) \frac{1}{x} H_m(x) \, dx \]  
\[ L_{n,m} = \int_{0}^{\infty} e^{-x^2} H_n(x) \frac{1}{x} H_m(x) \, dx \]  
\[ A_{n,m} = \int_{0}^{\infty} H_n(x) H_m(x) e^{-x^2} \, dx. \]

2. CALCULATION OF THE \( I_{n,m} \)

2.1. Convergence and Symmetry

An explicit expression of the Hermite polynomials is given by \[7, (4.9.2)\]

\[ H_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k n!}{k!(n-2k)!} (2x)^{n-2k}, \]  
where \( \lfloor v \rfloor \) denotes the integer part of \( v \). From Eq. (7) the behaviour of \( H_n(x) \) as \( x \to 0 \) can be derived easily.

\[ H_{2m}(x) = \frac{(-1)^m (2m)!}{m!} + O(x^3) \]  
\[ H_{2m+1}(x) = \frac{(-1)^m (2m+1)!}{m!} 2x + O(x^3). \]

It is obvious from (8) that for \( n \) and \( m \) even \( I_{n,m} \) is divergent, while for all other combinations of \( n \) and \( m \) the integral \( I_{n,m} \) is convergent because then the integrand \( \exp(-x^2) H_n(x) 1/x H_m(x) \) remains finite as \( x \to 0 \).

Since \( H_n(x) \) is an even (odd) function for \( n \) even (odd), it follows immediately that

\[ I_{2n+1, 2m+1} = 0 \]

\[ \int_{-\infty}^{+\infty} e^{-x^2} H_{2n}(x) \frac{1}{x} H_{2m}(x) \, dx = 0, \quad H: \text{principal value.} \]

2.2. Calculation of \( I_{n, n+1} \)

In this section I am going to consider the special integral \( J_n := I_{n, n+1} \). For Hermite polynomials the following recurrence relation holds \[7, \text{Eq. (4.10.1)}\]:

\[ H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x). \]
The integrals over the squares of the Hermite functions are given by [5, (7.374(1))]
\[ \int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x) \, dx = 2^n n! \sqrt{\pi} \delta_{nm}, \quad n, m \in \mathbb{N}_0. \] (11)

Inserting (10) into \( J_n \) and using (11), a recurrence relation for the \( J_n \) is obtained for \( n > 0 \):
\[ J_n = 2^{n+1} n! \sqrt{\pi} - 2n J_{n-1}. \] (12)

Starting from \( J_0 \), Eq. (12) allows us to calculate \( J_n \) for the lowest values of \( n \):
\[ J_0 = 2 \sqrt{\pi} \]
\[ J_1 = 0 \]
\[ J_2 = 2^3 2! \sqrt{\pi} \]
\[ J_3 = 0 \]
\[ J_4 = 2^5 4! \sqrt{\pi} \]
\[ J_5 = 0. \] (13)

The general formula for \( J_n \),
\[ J_n = 2^{n+1} n! \sqrt{\pi}; \quad n \in \mathbb{N}_0 \text{ and } n \text{ even} \] (14)
\[ J_n = 0; \quad n \in \mathbb{N} \text{ and } n \text{ odd}, \] (15)
can be proved easily by mathematical induction.

2.3. General Expression for \( I_{n,m} \)

Using Eqs. (10) and (11) the following recurrence relation can be obtained:
\[ I_{n,n+2m} = 2^{n+1} n! \sqrt{\pi} \delta_{m,0} - 2(n + 2m) I_{n,n+2m-1} \]
\[ n, m \in \mathbb{N}_0 \quad \text{and} \quad (n + m) \in \mathbb{N}. \] (16)

For \( m = 0 \), Eq. (16) gives (12). From (16) it can be seen that
\[ I_{o,e} = 0 \quad \text{for} \quad o < e, \] (17)
where \( o \) and \( e \) denote odd or even numbers, respectively. If the even subscript \( e \) is smaller than the odd one, the integral \( I_{o,e} \) remains finite. The general equation in this case,
\[ I_{n, n+2m+1} = (-1)^m \{n\}_{2m} n! 2^{n+m+1} \sqrt{\pi} \]
\[ \{n\}_{2m} = (n+2)(n+4) \cdots (n+2m) = \frac{(n+2m)!!}{n!!} \]
\[ n, m \in \mathbb{N}_0 \text{ and } n \text{ even} \]

It can be proved by mathematical induction using Eqs. (16) and (13). The values of the integral \( I_{n, m} \) for all possible subscripts \( n, m \) are given by Eqs. (9), (10), (17), and (18)

\[ I_{2n+1, 2m+1} = I_{2n+1, 2n+2m+2} = 0 \]
\[ I_{2n, 2m} \text{ is divergent,} \]
\[ \int_{-\infty}^{\infty} e^{-x^2} H_{2n}(x) \frac{1}{x} H_{2m}(x) \, dx = 0 \]
\[ I_{2n, 2n+2m+1} = (-1)^m \{2n\}! 2^{2n+m+1} \sqrt{\pi} \]
\[ n, m \in \mathbb{N}_0. \]

It is not evident from the symmetry of the integrand that the \( I_{0, e} \) vanish for \( o < e \). For the \( J_n \) this fact can be seen from a plot of the integrands. In Fig. 1 and 2 the integrands of \( I_{4, 5} \) and \( I_{5, 6} \) are shown. Most of the outer parts of the integrands are positive, only the large extremum located at

\[ H_4(x) \frac{1}{x} H_5(x) \exp(-x^2) \]

\[ -5 \quad 0 \quad 5 \]

**Fig. 1.** The integrand of \( J_4 \). The large maximum centered at \( x = 0 \) is added to the positive outer part of the integrand giving a large positive value of the integral \( J_4 \).
FIG. 2. The integrand of the integral $J_z$. The large minimum centered at $x = 0$ compensates the positive outer part of the integrand. The calculation outlined in Subsection 2.2 shows that $J_z$ is exactly zero.

$x = 0$ is positive or negative, respectively. The expansion of the integrands as $x \to 0$ of $J_e$ and $J_o$ can be easily derived from (8):

\[
e^{-x^2}H_e(x) \frac{1}{x} H_{e+1}(x) = 2(e+1) \left( \frac{e!}{(e/2)!} \right)^2 + O(x^2) \quad \text{as } x \to 0
\]

\[
e^{-x^2}H_o(x) \frac{1}{x} H_{o+1}(x) = -4 \left( \frac{o!}{(o-1)!/2} \right)^2 + O(x^2) \quad \text{as } x \to 0
\]

(20)

\(o: \text{ odd, } \quad e: \text{ even.}\)

Thus the area under the central extremum is added to the positive rest of $J_n$ (maximum for $n$ even) or is subtracted from it (minimum for $n$ odd). It cannot be seen from the plots that $J_o$ is exactly zero, but a strong alternation between adjacent $J_e$ and $J_o$ (normalized to the absolute value of the central extremum) can be expected.

For $I_{n,m}$ with $|n-m| > 1$ the plot of the integrands cannot be interpreted in the same clear way as for the $J_n$. 
3. Calculation of $K_{n,m}$

The results for $I_{n,m}$ will now be used to evaluate the integrals $K_{n,m}$ of the form

$$K_{n,m} = \int_{-\infty}^{\infty} e^{-x^2} H_n(x) \frac{1}{x^2} H_m(x) \, dx. \quad (21)$$

By a procedure similar to Subsection 2.1 it can be seen that only integrals $K_{n,m}$ with both $n$ and $m$ odd exist. The principal value of $K_{n,m}$ is zero. Using Eqs. (10), (11), and (17) a recurrence relation for the $K_{n,m}$ can be obtained.

$$K_{n,n} = 2^{n+1}(n-1)! \sqrt{\pi} + 4(n-1)^2 K_{n-2,n-2}, \quad n \geq 3 \text{ and odd.} \quad (22)$$

It can be used to prove an explicit expression for $K_{n,n}$ by induction

$$K_{n,n} = 2^{n+1} n! \sqrt{\pi}, \quad n \geq 1 \text{ and odd.} \quad (23)$$

By the same way, one finds

$$K_{n,n+2m} = (-1)^m n!! 2^{n+m+1}(n+2m-1)!! \sqrt{\pi}, \quad n \text{ odd; } m \in \mathbb{N}_0 \quad (24)$$

using Eqs. (10), (17), and (23). Again, the proof can be carried out by induction using a recurrence relation:

$$K_{n,n+2m} = -2(n+2m-1) K_{n,n+2m-2}, \quad n \text{ odd, } m \in \mathbb{N}. \quad (25)$$

4. Calculation of the $L_{n,m}$

I now consider integrals of the type

$$L_{n,m} = \int_{0}^{\infty} H_n(x) H_m(x) e^{-x^2} \, dx. \quad (26)$$

For odd $(n+m)$ the $L_{n,m}$ can be easily found from (19), whereas for even $(n+m)$, Eq. (19) cannot be used. Since $L_{2n,2m}$ is obviously divergent, one has to consider only the type $L_{2n+1,2m+1}$. Integrals of the type

$$A_{n,m} = \int_{0}^{\infty} H_n(x) H_m(x) e^{-x^2} \, dx$$

will turn out to be convenient for the calculation of the $L_{2n+1,2m+1}$. 
4.1. Calculation of the \(A_{n,m}\)

It is worth noting that the indefinite integrals \(\int H_n(x) H_m(x) e^{-x^2} \, dx\) can be solved in a closed form. By means of \([7, \text{p. 130}]\)

\[
H_p(x) H_q(x) = p! q! \sum_{n=0}^{\min(p, q)} \frac{2^n H_{p+q-2n}(x)}{n! (p-n)! (q-n)!}, \quad p, q \in \mathbb{N}_0
\]  

(28)

and \([5, \text{Vol. II, p. 223; 1, (7.1.1)}]\)

\[
\int H_n(x) e^{-x^2} \, dx = -H_{n-1}(x) e^{-x^2} + C; \quad n \in \mathbb{N}
\]  

(29)

\[
\int H_0(x) e^{-x^2} \, dx = \frac{\sqrt{\pi}}{2} \text{erf}(x) + C; \quad \text{erf: error function}
\]  

(30)

we get

\[
\int H_p(x) H_q(x) e^{-x^2} \, dx
= -p! q! e^{-x^2} \sum_{n=0}^{\min(p, q)} \frac{2^n}{n! (p-n)! (q-n)!} H_{p+q-2n-1}(x) + C
\]  

(31)

if \(p \neq q\) and

\[
\int [H_p(x)]^2 e^{-x^2} \, dx = - (p!)^2 e^{-x^2} \sum_{n=0}^{p-1} \frac{2^n}{n! [(p-n)!]^2} H_{2p-2n-1}(x)
\]

\[
+ p! 2^{p-1} \sqrt{\pi} \text{erf}(x) + C.
\]  

(32)

By multiple use of (28), all indefinite integrals of the type

\[
\int H_{n_1}(x) H_{n_2}(x) \cdots H_{n_m}(x) e^{-x^2} \, dx
\]  

(33)

can be, in principle, evaluated. Inserting (8)

\[
H_{2n}(0) = (-1)^n \frac{(2n)!}{n!}; \quad H_{2n+1}(0) = 0; \quad n \in \mathbb{N}_0
\]  

(34)

into (31) and (32) it can be easily seen that

\[
\int_0^\infty H_p(x) H_q(x) e^{-x^2} \, dx = 2^{p-1} p! \sqrt{\pi} \delta_{pq}. \quad (p + q) \text{ even}
\]  

(35)

For odd \((p + q)\) the summation of the series resulting from (34), (31), and (32) is involved, thus the integral is evaluated as follows. By application of Rodrigues' formula \([7, (4.9.1)]\)

\[
H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}; \quad n \in \mathbb{N}_0
\]  

(36)
to $H_n(x) \exp(-x^2)$, integration by parts, and use of Eq. (10) we obtain the recurrence relation,

$$A_{m,n} = 2mA_{m-1,n-1}, \quad n, m \in \mathbb{N} \text{ and } m \text{ odd} \quad (37)$$

which is used to prove general expressions for $A_{n,m}$, with $(n+m)$ odd:

$$A_{m,n} = \begin{cases} 
2^n \frac{m!!(n+1)!!}{(m-n)!!(n+1)} \left( -1 \right)^{(m-n-1)/2} \frac{(m-n-1)!}{((m-n-1)/2)!} & m > n; \quad m \text{ odd; } n \text{ even} \\
2^m \frac{m!!(n-1)!!}{(n-m)!!} \left( -1 \right)^{(n-m-1)/2} \frac{(n-m-1)!}{((n-m-1)/2)!} & m < n; \quad m \text{ odd; } n \text{ even.} 
\end{cases} \quad (38)$$

4.2. Calculation of the $L_{2n+1,2n+1}$

The recurrence relation

$$L_{2n+1,2n+1} = 2 \left\{ \frac{(2n)!}{n!} \right\}^2 + 16n^2L_{2n-1,2n-1}; \quad n \in \mathbb{N} \quad (40)$$

is obtained by inserting (10) into (26) and integrating by parts. Using (40), a general formula for the $L_{2n+1,2n+1}$ can be proved by mathematical induction:

$$L_{2n+1,2n+1} = 2^{4n+1}(n!)^2 \sum_{m=0}^{\infty} \left\{ \frac{(2m+1)!!}{(2m)!!} \right\}^2 \quad \sum_{m=0}^{\infty} \frac{\left( -1 \right)^{n-m}}{n!!} = 1. \quad (41)$$

4.3. Calculation of the $L_{2n+1,2m+1}$

The recurrence relation

$$L_{2n+1,2m+1} = 2^{m+n+1} \frac{(-1)^{n-m}}{(2n-2m+1)(2m+1)} \quad (2n+1)!! \quad (2m+1)!! \quad (42)$$

is obtained using (10), (38), and (39). It is used to prove

$$L_{2n+1,2m+1} = 2^{n+m+1} \frac{(-1)^{n-m}}{(2n+1)!!} \sum_{k=0}^{m} 2^k \frac{m!(2m-2k+1)!!}{(m-k)! \left[ 2(n+k-m) + 1 \right] (2m-2k+1)} \quad (43)$$
by induction, starting from \( m = 0 \) with (29), (34),

\[
L_{2n+1, 1} = 2^{n+1} (-1)^n \frac{(2n+1)!!}{(2n+1)}. \tag{44}
\]

The same procedure can be carried out starting from \( L_{1, 2m+1} \) with \( n = 0 \) giving

\[
L_{2n+1, 2m+1} = 2^{m+n+1} (-1)^m \frac{(2m+1)!!}{(2m+1)}
\cdot \sum_{k=0}^{n} 2^k \frac{n!(2m-2k+1)!!}{(n-k)! [2(m+k-n)+1](2n-2k+1)}. \tag{45}
\]

Comparing (43) and (45), a relation between finite sums is obtained:

\[
(2n+1)!! \cdot \sum_{k=0}^{n} 2^k \frac{m!(2m-2k+1)!!}{(m-k)! [2(n+k-m)+1](2m-2k+1)}
= (2m+1)!!
\cdot \sum_{j=0}^{n} 2^j \frac{n!(2n-2j+1)!!}{(n-j)! [2(m+j-n)+1](2n-2j+1)}, \quad n, m \in \mathbb{N}_0. \tag{46}
\]

In the special case \( m = n \), Eq. (43) reads

\[
L_{2n+1, 2n+1} = 2^{2n+1}(2n+1)!! \sum_{k=0}^{n} 2^k \frac{(2n-2k+1)!! n!}{(n-k)! (2k+1)(2n-2k+1)}. \tag{47}
\]

Comparing (41) and (47), another non-trivial relation

\[
2^{2n}! \sum_{m=0}^{n} \left[ \frac{(2m+1)!!}{(2m)!! (2m+1)} \right]^2
= (2n+1)!! \sum_{k=0}^{n} 2^k \frac{(2n-2k+1)!!}{(n-k)! (2k+1)(2n-2k+1)}, \quad n \in \mathbb{N}_0 \tag{48}
\]

is obtained.

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