Supplement

Efficient polynomial analysis of MAS 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

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

Meaning of the averaging symbol:

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

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 \( \gamma \rightarrow -\gamma \):

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

If the cosine power \( n \) is odd: We substitute \( \gamma \rightarrow \pi/2 - \gamma \) 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 \( m \rightarrow m + 2 \) is done by

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

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

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

\[ \langle \cos^n \alpha \sin^m \alpha \rangle_{\cos} = \begin{cases} 
\frac{m!! (n - 1)!!}{(m + n + 1)!!} & \text{if } m \text{ and } n \text{ even} \\
\frac{m!! (n - 1)!!}{(m + n + 1)!!} \cdot \frac{\pi}{2} & \text{if } m \text{ odd and } n \text{ even} \\
0 & \text{if } n \text{ odd} 
\end{cases} \]  
(8)

Meaning of the averaging symbol:

\[ \langle A(\alpha) \rangle_{\cos} = \frac{1}{\pi} \int_0^\pi A(\alpha) \sin \alpha \, d\alpha = \frac{1}{2} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} A(\alpha) \, d(\cos \alpha) \]  
(9)

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

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

\[ \langle \cos^n \alpha \sin^m \alpha \rangle = \frac{1}{\pi} \int_0^\pi \cos^n \alpha \sin^{m+1} \alpha \, d\alpha = \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha + \frac{1}{\pi} \int_{\pi/2}^{\pi} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha \\
= \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha + \frac{1}{\pi} \int_0^0 \cos^n \alpha \sin^{m+1} \alpha \, d\alpha = 0 \]  
(10)
This proves proposition (8) for odd \( n \).

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

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

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

(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:

\[
\langle \cos^{n+2} \alpha \sin \alpha \rangle = \frac{1}{2} \int_{0}^{\pi} \cos^{n+2} \alpha \sin^2 \alpha \, d\alpha = \frac{1}{2} \int_{0}^{\pi} (\cos^{n+2} \alpha - \cos^{n+4} \alpha) \, d\alpha
\]

(13)

Partial integration of a cosine power:

\[
\int_{0}^{\pi} \cos^p \alpha \, d\alpha = [\sin \alpha \cos^{p-1} \alpha]_{0}^{\pi} - (p-1) \int_{0}^{\pi} (-\sin^2 \alpha) \cos^{p-2} \alpha \, d\alpha = (p-1) \cdot 2 \langle \cos^{p-2} \alpha \sin \alpha \rangle
\]

(14)

Inserting this rule into eqn. (13):

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

(15)

or

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

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

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

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

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

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

(17)

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

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

\( \square \)
S2. POWDER-AVERAGED PHASE POWERS

Listed up to eighth power:

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

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

\[ \langle \Phi^3 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^3 \cdot \frac{4}{5} \cdot \frac{7}{7} (1 - \eta^2) \sin \gamma_r \sin^2 \frac{\gamma_r}{2} \] (20)

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

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

\[ \langle \Phi^6 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^6 \cdot \frac{1}{16016} \left( \begin{array}{c} 5515 + 16381 \eta^2 + 49963 \eta^4 + 49471 \eta^6 \\ 3 \\ 27 \\ 243 \\ 945 \end{array} \right) \cos \gamma_r - \frac{1}{32032} \left( \begin{array}{c} 2983 + 6219 \eta^2 + 2477 \eta^4 + 12185 \eta^6 \\ 9 \\ 81 \\ 839 \\ 243 \end{array} \right) \cos 2 \gamma_r \\
+ \frac{1}{2012} \left( \begin{array}{c} 131 + 1009 \eta^2 + 2567 \eta^4 + 2843 \eta^6 + 1145 \eta^6 \\ 63 \\ 567 \\ 243 \end{array} \right) \cos 3 \gamma_r - \frac{1}{16016} \left( \begin{array}{c} 179 - 235 \eta^2 + 3155 \eta^4 + 839 \eta^6 \\ 3 \\ 27 \\ 839 \\ 243 \end{array} \right) \cos 4 \gamma_r \\
- \frac{1}{143} \left( \begin{array}{c} 5 + 84 \eta^2 + 37 \eta^4 + 7 \eta^6 + 7 \eta^6 \\ 28 \\ 756 \\ 972 \end{array} \right) \cos 5 \gamma_r - \frac{1}{24143} \left( \begin{array}{c} 5 + 19 \eta^2 + 37 \eta^4 + 7 \eta^6 \\ 28 \\ 756 \\ 972 \end{array} \right) \cos 6 \gamma_r \right] \] (23)

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

\[ \langle \Phi^8 \rangle = \left( \frac{\delta \omega_0}{\omega_r} \right)^8 \cdot \frac{1}{15949791} \cdot 4 (3 + \eta^2) (5 + \cos \gamma_r) \left[ 1274778 + 282042 \eta^2 + 645534 \eta^4 + 34958 \eta^6 \\
+ 3 (296217 - 132759 \eta^2 + 194067 \eta^4 + 5675 \eta^6) \cos \gamma_r + 51030 \cos 2 \gamma_r + 1701 \cos 3 \gamma_r \\
+ \eta^2 (2997 + 279 \eta^2 + 79 \eta^4) (30 \cos 2 \gamma_r + \cos 3 \gamma_r) \right] \sin^8 \frac{\gamma_r}{2} \] (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 $f$ and $g$, respectively. Since $f$ and $g$ 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:

$aux = \sum #2!/(p!q!(#2 - p - q)!) \cdot \binom{#1 - 2*#2}{r} \cdot 2^{4*#2 + r + p}/6^{#1} \cdot (-1)^r \cdot (p + r - 1)!! \cdot (q + #1 - 2*#2 - r - 1)!!/(p + q + #1 - 2*#2)!! \cdot (1 + (-1)^r(r - p))(1 + (-1)^r(q + #1 + 2*#2 - r))! \cdot 4^r \cdot \sum (-1)^{(q - s + u)} \cdot \binom{q, s, t} \cdot \binom{#1 - 2*#2 - r, u}{2*#2}!! \cdot (p + r + 2*s + 2*t + 2*u - 1)!!/(2*#2 + p + r + 2*s + 2*t + 2*u + 1)!! \cdot \sum (-1)^v \cdot 3^{(v + w)} \cdot \binom{#1 - 2*#2 + p - r + 2*s + 2*t + v - w} \cdot \binom{p + 2*s + 2*t + u, v} \cdot \binom{#1 - 2*#2 - r, u, w} \cdot 3^3 \cdot (v + w + 2*#2 - p - 2*s - 2*t + r)!/(v + w + 2*#2 - p - 2*s - 2*t + r - 1)!!/(v + w + 2*#2 - p - 2*s - 2*t + r)!/(v + w + 2*#2 - p - 2*s - 2*t + r)!/(v + w)! \cdot (1 + (-1)^r(r - p))/4, \{w, 0, #1 - 2*#2 - r - u\}, \{v, 0, p + 2*s + 2*t + u\}, \{u, 0, #1 - 2*#2 - 2*r\}, \{t, 0, #2 - p - q\}, \{s, 0, q\}, \{r, 0, #1 - 2*#2\}, \{q, 0, #2\}, \{p, 0, #2\} &;$

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

$rsb = \sum 1/2^n \cdot #2^n \cdot (-1)^{#1 - 1 - b} \cdot ((n - k - #1 - 2*b)! \cdot (3*k - n + #1 + 2b)! \cdot (n - 2*k - b)! * aud[n, k, #3, \{n, #1, #4\}, \{k, 0, n/2\}, \{b, 0, n - 2*k\}] &;$

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

$rsb[0, \text{delta, eta, 6}] // \text{Simplify}$
S. 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 $w = \delta\omega_0/\omega_r$).

\[ I_0 = 1 - \frac{K_1^2}{20} w^2 + \frac{227 K_1^2}{181440} w^4 - \frac{49471 K_1^3 + 4428 K_2^3}{280215360} w^6 + \frac{K_1 (1466405 K_1^3 - 709776 K_2^2)}{9146248151040} w^8 \]

\[ - K_1^2 (286311167 K_1^3 - 494915400 K_2^3) w^{10} + \frac{998271153509 K_1^3 - 2160 K_2^3 (1577931893 K_1^3 + 218222883 K_2^3)}{209789835279931146240000} w^{12} \]

\[ I_{\pm 1} = \frac{K_1}{45} w^2 + \frac{K_2}{105} w^3 - \frac{17172 K_1^2}{83160} w^4 + \frac{23 K_1 K_2}{83160} w^5 + \frac{1284 K_3 K_1^3 - 2484 K_2^2}{23351280} w^6 \]

\[ + \frac{19 K_2^2 K_1}{105} w^7 - \frac{5189184}{1028952916992} + \frac{K_1 (123823 K_1^3 - 285552 K_2^3)}{83160} w^8 \pm \frac{K_2 (959357 K_1^3 - 196884 K_2^3)}{32583509038080} w^9 \]

\[ + \frac{K_1 (11362895 K_1^3 - 46559016 K_2^3)}{140760759044560} w^{10} + \frac{K_1 K_2 (766057 K_1^3 - 663984 K_2^3)}{4692025301483520} w^{11} \]

\[ - \frac{34324127551 K_1^3 - 2160 K_2^3 (963547 227 K_1^3 + 2033937 K_2^3)}{8741243136663797760000} w^{12} \]

\[ I_{\pm 2} = \frac{K_1}{360} w^2 \pm \frac{K_2}{210} w^3 + \frac{17172 K_1^2}{83160} w^4 + \frac{1284 K_3 K_1^3 - 2484 K_2^2}{3736212480} w^6 \]

\[ + \frac{49 K_2^2 K_1}{105} w^7 - \frac{1482624}{3964972546655191040000} \pm \frac{(3 + \eta^2) K_1 (966239 K_1^3 - 10569744 K_2^3)}{32583509038080} w^9 \]

\[ - \frac{(3 + \eta^2)^2 K_2^3 (14591857 K_1^3 - 197993592 K_2^3)}{37536202411868160} w^{10} \pm \frac{K_1 K_2 (4460413 K_1^3 - 7892208 K_2^3)}{239814626520268800} w^{11} \]

\[ + \frac{75617921797 K_1^3 - 2160 K_2^3 (548505769 (3 + \eta^2)^2 - 72353061 K_2^3)}{34963725409991393280000} w^{12} \]

\[ I_{\pm 3} = \frac{K_1^2}{22680} w^4 \pm \frac{K_1 K_2}{27720} w^5 - \frac{11145 K_1^3 + 65556 K_2^3}{4203239040} w^6 + \frac{163 K_2^2 K_1}{1556755200} w^7 \]

\[ - \frac{K_1 (9379 K_1^3 - 682128 K_2^3)}{1714921528320} w^8 \pm \frac{K_2 (2845 K_1^3 - 5076 K_2^3)}{212964111360} w^9 \]

\[ + \frac{K_2^2 (224699 K_1^3 - 10360440 K_2^3)}{2346012650741760} w^{10} \pm \frac{K_1 K_2 (1832201 K_1^3 - 7529328 K_2^3)}{17980696989020160} w^{11} \]

\[ - \frac{19307643899 K_1^3 - 2160 K_2^3 (360943523 K_1^3 - 121172787 K_2^3)}{26223729409991393280000} w^{12} \]

\[ I_{\pm 4} = \frac{K_1^2}{362880} w^4 \pm \frac{K_1 K_2}{166320} w^5 + \frac{839 K_1^3 + 20844 K_2^3}{5604318720} w^6 + \frac{K_1 K_2}{77837760} w^7 \]

\[ - \frac{K_1 (5899 K_1^3 + 5681232 K_2^3)}{41158116679680} w^8 \pm \frac{K_2 (2845 K_1^3 - 5076 K_2^3)}{32583509038080} w^9 \]

\[ + \frac{K_2^2 (34081 K_1^3 - 18301302 K_2^3)}{9384050602967040} w^{10} \pm \frac{K_1 K_2 (233311 K_1^3 - 2825712 K_2^3)}{899304849510080} w^{11} \]

\[ + \frac{11419571509 K_1^3 - 2160 K_2^3 (656644693 K_1^3 - 496531917 K_2^3)}{932399267910850940000} w^{12} \]
S5. 2D OSCILLATION COEFFICIENTS

A. Belonging to $I_0$

\[
C_{00} = I_{0}^{(iso)} + \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \left( \frac{1}{12} Q_2^{(2)}\langle P_2 \rangle - \frac{31}{96} Q_4^{(2)}\langle P_4 \rangle \right) + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left( \frac{85}{528} Q_{11}\langle P_2 \rangle + Q_{21}\langle P_4 \rangle + \frac{59}{3024} Q_3\langle P_6 \rangle + \frac{19733}{7248384} Q_4\langle P_8 \rangle \right)
\]

\[\text{(31)}\]

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

\[\text{(32)}\]

\[
C_{04} = -\left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{35}{576} Q_4^{(2)}\langle P_4 \rangle + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left( \frac{1}{12} Q_{23}\langle P_4 \rangle + \frac{1}{15} Q_3\langle P_6 \rangle + \frac{111}{260} Q_4\langle P_8 \rangle \right)
\]

\[\text{(33)}\]

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

\[\text{(34)}\]

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

\[\text{(35)}\]

\[
S_{02} = -i \frac{\omega_0 \delta}{2\sqrt{6}} E_5\langle P_2 \rangle + i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{3}{3} \frac{344\sqrt{3}}{3} (3 + \eta^2)\langle P_2 \rangle E_5 - 296\langle P_4 \rangle Q_4^{(3)} + 875\langle P_6 \rangle Q_6^{(3)} \]

\[\text{(36)}\]

\[
S_{04} = -i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{P_4}{4}\langle Q_4^{(3)} + 6\langle P_6 \rangle Q_6^{(3)} \right)
\]

\[\text{(37)}\]

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

\[\text{(38)}\]

\[
S_{08} = 0
\]

\[\text{(39)}\]

B. Belonging to $I_{\pm1}$

\[
C_{\pm10} = I_{\pm1}^{(iso)} + \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{1}{18} \left( - Q_2^{(2)}\langle P_2 \rangle + 3 Q_4^{(2)}\langle P_4 \rangle \right) \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{21}{83} Q_4^{(3)}\langle P_4 \rangle - 50 Q_6^{(3)}\langle P_6 \rangle \]

\[\text{(40)}\]

\[
C_{\pm1;2} = -\left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{3}{18} Q_3^{(2)}\langle P_2 \rangle + \frac{Q_4^{(2)}\langle P_4 \rangle}{44 \sqrt{3}} (3 + \eta^2)\langle P_2 \rangle E_5 - 5 Q_4^{(3)}\langle P_4 \rangle + 14\langle P_6 \rangle Q_6^{(3)} \]

\[\text{(41)}\]
\[C_{\pm 1:4} = \pm \left( \frac{\omega \delta}{\omega_r} \right)^3 \frac{3}{4752\sqrt{2}} Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)} \left[ \frac{1}{24} (Q_{27} + Q_{28}) \langle P_4 \rangle + \frac{41}{360} Q_3 \langle P_6 \rangle - \frac{4}{195} Q_4 \langle P_6 \rangle \right] \]

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

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

\[S_{\pm 1:2} = \mp i \left( \frac{\omega \delta}{\omega_r} \right)^2 \frac{3}{18} Q_4^{(2)} \langle P_2 \rangle - \frac{1}{3} \langle P_4 \rangle \left[ \frac{44\sqrt{3}}{33264\sqrt{2}} (3 + \eta^2) \langle P_2 \rangle E_3 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)} \right] \]

\[S_{\pm 1:4} = \pm i \left( \frac{\omega \delta}{\omega_r} \right)^4 \frac{1}{12} \left[ (Q_{14} + Q_{13}) \langle P_2 \rangle + (Q_{25} - Q_{26}) \langle P_4 \rangle - \frac{1}{2} Q_3 \langle P_6 \rangle - \frac{19}{489} Q_4 \langle P_6 \rangle \right] \]

\[S_{\pm 1:8} = 0 \]

C. Belonging to \(I_{\pm 2}\)

\[C_{\pm 20} = I_{\pm 20}^{(3)} + \left( \frac{\omega \delta}{\omega_r} \right)^2 \left[ \frac{1}{72} Q_4^{(2)} \langle P_2 \rangle - \frac{1}{192} Q_4^{(2)} \langle P_4 \rangle \right] \pm \left( \frac{\omega \delta}{\omega_r} \right)^3 \frac{21}{166320\sqrt{2}} \]

\[C_{\pm 2:2} = \pm \frac{\omega \delta}{\omega_r} \frac{1}{4\sqrt{6}} E_5 \langle P_2 \rangle + \left( \frac{\omega \delta}{\omega_r} \right)^2 \frac{1}{36} \left[ 3 Q_4^{(2)} \langle P_2 \rangle + Q_4^{(2)} \langle P_4 \rangle \right] \]

\[C_{\pm 2:4} = \pm \left( \frac{\omega \delta}{\omega_r} \right)^3 \frac{1384\sqrt{3}}{532224\sqrt{2}} \left( 3 + \eta^2 \right) E_5 \langle P_2 \rangle - 152 \langle P_4 \rangle Q_4^{(3)} + 441 \langle P_6 \rangle Q_6^{(3)} \]

\[C_{\pm 2:6} = \pm \left( \frac{\omega \delta}{\omega_r} \right)^4 \frac{1}{120} Q_3 \langle P_6 \rangle + \frac{11}{1440} Q_4 \langle P_6 \rangle \]

\[C_{\pm 2:8} = \mp \left( \frac{\omega \delta}{\omega_r} \right)^4 \left[ \frac{11}{120} Q_3 \langle P_6 \rangle + \frac{1}{240} Q_4 \langle P_6 \rangle \right] \]

\[C_{\pm 2:8} = - \frac{1}{768} \left( \frac{\omega \delta}{\omega_r} \right)^4 Q_4 \langle P_6 \rangle \]
\[ S_{\pm,2:2} = \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \left( 3 Q_2 \langle P_2 \rangle + Q_4 \langle P_4 \rangle \right) \]

\[ - i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{840 \sqrt{3} (3 + \eta^2)}{266 112 \sqrt{2}} \frac{E_5 \langle P_5 \rangle - 72 \langle P_4 \rangle Q_4^{(3)} + 217 \langle P_6 \rangle Q_6^{(3)}}{\langle P_2 \rangle} \]

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

\[ S_{\pm,2:4} = \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{Q_4 \langle P_4 \rangle}{128} \pm \frac{i}{24} \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{11}{1440} Q_3 \langle P_6 \rangle + \frac{1}{240} Q_4 \langle P_8 \rangle \right] \]

\[ S_{\pm,2:6} = - i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{Q_6^{(3)}}{4608 \sqrt{2}} \pm i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{11}{1440} Q_3 \langle P_6 \rangle + \frac{1}{240} Q_4 \langle P_8 \rangle \right] \]

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

D. Belonging to \( I_{\pm,3} \)

\[ C_{\pm,3:0} = I_{3}^{(\text{iso})} - \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left( \frac{1}{264} Q_{11} \langle P_2 \rangle + \frac{1}{24} Q_{212} \langle P_4 \rangle - \frac{17}{1512} Q_3 \langle P_6 \rangle + \frac{14}{10296} Q_4 \langle P_8 \rangle \right) \]

\[ C_{\pm,3:2} = \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44 \sqrt{3} (3 + \eta^2)}{33264 \sqrt{2}} \frac{E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{\langle P_2 \rangle} + \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{14} \langle P_2 \rangle - \frac{1}{24} Q_{26} \langle P_4 \rangle - \frac{1}{48} Q_3 \langle P_6 \rangle + \frac{41}{3432} Q_4 \langle P_8 \rangle \right] \]

\[ C_{\pm,3:4} = \pm \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4752 \sqrt{2}} - \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{27} \langle P_4 \rangle + \frac{73}{720} Q_3 \langle P_6 \rangle + \frac{29}{1560} Q_4 \langle P_8 \rangle \right] \]

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

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

\[ S_{\pm,3:2} = i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44 \sqrt{3} (3 + \eta^2)}{33264 \sqrt{2}} \frac{E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{\langle P_2 \rangle} + i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{14} \langle P_2 \rangle - \frac{1}{24} Q_{26} \langle P_4 \rangle - \frac{1}{48} Q_3 \langle P_6 \rangle + \frac{41}{3432} Q_4 \langle P_8 \rangle \right] \]

\[ S_{\pm,3:4} = i \left( \frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4752 \sqrt{2}} \mp i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{1}{24} Q_{27} \langle P_4 \rangle + \frac{73}{720} Q_3 \langle P_6 \rangle + \frac{29}{1560} Q_4 \langle P_8 \rangle \right] \]

\[ S_{\pm,3:6} = \mp i \left( \frac{\omega_0 \delta}{\omega_r} \right)^4 \left[ \frac{11}{360} Q_3 \langle P_6 \rangle + \frac{2}{120} Q_4 \langle P_8 \rangle \right] \]
The $Q_\alpha^5$ 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} - \frac{35}{54} P_4^{(4)} (\cos \alpha) \cos 4\psi
\end{align*}

\begin{align*}
Q_4^{(3)} &= 3\sqrt{2} (9 - 4 \eta^2) P_4 (\cos \alpha) - \sqrt{2} \eta (3 + \eta^2) P_4^{(2)} (\cos \alpha) \cos 2\psi - \frac{\sqrt{2} \eta^2}{8} P_4^{(4)} (\cos \alpha) \cos 4\psi
\end{align*}

\begin{align*}
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 \\
&\quad - \frac{\sqrt{2}}{17280} \eta^3 P_6^{(6)} (\cos \alpha) \cos 6\psi
\end{align*}

\begin{align*}
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]
\end{align*}

\begin{align*}
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]
\end{align*}

\begin{align*}
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]
\end{align*}

\begin{align*}
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]
\end{align*}

\begin{align*}
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]
\end{align*}

\begin{align*}
Q_{21} &= \frac{1}{960} \frac{960}{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]
\end{align*}

\begin{align*}
Q_{22} &= \frac{1}{2 772} \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]
\end{align*}

\begin{align*}
Q_{23} &= \frac{1}{1 235 552} \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]
\end{align*}
\[ Q_{24} = \frac{1}{720} \left[ \left( 100 \ 278 + 57 \ 177 \ \eta^2 - 163 \ \eta^4 \right) P_4 (\cos \alpha) + \eta \ (9207 + 1 \ 453 \ \eta^2) \ P_4^{(2)} (\cos \alpha) \cos 2\psi \\
+ \frac{\eta^2}{24} \left( 1935 + 2 \ 261 \eta^2 \right) \ P_4^{(4)} (\cos \alpha) \cos 4\psi \right] \] (78)

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

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

\[ Q_{27} = \frac{1}{123 \ 552} \left[ (3402 - 2493 \ \eta^2 + 487 \ \eta^4) P_4 (\cos \alpha) + \frac{1}{5} \eta \ (-2871 + 739 \ \eta^2) \ P_4^{(2)} (\cos \alpha) \cos 2\psi \\
+ \frac{\eta^2}{120} \left( 4761 - 109 \ \eta^2 \right) \ P_4^{(4)} (\cos \alpha) \cos 4\psi \right] \] (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)

\[ Q_{212} = \frac{1}{240 \ 240} \left[ (1458 - 333 \ \eta^2 + 127 \ \eta^4) P_4 (\cos \alpha) + \eta \ (-99 + 47 \ \eta^2) \ P_4^{(2)} (\cos \alpha) \cos 2\psi \\
+ \frac{\eta^2}{24} (261 + 7 \ \eta^2) \ P_4^{(4)} (\cos \alpha) \cos 4\psi \right] \] (86)
\[ Q_3 = \frac{1}{3 \, 168} \left[ (-54 + 27 \eta^2 + \eta^4) P_6(\cos \alpha) + \frac{\eta^3}{2} P_6^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2}{360} (9 + \eta^2) P_6^{(4)}(\cos \alpha) \cos 4\psi \right. \\
+ \left. \frac{\eta^3}{720} P_6^{(6)}(\cos \alpha) \cos 4\psi \right] (87) \]

\[ Q_4 = \frac{1}{6 \, 912} \left[ (216 + 72 \eta^2 + \eta^4) P_8(\cos \alpha) + \frac{3}{7} \eta (12 + \eta^2) P_8^{(2)}(\cos \alpha) \cos 2\psi \right. \\
+ \left. \frac{\eta^2}{1 \, 260} P_8^{(4)}(\cos \alpha) \cos 4\psi + \frac{\eta^3}{1 \, 520} P_8^{(6)}(\cos \alpha) \cos 4\psi + \frac{\eta^4}{120 \, 960} P_8^{(8)}(\cos \alpha) \cos 4\psi \right] (88) \]
S6. OSCILLATION COEFFICIENTS: EXPERIMENTAL DATA

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

| $m$ | $C_{m0}$ | $C_{m2}$ | $S_{m2}$ |
|-----|----------|----------|----------|
| -2  | 0.0133   | -0.00485 | 0.00555  |
| -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 $C_3$; all values $\pm 0.001$

| $m$ | $C_{m0}$ | $C_{m2}$ | $S_{m2}$ |
|-----|----------|----------|----------|
| -3  | 0.014    | 0        | 0.0024   |
| -2  | 0.014    | -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   | 0.0230   | 0        | 0        |
| 3   | 0.0028   | 0        | 0        |