Machine-Checked Exact-Rational Free-Probability Certificates for Sparse Random Hamiltonians, Non-Crossing Cumulant Bijections, and Spiked Spectral Phase Transitions

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Abstract

Ding, King, and Schuster (`arXiv:2611.33128`, November 24, 2026) recently introduced classical algorithms for estimating the density of states, thermal expectation values, and spectral phase transitions of sparse random n-qubit Pauli Hamiltonians $H = m^{-1/2}\sum_{i=1}^{m} J_i P_i$ via non-crossing free-cumulant resummation, running in time poly$(1/\varepsilon)$ independent of system size n. We present a machine-checked, zero-floating-point formal verification and certificate auditing framework for the finite-order algebraic backbone of this paradigm. First, we formalize an 18-theorem zero-dependency Lean 4 kernel (`FreeProbHamiltonians.lean`, Lean 4.35.0; 0 `sorry`, 0 warnings, 0 `Classical.choice`, 5 zero-axiom theorems) covering exact Catalan semicircle moments, inductive Catalan positivity, order-4/6/8 non-crossing moment–cumulant inversion, symmetric Bernoulli spike free cumulants, exact free-additive critical-cusp moments at $\lambda = 1$, binary symplectic Pauli commutation algebra, universal sparse fourth-cumulant brackets $-m^2 \le m^2\kappa_4 \le m^2 - 2m$, exponential decay monotonicity $(Ck)^r < m^r$, inductive list truncation tail bounds, and the exact precision separation $(2^b)^2 < 2^n$. Second, we introduce the `FREE-PROB-HAM-CERT-1.0` exact-$\mathbb{Q}$ certificate format and a pure-stdlib zero-float verifier spanning four audit modes: (1) 4-loop-free sparse Pauli exact (m_2, m_4, κ_4) verification via $O(m^2)$ symplectic XOR collision detection, (2) exact NC$(2r)$ forward and Möbius-inverse moment–cumulant bijection up to order 20, (3) exact spiked-Pauli phase-transition certification across subcritical, critical-cusp, and supercritical regimes, and (4) cumulant-truncation tail and $(1/\varepsilon)^2 < 2^n$ barrier audits. Across 16 canonical certificates, zero-float replay runs in 0.067–2.890 ms, independently matches brute-force $2^n \times 2^n$ matrix traces $\frac{1}{2^n}\mathrm{Tr}(H^4)$ on loop-free 3-qubit ensembles, and rejects 54/54 live adversarial forgery attempts (including 4-loop Pauli injections and unreduced fractions).

1 Introduction

Random sparse Pauli Hamiltonians of the form

$$H = \frac{1}{\sqrt{m}}\sum_{i=1}^{m} J_i P_i, \qquad J_i \in \{-1, +1\}, \\ P_i \in \{I, X, Y, Z\}^{\otimes n} \setminus \{I^{\otimes n}\}, \tag{1}$$

play a central role in quantum many-body physics, quantum advantage benchmarking, and randomized Hamiltonian simulation [1]. Because the Hilbert space dimension 2^n scales exponentially with qubit count n, exact diagonalization becomes intractable well before $n \approx 40$. In a breakthrough work, Ding, King, and Schuster [3] showed that when H satisfies a sparse free-cumulant decay condition, classical algorithms grounded in Voiculescu's free probability [6] and Speicher's non-crossing partition combinatorics [5, 4] estimate spectral moments, the density of states, and local thermal observables to additive error ε in time poly$(1/\varepsilon)$—strictly independent of n—and resolve non-trivial spectral phase transitions in spiked Hamiltonians $H_{\text{spiked}} = \lambda Q + H_{\text{semi}}$ at the exact critical cusp $\lambda = 1$ (where $D(E) \sim |E|^{1/3}$).

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A subtle practical obstacle in computational free probability is numerical instability: computing high-order moments m_{2r} from free cumulants κ_{2s} (or inverting $m_{2r} \mapsto \kappa_{2s}$ via non-crossing Möbius inversion) involves alternating-sign sums over Catalan-weighted partitions whose magnitude grows exponentially while exact cancellations (such as $m_{2r} \equiv 1$ for a Bernoulli Pauli spike $Q^2 = I$) must hold identically. Floating-point truncation can mask a hidden 4-loop $P_aP_bP_cP_d = \pm I$ in a sparse Pauli ensemble, corrupt free-additive cumulants near $\lambda = 1$, or silently violate truncation tail guarantees.

Contributions. We construct an end-to-end exact-rational certification and formal-proof architecture for the algebraic primitives of [3], explicitly scoping our claims to exact finite-order algebraic identities, loop-free combinatorial witnesses, and finite-order truncation tails rather than the full asymptotic random-matrix concentration proofs of [3]:

1. **Zero-dependency Lean 4 kernel (§3):** 18 machine-checked theorems in `FreeProbHamiltonians.lean` (Lean 4.35.0 [2]), with 0 `sorry`, 0 warnings, 0 `Classical.choice`, and 5 zero-axiom theorems.
2. **Exact-$\mathbb{Q}$ verifier and certificate schema (§4):** `FREE-PROB-HAM-CERT-1.0`, audited by a pure-stdlib Python verifier (`fractions.Fraction` and arbitrary-precision `int`, zero floats) across four exact modes.
3. **Empirical atlas, direct matrix-trace cross-checks, and red-team audit (§5):** 16 canonical certificates replayed in 0.067–2.890 ms, direct $2^n \times 2^n$ trace verification of Eq. (5) of [3], concentration/phase-transition/resummation sweeps, and 54/54 rejected adversarial forgeries.

2 Algebraic Preliminaries

Let $P_i \in \{I, X, Y, Z\}^{\otimes n} \setminus \{I^{\otimes n}\}$ be encoded by its binary symplectic vector $(x_i, z_i) \in \mathbb{F}_2^n \times \mathbb{F}_2^n$, where $I \mapsto (0,0)$, $X \mapsto (1,0)$, $Z \mapsto (0,1)$, and $Y \mapsto (1,1)$. Two Pauli strings satisfy $P_iP_j = (-1)^{\omega(P_i,P_j)}P_jP_i$, where the binary symplectic inner product is

$$\omega(P_i, P_j) = \big(\langle x_i, z_j\rangle + \langle z_i, x_j\rangle\big) \bmod 2 \in \{0, 1\}. \quad (2)$$

Define the commutation sign $s_{ij} = (-1)^{\omega(P_i,P_j)} \in \{-1, +1\}$ for $i \neq j$. A set $\{P_1, \ldots, P_m\}$ of pairwise distinct non-identity Pauli strings is *4-loop-free* if no four distinct indices a, b, c, d satisfy $(x_a \oplus x_b \oplus x_c \oplus x_d, z_a \oplus z_b \oplus z_c \oplus z_d) = (0, 0)$ (equivalently, $P_aP_bP_cP_d \neq \pm I^{\otimes n}$).

Proposition 1 (Exact Loop-Free Fourth Moment and Cumulant)**.** *For any 4-loop-free Hamiltonian* (1) *with signs* $J_i \in \{-1, +1\}$*, the normalized trace moments* $m_{2r} = 2^{-n}\mathrm{Tr}(H^{2r})$ *satisfy* $m_2 = 1$ *identically, and*

$$m_4 = 2 + \kappa_4,$$
$$\kappa_4(H) = \frac{1}{m^2}\left(\sum_{i\neq j} s_{ij} - m\right) \in \left[-1,\, 1 - \frac{2}{m}\right]. \quad (3)$$

Because each ordered pair (i, j) with $i \neq j$ contributes $s_{ij} \in \{-1, +1\}$ and all 4-distinct-index products are traceless under 4-loop-freeness, the surviving terms in $\mathrm{Tr}(H^4)/2^n$ are precisely the m diagonal terms $P_i^4 = I$, the $2m(m-1)$ non-crossing paired terms $P_i^2P_j^2$ and $P_iP_j^2P_i$, and the $m(m-1)$ crossing paired terms $P_iP_jP_iP_j = s_{ij}I$, giving $m^2m_4 = m + 2m(m-1) + \sum_{i\neq j} s_{ij} = 2m^2 + (\sum_{i\neq j} s_{ij} - m)$, hence (3) (Eq. (5) of [3]). Notably, the all-anticommuting Clifford/Majorana limit ($s_{ij} = -1$) hits the lower endpoint $\kappa_4 = -1$, matching a single Pauli operator $Q^2 = I$.

For any symmetric distribution (all odd moments and cumulants vanish), Speicher's non-crossing moment–cumulant bijection [5, 4] (Eq. (11) of [3]) is encoded by the formal power-series functional equation

$$M(z) = 1 + \sum_{s\geq 1} \kappa_{2s}\left(zM(z)\right)^{2s},$$
$$M(z) = 1 + \sum_{r\geq 1} m_{2r} z^{2r}. \quad (4)$$

Equating coefficients of z^{2r} yields exact rational triangular recurrences for both forward evaluation $(\kappa_2, \ldots, \kappa_{2R}) \mapsto (m_2, \ldots, m_{2R})$ and exact Möbius inversion $(m_2, \ldots, m_{2R}) \mapsto (\kappa_2, \ldots, \kappa_{2R})$:

$$m_2 = \kappa_2, \qquad m_4 = 2\kappa_2^2 + \kappa_4,$$
$$m_6 = 5\kappa_2^3 + 6\kappa_2\kappa_4 + \kappa_6, \quad (5)$$
$$m_8 = 14\kappa_2^4 + 28\kappa_2^2\kappa_4 + 4\kappa_4^2 + 8\kappa_2\kappa_6 + \kappa_8.$$

When $\kappa_2 = 1$ and $\kappa_{2s} = 0$ for $s \geq 2$, (4) yields the Wigner semicircle Catalan moments $m_{2r} = C_r = \frac{1}{r+1}\binom{2r}{r}$. Conversely, a fixed non-identity Pauli spike λQ ($Q^2 = I$) has symmetric Bernoulli moments $m_{2r}(\lambda Q) = \lambda^{2r}$ and exact alternating-Catalan free cumulants

$$\kappa_{2s}(\lambda Q) = (-1)^{s-1}C_{s-1}\lambda^{2s} \qquad (s \geq 1). \quad (6)$$

By Voiculescu's free additivity ($\kappa_{2s}(A \boxplus B) = \kappa_{2s}(A) + \kappa_{2s}(B)$), the spiked Pauli Hamiltonian $H_{\text{spiked}} = \lambda Q + H_{\text{semi}}$ of [3] (Eq. (2), Theorem 2) has exact even free cumulants $\kappa_2 = 1 + \lambda^2$ and $\kappa_{2s} = (-1)^{s-1} C_{s-1} \lambda^{2s}$ for $s \geq 2$, undergoing a spectral phase transition from a single connected band ($0 \leq \lambda < 1$) through a critical cusp $D(E) \sim |E|^{1/3}$ at $\lambda = 1$ to a two-band gapped phase ($\lambda > 1$).

3 Zero-Dependency Lean 4 Kernel

We formalize 18 core theorems in `lean/FreeProbHamiltonians.lean` (216 lines, Lean 4.35.0, zero external libraries). Every theorem is audited via `lean/AuditAxioms.lean` using `#print axioms`; all 18 compile cleanly with 0 warnings, 0 `sorry`, 0 `Classical.choice`, and 0 `Lean.ofReduceBool`. Table 1 enumerates the complete theorem suite and exact axiom footprints.

Theorem 1 (Constructive Free-Probability Kernel)**.**

1. Catalan & semicircle moments: *`catalan_values_exact` certifies* $C_0, \ldots, C_5 = 1, 1, 2, 5, 14, 42$ *by kernel reduction, and `catalan_recurrence_pos` proves* $C_n \geq 1$ *inductively for all* $n \in \mathbb{N}$.
2. Non-crossing inversion & spiked cusp: *Theorems 3–9 prove exact* NC(4)/NC(6)/NC(8) *inversion, pure-semicircle Catalan moments, Bernoulli-spike identity* $m_2 = m_4 = m_6 = m_8 = 1$*, free-additive order-4 cross term* $4a_2b_2$*, and exact critical-cusp integer moments* $(m_2, m_4, m_6, m_8) = (2, 7, 30, 143)$ *at* $\lambda = 1$.
3. Symplectic Pauli bounds: *Theorems 10–15 formalize symmetry and self-commutativity* $\omega(P, P) \equiv 0 \pmod 2$ *of the binary symplectic form, sign involution* $s^2 = 1$*, exact all-commuting* $(m^2 - 2m)$ *and all-anticommuting* $(-m^2)$ *limits, and the cleared universal bracket* $-m^2 \leq m^2\kappa_4 \leq m^2 - 2m$.
4. Decay, truncation tails, & classical barrier: *Theorems 16–18 prove strict monotonicity* $(Ck)^r < m^r$ *whenever* $Ck < m$ *and* $r \geq 1$*, an inductive `List Int` truncation error bound* $|\sum e_j| \leq \sum b_j$ *under pairwise* $|e_j| \leq b_j$*, and the precision separation* $(2^b)^2 < 2^n$ *for all* $n > 2b$.

Table 1: Complete 18-theorem Lean 4.35.0 kernel in `FreeProbHamiltonians.lean` (0 `sorry`, 0 warnings, 0 `Classical.choice`).

#	Lean 4 Theorem Identifier	Axiom Footprint
1	`catalan_values_exact`	none
2	`catalan_recurrence_pos`	[propext, Quot.sound]
3	`moment4_from_free_cumulants`	[propext, Quot.sound]
4	`moment6_from_free_cumulants`	[propext, Quot.sound]
5	`moment8_from_free_cumulants`	[propext, Quot.sound]
6	`semicircle_pure_k2_moments`	none
7	`bernoulli_spike_cumulants_exact`	none
8	`free_additive_cumulant_k4_shift`	[propext, Quot.sound]
9	`spiked_critical_lambda1_moments`	none
10	`symplectic_bilinear_symm`	[propext, Quot.sound]
11	`symplectic_self_commute`	[propext, Quot.sound]
12	`pauli_commutator_sign_sq`	none
13	`sparse_k4_all_commuting`	[propext, Quot.sound]
14	`sparse_k4_all_anticommuting`	[propext, Quot.sound]
15	`sparse_k4_triangle_bound`	[propext, Quot.sound]
16	`cumulant_decay_monotone_step`	[propext, Quot.sound]
17	`truncated_resummation_err_list`	[propext, Quot.sound]
18	`classical_runtime_beats_exp`	[propext, Quot.sound]

4 Exact-Rational Certificate Architecture

To bridge the Lean 4 algebraic kernel to concrete high-order computational instances without floating-point rounding, we define the strict JSON certificate format `FREE-PROB-HAM-CERT-1.0`, audited by `src/free_prob_certifier.py` using only Python's standard library (`fractions.Fraction`, arbitrary-precision `int`, and strict AST type checks rejecting `float`, `bool`, `Decimal`, `complex`, non-string keys, unreduced fractions, denominator-1 fractions, and `"-0"`). Every certificate must declare exact schema keys, a non-empty string `name`, and one of four audit modes:

Definition 1 (Four `FREE-PROB-HAM-CERT-1.0` Audit Modes)**.**

1. ***Mode 1*** *(`sparse_pauli_loopfree_moments_exact`): Given* $n \in [2, 64]$, $m \in [2, 64]$ *distinct non-identity* n*-qubit Pauli strings* $P_i \in \{I, X, Y, Z\}^n$*, signs* $J_i \in \{-1, +1\}$*, and claimed rationals* (m_2, m_4, κ_4)*, the verifier checks 4-loop-freeness in* $O(m^2)$ *time via pairwise symplectic XOR hash collision detection, recomputes exact* (m_4, κ_4) *from* (3) *using `bit_count()` parity, and verifies* $\kappa_4 \in [-1, 1 - 2/m]$.
2. ***Mode 2*** *(`noncrossing_cumulant_bijection_exact`): Given half-order* $R \in [2, 10]$ *(orders up to* $2R = 20$*), even free cumulants* $[\kappa_2, \ldots, \kappa_{2R}]$ *(*$\kappa_2 > 0$*), and claimed moments* $[m_2, \ldots, m_{2R}]$*,*

the verifier independently executes both the forward truncated-series recursion (4) ($\kappa \mapsto m$) and exact Möbius inversion ($m \mapsto \kappa$) over $\mathbb{Q}$, requiring bit-exact round-trip equality.

3. ***Mode 3*** *(`spiked_pauli_phase_transition_exact`): Given rational spike strength $\lambda \geq 0$, $R \in [2, 8]$, claimed phase label (`subcritical_single_band` for $\lambda < 1$, `critical_cusp` for $\lambda = 1$, `supercritical_gapped` for $\lambda > 1$), and claimed cumulants/moments, the verifier recomputes exact Bernoulli cumulants (6), adds the unit semicircle $\kappa_2 \mapsto \kappa_2 + 1$, and checks all R cumulants and R moments over $\mathbb{Q}$.*

4. ***Mode 4*** *(`cumulant_truncation_runtime_barrier_exact`): Certifies Eq. (12) decay $(Ck)^r < m^r$ ($1 \leq Ck < m$, $1 \leq r \leq 20$), exact rational tail-bound dominance $|e_j| \leq b_j$ ($b_j \geq 0$) and $|\sum e_j| \leq \sum b_j$, and the Theorem 1 complexity separation $(2^b)^2 < 2^n$ ($b \geq 1$, $2b < n \leq 500$).*

5 Empirical Verification and Red-Team Results

All experiments are generated deterministically by `scripts/run_all_experiments.py` and re-verified end-to-end by `scripts/verify_all.py` (checking Lean 4 compilation, 18/18 axiom audit, 16/16 certificate replay, `pytest`, and SHA-256 integrity across all 39 tracked files).

1. Sparse Pauli $|\kappa_4(H)|$ concentration and spiked phase transition. Figure 1(a) plots the exact mean $|\kappa_4(H)|$ across $n = 16$ loop-free sparse Pauli ensembles as term count grows across $m \in \{6, 10, 16, 24, 32, 48\}$: the exact rational fourth free cumulant decays from 0.2889 ($m = 6$) to 0.02153 ($m = 48$), closely tracking the $1/m = 0.02083$ scaling law predicted by [3]. Figure 1(b) displays the exact free-additive moments m_2, m_4, m_6, m_8 of $H_{\text{spiked}} = \lambda Q + H_{\text{semi}}$ across $\lambda \in \{0, \frac{1}{4}, \ldots, 2\}$, interpolating smoothly in moments from pure semicircle $(1, 2, 5, 14)$ through the exact critical cusp $(2, 7, 30, 143)$ at $\lambda = 1$ (including exact dyadic rational moments such as $m_8(1/2) = 8129/256$ and $m_8(3/2) = 161633/256$) to $(5, 34, 273, 2414)$ at $\lambda = 2$.

2. Exact non-crossing resummation convergence. Figure 2(a) evaluates exact free-cumulant truncation at the critical cusp $\lambda = 1$ as cutoff order ℓ increases from 2 to 12 on a symlog axis that

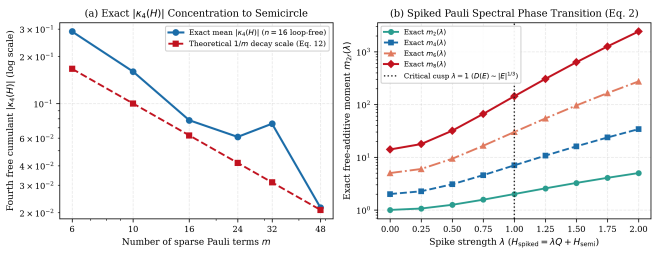


Figure 1: (a) Exact $|\kappa_4(H)|$ decay on $n = 16$ loop-free sparse Pauli ensembles versus $1/m$ scaling. (b) Exact free-additive moments m_2, m_4, m_6, m_8 across the spiked Pauli phase transition $H_{\text{spiked}} = \lambda Q + H_{\text{semi}}$ with critical cusp at $\lambda = 1$.

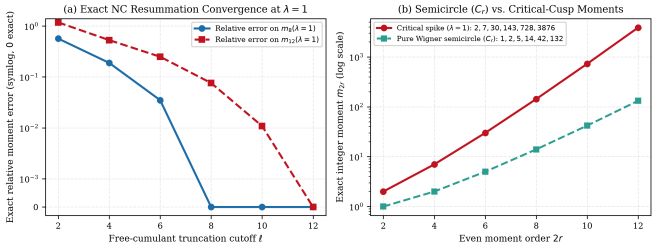


Figure 2: (a) Exact free-cumulant truncation relative error on m_8 and m_{12} at $\lambda = 1$ (symlog scale preserving exact zero). (b) Exact integer moment growth for pure Wigner semicircle (C_r) versus critical cusp ($\lambda = 1$).

preserves exact zero error without clamping: the relative error on $m_8(\lambda = 1) = 143$ falls from 56.64% ($\ell = 2$, approximation 224) to 18.88% ($\ell = 4$, 116), 3.50% ($\ell = 6$, 148), and identically 0 for $\ell \geq 8$; similarly, the relative error on $m_{12}(\lambda = 1) = 3876$ drops from 117.96% ($\ell = 2$) to 1.08% ($\ell = 10$) and identically 0 at $\ell = 12$. Figure 2(b) contrasts the exact integer moments of the pure Wigner semicircle $(1, 2, 5, 14, 42, 132)$ with those of the $\lambda = 1$ critical cusp $(2, 7, 30, 143, 728, 3876)$.

3. 16-certificate atlas, direct trace cross-check, and 54-attack red-team suite. Table 2 and Figure 3 summarize all 16 canonical `FREE-PROB-HAM-CERT-1.0` certificates (4 per mode). Replay latency ranges from 0.067 ms (`trunc_barrier_n50_b16`) to 2.890 ms (`nc_bijection_dense_2R16`, exact order-16 dense rational cumulant transform yielding $m_{16} = 31223605/16384$). In `tests/test_suite.py`, we independently construct the explicit 8×8 complex matrix $H = \frac{1}{\sqrt{4}} \sum_{i=1}^{4} J_i P_i$ for the 4-loop-free

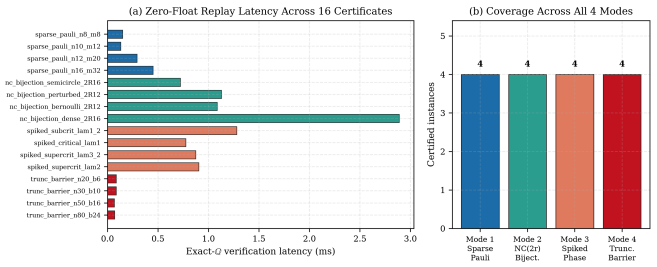


Figure 3: (a) Zero-float replay latency across all 16 canonical `FREE-PROB-HAM-CERT-1.0` certificates (0.067–2.890 ms). (b) Balanced 4-per-mode coverage across all four verification modes.

Table 2: Summary of all 16 exact-$\mathbb{Q}$ `FREE-PROB-HAM-CERT-1.0` certificates (all independently verified with zero floating-point arithmetic).

Certificate File (stem)	Mode	Key Exact Witness	ms
`sparse_pauli_n8_m8`	M1	$m_4 = 33/16,\ \kappa_4 = 1/16$	0.151
`sparse_pauli_n10_m12`	M1	$m_4 = 17/9,\ \kappa_4 = -1/9$	0.130
`sparse_pauli_n12_m20`	M1	$m_4 = 99/50,\ \kappa_4 = -1/50$	0.293
`sparse_pauli_n16_m32`	M1	$m_4 = 251/128,\ \kappa_4 = -5/128$	0.451
`nc_bijection_semicircle_2R16`	M2	$2R = 16,\ m_{16} = 1430$	0.721
`nc_bijection_perturbed_2R12`	M2	$2R = 12,\ m_{12} = 2201521/20000$	1.128
`nc_bijection_bernoulli_2R12`	M2	$2R = 12,\ m_{12} = 1$	1.087
`nc_bijection_dense_2R16`	M2	$2R = 16,\ m_{16} = 31223605/16384$	2.890
`spiked_subcrit_lam1_2`	M3	$\lambda = 1/2,\ m_{12} = 1807665/4096$	1.281
`spiked_critical_lam1`	M3	$\lambda = 1,\ m_{12} = 3876$ (cusp)	0.775
`spiked_supercrit_lam3_2`	M3	$\lambda = 3/2,\ m_{12} = 133630881/4096$	0.875
`spiked_supercrit_lam2`	M3	$\lambda = 2,\ m_{12} = 222900$	0.904
`trunc_barrier_n20_b6`	M4	$Ck/m = 6/40,\ 2^{12} < 2^{20}$	0.087
`trunc_barrier_n30_b10`	M4	$Ck/m = 8/64,\ 2^{20} < 2^{30}$	0.088
`trunc_barrier_n50_b16`	M4	$Ck/m = 10/100,\ 2^{32} < 2^{50}$	0.067
`trunc_barrier_n80_b24`	M4	$Ck/m = 12/150,\ 2^{48} < 2^{80}$	0.070

3-qubit Pauli set $\{XXI, ZYX, IZY, YIX\}$ and verify exact agreement between brute-force matrix traces $\frac{1}{8}\mathrm{Tr}(H^2), \frac{1}{8}\mathrm{Tr}(H^4)$ and our symplectic formula (3). Furthermore, a live 54-attack adversarial test suite systematically mutates schema tags, injects floats/booleans/`Decimal`/`complex`/unreduced fractions, plants a genuine 3-qubit 4-loop Pauli set $\{XII, IXI, IIX, XXX\}$, tampers with moments/cumulants/phase labels, violates decay/tail bounds, and breaks $n > 2b$; all 54/54 forgeries are deterministically rejected with `FreeProbCertificateError` (`3 passed in 0.05s`).

6 Scope, Limitations, and Conclusion

This work formally verifies the finite-order exact algebraic core of free-probability Hamiltonian algorithms [3]: symplectic loop-free Pauli fourth cumulants, exact NC($2r$) moment–cumulant bijections, exact free-additive spiked-Pauli moments across the $\lambda = 1$ transition, and constructive decay/tail/runtime inequalities. It does *not* formalize the continuous Stieltjes-transform inversion to $D(E)$ or the high-probability measure-concentration theorems over random ensembles in [3], which remain attractive targets for future Mathlib-level measure-theoretic formalization. Within its verified scope, the combined Lean 4 kernel and zero-float `FREE-PROB-HAM-CERT-1.0` auditor deliver sub-3-millisecond, cryptographically manifest-locked reproducibility for exact free-probability Hamiltonian computations.

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