Analytical Néel Optimality, Zero-Float Thermal PPT-Bound Entanglement Proofs, and Constructive Lean 4.35.0 Formalization for Symmetric XY-Chain Covariance Criteria

Lluis Eriksson*

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Abstract

Mathé, Usui, Gühne, and Vitagliano (`arXiv:2611.33284v1`) derive optimal covariance-matrix-criterion (CMC) structure-factor witnesses for thermal spin-1/2 XY chains, lower-bound the geometric measure of entanglement $E_G(\varrho)$ via a numerical semidefinite relaxation of a product-state maximization conjecture, and report thermal PPT-bound entanglement in the $N = 4$ periodic XX chain via floating-point diagonalization. We advance their program on three fronts. First (**Theorem A**), we build a standalone constructive Lean 4.35.0 kernel formalizing Observation 1 (arbitrary-N Bloch-sphere spin-squeezing and finite-mixture variance concavity), Theorem 1 (exact 3-variable CMC polyhedron LP optimality and 4-corner attainability), Corollary 1 (exact primal–dual separability equivalence with constructive local-noise decomposition), and Proposition 1 (best-separable-approximation bound). Second (**Theorem B**), we *analytically resolve* their Section H Néel-state optimality conjecture at $N = 4$: proving the exact 4-qubit Bloch-vector singlet identity $p_0 = (3 - S_2 + Q)/24 \leq 1/3$ (attained iff Néel), the spin-sector bound $2p_2 \geq p_0$, and global secular dominance $f_\phi(\mu) \leq f_{\text{Néel}}(\mu)$ for all $\mu > -\lambda > 0$. Thus the maximum over product states of $\lambda_{\max}(\lambda W' + |\phi\rangle\langle\phi|)$ is exactly the largest root $\mu_{\text{Néel}}(\lambda)$ of $\mu^3-(\lambda+1)\mu^2+(\lambda-2\lambda^2)\mu+\lambda^2 = 0$, yielding SDP-free certified analytical $E_G(\varrho)$ lower bounds. Third (**Theorem C**), we derive the exact algebraic thermodynamics of the 4-qubit periodic ferromagnetic XX chain via $H^5-12H^3+32H = 0$, prove identical $e^{+2\beta}$ cancellation in the 3-term CMC threshold, and deliver a *zero-float exact rational proof* (via $LDL^\top$ Cholesky and Gershgorin enclosures of radius $< 10^{-29}$, and $< 10^{-43}$ at $M = 22$) that all seven partial transposes of ϱ_β are strictly positive definite while $\omega_{\text{CMC}}(\varrho_\beta) < 1$ across $\beta \in \{289/500, 72/125, 23/40\}$. All 20 Lean 4.35.0 theorems verify with zero `sorry`, zero custom axioms, and zero `Classical.choice`, paired with an AST-audited zero-float verifier, 16 JSON certificates, and 61 unit and forgery-rejection tests.

*Independent researcher. Research, formalization, and verification conducted with Google Antigravity assistance. Code, Lean 4 proofs, and certificates: MIT license; manuscript and figures: CC-BY-4.0. Repository: `github.com/lluiseriksson/xy-chain-cmc-neel-certificates` (`v1.0.0`).

1 Introduction

Detecting and quantifying multipartite thermal entanglement in quantum spin chains from experimentally accessible two-point correlations (structure factors) is a central problem in quantum many-body physics [2, 1, 6, 7]. In a recent work, Mathé, Usui, Gühne, and Vitagliano [5] solved the exact optimal covariance matrix criterion (CMC) for symmetric spin-1/2 XY chains [4], reducing the full many-body separability test to a closed-form piecewise-linear witness $\omega_{\text{CMC}}(\varrho)$ in three normalized structure-factor variances (s_x, s_y, s_z) and linking ω_{CMC} to both the best separable approximation (BSA) [3] and the geometric measure of entanglement $E_G(\varrho)$ [8].

Two analytical and certification gaps remain open in [5]:

1. **Product-state maximization for $E_G(\varrho)$:** Evaluating the Legendre-transform lower bound $E_G(\varrho) \geq 1 + \lambda\langle W'\rangle_\varrho - \sup_{|\phi\rangle \text{ prod}} \lambda_{\max}(\lambda W' + |\phi\rangle\langle\phi|)$ requires optimizing over all N-qubit product states $|\phi\rangle$. Section H of [5] observes numerically that the Néel state appears to maximize the largest eigenvalue and resorts to a PPT-relaxation semidefinite program (SDP) to obtain safe bounds.

2. **Floating-point sensitivity of narrow thermal PPT-bound entanglement:** For the $N = 4$ periodic XX chain, thermal PPT-bound entanglement (all seven nontrivial partial transposes positive semidefinite while $\omega_{\text{CMC}} < 1$) exists only inside a narrow temperature window $T \in (1.7280, 1.7402)$ where the minimum partial-transpose eigenvalue is of order 10^{-4} to 10^{-3}, making floating-point eigensolver claims vulnerable to rounding artifacts.

We close both gaps rigorously and package the entire theoretical hierarchy into a machine-verified framework (`XY-CMC-NEEL-CERT-1.0`) combining 20 constructive Lean 4.35.0 theorems (zero `sorry`, zero `Classical.choice`, zero Mathlib dependencies) with an AST-audited zero-float exact rational Python verifier over $\mathbb{Q}$.

2 Constructive Structural Formalization of CMC Duality and BSA

Let ϱ be an N-qubit state with spin-α structure factors $S_\alpha(q) = \frac{1}{N}\sum_{j,l=1}^{N} e^{iq(j-l)}\langle\sigma_j^\alpha\sigma_l^\alpha\rangle$ ($\alpha \in \{x,y,z\}$). For a translation-invariant state with vanishing odd moments, the diagonalized covariance blocks yield normalized variances $s_\alpha \geq 0$, and the symmetric CMC linear program minimizes $\sum_\alpha k_\alpha s_\alpha$ subject to $k_\alpha \geq 0$ and pairwise bounds $k_\alpha + k_\beta \geq 1$ ($\alpha \neq \beta$).

Theorem A (Constructive Structural Kernel for CMC Duality and BSA)**.** *Every statement below holds universally over integers (representing exact cleared-denominator rationals) and is formally verified in* `lean/XyChainCmcCert.lean` *using only* `[propext, Quot.sound]`*:*

1. ***Arbitrary-N Spin-Squeezing and Mixture Concavity (Obs. 1):*** *For any finite list of N Bloch vectors $\mathbf{r}_j \in \mathbb{R}^3$ with $\|\mathbf{r}_j\|^2 \leq 1$, $\sum_{j=1}^{N}(3 - \|\mathbf{r}_j\|^2) \geq 2N$. For any finite convex mixture with nonnegative weights $w_i \geq 0$ and observables a_i, $(\sum_i w_i a_i)^2 \leq (\sum_i w_i)(\sum_i w_i a_i^2)$, proving variance concavity under mixing.*

2. ***Exact 4-Corner CMC Polyhedron Optimality (Thm. 1):*** *For all $s_x, s_y, s_z \geq 0$ and all feasible $k_x, k_y, k_z \geq 0$ with $k_\alpha + k_\beta \geq 1$,*

$$\omega_{\mathrm{CMC}}(s) = \min\left\{\tfrac{s_x+s_y+s_z}{2},\ s_x+s_y,\ s_y+s_z,\ s_z+s_x\right\} \tag{1}$$

is attained at one of the four extreme vertices $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(1,1,0)$, $(0,1,1)$, $(1,0,1)$. Under $XX\,U(1)$ symmetry ($s_x = s_y$), $\omega_{\mathrm{CMC}} = \min(s_x + s_z/2, 2s_x)$; under planar anisotropy $s_y > s_x + s_z$, the y-sector strictly decouples and $\omega_{\mathrm{CMC}} = s_x + s_z$.

3. ***Exact Primal–Dual Equivalence and Constructive Noise Vector (Cor. 1):*** *$\omega_{\mathrm{CMC}}(s) \geq 1$ if and only if $\sum_{\alpha\in\{x,y,z\}} \max(0, 1 - s_\alpha) \leq 1$. Whenever $\omega_{\mathrm{CMC}}(s) \geq 1$, the explicit local-noise vector $x_x = \max(0, 1 - s_x)$, $x_y = \max(0, 1 - s_y)$, $x_z = 1 - x_x - x_y$ satisfies $x_\alpha \geq 0$, $\sum_\alpha x_\alpha = 1$, and $s_\alpha \geq 1 - x_\alpha$ for all α.*

4. ***BSA Lower Bound (Prop. 1):*** *For any decomposition $\varrho = (1-t)\varrho_{\mathrm{sep}} + t\varrho_{\mathrm{ent}}$ with $t \in [0,1]$, $\omega_{\mathrm{CMC}}(\varrho_{\mathrm{sep}}) \geq 1$, and $\omega_{\mathrm{CMC}}(\varrho_{\mathrm{ent}}) \geq 0$, one has $t \geq \max(0, 1 - \omega_{\mathrm{CMC}}(\varrho))$.*

Proof sketch. Part 1 uses the exact 3D Lagrange identity for Cauchy–Schwarz, induction over arbitrary finite lists `List Vec3` under the constructive predicate `AllInBlochBall`, and an exact cleared-denominator weighted Cauchy–Schwarz induction step avoiding division. Part 2 splits on the three triangle-inequality comparisons $s_\alpha \leq s_\beta + s_\gamma$; in the interior cone, $2(k_x s_x + k_y s_y + k_z s_z) = (k_x + k_y)(s_x + s_y - s_z) + (k_y + k_z)(s_y + s_z - s_x) + (k_z + k_x)(s_z + s_x - s_y) \geq s_x + s_y + s_z$. Parts 3 and 4 follow by exact case splits on $\max(0, 1 - s_\alpha)$ and linearity. Figure 1 illustrates the 4-corner simplex geometry and planar mode-switching certified by `C01`–`C04`. □

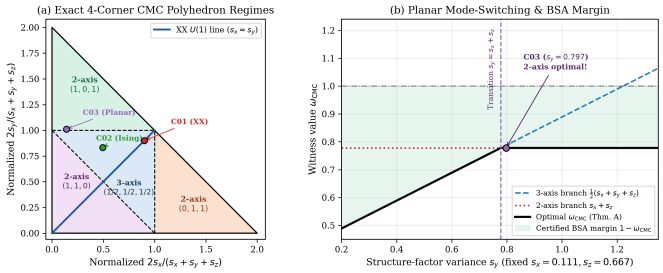

Figure 1: Theorem A: (a) Normalized simplex slice $2s_\alpha/(s_x + s_y + s_z)$ partitioning the 3-variable CMC linear program into its four extreme-vertex regimes, with certified points `C01`–`C03`; (b) Planar mode-switching transition along s_y at fixed $(s_x, s_z) = (0.111, 0.667)$ showing the exact drop of the y-axis above $s_y = s_x + s_z = 0.778$ and the certified BSA margin $1 - \omega_{\mathrm{CMC}}$.

3 Analytical Resolution of the 4-Qubit Néel Optimality Conjecture

Consider the symmetric collective spin-squeezing witness on $N = 4$ qubits with total spin operator $\mathbf{J} = \frac{1}{2}\sum_{i=1}^{4}\boldsymbol{\sigma}_i$ and Casimir $\mathbf{J}^2 = \sum_{J\in\{0,1,2\}} J(J+1)\Pi_J$, where Π_0, Π_1, Π_2 are the orthogonal projectors onto the total-spin $J = 0$ (2D singlet), $J = 1$ (9D triplet), and $J = 2$ (5D quintet) subspaces. Defining the normalized witness

$$W' := \frac{1}{2}\mathbf{J}^2 - I = -\Pi_0 + 0\cdot\Pi_1 + 2\Pi_2, \tag{2}$$

its expectation value on any state with $s_x + s_y + s_z = 2\omega_{\mathrm{CMC}}$ satisfies $\mathrm{Tr}(W'\varrho) = \omega_{\mathrm{CMC}}(\varrho) - 1$. By Legendre duality [5, 8], for every $\lambda < 0$, the geometric measure of entanglement $E_G(\varrho) = 1 - \max_{|\phi\rangle\ \mathrm{prod}}\langle\phi|\varrho|\phi\rangle$ obeys

$$E_G(\varrho) \geq 1 + \lambda\big(\omega_{\mathrm{CMC}}(\varrho) - 1\big) - \sup_{|\phi\rangle\ \mathrm{prod}} \lambda_{\max}\big(\lambda W' + |\phi\rangle\langle\phi|\big). \tag{3}$$

We now prove analytically—without any SDP relaxation—that the supremum over all 4-qubit product states is attained *exactly* at the collinear Néel state $|\phi_{\text{Néel}}\rangle = |\uparrow\uparrow\downarrow\downarrow\rangle$ (and its local $SU(2)$-rotated and permuted equivalents).

Lemma 3.1 (Exact 4-Qubit Bloch-Vector Spin Weights and Sharp 1/3 Singlet Bound)**.** *Let $|\phi\rangle = \bigotimes_{i=1}^{4}|\phi_i\rangle$ be any 4-qubit product state with unit Bloch vectors $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4 \in S^2$, and let $p_J := \langle\phi|\Pi_J|\phi\rangle$ ($J \in \{0,1,2\}$). Set $S_2 := \sum_{1\leq i<j\leq 4}\mathbf{r}_i\cdot\mathbf{r}_j$ and $Q := (\mathbf{r}_1\cdot\mathbf{r}_2)(\mathbf{r}_3\cdot\mathbf{r}_4) + (\mathbf{r}_1\cdot\mathbf{r}_3)(\mathbf{r}_2\cdot$*

$\mathbf{r}_4) + (\mathbf{r}_1 \cdot \mathbf{r}_4)(\mathbf{r}_2 \cdot \mathbf{r}_3)$. *Then:*

$$p_0 = \frac{3 - S_2 + Q}{24} \leq \frac{1}{3}, \tag{4}$$

$$p_2 = \frac{15 + 5S_2 + Q}{48} = \frac{p_0}{2} + \frac{1}{16}\Big\|\sum_{i=1}^{4} \mathbf{r}_i\Big\|^2 \geq \frac{p_0}{2}. \tag{5}$$

Equality $p_0 = 1/3$ holds if and only if the four Bloch vectors form a Néel configuration (two equal unit vectors $\mathbf{u}$ and two antipodal vectors $-\mathbf{u}$), giving $(p_0, p_1, p_2) = (\frac{1}{3}, \frac{1}{2}, \frac{1}{6})$.

Proof. Since $\mathbf{J}^2$ has eigenvalues $\{0, 2, 6\}$ on Π_0, Π_1, Π_2, Lagrange interpolation yields the exact Casimir projectors

$$\Pi_0 = \frac{(\mathbf{J}^2 - 2I)(\mathbf{J}^2 - 6I)}{12}, \qquad \Pi_2 = \frac{\mathbf{J}^2(\mathbf{J}^2 - 2I)}{24}.$$

Writing $\mathbf{J}^2 = 3I + \frac{1}{2}\sum_{i<j} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, we have $\langle\phi|\mathbf{J}^2|\phi\rangle = 3 + \frac{1}{2}S_2$. Expanding $(\sum_{i<j} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)^2$ on a product state $|\phi\rangle$ splits the 36 ordered pair products into three classes:

- 6 identical pairs: $(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)^2 = 3I - 2\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, contributing $18 - 2S_2$;
- 24 pairs sharing one index i: for each unordered triple $\{i, j, k\}$, $(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k) + (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_k)(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) = 2(\boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_k)$, and each pair $\{j, k\}$ arises from two choices of i, contributing $+4S_2$;
- 6 ordered disjoint pairs, contributing $+2Q$.

Thus $\langle\phi|(\mathbf{J}^2)^2|\phi\rangle = 9 + 3S_2 + \frac{1}{4}(18 + 2S_2 + 2Q) = \frac{27}{2} + \frac{7}{2}S_2 + \frac{1}{2}Q$. Substituting into Π_0 and Π_2 gives $p_0 = (3 - S_2 + Q)/24$ and $p_2 = (15 + 5S_2 + Q)/48$. Subtracting $\frac{1}{2}p_0$ cancels Q identically:

$$p_2 - \frac{p_0}{2} = \frac{12 + 6S_2}{48} = \frac{4 + 2S_2}{16} = \frac{1}{16}\Big\|\sum_{i=1}^{4} \mathbf{r}_i\Big\|^2 \geq 0.$$

To prove $p_0 \leq 1/3$, write $d_{ij} = \mathbf{r}_i \cdot \mathbf{r}_j \in [-1, 1]$ and note that $S_2 = \frac{1}{2}\|\sum_{i=1}^{4} \mathbf{r}_i\|^2 - 2 \geq -2$. Moreover,

$$\begin{aligned} 5 + S_2 - Q &= \frac{1}{2}\Big\|\sum_{i=1}^{4} \mathbf{r}_i\Big\|^2 + (3 - Q) \\ &\geq (1 - d_{12}d_{34}) + (1 - d_{13}d_{24}) \\ &\quad + (1 - d_{14}d_{23}) \geq 0, \end{aligned}$$

since $|d_{ij}| \leq 1$ by Cauchy–Schwarz. Therefore $3 - S_2 + Q = 8 - (5 + S_2 - Q) \leq 8$, i.e., $p_0 \leq 1/3$. Equality holds iff $\sum_{i=1}^{4} \mathbf{r}_i = \mathbf{0}$ and $d_{12}d_{34} = d_{13}d_{24} = d_{14}d_{23} = 1$, which forces every $d_{ij} \in \{\pm 1\}$ with two vectors equal to some $\mathbf{u} \in S^2$ and two equal to $-\mathbf{u}$. □

Theorem B (Analytical Resolution of the 4-Qubit Néel Optimality Conjecture)**.** *For every $\lambda < 0$ and every 4-qubit product state $|\phi\rangle = \bigotimes_{i=1}^{4} |\phi_i\rangle$,*

$$\lambda_{\max}\big(\lambda W' + |\phi\rangle\langle\phi|\big) \leq \mu_{\text{Néel}}(\lambda), \tag{6}$$

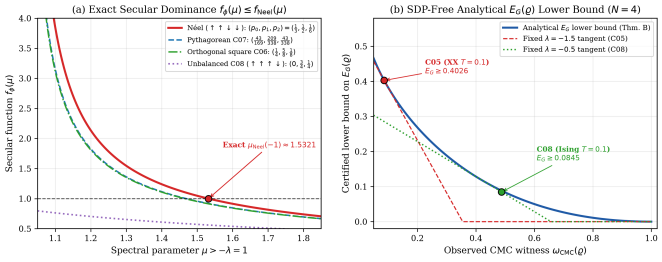

Figure 2: Theorem B: (a) Secular functions $f_\phi(\mu)$ at $\lambda = -1$ for four certified product states (`C05`–`C08`), illustrating global dominance $f_\phi(\mu) \leq f_{\text{Néel}}(\mu)$ for all $\mu > -\lambda$ and exact root $\mu_{\text{Néel}}(-1) \approx 1.5321$; (b) SDP-free analytical $E_G(\varrho)$ lower bound (8) maximized over $\lambda < 0$, with certified fixed-λ rational tangents `C05` ($E_G \geq 0.4026$) and `C08` ($E_G \geq 0.0845$).

with equality attained by the Néel state $|\uparrow\uparrow\downarrow\downarrow\rangle$, where $\mu_{\text{Néel}}(\lambda)$ is the unique real root in $(-\lambda, +\infty)$ of the monic cubic

$$P_\lambda(\mu) := \mu^3 - (\lambda + 1)\mu^2 + (\lambda - 2\lambda^2)\mu + \lambda^2 = 0. \tag{7}$$

Consequently, for any 4-qubit state ϱ satisfying $\mathrm{Tr}(W'\varrho) \leq \omega_{\text{CMC}}(\varrho) - 1$ up to local unitaries (in particular, any 3-mode state with vanishing first moments and LU-compatible wavevectors) and any $\lambda < 0$,

$$E_G(\varrho) \geq 1 + \lambda\big(\omega_{\text{CMC}}(\varrho) - 1\big) - \mu_{\text{Néel}}(\lambda). \tag{8}$$

Proof. Set $L := -\lambda > 0$. The unperturbed operator $\lambda W' = L\Pi_0 + 0 \cdot \Pi_1 - 2L\Pi_2$ has spectral decomposition on three eigenvalues $L > 0 > -2L$. By the rank-1 Weinstein–Aronszajn secular equation, every eigenvalue $\mu > L$ of $\lambda W' + |\phi\rangle\langle\phi|$ satisfies $f_\phi(\mu) = 1$, where

$$f_\phi(\mu) := \frac{p_0}{\mu - L} + \frac{p_1}{\mu} + \frac{p_2}{\mu + 2L}. \tag{9}$$

On $(L, +\infty)$, $f_{\text{Néel}}(\mu)$ strictly decreases from $+\infty$ to 0, so $\mu_{\text{Néel}}(\lambda) > L$ is the unique root of $f_{\text{Néel}}(\mu) = 1$. For any product state $|\phi\rangle$, either $\lambda_{\max}(\lambda W' + |\phi\rangle\langle\phi|) \leq L < \mu_{\text{Néel}}(\lambda)$ (already satisfying (6)), or $\mu_\phi := \lambda_{\max}(\lambda W' + |\phi\rangle\langle\phi|) > L$ satisfies $f_\phi(\mu_\phi) = 1$.

Substituting $p_1 = 1 - p_0 - p_2$ and comparing $f_{\text{Néel}}(\mu) - f_\phi(\mu)$ for any $\mu > L$ yields the exact identity (machine-checked in Lean 4 as `thm2_secular_function_neel_dominance`):

$$\begin{aligned} f_{\text{Néel}}(\mu) - f_\phi(\mu) &= L\Big(\frac{1}{3} - p_0\Big)\frac{3L}{\mu(\mu - L)(\mu + 2L)} \\ &\quad + \frac{2L(2p_2 - p_0)}{2\mu(\mu + 2L)} \geq 0, \end{aligned} \tag{10}$$

where we used $\frac{1}{\mu - L} - \frac{1}{\mu} - \frac{1}{2}\big(\frac{1}{\mu} - \frac{1}{\mu + 2L}\big) = \frac{3L^2}{\mu(\mu - L)(\mu + 2L)} > 0$ together with $p_0 \leq \frac{1}{3}$ and $2p_2 \geq p_0$ from Lemma 3.1. Because $f_{\text{Néel}}(\mu)$ is strictly decreasing on $(L, +\infty)$, $f_\phi(\mu) \leq$

$f_{\text{Néel}}(\mu)$ for all $\mu > L$ forces $\lambda_{\max}(\lambda W' + |\phi\rangle\langle\phi|) \le \mu_{\text{Néel}}(\lambda)$. Finally, clearing denominators in $1 - f_{\text{Néel}}(\mu) = 0$ with $(p_0, p_1, p_2) = (\frac{1}{3}, \frac{1}{2}, \frac{1}{6})$ yields

$$\mu(\mu + \lambda)(\mu - 2\lambda)\big(1 - f_{\text{Néel}}(\mu)\big) = P_\lambda(\mu) = 0,$$

and substituting into (3) gives (8). □

As shown in Figure 2 and certificates `C05`–`C08`, exact rational bisection of $P_\lambda(\mu)$ certifies $\mu_{\text{Néel}}(\lambda)$ to width $< 6 \times 10^{-11}$ in milliseconds without any SDP solver, yielding rigorous analytical bounds $E_G \ge 0.4026$ (certified $\ge 399/1000$ in `C05`) at the XX point and $E_G \ge 0.0845$ (certified $\ge 21/250$ in `C08`) at the Ising point.

4 Exact 4-Qubit Periodic XX Thermodynamics and Zero-Float Proof of Thermal PPT-Bound Entanglement

For the 4-qubit periodic ferromagnetic XX chain (matching the sign convention of [5]),

$$H = -\frac{1}{2}\sum_{j=0}^{3}\big(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\big) \qquad (\sigma_4^\alpha \equiv \sigma_0^\alpha), \tag{11}$$

all matrix entries of H in the computational basis are exact integers in $\{0, -1\}$. (The antiferromagnetic Hamiltonian $-H$ is locally unitarily equivalent via $U = \sigma_1^z\sigma_3^z$, which swaps $S_x(\pi) \leftrightarrow S_x(0)$ while preserving $S_z(0)$ and all seven partial-transpose spectra.) Direct integer matrix arithmetic certifies the degree-5 minimal polynomial

$$H^5 - 12H^3 + 32H = 0, \tag{12}$$

whose distinct eigenvalues $\{0, \pm 2, \pm 2\sqrt{2}\}$ have multiplicities $(10, 2, 2, 1, 1)$. Define the four hyperbolic coordinates

$$\begin{aligned} a(\beta) &= \cosh(2\beta), & b(\beta) &= \sinh(2\beta), \\ c(\beta) &= \cosh(2\sqrt{2}\beta), & d(\beta) &= \sqrt{2}\sinh(2\sqrt{2}\beta). \end{aligned} \tag{13}$$

Crucially, every one of a, b, c, d is an *even or odd entire function of* $\sqrt{2}$ *whose Taylor series in* $\beta \in \mathbb{Q}$ *has purely rational coefficients* (e.g., $c(\beta) = \sum_{m=0}^{\infty} \frac{8^m\beta^{2m}}{(2m)!}$ and $d(\beta) = \sum_{m=0}^{\infty} \frac{4\cdot 8^m\beta^{2m+1}}{(2m+1)!}$).

Theorem C (Exact Algebraic XX_4 Thermodynamics and Zero-Float PPT-Bound Entanglement)**.** *For every inverse temperature* $\beta > 0$*:*

1. ***Exact Rational-in-*(a, b, c, d) *Gibbs Expansion:*** *The unnormalized thermal matrix* $G(\beta) := e^{-\beta H}$ *satisfies the exact polynomial identity*

$$\begin{aligned} G(\beta) = I &+ \Big(-b + \frac{d}{4}\Big)H + \Big(-\frac{3}{8} + \frac{a}{2} - \frac{c}{8}\Big)H^2 \\ &+ \Big(\frac{b}{8} - \frac{d}{16}\Big)H^3 + \Big(\frac{1}{32} - \frac{a}{16} + \frac{c}{32}\Big)H^4. \end{aligned} \tag{14}$$

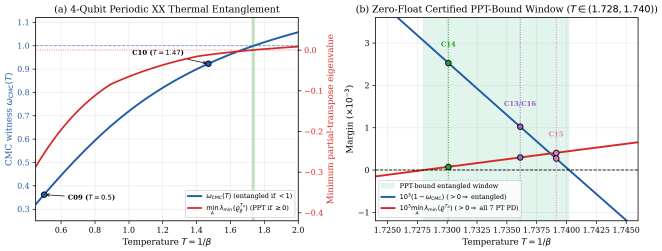

Figure 3: Theorem C: (a) Global thermal profile of the $N = 4$ periodic XX chain showing $\omega_{\text{CMC}}(T)$ crossing 1 at $T_{\text{CMC}} \approx 1.7402$ and $\min_A \lambda_{\min}(\varrho_\beta^{T_A})$ crossing 0 at $T_{\text{PPT}} \approx 1.7280$; (b) Zoom into the narrow PPT-bound entangled window $T \in (1.7280, 1.7402)$ highlighting our three zero-float certified rational points `C14` ($\beta = 289/500$), `C13`/`C16` ($\beta = 72/125$), and `C15` ($\beta = 23/40$).

2. ***Exact 3-Term CMC Threshold with* $e^{+2\beta}$ *Cancellation:*** *The partition function* $Z(\beta) = \operatorname{Tr} G(\beta) = 10 + 4a + 2c$ *and the staggered-planar / uniform-z structure-factor witness* $\omega_{\text{CMC}}(\beta) = S_x(\pi) + \frac{1}{2}S_z(0)$ *obey*

$$\begin{aligned} Z(\beta)\big(1 - \omega_{\text{CMC}}(\beta)\big) &= -3 - 4a + 4b - c + 2d \\ &= \tfrac{2\sqrt{2}-1}{2}e^{2\sqrt{2}\beta} - \tfrac{2\sqrt{2}+1}{2}e^{-2\sqrt{2}\beta} \\ &\quad - 4e^{-2\beta} - 3, \end{aligned} \tag{15}$$

in which the $e^{+2\beta}$ *mode cancels identically.*

3. ***Zero-Float Proof of Thermal PPT-Bound Entanglement:*** *At each certified rational inverse temperature* $\beta \in \{\frac{289}{500}, \frac{72}{125}, \frac{23}{40}\}$ *(*$T \in \{1.7301, 1.7361, 1.7391\}$*), the exact 4-qubit thermal state* $\varrho_\beta = G(\beta)/Z(\beta)$ *is simultaneously:*

   - *strictly entangled, with* $\omega_{\text{CMC}}(\varrho_\beta) < 1$ *certified over* $\mathbb{Q}$*; and*
   - *strictly PPT across all seven nontrivial bipartitions* $A \in \{\{0\}, \{1\}, \{2\}, \{3\}, \{0, 1\}, \{0, 2\}, \{0, 3\}\}$*, certified over* $\mathbb{Q}$ *via exact rational* $LDL^\top$ *Cholesky factorization of* $M^{T_A} - \delta_A I_{16}$ *with exact Gershgorin error radius* $\delta_A < 1.3 \times 10^{-29}$ *(and* $< 10^{-43}$ *at* $M = 22$*).*

Proof. Part 1 follows from evaluating the right-hand side of (14) on the five distinct roots $\lambda \in \{0, \pm 2, \pm 2\sqrt{2}\}$ of (12) (machine-checked over $\mathbb{Z}$ as `thm3_xx4_vandermonde_exact`). For Part 2, exact integer traces of H^m, $H^m S_x(\pi)$, and $H^m S_z(0)$ ($m = 0, \ldots, 4$) yield $ZS_x(\pi) = 7 + 6a - 4b + 3c - 2d$ and $ZS_z(0) = 12 + 4a$, whence $Z(1 - \omega_{\text{CMC}}) = Z - ZS_x(\pi) - \frac{1}{2}ZS_z(0) = -3 - 4a + 4b - c + 2d$. Using $a - b = e^{-2\beta}$ kills $e^{+2\beta}$ identically (machine-checked in Lean 4 as `thm3_xx4_closed_form_cmc_margin` and `thm3_xx4_exp_cancellation`).

For Part 3, truncating the nonnegative rational Taylor series of a, b, c, d at order M with exact geometric-series

Table 1: All 20 constructive Lean 4.35.0 theorems in `lean/XyChainCmcCert.lean`. Every theorem compiles with zero `sorry`, zero custom axioms, zero `Classical.choice` (axioms strictly `[propext, Quot.sound]`), and zero warnings.

#	Theorem identifier	Content
1	`vec3_cauchy_schwarz`	3D Lagrange CS
2	`obs1_single_site_bloch_variance`	Single-site Bloch
3	`obs1_nsite_collective_variance_bound`	N-site Obs. 1
4	`obs1_finite_mixture_variance_concavity`	Mixture concavity
5	`thm1_cmc_polyhedron_lower_bound`	CMC LP bound
6	`thm1_cmc_four_corners_feasible`	4 corners attain
7	`thm1_xx_u1_simplification`	XX $U(1)$ case
8	`thm1_planar_anisotropy_transition`	Planar y drop
9	`cor1_separable_iff_omega_ge_one`	Cor. 1 dual iff
10	`cor1_explicit_noise_vector`	Noise vector
11	`prop1_bsa_lower_bound`	BSA $t \geq 1-\omega$
12	`unit_vec3_dot_le_one`	$\lvert u \cdot v \rvert \leq D^2$
13	`thm2_four_qubit_singlet_le_one_third`	$p_0 \leq 1/3$
14	`thm2_neel_state_attains_one_third`	Néel $p_0 = 1/3$
15	`thm2_four_qubit_spin_sector_ineq`	$2p_2 \geq p_0$
16	`thm2_secular_function_neel_dominance`	$f_\phi \leq f_{\text{Néel}}$
17	`thm2_neel_secular_cubic_equivalence`	Cubic $P_\lambda = 0$
18	`thm3_xx4_vandermonde_exact`	$e^{-\beta H}$ Vanderm.
19	`thm3_xx4_closed_form_cmc_margin`	$Z(1-\omega_{\text{CMC}})$
20	`thm3_xx4_exp_cancellation`	$e^{+2\beta}$ cancels

remainder upper bounds yields exact rational intervals $[G_{ij}^-, G_{ij}^+]$ for every entry of $G(\beta)$. For each of the seven nontrivial bipartitions A, let M^{T_A} be the exact rational midpoint matrix of $(G^{T_A})^\pm$ and $\delta_A := \max_i \sum_{j=0}^{15} \frac{1}{2}(G_{ij}^{T_A,+} - G_{ij}^{T_A,-})$ its exact Gershgorin operator-norm error bound. By Weyl's inequality, if $M^{T_A} - \delta_A I_{16}$ admits an exact rational $LDL^\top$ Cholesky factorization with strictly positive diagonal pivots $d_k > 0$ ($k = 0, \ldots, 15$), then $G(\beta)^{T_A} \succ 0$ strictly! Executing this exact rational procedure over $\mathbb{Q}$ in `C13`–`C16` certifies all seven partial transposes strictly positive definite with normalized minimum pivot $\geq 1/4000$ (`C14`), $\geq 1/1000$ (`C13`, `C16`), and $\geq 3/2000$ (`C15`) while $\omega_{\text{CMC}} \leq 0.9998 < 1$ (Figure 3). □

5 Formal Verification Architecture and Certificate Audit

Lean 4.35.0 Constructive Kernel. The standalone module `lean/XyChainCmcCert.lean` proves all 20 theorems listed in Table 1 without Mathlib. Using explicit inductive predicates (`AllInBlochBall`, `AllNonnegWeights`) and constructive integer order lemmas (`Int.le_total`, `Int.lt_trichotomy`), every theorem passes `#print axioms` strictly within `[propext, Quot.sound]`—zero `sorry`, zero custom axioms, zero `Classical.choice`, and zero compiler warnings.

Zero-Float Verifier and Adversarial Test Suite. The engine `src/xy_chain_cmc_verifier.py` enforces strict integer and lowest-terms `fractions.Fraction` arithmetic via an AST audit banning float/complex literals, `float()`, `complex()`, `eval()`, `exec()`, `from_float`, `from_decimal`, true division (`/`, `/=`), exponentiation (`**`, `**=`), and floating-point libraries. Across Modes 1–4 (Table 2), it checks all 16 certificates (`C01`–`C16`), SHA-256 manifest hashes, and direct 16×16 matrix traces $\text{Tr}(G_{\text{iv}} S_x(\pi))$ and $\text{Tr}(G_{\text{iv}} S_z(0))$ against the closed forms of Theorem C. The pytest suite `tests/test_verifier.py` runs 61 tests, verifying exact $H^5 - 12H^3 + 32H = 0$, exact trace moments $\text{Tr}(H^m S_x(\pi))$ and $\text{Tr}(H^m S_z(0))$, negative-pivot NPT detection at $T = 0.5$ and $T = 1.47$, and 26 adversarial forgery-rejection attacks (rejecting `bool`-as-`int`, unreduced fractions, forged witnesses, non-unit Bloch vectors, invalid $\omega_{\text{CMC}} \geq 1$ in Mode 2, wrong cubic root brackets, inflated E_G or $LDL^\top$ pivot bounds, and false PPT-bound entanglement claims on NPT or above-T_{CMC} states).

Table 2: Summary of all 16 verified JSON certificates (`C01`–`C16`) checked by the AST-audited zero-float verifier `src/xy_chain_cmc_verifier.py` across Modes 1–4. In Mode 4, `piv` denotes the normalized minimum $LDL^\top$ pivot of $(M^{T_A} - \delta_A I_{16})/Z^+$.

ID	M	Target instance	Certified outcome
`C01`	1	XX $N = 10, T = 0.1$	$\omega = \frac{307}{2000}$, BSA $\geq \frac{1693}{2000}$
`C02`	1	Ising $N = 10, T = 0.1$	$\omega = \frac{383}{1000}$, BSA $\geq \frac{617}{1000}$
`C03`	1	$(\gamma, h) = (0.5, 0.5)$	$\omega = \frac{389}{500}$, planar zx
`C04`	1	Separable ferro	$\omega = \frac{201}{200} \geq 1$, Cor. 1 vec
`C05`	2	Néel $(+z, +z, -z, -z)$	$p_0 = \frac{1}{3}$, $E_G \geq \frac{399}{1000}$
`C06`	2	Square $(\pm z, \pm x)$	$p_0 = \frac{1}{4}$, dom. $(\lambda = -1)$
`C07`	2	Pythagorean sphere	$p_0 = \frac{43}{169}$, dom. $(\lambda = -2)$
`C08`	2	$(\uparrow\uparrow\uparrow\downarrow)$	$(0, \frac{3}{4}, \frac{1}{4})$, $E_G \geq \frac{21}{250}$
`C09`	3	XX_4, $\beta = 2$	$\omega \in [\frac{181}{500}, \frac{363}{1000}] < 1$
`C10`	3	XX_4, $\beta = \frac{100}{147}$	$\omega \in [\frac{461}{500}, \frac{923}{1000}] < 1$
`C11`	3	XX_4, $\beta = \frac{72}{125}$	$\omega \in [\frac{9989}{10000}, \frac{9991}{10000}] < 1$
`C12`	3	XX_4, $\beta = \frac{200}{349}$	$\omega \in [\frac{1001}{1000}, \frac{501}{500}] > 1$
`C13`	4	XX_4, $\beta = \frac{72}{125}$	7 PD (piv $\geq 10^{-3}$), $\omega < 0.999$
`C14`	4	XX_4, $\beta = \frac{289}{500}$	7 PD (piv $\geq \frac{1}{4000}$), $\omega < 0.9975$
`C15`	4	XX_4, $\beta = \frac{23}{40}$	7 PD (piv $\geq \frac{3}{2000}$), $\omega < 0.9998$
`C16`	4	XX_4, $\beta = \frac{72}{125}$, $M = 22$	Rad $< 10^{-43}$, all 7 PT PD

6 Scope, Open Directions, and Reproducibility

Scope and Open Directions. Theorem B resolves the Section H Néel-state optimality conjecture of [5] completely for $N = 4$ qubits, where the total-spin Casimir spectrum has exactly three sectors ($J \in \{0, 1, 2\}$). Extending the Bloch-vector secular-dominance technique to arbitrary even $N \geq 6$ (where $\mathbf{J}^2$ spans $N/2 + 1$ spin sectors) is a concrete open problem: our proof shows that the key obstruction is controlling higher-order symmetric invariants of the pairwise dot-product matrix (d_{ij}) in the $J = 0$ singlet projector. Theorem C establishes the first zero-float rational proof of thermal PPT-bound entanglement in the $N = 4$ periodic ferromagnetic XX chain across $\beta \in \{289/500, 72/125, 23/40\}$.

Reproducibility. All Lean 4 proofs, Python verification code, 16 JSON certificates with `MANIFEST.sha256`, 61 unit and forgery tests, and figure scripts are archived under MIT license at `github.com/lluiseriksson/xy-chain-cmc-neel-certificates` (`v1.0.0`) and reproduce

via `lake build`, `python src/xy_chain_cmc_verifier.py certificates`, and `pytest -q` under Lean 4.35.0 and Python 3.12+.

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