The general formula for rotational averages

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Spectroscopic applications require finding uniform rotational averages of $n$th rank three-dimensional tensor quantities. This problem reduces to calculating a tensor $I^{(n)}$ formed by averaging products of $n$ direction cosines:

$$I^{(n)}_i \cdots i_n \lambda_1 \cdots \lambda_n = \langle l_i \lambda_1 \cdots l_n \lambda_n \rangle = \int_{SO(3)} dg \ l_i \lambda_1(g) \cdots l_n \lambda_n(g).$$

Previous writers$^{[1]}$ express $I^{(n)}$ as a trigonometric integral over Euler angles only to shy away from integrating it: instead they find a systematic expansion in “basic” (Kronecker and Levi-Civita) isotropic tensors. While ingenious this method has not been extended past rank $n = 8$, where it already entails a coefficient matrix that occupies an entire page of typescript.$^{[2]}$

We by contrast find a formula for $I^{(n)}$ that is valid for all ranks, fits within a few lines of print or code, and is trivial to run on a computer. In short we decompose the Euler integral representation into a sum of Euler beta integrals, then perform some manipulations to obtain a completely elementary expression.

Beyond clearing the path for any three-dimensional cartesian tensor to be averaged, our formula provides a friendly base for deriving further results. As illustration we obtain simple criteria to determine when $I^{(n)} = 0$ and observe a connection to Wigner’s $D$-matrix.

Figure: the component $\langle l_{18} l_{16} l_{13} l_{14} l_{15} l_{16} l_{17} l_{18} l_{19} l_{21} l_{22} l_{23} l_{24} l_{25} l_{26} l_{27} l_{28} l_{29} l_{30} l_{31} l_{32} l_{33} l_{34} l_{35} l_{36} l_{37} l_{38} l_{39} l_{40} l_{41} l_{42} l_{43} l_{44} l_{45} l_{46} l_{47} l_{48} l_{49} l_{50} l_{51} l_{52} l_{53} \rangle$ of $I^{(195)}$, a number that we wager is making its print debut here. Our program finds it within seconds.