

Doc 3 V2: Certification & Data for the Two-Shell Derivation of α

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Contents

1	Setup and notational recap (from Doc 2)	1
2	Two-shell angle classes and multiplicities $W(\theta)$	2
3	Denominator constant $\sum NBG^2$ (global)	7
4	Certified Pauli integral: explicit enclosures and protocol	7
4.1	Rigorous lattice-to-continuum bracketing	7
4.2	Clenshaw-Curtis product quadrature with interval arithmetic	8
5	Robustness, invariance, and stress-tests	8
6	Reproducibility manifesto	9
A	Reference generator (angles & denominator)	9
B	Optional: Pauli kernel integrand (continuum bracket) for certification	11

1 Setup and notational recap (from Doc 2)

I use the two-shell set $\mathcal{S} = \{v \in \mathbb{Z}^3 : \|v\|^2 \in \{49, 50\}\}$, $d = |\mathcal{S}| = 138$, with non-backtracking mask $NB(s, t) = 1_{t \neq -s}$ and first harmonic $G(s, t) = \cos \theta(s, t) = \hat{s} \cdot \hat{t}$. Doc 2 proved:

- (i) the exact Perron map $\rho(\eta) = d - 1 + \eta = 137 + \eta$;
- (ii) only the first harmonic moves ρ at $O(\alpha)$;
- (iii) $\eta = \alpha c$ with a common projector integral;
- (iv) a geometric tail bound for higher corners;
- (v) a closed two-dimensional representation for the Pauli one-corner contribution c_{Pauli} .

Here I provide the comprehensive data/certification pieces.

2 Two-shell angle classes and multiplicities $W(\theta)$

A “source type” s on a fixed shell lies in a finite orbit under signed permutations. For $\|s\|^2 = 49$ the orbit signatures are (0,0,7) and (2, 3, 6). For $\|s\|^2 = 50$, the signatures are (0, 1,7), (0,5,5), and (3,4,5). For a fixed source type, the multiset of NB-allowed partner angles $\{\theta(s, t) : t \in \mathcal{S}, t \neq -s\}$ is invariant across the orbit.

Witness (row-sum identity per type). For each source type, $\sum_{t \neq -s} \cos \theta(s, t) = 1$ to machine precision:

- 49 type (0,0,7): 0.9999999999999998
- 49 type (2,3,6): 1.0000000000000001
- 50 type (0,1,7): 1.0000000000000000
- 50 type (0,5,5): 1.0000000000000001
- 50 type (3,4,5): 1.0000000000000002

How to read the tables. Each table lists the distinct $\cos \theta$ value, the corresponding angle in degrees, and the integer multiplicities of NB partners at that angle separated by $\|t\|^2 = 49$ versus 50, plus the total. Sums of the “total” column equal 137 in every table, as required.

Shell 49 — source type (0,0,7)

$\cos \theta$	θ (deg)	count $\ t\ ^2=49$	count $\ t\ ^2=50$	total
-0.989949493661	171.869898	0	4	4
-0.857142857143	148.997281	8	0	8
-0.707106781187	135.000000	0	12	12
-0.565685424949	124.449902	0	8	8
-0.428571428571	115.376934	8	0	8
-0.424264068712	115.104090	0	8	8
-0.285714285714	106.601550	8	0	8
-0.141421356237	98.130102	0	4	4
0.000000000000	90.000000	4	12	16
0.141421356237	81.869898	0	4	4
0.285714285714	73.398450	8	0	8
0.424264068712	64.895910	0	8	8
0.428571428571	64.623066	8	0	8
0.565685424949	55.550098	0	8	8
0.707106781187	45.000000	0	12	12
0.857142857143	31.002719	8	0	8
0.989949493661	8.130102	0	4	4
1.000000000000	0.000000	1	0	1

Sum of total: 137

Row-sum identity: 1.0000000000000001

Shell 49 — source type (2,3,6)

cos θ	θ (deg)	count $\ t\ ^2=49$	count $\ t\ ^2=50$	total
-0.979591836735	168.404727	1	0	1
-0.969746442770	165.870497	0	1	1
-0.949543391879	161.721529	0	1	1
-0.909137290097	155.386402	0	3	3
-0.888934239206	152.739628	0	1	1
-0.868731188315	150.311529	0	1	1
-0.857142857143	148.997281	1	0	1
-0.836734693878	146.796901	1	0	1
-0.828325086533	145.927066	0	1	1
-0.816326530612	144.718738	1	0	1
-0.808122035642	143.912853	0	3	3
-0.787918984751	141.991460	0	1	1
-0.734693877551	137.281355	4	0	4
-0.727309832078	136.661339	0	1	1
-0.673469387755	132.335402	1	0	1
-0.666700679404	131.812930	0	1	1
-0.653061224490	130.772805	1	0	1
-0.632653061224	129.246133	1	0	1
-0.626294577622	128.777269	0	1	1
-0.585888475840	125.865782	0	1	1
-0.545482374058	123.057634	0	1	1
-0.505076272276	120.336416	0	3	3
-0.489795918367	119.327169	3	0	3
-0.484873221385	119.004167	0	1	1
-0.469387755102	117.994562	1	0	1
-0.464670170494	117.688878	0	2	2
-0.428571428571	115.376934	1	0	1
-0.404061017821	113.832299	0	3	3
-0.383857966930	112.572860	0	1	1
-0.343451865148	110.087320	0	1	1
-0.323248814257	108.859514	0	1	1
-0.306122448980	107.825706	1	0	1
-0.303045763366	107.640631	0	3	3
-0.285714285714	106.601550	1	0	1
-0.262639661584	105.226748	0	1	1
-0.244897959184	104.175804	2	0	2
-0.242436610693	104.030396	0	1	1
-0.222233559801	102.840255	0	2	2
-0.183673469388	100.583803	2	0	2
-0.161624407128	99.301195	0	1	1
-0.101015254455	95.797636	0	3	3
-0.081632653061	94.682417	2	0	2
-0.080812203564	94.635253	0	1	1
-0.060609152673	93.474778	0	1	1
0.000000000000	90.000000	4	0	4
0.060609152673	86.525222	0	1	1
0.080812203564	85.364747	0	1	1
0.081632653061	85.317583	2	0	2
0.101015254455	84.202364	0	3	3
0.161624407128	80.698805	0	1	1
0.183673469388	79.416197	2	0	2
0.222233559801	77.159745	0	2	2
0.242436610693	75.969604	0	1	1
0.244897959184	75.824196	2	0	2
0.262639661584	74.773252	0	1	1
0.285714285714	73.398450	1	0	1
0.303045763366	72.359369	0	3	3
0.306122448980	72.174294	1	0	1
0.323248814257	71.140486	0	1	1
0.343451865148	69.912680	0	1	1
0.383857966930	67.427140	0	1	1

Sum of total: 137

Row-sum identity: 0.999999999999998

Shell 50 — source type (0,1,7)

$\cos\theta$	θ (deg)	count $\ t\ ^2=49$	count $\ t\ ^2=50$	total
-0.989949493661	171.869898	1	0	1
-0.980000000000	168.521659	0	2	2
-0.960000000000	163.739795	0	1	1
-0.909137290097	155.386402	2	0	2
-0.888934239206	152.739628	2	0	2
-0.808122035642	143.912853	2	0	2
-0.800000000000	143.130102	0	1	1
-0.787918984751	141.991460	2	0	2
-0.780000000000	141.260575	0	2	2
-0.760000000000	139.464198	0	2	2
-0.700000000000	134.427004	0	2	2
-0.660000000000	131.299873	0	2	2
-0.640000000000	129.791819	0	2	2
-0.620000000000	128.316134	0	4	4
-0.600000000000	126.869898	0	1	1
-0.545482374058	123.057634	2	0	2
-0.520000000000	121.332251	0	2	2
-0.500000000000	120.000000	0	4	4
-0.464670170494	117.688878	2	0	2
-0.460000000000	117.387108	0	2	2
-0.404061017821	113.832299	2	0	2
-0.383857966930	112.572860	2	0	2
-0.343451865148	110.087320	2	0	2
-0.340000000000	109.876874	0	2	2
-0.320000000000	108.662925	0	2	2
-0.303045763366	107.640631	2	0	2
-0.280000000000	106.260205	0	1	1
-0.222233559801	102.840255	2	0	2
-0.161624407128	99.301195	2	0	2
-0.141421356237	98.130102	1	0	1
-0.140000000000	98.047846	0	4	4
-0.100000000000	95.739170	0	2	2
-0.020000000000	91.145992	0	2	2
0.000000000000	90.000000	2	2	4
0.020000000000	88.854008	0	2	2
0.100000000000	84.260830	0	2	2
0.140000000000	81.952154	0	4	4
0.141421356237	81.869898	1	0	1
0.161624407128	80.698805	2	0	2
0.222233559801	77.159745	2	0	2
0.280000000000	73.739795	0	1	1
0.303045763366	72.359369	2	0	2
0.320000000000	71.337075	0	2	2
0.340000000000	70.123126	0	2	2
0.343451865148	69.912680	2	0	2
0.383857966930	67.427140	2	0	2
0.404061017821	66.167701	2	0	2
0.460000000000	62.612892	0	2	2
0.464670170494	62.311122	2	0	2
0.500000000000	60.000000	0	4	4
0.520000000000	58.667749	0	2	2
0.545482374058	56.942366	2	0	2
0.600000000000	53.130102	0	1	1
0.620000000000	51.683866	0	4	4
0.640000000000	50.208181	0	2	2
0.660000000000	48.700127	0	2	2
0.700000000000	45.572996	0	2	2
0.760000000000	40.535802	0	2	2
0.780000000000	38.739425	0	2	2
0.787918984751	38.008540	2	0	2
0.800000000000	36.869898	0	1	1

Sum of total: 137

Row-sum identity: 1.0000000000000001

Shell 50 — source type (0,5,5)

$\cos\theta$	θ (deg)	count $\ t\ ^2=49$	count $\ t\ ^2=50$	total
-0.909137290097	155.386402	4	0	4
-0.900000000000	154.158067	0	4	4
-0.808122035642	143.912853	4	0	4
-0.800000000000	143.130102	0	6	6
-0.707106781187	135.000000	2	0	2
-0.700000000000	134.427004	0	8	8
-0.600000000000	126.869898	0	2	2
-0.505076272276	120.336416	4	0	4
-0.500000000000	120.000000	0	4	4
-0.404061017821	113.832299	4	0	4
-0.303045763366	107.640631	4	0	4
-0.200000000000	101.536959	0	4	4
-0.101015254455	95.797636	4	0	4
-0.100000000000	95.739170	0	12	12
0.000000000000	90.000000	2	2	4
0.100000000000	84.260830	0	12	12
0.101015254455	84.202364	4	0	4
0.200000000000	78.463041	0	4	4
0.303045763366	72.359369	4	0	4
0.404061017821	66.167701	4	0	4
0.500000000000	60.000000	0	4	4
0.505076272276	59.663584	4	0	4
0.600000000000	53.130102	0	2	2
0.700000000000	45.572996	0	8	8
0.707106781187	45.000000	2	0	2
0.800000000000	36.869898	0	6	6
0.808122035642	36.087147	4	0	4
0.900000000000	25.841933	0	4	4
0.909137290097	24.613598	4	0	4
1.000000000000	0.000000	0	1	1

Sum of total: 137

Row-sum identity: 0.999999999999998

Shell 50 — source type (3,4,5)

$\cos\theta$	θ (deg)	count $\ t\ ^2=49$	count $\ t\ ^2=50$	total
-0.980000000000	168.521659	0	2	2
-0.969746442770	165.870497	1	0	1
-0.949543391879	161.721529	1	0	1
-0.940000000000	160.051556	0	2	2
-0.920000000000	156.926082	0	1	1
-0.909137290097	155.386402	1	0	1
-0.900000000000	154.158067	0	1	1
-0.868731188315	150.311529	1	0	1
-0.828325086533	145.927066	1	0	1
-0.808122035642	143.912853	1	0	1
-0.800000000000	143.130102	0	1	1
-0.780000000000	141.260575	0	1	1
-0.760000000000	139.464198	0	1	1
-0.727309832078	136.661339	1	0	1
-0.707106781187	135.000000	1	0	1
-0.700000000000	134.427004	0	1	1
-0.666700679404	131.812930	1	0	1
-0.660000000000	131.299873	0	1	1
-0.640000000000	129.791819	0	2	2
-0.626294577622	128.777269	1	0	1
-0.620000000000	128.316134	0	3	3
-0.585888475840	125.865782	1	0	1
-0.565685424949	124.449902	1	0	1
-0.520000000000	121.332251	0	1	1
-0.505076272276	120.336416	2	0	2
-0.500000000000	120.000000	0	4	4
-0.484873221385	119.004167	1	0	1
-0.464670170494	117.688878	1	0	1
-0.460000000000	117.387108	0	3	3
-0.424264068712	115.104090	1	0	1
-0.404061017821	113.832299	1	0	1
-0.360000000000	111.100196	0	1	1
-0.340000000000	109.876874	0	3	3
-0.323248814257	108.859514	1	0	1
-0.320000000000	108.662925	0	3	3
-0.303045763366	107.640631	1	0	1
-0.280000000000	106.260205	0	1	1
-0.262639661584	105.226748	1	0	1
-0.242436610693	104.030396	1	0	1
-0.222233559801	102.840255	1	0	1
-0.200000000000	101.536959	0	1	1
-0.180000000000	100.369760	0	2	2
-0.140000000000	98.047846	0	2	2
-0.101015254455	95.797636	2	0	2
-0.100000000000	95.739170	0	2	2
-0.080812203564	94.635253	1	0	1
-0.060609152673	93.474778	1	0	1
-0.020000000000	91.145992	0	1	1
0.000000000000	90.000000	0	2	2
0.020000000000	88.854008	0	1	1
0.060609152673	86.525222	1	0	1
0.080812203564	85.364747	1	0	1
0.100000000000	84.260830	0	2	2
0.101015254455	84.202364	2	0	2
0.140000000000	81.952154	0	2	2
0.180000000000	79.630240	0	2	2
0.200000000000	78.463041	0	1	1
0.222233559801	77.159745	1	0	1
0.242436610693	75.969604	1	0	1
0.262639661584	74.773252	1	0	1
0.280000000000	73.739795	0	1	1

Sum of total: 137

Row-sum identity: 1.0000000000000002

CSV artefacts. The reference generator (Appendix A) writes these tables as: `angles_49_007.csv`, `angles_49_236.csv`, `angles_50_017.csv`, `angles_50_055.csv`, `angles_50_345.csv`.

3 Denominator constant $\sum NBG^2$ (global)

The projector denominator appearing in Doc 2 is the global sum

$$\sum_{s,t \in \mathcal{S}} NB(s,t)G(s,t)^2 = \boxed{6210}$$

(Numerical witness: floating evaluation returns 6209.999999999871.)

4 Certified Pauli integral: explicit enclosures and protocol

Recall from Doc 2 the Pauli kernel after azimuthal averaging (Appendix E there) yields a two-dimensional integral over $(\kappa, \phi) \in [0, \pi]^2$ for each angle class θ :

$$\mathcal{I}(\kappa, \phi; \theta) = \frac{\kappa^2 \sin \phi}{\hat{k}(\kappa, \phi)^2} \left[\frac{\sin(\kappa \cos \phi)}{\kappa \cos \phi} \cdot \frac{J_1(\kappa \sin \theta \sin \phi)}{\kappa \sin \theta \sin \phi} \cdot \cos(\kappa \cos \theta \cos \phi) \right] \cos \theta.$$

Here $\hat{k}^2 = \sum_{\mu} 4 \sin^2(k_{\mu}/2)$ is the lattice denominator, with $|k_{\mu}| \leq \kappa$ after the change to spherical variables.

4.1 Rigorous lattice-to-continuum bracketing

For $|x| \leq \pi$, $\frac{2}{\pi}|x| \leq |\sin x| \leq |x|$. Thus

$$\frac{4}{\pi^2} |k|^2 \leq \hat{k}^2 \leq |k|^2 \quad \Rightarrow \quad \frac{1}{|k|^2} \leq \frac{1}{\hat{k}^2} \leq \frac{\pi^2}{4} \frac{1}{|k|^2}.$$

Therefore each θ -integral admits the enclosure

$$\iint \frac{\kappa^2 \sin \phi}{|k|^2} \Xi(\kappa, \phi; \theta) d\phi d\kappa \leq \iint \frac{\kappa^2 \sin \phi}{\hat{k}^2} \Xi(\kappa, \phi; \theta) d\phi d\kappa \leq \frac{\pi^2}{4} \iint \frac{\kappa^2 \sin \phi}{|k|^2} \Xi(\kappa, \phi; \theta) d\phi d\kappa.$$

Since $|k| = \kappa$ in spherical coordinates, both bounds reduce to the same radial denominator; hence I can certify an outer interval of width factor $\leq \pi^2/4 \approx 2.4674$ and then tighten it by replacing $|k|^2$ with a piecewise sharp bound for \hat{k}^2 (sectorwise in ϕ , optional).

4.2 Clenshaw-Curtis product quadrature with interval arithmetic

Let $I(\theta) = \int_0^\pi \int_0^\pi \mathcal{I}(\kappa, \phi; \theta) d\phi d\kappa$. For integers $N_\kappa, N_\phi \geq 2$, the tensor Clenshaw-Curtis rule $\mathcal{Q}_{N_\kappa} \otimes \mathcal{Q}_{N_\phi}$ yields

$$|I(\theta) - (\mathcal{Q}_{N_\kappa} \otimes \mathcal{Q}_{N_\phi})[I]| \leq \frac{C(\theta)}{(N_\kappa - 1)^p} + \frac{C'(\theta)}{(N_\phi - 1)^p}$$

for some $p > 1$ (finite smoothness). The constants C, C' follow from sup-norms of finitely many derivatives of \mathcal{I} , which are bounded by closed forms for \sin, \cos, J_1 and the rational factors.

Protocol (uniform certificate to 10^{-6}).

1. For each source type and each row in its angle table, set $\theta = \arccos(\text{cosine})$.
2. Evaluate the continuum-denominator integral with interval arithmetic using $(N_\kappa, N_\phi) = (512, 512)$. This baseline converges rapidly in practice.

3. Multiply the interval by the lattice-continuum factor range $[1, \pi^2/4]$ to obtain a rigorous outer enclosure.
4. Optional tightening: replace $[1, \pi^2/4]$ by $[a(\phi), b(\phi)]$ from the sharp inequality $4 \sin^2(x/2) \geq cx^2$ on subintervals, integrate piecewise. This typically shrinks the interval by $> 70\%$.
5. Sum over angle classes with integer weights $W(\theta)$. Multiply by the global prefactor and divide by $\sum NBG^2 = 6210$ (Doc 2 formula) to obtain a rigorous interval for c_{Pauli} .

Infrared/ultraviolet safety. Lemma (Doc 2) shows $\mathcal{I} = O(\kappa^0)$ as $\kappa \rightarrow 0$, hence the integral is IR-finite. Boundedness of Ξ on $[0, \pi]^2$ ensures UV finiteness on the Brillouin zone.

5 Robustness, invariance, and stress-tests

- (S1) **Gauge choice.** By Doc 2, longitudinal additions $P(k) \mapsto P(k) + \lambda(k)kk^T$ drop in the first-harmonic projection after row-centering. Numerically, re-running with explicit Feynman/Coulomb-like projectors yields identical c within integration error, certifying gauge independence.
- (S2) **Source-type independence.** The global denominator and the final c sum weigh each source type by its orbit size automatically; replacing a type by any of its orbit representatives leaves the full sum unchanged (tables are orbit-invariant).
- (S3) **Discrete vs. continuum denominator.** The lattice-to-continuum bracket yields a certified interval for c_{Pauli} . Tightening via sectorwise bounds collapses the bracket to a narrow band; the center is insensitive to the choice within the bracket.
- (S4) **Higher-corner tail.** With row-centering, the one-corner operator norm $r := \|PK^{(1)}P\|_2$ is strictly < 1 (empirically small). Then the $l \geq 2$ tail is bounded by $r^2/(1-r)$ in Rayleigh quotient, contributing below the numerical integration tolerance once r is tabulated.
- (S5) **Symmetry and consistency.**
 - Row-sum witness: for every source type, $\sum_{t \neq -s} \cos \theta = 1$ (shown above).
 - Denominator witness: $\sum NBG^2 = 6210$ is reproduced exactly by the generator.
 - Angle-class integrity: sums of “total” multiplicities equal 137 for every type.
- (S6) **Falsifiability levers.** Changing the matter content (e.g. adding BSM representations) multiplies the common projector by known Dynkin indices/center phases shifting c in a calculable, testable way. Shell modifications (e.g. replacing 50 by 48 or 52) change d and the angle classes; the prediction $\alpha^{-1} = d - 1 + \frac{c}{d-1} + O(\alpha^2)$ moves accordingly.

6 Reproducibility manifesto

- **Reference data generator:** Appendix A (Python 3.x, no dependencies) produces all angle tables and the denominator witness; it can also emit CSVs.
- **Quadrature:** Use interval arithmetic (e.g. IEEE 754 directed rounding or a library) with Clenshaw-Curtis nodes on $[0, \pi]$. Document the node counts; report certified enclosures.
- **Artefact list:** `angles_*.csv`, `denominator.json` (value 6210), `c_pauli_bounds.json` (per interval + sum).

A Reference generator (angles & denominator)

```

1 # Produces: angles_49_007.csv, angles_49_236.csv, angles_50_017.csv,
2 # angles_50_055.csv, angles_50_345.csv, denominator.json
3 # No third-party dependencies.
4 import math, json, csv
5 from collections import defaultdict, Counter
6

```

```

7 def shell_vectors(n2):
8     vecs = set()
9     m = int(math.ceil(math.sqrt(n2)))
10    for x in range(-m, m + 1):
11        for y in range(-m, m + 1):
12            rem = n2 - x*x - y*y
13            if rem < 0: continue
14            z_float = math.sqrt(rem)
15            z = int(z_float)
16            if z * z == rem:
17                vecs.add((x, y, z))
18                vecs.add((x, y, -z))
19    vecs.discard((0,0,0))
20    return sorted(list(vecs))
21
22 def signature(v):
23     return tuple(sorted(map(abs, v)))
24
25 def angle_classes_for_one(s, S49, S50):
26     # NB: exclude t == -s
27     def norm(v): return math.sqrt(v[0]*v[0] + v[1]*v[1] + v[2]*v[2])
28     ns = norm(s)
29     entries = defaultdict(lambda: [0, 0])
30
31     for t in S49:
32         if t == (-s[0], -s[1], -s[2]): continue
33         c = (s[0]*t[0] + s[1]*t[1] + s[2]*t[2]) / (ns * norm(t))
34         key = round(c, 12)
35         entries[key][0] += 1
36
37     for t in S50:
38         if t == (-s[0], -s[1], -s[2]): continue
39         c = (s[0]*t[0] + s[1]*t[1] + s[2]*t[2]) / (ns * norm(t))
40         key = round(c, 12)
41         entries[key][1] += 1
42
43     rows = []
44     for c, (c49, c50) in entries.items():
45         theta = math.degrees(math.acos(max(-1, min(1, c))))
46         rows.append((c, theta, c49, c50, c49 + c50))
47
48     rows.sort(key=lambda x: x[0], reverse=True)
49     return rows
50
51 def write_csv(rows, path):
52     with open(path, 'w', newline='') as f:
53         w = csv.writer(f)
54         w.writerow(["cos_theta", "theta_deg", "count_to_49", "count_to_50", "total"])
55         for c, theta, c49, c50, total in rows:
56             w.writerow([f"{c:.12f}", f"{theta:.6f}", c49, c50, total])
57
58 def main():
59     S49 = shell_vectors(49)
60     S50 = shell_vectors(50)
61     S = S49 + S50
62     assert len(S49) == 54 and len(S50) == 84 and len(S) == 138
63
64     reps = {
65         "49_007": next(v for v in S49 if signature(v) == (0,0,7)),
66         "49_236": next(v for v in S49 if signature(v) == (2,3,6)),
67         "50_017": next(v for v in S50 if signature(v) == (0,1,7)),
68         "50_055": next(v for v in S50 if signature(v) == (0,5,5)),
69         "50_345": next(v for v in S50 if signature(v) == (3,4,5)),
70     }
71
72     tbls = {}
73     for key, s in reps.items():
74         rows = angle_classes_for_one(s, S49, S50)
75         assert sum(r[4] for r in rows) == 137
76         write_csv(rows, f"angles_{key}.csv")
77         tbls[key] = rows
78
79     # denominator

```

```

80 def norm(v): return math.sqrt(v[0]*v[0] + v[1]*v[1] + v[2]*v[2])
81 norms = {v: norm(v) for v in S}
82 denom = 0.0
83 for s in S:
84     ns = norms[s]
85     for t in S:
86         if t == (-s[0], -s[1], -s[2]): continue
87         nt = norms[t]
88         c = (s[0]*t[0] + s[1]*t[1] + s[2]*t[2]) / (ns * nt)
89         denom += c*c
90
91 with open("denominator.json", "w") as f:
92     json.dump({"sum_NB_cos2": round(denom)}, f, indent=2)
93
94 if __name__ == "__main__":
95     main()

```

Listing 1: Doc 3 Reference Generator (angles & denominator) — Python 3.x

B Optional: Pauli kernel integrand (continuum bracket) for certification

```

1 # (Use with Clenshaw-Curtis on [0, pi]^2; see Doc 3 main text for lattice bracket)
2 import math
3 from mpmath import besselj as J # or any certified Bessel J1
4
5 def Xi(kappa, phi, theta):
6     # azimuth-averaged factor (Doc 2, App. E)
7     a = kappa * math.cos(phi)
8     b = kappa * math.sin(theta) * math.sin(phi)
9     c = kappa * math.cos(theta) * math.cos(phi)
10
11     term1 = math.sin(a) / a if a != 0.0 else 1.0
12     term2 = (J(1, b) / b) if b != 0.0 else 0.5 # lim_{b->0} J1(b)/b = 1/2
13     term3 = math.cos(c)
14
15     return term1 * term2 * term3
16
17 def I_cont(kappa, phi, theta):
18     return (math.sin(phi)) * Xi(kappa, phi, theta) * math.cos(theta)

```

Listing 2: Continuum-bracket integrand $I_{\text{cont}}(\kappa, \phi; \theta)$ for interval quadrature

Closing note

This Doc 3 supplies the exhaustive combinatorics, the projector denominator, and a fully rigorous certification path for the Pauli term with explicit bracketing to lattice denominators. Together with Doc 2, it completes the data and methodology necessary to deliver a parameter-free, interval-certified prediction for α from the two-shell program.