Some Integrals Involving Symmetric-Top Eigenfunctions

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Using closure over a complete set of rotational states for methane to evaluate the intensity for quasi-elastic electron scattering in the first Born approximation, a number of integrals were encountered that appear not to have been evaluated previously. Mathematica was employed to evaluate these and similar integrals, and it was discovered that in all the cases studied the results could be represented by simple formulas.

Details of the Integral Evaluations

The integrals discussed here are related to averages over the spherical matrix elements $D_{M_1M_2}(a, x, \gamma)$ [1, 2] defined by

$$D_{M_1M_2}^J (a, x, \gamma) = e^{-iaM_1} d_{M_1M_2}^J (x) e^{-i\gamma M_2},$$

which are symmetric-top eigenfunctions with eigenvalues $J(J+1)$ and a degeneracy $(2J+1)^2$. The function $d_{M_1M_2}^J (x)$ is defined [1, 2] as

$$d_{M_1M_2}^J (x) = \sum_t (-1)^t \frac{\sqrt{(J + M_1)! (J - M_1)! (J + M_2)! (J - M_2)!}}{2^J (J + M_1 - t)! (J - M_2 - t)! t! (t + M_2 - M_1)!} (1 + x)^{J + M_2 - t} (1 - x)^{J + M_2 - t},$$

where the sum is over all integer values of $t$ from 0 to the first negative factorial that occurs in the denominator. In the impulse approximation for quasi-elastic electron scattering [3], averages over the rotational motion of a spherical top molecule such as methane are integrals of the following form:

$$I_{JM_1M_2}(n) = \frac{1}{2} \int_{-1}^{1} d_{M_1M_2}^J (x) (1 - x^n)^n H(x) d_{M_1M_2}^J (x) dx,$$

where
\[ H = -\left(1 - x^2\right) \frac{d^2}{dx^2} - 2x \frac{d}{dx} \]  

is the Hamiltonian operator whose eigenfunctions are the Legendre polynomials \( P_J(x) \) with eigenvalues \( J(J + 1) \). Equation (4) is also a part of the Hamiltonian for which the \( D^{(a)}_{M_1 M_2}(\alpha, x, \gamma) \) are solutions, but the \( d^{(a)}_{M_1 M_2}(x) \) are not eigenfunctions of \( H(x) \). The occurrence of \( H \) arises in the treatment of the scattering problem in the impulse approximation [3]. By use of Mathematica it was possible to prove that

\[ \sum_{M_1 = -J}^{J} \sum_{M_2 = -J}^{J} N_{JM_1 M_2} I_{JM_1 M_2}(0) = \frac{1}{3} J(J + 1) (2J + 1)^2, \]

where the normalization factor \( N_{JM_1 M_2} \) is given by

\[ N_{JM_1 M_2} = \frac{1}{\frac{1}{2} \int_{-1}^{1} d^{(a)}_{M_1 M_2}(x) d^{(a)}_{M_1 M_2}(x) dx} = 2J + 1 \]

for all values of \( M_1 \) and \( M_2 \). For integer \( n > 0 \) the results are

\[ \sum_{M_1 = -J}^{J} \sum_{M_2 = -J}^{J} N_{JM_1 M_2} I_{JM_1 M_2}(n) = C(n) J(J + 1) (2J + 1)^2, \]

where

\[ C(n) = \frac{1}{3} \frac{2^n n!}{(2n + 1)!!}. \]

The use of the word “prove” is based on the results from a Mathematica program. All of these expressions occur as ratios of positive integers and were found to be in exact agreement with the results on the right-hand sides in equation (7) for values of \( J \) from 0 through 18.

Note that the same result can be obtained for the case where \( (1 - x^2)^n \) is replaced by \( x^{2n} \) if \( C(n) \) is replaced by

\[ C(n) = \frac{1}{3(2n + 1)}. \]

Except for the factor of \( \frac{1}{3} \) for \( (1 - x^2)^n \) and for \( x^{2n} \) in the definitions of the \( C(n) \), the remaining parts are equivalent to the integrals

\[ \frac{1}{2} \int_{-1}^{1} (1 - x^2)^n dx = \frac{2^n n!}{(2n + 1)!!}, \]

and

\[ \frac{1}{2} \int_{-1}^{1} x^{2n} dx = \frac{1}{(2n + 1)}. \]
Further investigation using \( \sqrt{1 - x^2}^{2n+1} \) found the same result with

\[
C(n) = \frac{1}{3} \frac{\pi (2n + 1)!!}{2^{n+2} (n+1)!},
\]

where it is noted that

\[
\frac{1}{2} \int_{-1}^{1} \left( \sqrt{1 - x^2} \right)^{2n+1} dx = \frac{\pi (2n + 1)!!}{2^{n+2} (n+1)!}.
\]

Define the double sum over the integral

\[
I_J(m, n) = \sum_{M_1=-J}^{J} \sum_{M_2=-J}^{J} \frac{1}{2} \int_{-1}^{1} d_{M_1M_2}^J(x) (1-x^2)x^{2n} Hd_{M_1M_2}^J(x) dx,
\]

and

\[
I_C(m, n) = J(J+1)(2J+1)^2 \frac{1}{2} \int_{-1}^{1} (1-x^2)x^{2n} dx.
\]

These results suggest the conjecture that \( I_J(m, n) = C_0 I_C(m, n) \), where \( C_0 \) is a constant. For \( m = 0, 1 \) and \( n = 0, 1 \), the constant factor \( C_0 \) was found to be \( \frac{1}{3} \) for \( J = 1, 2, 3, 4 \), as shown in the next section.

### Implementation

The function \( d \) is \( d_{M_1M_2}^J(x) \).

\[
d[j, m1_, m2_, x_] := \text{Module}[(t, \text{tmin}, \text{tmax}),
\text{tmin} = \text{Max}[m1 - m2, 0];
\text{tmax} = \text{Max}[\text{Min}[j + m1, j - m2], \text{tmin}];
\text{Sqrt}[(j + m1)! (j - m1)! (j + m2)! (j - m2)!] / 2^j
\text{Sum}[-1]^t (1 + x)^{(j - t + (m1 - m2) / 2)}
(1 - x)^{(t - (m1 - m2) / 2) /}
((j + m1 - t)!(j - m2 - t)! t!(t - 2 (m1 - m2) / 2)!),
\{t, \text{tmin}, \text{tmax}\})]
\]

The functions \( d1 \) and \( d2 \) are the first and second derivatives of \( d_{M_1M_2}^J(x) \) with respect to \( x \).

\[
d1[j, m1_, m2_, x_] := D[d[j, m1, m2, x], x]
d2[j, m1_, m2_, x_] := D[d1[j, m1, m2, x], x]
\]
The function \( h \) is the result of the Hamiltonian \( H \) operating on \( d \).

\[
\begin{align*}
  h[j_\_, m1_\_, m2_\_, x_\_] := \\
  (1 - x^2) d2[j_\_, m1_\_, m2_\_, x_\_] - 2 x d1[j_\_, m1_\_, m2_\_, x_\_]
\end{align*}
\]

Define the integral \( a \).

\[
\begin{align*}
  a[m_\_, n_\_] := \\
  & \text{Module}[\{x\},] \\
  & \quad 1/2 \text{Integrate}[ (1 - x^2) (m/2) (x^2)^n, \{x, -1, 1\}]
\end{align*}
\]

The function \( \text{int1} \) is the integral in equation (14).

\[
\begin{align*}
  \text{int1}[j_\_, m1_\_, m2_\_, m_\_, n_\_] := \\
  & \text{Module}[\{x\},] \\
  & \quad 1/2 \text{Integrate}[ (1 - x^2) (m/2) (x^2)^n d[j_\_, m1_\_, m2_\_, x_\_] h[j_\_, m1_\_, m2_\_, x_\_, \{x, -1, 1\}]]
\end{align*}
\]

The function \( \text{int2} \) is the normalization integral of the square of \( d_{M_1M_2}(x) \).

\[
\begin{align*}
  \text{int2}[j_\_, m1_\_, m2_\_] := \\
  & \text{Module}[\{x\},] \\
  & \quad 1/2 \text{Integrate}[d[j_\_, m1_\_, m2_\_, x]^2, \{x, -1, 1\}]
\end{align*}
\]

The function \( s \) is the sum of the ratios of the integrals \( \text{int1} \) and \( \text{int2} \) over \( M_1 \) and \( M_2 \).

\[
\begin{align*}
  s[j_\_, m_\_, n_\_] := \\
  & \text{Module}[\{m1, m2\},] \\
  & \quad \text{Sum}[\text{Sum}[\text{int1}[j_\_, m1, m2, m, n] / \text{int2}[j_\_, m1, m2], \{m2, -j, j\}], \{m1, -j, j\}]
\end{align*}
\]

For various choices of \( m, n, \) and \( J \), the table compares the exact evaluation of \( I_J(m, n) \) (equation (14)) with the proposed result \( I_c(m, n) \) (equation (15)) and shows that the ratio of the two is a constant, which in this case is \( C_0 = \frac{1}{3} \). The evaluation of \( \text{table}[1, 1] \) takes some time.

\[
\begin{align*}
  \text{table}[mmax_\_, nmax_\_] := \\
  & \text{Text@} \\
  & \quad \text{Grid[} \\
  & \quad \quad \text{Prepend[} \\
  & \quad \quad \quad \text{Flatten[} \\
  & \quad \quad \quad \quad \text{Table}[m, n, j, s[j, m, n], -j (j + 1) ((2 j + 1)^2) a[m, n], \\
  & \quad \quad \quad \quad \quad s[j, m, n] / (-j (j + 1) ((2 j + 1)^2) a[m, n]), \\
  & \quad \quad \quad \quad \quad \{m, 0, mmax\}, \{n, 0, nmax\}, \{j, 4\}], 2], \\
  & \quad \quad \quad \quad \{\text{Style["m", Italic], Style["n", Italic],} \\
  & \quad \quad \quad \quad \quad \text{Style["J", Italic],} \\
  & \quad \quad \quad \quad \quad \text{Row[} \{\text{Style["I", Italic]} \text{Style["J", Italic]} \}, "\text{)}], \\
  & \quad \quad \quad \quad \text{\}} \\
  & \quad \quad \text{\}]} \\
  & \quad \text{\}]
\end{align*}
\]
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\[
\begin{array}{cccc}
\text{Style}["m", \text{Italic}], "", \text{Style}["n", \text{Italic}], ")")}]
, \\
\text{Row}[\{\text{Style}["I", \text{Italic}]\text{Style}["C", \text{Italic}], "",
\text{Style}["m", \text{Italic}], "", \text{Style}["n", \text{Italic}], ")")}]
, \\
\text{Row}[\{\text{Style}["I", \text{Italic}]\text{Style}["J", \text{Italic}], "",
\text{Style}["m", \text{Italic}], "", \text{Style}["n", \text{Italic}], ")")}]
/ \\
\text{Row}[\{\text{Style}["I", \text{Italic}]\text{Style}["C", \text{Italic}], "",
\text{Style}["m", \text{Italic}], "", \text{Style}["n", \text{Italic}], ")")}]]
\]

table[1, 1]

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# References


## About the Author

Russell A. Bonham received his Ph.D. in physical chemistry from Iowa State University in 1957. He is the author of more than 200 articles on all aspects of electron scattering from free atoms and molecules. He is currently a professor emeritus at Indiana University and an adjunct professor at the Illinois Institute of Technology.

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