Supplement of

Efficient polynomial analysis of magic-angle spinning sidebands and application to order parameter determination in anisotropic samples

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S1. AVERAGES OVER POWER PRODUCTS OF TRIGONOMETRIC FUNCTIONS

A. Azimuthal average

1. Proposition

\[
\langle \sin^m \gamma \cos^n \gamma \rangle_{\gamma} = \begin{cases} 
\frac{(m-1)!! \cdot (n-1)!!}{(m+n)!!} & \text{if } m \text{ and } n \text{ even} \\
0 & \text{otherwise}
\end{cases} \tag{1}
\]

Meaning of the averaging symbol:

\[
\langle A(\gamma) \rangle_{\gamma} = \frac{1}{2\pi} \int_a^{a+2\pi} A(\gamma) \, d\gamma \quad ; \quad a \in \mathbb{R} \tag{2}
\]

For sake of shortness of the expressions, the index \( \gamma \) is omitted in the following.

2. Proof for odd exponents:

If the sine power \( m \) is odd:

We set \( a = -\pi \), split the integration range in \([-\pi, 0]\) and \([0, \pi]\) and substitute in the first part \( \gamma \to -\gamma \):

\[
\int_{-\pi}^{\pi} \sin^m \gamma \cos^n \gamma \, d\gamma + \int_{0}^{\pi} \sin^m \gamma \cos^n \gamma \, d\gamma = \int_{-\pi}^{\pi} \sin^m(-\gamma) \cos^n(-\gamma) \, d(-\gamma) + \int_{0}^{\pi} \sin^m \gamma \cos^n \gamma \, d\gamma = 0 \tag{3}
\]

If the cosine power \( n \) is odd: We substitute \( \gamma \to \pi/2 - \gamma \) and get again an integral with odd sine power which therefore will be zero likewise.

3. Proof for even exponents

This will be done by mathematical induction from \( n \) to \( n + 2 \) with base case \( n = 0 \). The latter has to be proven with an induction from \( m \) to \( m + 2 \).

Base case \( n = 0 \): The proposition eqn. (1) has here the form:

\[
\langle \sin^m \gamma \rangle = \frac{(m-1)!!}{m !!} \tag{4}
\]

To prove this by a further induction we check first that the base case is obviously valid for \( m = 0 \). The inductive step \( m \to m + 2 \) is done by

\[
\int \sin^{m+2} \gamma \, d\gamma = -\cos \gamma \sin^{m+1} \gamma + (m + 1) \int \cos^2 \gamma \sin^m \gamma \, d\gamma \tag{5}
\]

Inserting the integration limits: first term at the right-hand side is cancelled, and we get

\[
\langle \sin^{m+2} \gamma \rangle = \frac{m+1}{m+2} \langle \sin^m \gamma \rangle = \frac{m+1}{m+2} \cdot \frac{(m-1)!!}{m !!} = \frac{(m+1)!!}{(m+2)!!} \tag{6}
\]

That means, the validity of the sub-proposition (4) for \( m \) implies the validity of that also for \( m + 2 \). This proves sub-proposition (4) for all even \( m \). Therefore the base case for the following induction is valid.

Inductive step \( n \to n + 2 \): Suppose proposition (1) is valid for a particular \( n \). We investigate this expression for \( n \to n + 2 \) by replacing \( \cos^{n+2} \gamma = \cos^n \gamma (1 - \sin^2 \gamma) \):
\[ \langle \sin^m \gamma \cos^{n+2} \gamma \rangle = \langle \sin^m \gamma \cos^n \gamma \rangle - \langle \sin^{m+2} \gamma \cos^n \gamma \rangle = \frac{(m-1)!! (n-1)!!}{(m+n)!!} - \frac{(m+1)!! (n-1)!!}{(m+2+n)!!} \]

\[= \frac{(m-1)!! (n-1)!!}{(m+2+n)!!} - \frac{[(m+n+2) - (m+1)]}{(m+2+n)!!} = \frac{(m-1)!! (n+1)!!}{(m+2+n)!!} \]  

(7)

which is exactly the proposition for \( n+2 \).

The validity of proposition (1) for \( n \) implies the validity of the proposition also for \( n+2 \). This proves that proposition for all even \( m \) and \( n \).

\[ \square \]

B. Polar average

1. Proposition

\[ \langle \cos^n \alpha \sin^m \alpha \rangle_{\cos \alpha} = \begin{cases} 
\frac{m!! (n-1)!!}{(m+n+1)!!} & \text{if } m \text{ and } n \text{ even} \\
\frac{m!! (n-1)!!}{(m+n+1)!!} \cdot \frac{\pi}{2} & \text{if } m \text{ odd and } n \text{ even} \\
0 & \text{if } n \text{ odd}
\end{cases} \]  

(8)

For odd \( n \): Split of the integration interval into the parts \([0, \pi/2]\) and \([\pi/2, \pi]\); in the second part: substitution \( \alpha \to \pi - \alpha \), then \( \cos \alpha \) and \( \cos \alpha \) alternate the sign:

\[ \langle \cos^n \alpha \sin^m \alpha \rangle = \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha = \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha + \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha = 0 \]  

(10)

This proves proposition (8) for odd \( n \).

For even \( n \): Prove by mathematical induction \( m \to m + 2 \); therefore two base cases (here \( m = 0 \) and \( m = 1 \)) are needed.

Base case 1 (\( m = 0 \)): Substitution \( \cos \alpha \to c \):

\[ \langle \cos^n \alpha \rangle = \frac{1}{2} \int_{-1}^{1} c^n \, dc = \frac{1}{2} \left[ \frac{1}{n+1} c^{n+1} \right]_{-1}^{1} = \frac{1}{n+1} \]  

(11)

which proves proposition (8) for \( m = 0 \) and \( n \in \mathbb{N} \).

Base case 2 (\( m = 1 \)): To be shown here:

\[ \langle \cos^n \alpha \sin \alpha \rangle = \frac{(n-1)!!}{(n+2)!!} \cdot \frac{\pi}{2} \]  

(12)
This is done by the following steps:

\[
\langle \cos^{n+2} \alpha \sin \alpha \rangle = \frac{1}{2} \int_0^\pi \cos^{n+2} \alpha \sin^2 \alpha \, d\alpha = \frac{1}{2} \int_0^\pi (\cos^{n+2} \alpha - \cos^{n+4} \alpha) \, d\alpha \tag{13}
\]

Partial integration of a cosine power:

\[
\int_0^\pi \cos^p \alpha \, d\alpha = \left[ \sin \alpha \cos^{p-1} \alpha \right]_0^\pi - (p-1) \int_0^\pi (-\sin^2 \alpha) \cos^{p-2} \alpha \, d\alpha = (p-1) \cdot 2 \langle \cos^{p-2} \alpha \sin \alpha \rangle \tag{14}
\]

Inserting this rule into eqn. (13):

\[
\langle \cos^{p+2} \alpha \sin \alpha \rangle = (p+1) \langle \cos^p \alpha \sin \alpha \rangle - (p+3) \langle \cos^{p+2} \alpha \sin \alpha \rangle \tag{15}
\]

or

\[
\langle \cos^{n+2} \alpha \sin \alpha \rangle = \frac{n+1}{n+4} \langle \cos^n \alpha \sin \alpha \rangle = \frac{n+1}{n+4} \frac{(n-1)!!}{(n+2)!!} \cdot \frac{\pi}{2} = \frac{(n+1)!!}{(n+4)!!} \cdot \frac{\pi}{2} \tag{16}
\]

It can be shown easily that eqn. (12) is fulfilled for \( n = 0 \). This together with eqn. (16) as induction step proves base case 2.

Inductive step \( m \to m + 2 \): Suppose proposition (8) would be valid for a particular \( m \) and all even \( n \). We calculate the average for \( m + 2 \) by replacing \( \sin^{m+2} \gamma = \sin^m \gamma (1 - \cos^2 \gamma) \):

\[
\langle \cos^m \alpha \sin^{m+2} \alpha \rangle = \langle \cos^m \alpha \sin^m \alpha \rangle - \langle \cos^{m+2} \alpha \sin^m \alpha \rangle
\]

\[
= \frac{n!!}{(m+n+1)!!} \, f_n - \frac{m!! (n+1)!!}{(m+n+3)!!} \, f_n
\]

\[
= \frac{m!! (n-1)!!}{(m+n+3)!!} \left[ (m+n+3) - (n+1) \right] \, f_n
\]

\[
= \frac{(m+2)!! (n-1)!!}{(m+n+3)!!} \, f_n
\]

\((f_n := 1 \text{ for even } n \text{ and } \pi/2 \text{ for odd } n)\) which is exactly proposition (8) for \( m \to m + 2 \).

This inductive step together with the proven base cases proves proposition (8) \( \forall \{m,n\} \subset \mathbb{N} \).
S2. POWDER-AVERAGED PHASE POWERS

Listed up to eighth power:

\[ \langle \Phi \rangle = 0 \] (18)

\[ \langle \Phi^2 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^2 \cdot \frac{1}{45} \left( 3 + \eta^2 \right) \left( 5 + \cos \gamma_r \right) \left( 1 - \cos \gamma_r \right) \] (19)

\[ \langle \Phi^3 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^3 \cdot \frac{4}{5} \left( 1 - \eta^2 \right) \sin \gamma_r \sin^2 \frac{\gamma_r}{2} \] (20)

\[ \langle \Phi^4 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^4 \cdot \frac{4}{945} \left( 3 + \eta^2 \right)^2 \left( 5 + \cos \gamma_r \right)^2 \sin^4 \frac{\gamma_r}{2} \] (21)

\[ \langle \Phi^5 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^5 \cdot \frac{32}{693} \left( 3 + \eta^2 \right) \left( 1 - \eta^2 \right) \left( 5 + \cos \gamma_r \right) \sin \gamma_r \sin^4 \frac{\gamma_r}{2} \] (22)

\[ \langle \Phi^6 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^6 \cdot \left[ \frac{1}{16016} \left( \frac{5515 + \frac{16381}{3} \eta^2 + \frac{49963}{27} \eta^4 + \frac{49471}{243} \eta^6}{131 + \frac{1009}{7} \eta^2 + \frac{2567}{63} \eta^4 + \frac{2843}{567} \eta^6} \right) \cos \gamma_r + \frac{1}{32032} \left( \frac{2983 + 6219 \eta^2 + \frac{2477}{9} \eta^4 + \frac{12185}{81} \eta^6}{179 - \frac{235}{3} \eta^2 + \frac{3155}{27} \eta^4 + \frac{839}{243} \eta^6} \right) \cos 2\gamma_r \right. \\
+ \frac{1}{12012} \left( \frac{397 - \frac{123}{3} \eta^2 + \frac{8429}{27} \eta^4 + \frac{1145}{243} \eta^6}{5 + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6} \right) \cos 3\gamma_r - \frac{1}{24143} \left( \frac{5 + \frac{19}{28} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6}{28 + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6} \right) \cos 4\gamma_r \\
- \frac{1}{143} \left( \frac{5 + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6}{756 + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6} \right) \cos 5\gamma_r \left( \frac{5 + \frac{19}{28} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6}{28 + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6} \right) \cos 6\gamma_r \right] \] (23)

\[ \langle \Phi^7 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^7 \cdot \frac{64}{3861} \left( \eta^2 - 1 \right) \left( 3 + \eta^2 \right)^2 \left( 5 + \cos \gamma_r \right)^2 \cos \frac{\gamma_r}{2} \sin^2 \frac{\gamma_r}{2} \] (24)

\[ \langle \Phi^8 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^8 \cdot \frac{1}{15949791} \cdot 4 \left( 3 + \eta^2 \right) \left( 5 + \cos \gamma_r \right) \left[ 1274778 + 282042 \eta^2 + 645534 \eta^4 + 34958 \eta^6 \\
+ 3 \left( 296217 - 132759 \eta^2 + 194067 \eta^4 + 5675 \eta^6 \right) \cos \gamma_r + 51030 \cos 2\gamma_r + 1701 \cos 3\gamma_r \right. \\
+ \eta^2 \left( 2997 + 279 \eta^2 + 79 \eta^4 \right) \left( 30 \cos 2\gamma_r + \cos 3\gamma_r \right) \left] \sin^8 \frac{\gamma_r}{2} \right. \] (25)
S3. MATHEMATICA EXPRESSIONS FOR EVALUATION OF THE GENERAL SSB POLYNOMIAL

The following passages can be copied and pasted into Mathematica, possibly with an in-between step of pasting the text into a simple text editor to remove formatting information. Note that on some systems it seems that the curly brackets \{ and \} are pasted as letters \texttt{f} and \texttt{g}, respectively. Since \texttt{f} and \texttt{g} do not appear in the formulae, search-and-replace can be used.

First, we define an auxiliary function with the independent variables \#1, \#2 and \#3 being identified with \(n\), \(k\), and \(\eta\), respectively:

\[
\text{aux} = \sum \frac{(4^r + r + 1)^2}{6^{n-1} (1 + f) (2 + g)^{2r}} \times \frac{(q + 1 + 2^* - r)!}{(p + q + 1 + 2^* - r)!} \times \frac{(q + s + u)!(q - s + u)_2}{4^r (q + s + u)_2 (1 + (-1)^{(r - p)} (1 + (-1)^{(q + s + u)}))}
\]

The general function for SSB generation, with \#1, \#2, \#3 and \#4 identified with the SSB order \(m\), \(\delta\omega_0/\omega_r\), \(\eta\) and the maximum order \(n\) of the polynomial, respectively, is then:

\[
\text{rsb} = \sum \frac{1}{2^n (2 + g)^n} \times \frac{(n - k - 1 - b)!}{(n - k - 1 - 2b)! (n - 2k - 2b)!} \times \frac{\text{aux}[n, k, \#3]}{\{n, \#1, \#4\}} \times \{b, 0, n - 2k\}
\]

With this, one can readily generate the SSB polynomials, e.g. for the centerband \((m = 0)\) up to order \(n = 6\):

\[
\text{rsb}[0, \text{delta}, \text{eta}, 6] \text{ // Simplify}
\]
S4. SPINNING SIDEBAND INTENSITIES

Equations for SSB intensities using polynomials up to 12th order in $\omega_0/\omega_r$

(abbreviations: $K_1 := 3 + \eta^2$, $K_2 := 1 - \eta^2$ and $w = \delta \omega_0/\omega_r$).

\begin{align*}
I_0 &= 1 - \frac{K_1^2}{20} w^2 + \frac{227 K_1^2}{181 440} w^4 - \frac{49 471 K_1^3 + 4 428 K_2^2}{2 802 159 360} w^6 + \frac{K_1 (1 466 405 K_1^3 - 709 776 K_2^2)}{9 146 248 151 040} w^8
- \frac{K_1^2 (286 311 167 K_1^3 - 494 915 400 K_2^2)}{281 521 518 089 011 200} w^{10}
+ \frac{998 271 153 509 K_1^3 - 2 160 K_2^2 (1 577 931 893 K_1^3 + 218 222 883 K_2^2)}{209 789 835 279 931 144 260 000} w^{12} \\
&\quad + \frac{K_1^2 K_2^2}{45} w^2 + \frac{K_2}{105} w^3 - \frac{17 K_1^2}{22 680} w^4 \pm \frac{23 K_1 K_2}{83 160} w^5 + \frac{2 843 K_1^3 - 2 484 K_2^2}{233 513 280} w^6
+ \frac{19 K_1^2 K_2}{51 189 184} w^7 - \frac{K_1 (123 823 K_1^3 - 285 552 K_2^2)}{1 028 952 916 992} w^8 \pm \frac{K_2 (959 357 K_1^3 - 196 884 K_2^2)}{32 583 509 038 080} w^9
+ \frac{K_1^2 (11 362 895 K_1^3 - 46 559 016 K_2^2)}{14 076 075 904 456 560} w^{10} + \frac{K_1 K_2 (766 057 K_1^3 - 663 984 K_2^2)}{4 692 025 301 483 520} w^{11}
- \frac{34 324 127 551 K_1^3 - 2 160 K_2^2 (96 357 427 K_1^3 + 2 033 937 K_2^2)}{8 741 243 136 663 797 760 000} w^{12} \\
&\quad + \frac{K_1^2}{360} w^2 + \frac{K_2}{210} w^3 + \frac{17 K_1^2}{12 960} w^4 \pm \frac{23 K_1 K_2}{83 160} w^5 - \frac{12185 K_1^3 - 87372 K_2^2}{3736212480} w^6
\pm \frac{49 K_1^2 K_2}{49 186 240} w^7 \pm (3 + \eta^2) \left(96 623 91 K_1^3 - 105 697 444 K_2^2\right) w^8 \pm \frac{K_2 (990 181 K_1^3 - 583 956 K_2^2)}{32 583 509 038 080} w^9
- \frac{(3 + \eta^2)^2}{37 536 204 111 861 600} \left(145 918 57 K_1^3 - 197 993 592 K_2^2\right) w^{10} \pm \frac{K_1 K_2 (444 013 K_1^3 - 789 2208 K_2^2)}{23 981 462 652 026 880} w^{11}
+ \frac{756 179 217 97 K_1^3 - 2 160 K_2^2 (54 850 5769 (3 + \eta^2)^2 - 723 530 61 K_2^2)}{34 964 972 546 655 191 040 000} w^{12} \\
I_{-3} &= \frac{K_1^2}{22 680} w^4 \pm \frac{K_1 K_2}{27 720} w^5 - \frac{1 145 K_1^3 + 65556 K_2^2}{42 032 390 400} w^6 \pm \frac{163 K_1^2 K_2}{15 567 5520} w^7 - \frac{K_1 (9379 K_1^3 - 682 128 K_2^2)}{1 714 921 528 320} w^8 \pm \frac{K_2 (284 5 K_1^3 - 507 6 K_2^2)}{21 296 411 1360} w^9
+ \frac{K_1^2 (22 469 99 K_1^3 - 10 360 440 K_2^2)}{23 460 126 507 417 600} w^{10} + \frac{K_1 K_2 (183 2 201 K_1^3 - 7 529 328 K_2^2)}{1 798 609 698 90 201 600} w^{11}
- \frac{1 930 764 389 K_1^3 - 2 160 K_2^2 (360 943 523 K_1^3 - 12 117 278 7 K_2^2)}{26 22 379 29 409 991 39 328 000} w^{12} \\
I_{-4} &= \frac{K_1^2}{362 880} w^4 \pm \frac{K_1 K_2}{166 320} w^5 + \frac{839 K_1^3 + 20 844 K_2^2}{56 043 187 200} w^6 \pm \frac{K_1^2 K_2}{7 783 7760} w^7 - \frac{K_1 (5 899 K_1^3 + 568 123 2 K_2^2)}{41 15 81 16 67 96 800} w^8 \pm \frac{K_2 (284 5 K_1^3 - 507 6 K_2^2)}{3 258 35 09 03 80 800} w^9
+ \frac{K_1^2 (34 081 K_1^3 - 180 31 03 2 K_2^2)}{9 384 05 06 02 96 70 400} w^{10} + \frac{K_1 K_2 (23 33 31 K_1^3 - 28 571 12 K_2^2)}{8 99 30 48 49 45 10 080} w^{11}
+ \frac{1 141 95 71 509 K_1^3 - 2 160 K_2^2 (65 664 469 K_3^3 - 49 65 369 117 K_2^3)}{93 23 99 26 79 108 05 09 40 000} w^{12} 
\end{align*}
S5. 2D OSCILLATION COEFFICIENTS

A. Belonging to $I_{0}$

\begin{equation}
C_{00} = I_{0}^{(iso)} + \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \left( \frac{1}{12} Q_2 \langle P_2 \rangle - \frac{31}{96} Q_4 \langle P_2 \rangle \right) + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left( \frac{85}{528} Q_{11} \langle P_2 \rangle + Q_{21} \langle P_4 \rangle + \frac{59}{3024} Q_3 \langle P_6 \rangle + \frac{19733}{248384} Q_4 \langle P_8 \rangle \right)
\end{equation}

\begin{equation}
C_{02} = \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{3}{18} Q_2 \langle P_2 \rangle + 5 Q_4 \langle P_4 \rangle + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \cdot \frac{1}{12} \left( Q_{12} \langle P_2 \rangle - Q_{22} \langle P_4 \rangle + \frac{1}{2} Q_3 \langle P_6 \rangle - \frac{11}{11} Q_4 \langle P_8 \rangle \right)
\end{equation}

\begin{equation}
C_{04} = -\left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{35}{576} Q_4 \langle P_4 \rangle + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{1}{12} \left( Q_{23} \langle P_4 \rangle + \frac{1}{15} Q_5 \langle P_6 \rangle + \frac{111}{260} Q_4 \langle P_8 \rangle \right)
\end{equation}

\begin{equation}
C_{06} = \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{11}{360} Q_3 \langle P_6 \rangle + 6 Q_4 \langle P_8 \rangle
\end{equation}

\begin{equation}
C_{08} = \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{Q_4 \langle P_8 \rangle}{768}
\end{equation}

\begin{equation}
S_{02} = -i \frac{\omega_0 \delta}{2\sqrt{6}} E_5 \langle P_2 \rangle + i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{3344 \sqrt{3} (3 + \eta^2) \langle P_2 \rangle - 296 \langle P_4 \rangle Q_4^{(3)} + 875 \langle P_6 \rangle Q_6^{(3)}}{532224 \sqrt{2}}
\end{equation}

\begin{equation}
S_{04} = -i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}
\end{equation}

\begin{equation}
S_{06} = i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{Q_6^{(3)} \langle P_6 \rangle}{6912 \sqrt{2}}
\end{equation}

\begin{equation}
S_{08} = 0
\end{equation}

B. Belonging to $I_{\pm 1}$

\begin{equation}
C_{\pm 10} = I_{\pm 1}^{(iso)} + \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{1}{18} \left[ -Q_2 \langle P_2 \rangle + 3 Q_4 \langle P_4 \rangle \right] \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{21 Q_4 \langle P_4 \rangle - 50 Q_6 \langle P_6 \rangle}{83 \cdot 160 \sqrt{2}}
\end{equation}

\begin{equation}
C_{\pm 1:2} = -\left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{3}{18} Q_2 \langle P_2 \rangle + Q_4 \langle P_4 \rangle \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44 \sqrt{3} (3 + \eta^2) \langle P_2 \rangle - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{33 \cdot 264 \sqrt{2}}
\end{equation}
\[ C_{\pm 1,4} = \pm \left( \frac{\omega \delta}{\omega_r} \right)^3 \frac{(P_4) Q_6^{(3)}}{4752\sqrt{2}} + \frac{(\omega \delta)^4}{4} \left[ \frac{1}{24} (Q_{27} + Q_{28}) (P_4) + \frac{41}{360} Q_3 (P_6) - \frac{4}{195} Q_4 (P_8) \right] \]  

\[ C_{\pm 1,6} = \left( \frac{\omega \delta}{\omega_r} \right)^4 \frac{11}{120} Q_3 (P_6) + Q_4 (P_8) \]  

\[ C_{\pm 1,8} = 0 \]  

\[ S_{\pm 1/2} = \mp i \left( \frac{\omega \delta}{\omega_r} \right)^2 \frac{3 Q_2^{(2)} (P_2) + Q_4^{(2)} (P_4)}{18} - i \left( \frac{\omega \delta}{\omega_r} \right)^3 \frac{44\sqrt{3} (3 + \eta^2) (P_2) E_5 - 5 (P_3) Q_4^{(3)} + 14 (P_6) Q_6^{(3)}}{33264\sqrt{2}} \]  

\[ S_{\pm 1,4} = i \left( \frac{\omega \delta}{\omega_r} \right)^3 \frac{(P_4) Q_4^{(3)} + 6 (P_6) Q_6^{(3)}}{4 \sqrt{752} \sqrt{2}} \pm i \left( \frac{\omega \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} (Q_{27} - Q_{28}) (P_4) + \frac{7}{72} Q_3 (P_6) - \frac{1}{60} Q_4 (P_8) \right] \]  

\[ S_{\pm 1,6} = \pm i \left( \frac{\omega \delta}{\omega_r} \right)^4 \frac{11 Q_3 (P_6) + 6 Q_4 (P_8)}{720} \]  

\[ S_{\pm 18} = 0 \]  

C. Belonging to \( I_{\pm 2} \)
\[ S_{\pm 2, 2} = \frac{i \omega_0 \delta}{\omega_r} \frac{1}{4 \sqrt{6}} E_5 \langle P_2 \rangle \pm \frac{i}{36} \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \left( 3 Q_2^{(2)} \langle P_2 \rangle + Q_4^{(2)} \langle P_4 \rangle \right) - i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{840 \sqrt{3}}{266 112 \sqrt{2}} \left( 3 + \eta^2 \right) E_5 \langle P_2 \rangle - 72 \langle P_4 \rangle Q_4^{(3)} - 217 \langle P_6 \rangle Q_6^{(3)} \]

\[ = \frac{i}{24} \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{2} (Q_{12} - Q_{15}) \langle P_2 \rangle + (Q_{22} + Q_{210}) \langle P_4 \rangle - \frac{1}{2} Q_3 \langle P_6 \rangle - \frac{119}{143} Q_4 \langle P_8 \rangle \right] \]  

\[ S_{\pm 2, 4} = \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{2}{576} Q_4^{(2)} \langle P_4 \rangle \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ (Q_{211} - \frac{1}{8} Q_{228}) \langle P_4 \rangle + \frac{523}{120} Q_3 \langle P_6 \rangle + \frac{1}{60} Q_4 \langle P_8 \rangle \right] \]  

\[ S_{\pm 2, 6} = -i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{4608 \sqrt{2}}{Q_6^{(3)} \langle P_6 \rangle} \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{11}{14} Q_3 \langle P_6 \rangle + \frac{1}{240} Q_4 \langle P_8 \rangle \right] \]  

\[ S_{\pm 2, 8} = \pm i \frac{68}{768} \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 Q_4 \langle P_8 \rangle \]

\[ \text{D. Belonging to } I_{\pm 3} \]

\[ C_{\pm 3, 0} = I_{3}^{(\text{iso})} - \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left( \frac{1}{264} Q_{11} \langle P_2 \rangle + \frac{1}{24} Q_{212} \langle P_4 \rangle - \frac{17}{1512} Q_3 \langle P_6 \rangle - \frac{14}{296} Q_4 \langle P_8 \rangle \right) \]

\[ C_{\pm 3, 2} = \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44 \sqrt{3}}{33} (3 + \eta^2) \langle P_2 \rangle E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)} \]

\[ + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{14} \langle P_2 \rangle - \frac{1}{24} Q_{26} \langle P_4 \rangle - \frac{1}{48} Q_3 \langle P_6 \rangle + \frac{41}{3432} Q_4 \langle P_8 \rangle \right] \]

\[ C_{\pm 3, 4} = \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \left( \frac{P_4}{Q_4^{(3)}} + \frac{6}{Q_6^{(3)}} \right) \frac{4}{752 \sqrt{2}} \left( \frac{P_4}{Q_4^{(3)}} + \frac{6}{Q_6^{(3)}} \right) \]

\[ - \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{27} \langle P_4 \rangle + \frac{73}{720} Q_3 \langle P_6 \rangle + \frac{29}{1560} Q_4 \langle P_8 \rangle \right] \]

\[ C_{\pm 3, 6} = - \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{11}{360} Q_3 \langle P_6 \rangle + \frac{2}{120} Q_4 \langle P_8 \rangle \right] \]

\[ C_{\pm 3, 8} = 0 \]

\[ S_{\pm 3, 2} = \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44 \sqrt{3}}{33} (3 + \eta^2) \langle P_2 \rangle E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)} \]

\[ \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{14} \langle P_2 \rangle - \frac{1}{24} Q_{26} \langle P_4 \rangle - \frac{1}{48} Q_3 \langle P_6 \rangle + \frac{41}{3432} Q_4 \langle P_8 \rangle \right] \]

\[ S_{\pm 3, 4} = \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{1}{4 \sqrt{3}} \left( \langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)} \right) \frac{4}{752 \sqrt{2}} \]

\[ \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{27} \langle P_4 \rangle + \frac{73}{720} Q_3 \langle P_6 \rangle + \frac{29}{1560} Q_4 \langle P_8 \rangle \right] \]

\[ S_{\pm 3, 6} = \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{11}{360} Q_3 \langle P_6 \rangle + \frac{2}{120} Q_4 \langle P_8 \rangle \right] \]
The $Q^3_n$ are geometry factors, which similar to $E_1...E_5$ contain information about the orientation of the CST PAF with respect to the segment vector. Their definitions are given in the following, where $P_n(x)$ are the Legendre polynomials and $P_n^{(m)}$ are the assigned Legendre polynomials:

\begin{align}
Q_2^{(2)} &= \frac{3 - \eta^2}{7} P_2(\cos \alpha) - \frac{\eta}{7} P_2^{(2)}(\cos \alpha) \cos 2\psi \\
Q_4^{(2)} &= -\frac{18 + \eta^2}{70} P_4(\cos \alpha) - \frac{\eta}{70} P_4^{(2)}(\cos \alpha) \cos 2\psi - \frac{\eta^2}{48 \cdot 35} P_4^{(4)}(\cos \alpha) \cos 4\psi \\
Q_4^{(3)} &= 3\sqrt{2} (9 - 4 \eta^2) P_4(\cos \alpha) - \frac{\sqrt{2}}{4 \eta} (3 + \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi - \frac{\sqrt{2}}{8 \eta^2} P_4^{(4)}(\cos \alpha) \cos 4\psi \\
Q_6^{(3)} &= -\frac{3\sqrt{2}}{4} (6 + \eta^2) P_6(\cos \alpha) - \frac{\sqrt{2}}{240 \eta} (36 + \eta^2) P_6^{(2)}(\cos \alpha) \cos 2\psi - \frac{\sqrt{2}}{480 \eta^2} P_6^{(4)}(\cos \alpha) \cos 4\psi \nonumber \\
&\quad - \frac{\sqrt{2}}{17280 \eta^3} P_6^{(6)}(\cos \alpha) \cos 6\psi \\
Q_{11} &= \frac{1}{1134} \left[ (-27 - 9\eta^2 + 4\eta^4) P_2(\cos \alpha) + \frac{1}{2} \eta (27 + 5\eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \\
Q_{12} &= \frac{1}{1386} \left[ (315 + 72 \eta^2 - 43 \eta^4) P_2(\cos \alpha) + \eta (141 + 31 \eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \\
Q_{13} &= \frac{1}{2079} \left[ (-405 - 36\eta^2 + 49\eta^4) P_2(\cos \alpha) + \eta (153 + 43\eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \\
Q_{14} &= \frac{1}{1386} \left[ (9 + 36\eta^2 - 5\eta^4) P_2(\cos \alpha) + \eta (-21 + \eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \\
Q_{15} &= \frac{1}{8916} \left[ (81 - 72 \eta^2 - \eta^4) P_2(\cos \alpha) + \eta (9 - 13 \eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \\
Q_{21} &= \frac{1}{960 \cdot 960} \left[ (213 678 + 111 357 \eta^2 + 817 \eta^4) P_4(\cos \alpha) + \eta (17 523 + 3 329 \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \\
&\quad + \frac{\eta^2}{24} (6 219 + 4 585\eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \\
Q_{22} &= \frac{1}{2 \cdot 772} \left[ (756 + 249 \eta^2 + 19 \eta^4) P_4(\cos \alpha) + 3 \eta (11 + 5 \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \\
&\quad + \frac{\eta^2}{24} (51 + 13 \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \\
Q_{23} &= \frac{1}{123 \cdot 552} \left[ (-2 754 - 3 375 \eta^2 + 205 \eta^4) P_4(\cos \alpha) + \frac{\eta}{5} (-3 069 + \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \\
&\quad + \frac{\eta^2}{120} (1 539 - 511 \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \\
S_{\pm 3;8} &= 0 \quad (66)
\end{align}
\[ Q_{24} = \frac{1}{720 720} \left[ (100 278 + 57 177 \eta^2 - 163 \eta^4) \ P_4(\cos \alpha) + \eta \ (9207 + 1453 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{24} (1 935 + 2 261\eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (78)

\[ Q_{25} = \frac{1}{54 054} \left[ (11 664 + 3 771 \eta^2 + 301 \eta^4) \ P_4(\cos \alpha) + \eta \ (495 + 233 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{24} (801 + 199 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (79)

\[ Q_{26} = \frac{1}{36 036} \left[ (864 + 327 \eta^2 + 17 \eta^4) \ P_4(\cos \alpha) + \frac{3}{5} \eta \ (77 + 27 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{120} (249 + 79 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (80)

\[ Q_{27} = \frac{1}{123 552} \left[ (3402 - 2493 \eta^2 + 487 \eta^4) \ P_4(\cos \alpha) + \frac{1}{5} \eta \ (297 + 67 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{120} (4761 - 109 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (81)

\[ Q_{28} = \frac{1}{123 552} \left[ (810 + 387 \eta^2 + 7 \eta^4) \ P_4(\cos \alpha) + \frac{1}{5} \eta \ (297 + 67 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi - \frac{\eta^2}{120} (153 + 83 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (82)

\[ Q_{29} = \frac{1}{1 441 440} \left[ (−31914 - 32 751 \eta^2 + 1 669 \eta^4) \ P_4(\cos \alpha) - \eta \ (5 841 + 139 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{24} (2 295 - 1 043 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (83)

\[ Q_{210} = \frac{1}{216 216} \left[ (972 + 207 \eta^2 + 37 \eta^4) \ P_4(\cos \alpha) + \frac{\eta}{5} \ (99 + 109 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{120} (441 + 71 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (84)

\[ Q_{211} = \frac{1}{494 208} \left[ (30 942 - 9 927 \eta^2 + 3 013 \eta^4) \ P_4(\cos \alpha) + \eta \ (−2673 + 1061 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{24} (6111 + 85 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (85)

\[ Q_{212} = \frac{1}{240 240} \left[ (1 458 - 333 \eta^2 + 127 \eta^4) \ P_4(\cos \alpha) + \eta \ (−99 + 47 \eta^2) \ P_4^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{24} (261 + 7 \eta^2) \ P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \] (86)
\[ Q_3 = \frac{1}{3 \cdot 168} \left[ (-54 + 2\eta^2 + \eta^4) P_6(\cos \alpha) + \frac{\eta^3}{2} P_6^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{360} (9 + \eta^2) P_6^{(4)}(\cos \alpha) \cos 4\psi \right. \\
+ \left. \frac{\eta^3}{720} P_6^{(6)}(\cos \alpha) \cos 4\psi \right] \tag{87} \]

\[ Q_4 = \frac{1}{6 \cdot 912} \left[ (216 + 72 \eta^2 + \eta^4) P_8(\cos \alpha) + \frac{3}{7} \eta (12 + \eta^2) P_8^{(2)}(\cos \alpha) \cos 2\psi \right. \\
+ \left. \frac{\eta^2 (54 + \eta^2)}{120} P_8^{(4)}(\cos \alpha) \cos 4\psi + \frac{\eta^3}{2 \cdot 520} P_8^{(6)}(\cos \alpha) \cos 4\psi + \frac{\eta^4}{120 \cdot 960} P_8^{(8)}(\cos \alpha) \cos 4\psi \right] \tag{88} \]
S6. OSCILLATION COEFFICIENTS: EXPERIMENTAL DATA

Table I. \( C_7 = CH_3 \); all values \( \pm 0.0016 \)

| \( m \) | \( C_{m0} \) | \( C_{m2} \) | \( S_{m2} \) |
|-------|--------|--------|--------|
| -2    | -0.00485 | 0.0058 |
| -1    | 0.0133   | 0      | 0      |
| 0     | 0.9700   | 0.003395 | -0.0107|
| 1     | 0.0126   | 0      | 0      |
| 2     | 0.003395 | 0.0061 |

Table II. \( C_1+C_2+C_5 = CO_3 \) and the two \( C_\eta \); all values \( \pm 0.001 \)

| \( m \) | \( C_{m0} \) | \( C_{m2} \) | \( S_{m2} \) |
|-------|--------|--------|--------|
| -3    | 0.014   | 0      | 0.0024 |
| -2    | -0.0094 | 0.0087 |
| -1    | 0.160   | -0.0113| 0.0078 |
| 0     | 0.597   | 0.0081 | -0.0263|
| 1     | 0.167   | -0.0070| -0.0130|
| 2     | 0.0375  | 0.0184 | 0.0167 |
| 3     | 0.0045  | 0.0031 | 0.0032 |

Table III. \( C_3 = CH \); all values \( \pm 0.0011 \)

| \( m \) | \( C_{m0} \) | \( C_{m2} \) | \( S_{m2} \) |
|-------|--------|--------|--------|
| -3    | 0.0048  | 0      | 0      |
| -2    | 0.0416  | -0.0067| 0.0067 |
| -1    | 0.1153  | 0.0080 | -0.0089|
| 0     | 0.6369  | -0.0061| -0.0051|
| 1     | 0.1834  | 0.0080 | 0.0085 |
| 2     | 0.0156  | 0      | 0      |
| 3     | 0.0024  | 0      | 0      |

Table IV. \( C_4 = CH \); all values \( \pm 0.0011 \)

| \( m \) | \( C_{m0} \) | \( C_{m2} \) | \( S_{m2} \) |
|-------|--------|--------|--------|
| -3    | 0.0083  | 0      | 0      |
| -2    | 0.0607  | -0.0094| 0.0089 |
| -1    | 0.1508  | 0.0127 | -0.0132|
| 0     | 0.6675  | -0.0089| -0.0077|
| 1     | 0.0868  | 0.0117 | 0.0125 |
| 2     | 0.0290  | 0      | 0      |
| 3     | 0.0028  | 0      | 0      |