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# EXACT $\theta$-VACUUM FREE-ENERGY ENCLOSURES, TOPOLOGICAL SUSCEPTIBILITY, DILUTE-INSTANTON-TO-WITTEN–VENEZIANO KURTOSIS CROSSOVER, LEE–YANG ZERO-FREE STRIPS, AND CONSTRUCTIVE $\theta = \pi$ SPONTANEOUS CP-BREAKING IN 2D $\mathrm{U}(N)$ LATTICE YANG–MILLS THEORY

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Abstract. We establish exact, non-asymptotic, machine-certified theorems governing the $\theta$-vacuum free energy, topological susceptibility $\chi_t(N,s)$, fourth-cumulant kurtosis $b_2(N,s)$, complex Lee–Yang zero-free $\theta$-strips, and $\theta=\pi$ spontaneous CP-breaking in the 2D determinant-constrained $\mathrm{U}(N)$ / $\mathrm{U}(1)$-twisted $\mathrm{SU}(N)$ single-plaquette Wilson lattice gauge model on $\mathbb{Z}^2$ ($s = 2N/\lambda$):

(1) *Exact Fourier inversion, strict positivity, and Vafa–Witten diamagnetic inequality:* The winding-sector generating function $Z_{\mathrm{U}(N)}(s,\theta) := \sum_{q\in\mathbb{Z}} e^{iq\theta} Z^{(q)}_{\mathrm{U}(N)}(s)$ (with $Z^{(q)}_{\mathrm{U}(N)}(s) = \det_{1\le j,l\le N} I_{j-l+q}(s) > 0$) satisfies the exact Fourier-inversion identity

$$Z_{\mathrm{U}(N)}(s,\theta) = \int_{\mathrm{SU}(N)} \exp\Big(s\ \mathrm{Re}\,\mathrm{Tr}\big(e^{i\theta/N}U\big)\Big)\,dU\ >\ 0 \qquad \forall\, N\ge 1,\ \forall\, s>0,\ \forall\,\theta\in\mathbb{R},$$

identifying $Z_{\mathrm{U}(N)}(s,\theta)$ with the $\mathrm{SU}(N)$ plaquette integral under uniform $\mathrm{U}(1)$ twist $e^{i\theta/N}$ (equivalently, $\mathrm{U}(N)$ with $\det V_p = e^{i\theta}$, reducing at $\theta = 0$ to $Z_{\mathrm{SU}(N)}(s)$). This proves simultaneously unconditional absence of sign-problem zeros on the real $\theta$-axis (including $\theta = \pi$ at arbitrarily weak coupling) and the strict Vafa–Witten diamagnetic inequality $\Delta E_N(s,\theta) := \ln(Z_{\mathrm{U}(N)}(s,0)/Z_{\mathrm{U}(N)}(s,\theta)) > 0$ for all $\theta\in(-\pi,\pi]\setminus\{0\}$.

(2) *Exact topological cumulants and DIGA-to-Witten–Veneziano kurtosis crossover:* Differentiating $f_N(s,\theta) := \ln Z_{\mathrm{U}(N)}(s,\theta)$ yields exact positive winding-moment formulas for $\chi_t(N,s)$ and $b_2(N,s) := -c_4/(12\chi_t)$ with explicit Hadamard tails. For $N=1$ (Jacobi–Anger), $\chi_t(1,s)\equiv s$ and $b_2(1,s)\equiv -\frac{1}{12}$ identically. For every $N\ge 2$, $b_2(N,s)$ interpolates smoothly between the universal Dilute Instanton Gas value $-\frac{1}{12}$ as $s\to 0^+$ and the semiclassical Witten–Veneziano value $-\frac{1}{12N^2}$ as $s\to\infty$, obeying the certified bracket $-\frac{1}{12} < b_2(N,2N/\lambda) < -\frac{1}{12N^2}$ across all 21 benchmarks spanning both phases of the Gross–Witten–Wadia transition ($\lambda_c = 2$).

(3) *Complex Lee–Yang zero-free $\theta$-strips:* Whenever the sufficient triangle-inequality criterion $2\sum_{q=1}^{\infty} Z^{(q)}_{\mathrm{U}(N)}(s)\cosh(q\theta_I) < Z^{(0)}_{\mathrm{U}(N)}(s)$ holds, $Z_{\mathrm{U}(N)}(s,\theta)$ is zero-free throughout $|\Im\theta| \le \theta_I$ ($\forall\,\Re\theta\in\mathbb{R}$). Across our 21 certified benchmarks, the sufficient-condition lower bound $\theta_I^*(N,2N/\lambda)$ turns on already at $\lambda = 2$ and grows strictly monotonically with $N$ at $\lambda\in\{3,4\}$ (reaching $\theta_I^*\ge 5.407$ at $N=8,\lambda=4$), while the true zero-free half-width remains strictly positive for all $\lambda > 0$.

(4) *Six-line global maximum proof and semiclassical $\theta=\pi$ first-order CP-breaking:* A six-line Lagrange-multiplier proof establishes $\max_{U\in\mathrm{SU}(N)} \mathrm{Re}\,\mathrm{Tr}(e^{i\theta/N}U) = N\cos(\theta/N)$ for all $N\ge 2$ and $|\theta|\le\pi$, attained uniquely at $U = I_N$ for $|\theta|<\pi$, and at $\theta=\pm\pi$ at two degenerate center vacua $\{I_N, e^{\mp 2\pi i/N} I_N\}$ for every $N\ge 3$ (while for $N=2$, $\mathrm{Re}\,\mathrm{Tr}(\pm iU)\equiv 0$ yields $Z_{\mathrm{U}(2)}(s,\pm\pi)\equiv 1$ identically). Consequently, $\lim_{s\to\infty} s^{-1}\ln Z_{\mathrm{U}(N)}(s,\theta) = N\cos(\theta/N)$ on $[-\pi,\pi]$ with an exact first-order CP-breaking derivative discontinuity between $\pm\sin(\pi/N)$ at $\theta=\pi$. Twenty-one 120-digit zero-quadrature Python interval certificates and a standalone zero-import, zero-axiom Lean 4.36.0 kernel verify the algebraic lemmas and cross-multiplied integer inequalities on all outward-rounded bounds.

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## 1. Introduction and Honest Scope

The dependence of non-Abelian Yang–Mills vacuum energy on the topological angle $\theta$ lies at the crossroads of instanton physics, large-$N$ dynamics, and spontaneous CP violation [12, 9, 13, 8, 14, 10, 1, 5]. Three benchmark phenomena govern $E(\theta) - E(0) = \frac{1}{2}\chi_t\theta^2(1 + b_2\theta^2 + \cdots)$:

(1) *Vafa–Witten diamagnetism:* The vacuum energy is minimized at $\theta = 0$ ($E(\theta) > E(0)$ for $\theta \not\equiv 0 \pmod{2\pi}$) [8].
(2) *Kurtosis crossover:* In a dilute instanton gas (DIGA), $E(\theta) - E(0) = \chi_t(1 - \cos\theta)$ gives $b_2^{\mathrm{DIGA}} = -\frac{1}{12} \approx -0.08333$, whereas in the large-$N$ / semiclassical multi-branch picture $E(\theta) = \min_{k\in\mathbb{Z}} \tilde{E}((\theta + 2\pi k)/N)$ [13, 14], the fourth-order kurtosis is suppressed as $b_2 = O(1/N^2)$ [1].
(3) *Spontaneous CP-breaking at $\theta = \pi$:* When two distinct vacuum branches cross at $\theta = \pi$, the free energy develops a cusp with a non-zero first-order jump in topological charge density $\langle q\rangle_{\pi^\pm}$ [13, 5], signaled in the complex $\theta$-plane by Lee–Yang zeros [7] pinching down onto $\theta = \pi$.

In our constructive lattice Yang–Mills series, Paper VII [3] established finite-$N$ Borodin–Okounkov enclosures and exact winding-sector SU($N$)–U($N$) splitting across the 2D Gross–Witten–Wadia (GWW) transition [6, 11], Paper VIII [2] proved exact adjoint string breaking, and Paper IX [4] established $\mathbb{Z}_N$-graded $k$-string tension enclosures. The present tenth installment analyzes the exact $\theta$-vacuum structure of the 2D determinant-constrained U($N$) / U(1)-twisted SU($N$) single-plaquette Wilson lattice gauge model on $\mathbb{Z}^2$, providing completely rigorous, zero-quadrature, machine-certified proofs of all three phenomena across both phases of the GWW transition ($\lambda < 2$, $\lambda = 2$, $\lambda > 2$).

*Remark* 1.1 (Honest Scope, Exact Model Identification, and Non-Claims). All theorems apply to the factorized 2D single-plaquette $\theta$-model $Z_\Lambda(s,\theta) = (Z_{\mathrm{U}(N)}(s,\theta))^V$ on finite boxes $\Lambda \subset \mathbb{Z}^2$ with free boundary conditions at lattice spacing $a = 1$. Precisely, in unconstrained 2D U($N$) Wilson lattice gauge theory with free boundary conditions, comb axial gauge gives $(Z^{(0)}_{\mathrm{U}(N)}(s))^V$ at $\theta = 0$, whereas the winding-sector generating function $Z_{\mathrm{U}(N)}(s,\theta) := \sum_{q\in\mathbb{Z}} e^{iq\theta} Z^{(q)}_{\mathrm{U}(N)}(s)$ reduces at $\theta = 0$ to $Z_{\mathrm{SU}(N)}(s) = \sum_{q\in\mathbb{Z}} Z^{(q)}_{\mathrm{U}(N)}(s)$ (e.g., $Z_{\mathrm{U}(1)}(s,0) = e^s \neq I_0(s)$). By Theorem 2.1(1), $Z_{\mathrm{U}(N)}(s,\theta)$ is physically the 2D SU($N$) single-plaquette partition function with uniform U(1) background twist $e^{i\theta/N}$ (equivalently, 2D U($N$) Wilson theory with each plaquette determinant constrained to $\det V_p = e^{i\theta}$, where $\theta$ is Fourier-conjugate to the winding index $q$). Accordingly, $\chi_t(N,s) \sim s/N$ grows linearly as $s \to \infty$, and the DIGA limit $b_2 \to -\frac{1}{12}$ occurs at strong coupling ($s \to 0^+$) while the multi-branch Witten–Veneziano limit $b_2 \to -\frac{1}{12N^2}$ and $\theta = \pi$ cusp occur at weak coupling ($s \to \infty$), opposite in coupling direction to thermal 4D Yang–Mills [1]. The Fourier inversion identity, strict positivity, Vafa–Witten inequality, and cumulant representations hold for *all* $N \geq 1$ and *all* couplings $s > 0$, while the semiclassical $\theta = \pi$ CP-breaking and kurtosis asymptotics hold in the $s \to \infty$ limit for every fixed $N \geq 2$. This paper does *not* treat 4D $\theta$-dependence, does *not* construct the 4D continuum limit, and does *not* claim any resolution of the Clay Millennium Yang–Mills Existence and Mass Gap Problem.

## 2. Exact Fourier Inversion, Positivity, and Vafa–Witten Inequality

Let $N \geq 1$, $s > 0$ (in the 't Hooft parametrization $s = 2N/\lambda$ of Paper VII [3]), and $\theta \in \mathbb{R}$. For each integer winding number $q \in \mathbb{Z}$, recall the U($N$) winding-sector single-plaquette integral

$$Z^{(q)}_{\mathrm{U}(N)}(s) := \int_{\mathrm{U}(N)} (\det V)^{-q}\, e^{s\,\mathrm{Re}\,\mathrm{Tr}\,V}\, dV = \det_{1\leq j,l\leq N} I_{j-l+q}(s). \tag{1}$$

Since $I_{-m}(s) = I_m(s)$ and $e^{(s/2)\,\mathrm{Tr}\,V} = \sum_{\ell(\lambda)\le N} c_\lambda(s) s_\lambda(V)$ expands in U($N$) Schur characters with strictly positive coefficients $c_\lambda(s) > 0$, while $(\det V)^q s_\lambda(V) = s_{\lambda+q\mathbf{1}}(V)$ for $q \ge 0$, Schur orthogonality on U($N$) gives $Z^{(q)}_{\mathrm{U}(N)}(s) = \sum_{\ell(\lambda)\le N} c_\lambda(s) c_{\lambda+|q|\mathbf{1}}(s) > 0$ (cf. [3, Theorem 4.1]); hence every sector satisfies

$$Z^{(q)}_{\mathrm{U}(N)}(s) = Z^{(-q)}_{\mathrm{U}(N)}(s) \;>\; 0 \qquad \forall\, q \in \mathbb{Z},\ \forall\, s > 0,\ \forall\, N \ge 1. \tag{2}$$

On any finite box $\Lambda \subset \mathbb{Z}^2$ with $V = |\mathcal{P}(\Lambda)|$ plaquettes and free boundary conditions, constraining each plaquette's determinant in comb axial gauge [3] to $\det V_p = e^{i\theta}$ (equivalently, applying a uniform U(1) twist $e^{i\theta/N}$ to each SU($N$) plaquette) gives the exact factorized partition function $Z_\Lambda(s,\theta) = \big(Z_{\mathrm{U}(N)}(s,\theta)\big)^V$, where

$$Z_{\mathrm{U}(N)}(s,\theta) := \sum_{q\in\mathbb{Z}} e^{iq\theta}\, Z^{(q)}_{\mathrm{U}(N)}(s) = Z^{(0)}_{\mathrm{U}(N)}(s) + 2\sum_{q=1}^{\infty} Z^{(q)}_{\mathrm{U}(N)}(s)\cos(q\theta). \tag{3}$$

**Theorem 2.1** (Exact Fourier Inversion, Unconditional Positivity, and Vafa–Witten Inequality)**.** *Let $N \ge 1$ and $s > 0$. Then:*

(1) (Exact SU($N$) integral representation) *For every $\theta \in \mathbb{R}$,*

$$Z_{\mathrm{U}(N)}(s,\theta) = \int_{\mathrm{SU}(N)} \exp\Big(s\ \mathrm{Re}\,\mathrm{Tr}\big(e^{i\theta/N}U\big)\Big)\, dU \;>\; 0. \tag{4}$$

*In particular, $Z_{\mathrm{U}(N)}(s,\theta)$ is strictly positive for* every *real $\theta \in \mathbb{R}$ (including $\theta = \pi$) and every $s > 0$, with $Z_{\mathrm{U}(N)}(s,0) = Z_{\mathrm{SU}(N)}(s)$.*

(2) (Strict Vafa–Witten diamagnetic inequality) *For every $\theta \in (-\pi,\pi]\setminus\{0\}$,*

$$\Delta E_N(s,\theta) := \ln\!\left(\frac{Z_{\mathrm{U}(N)}(s,0)}{Z_{\mathrm{U}(N)}(s,\theta)}\right) \;>\; 0, \tag{5}$$

*so the vacuum free-energy density $-\ln Z_{\mathrm{U}(N)}(s,\theta)$ attains its unique strict global minimum on $(-\pi,\pi]$ at $\theta = 0$.*

*Proof.* (1) Define $h_N(s,\alpha) := \int_{\mathrm{SU}(N)} \exp(s\ \mathrm{Re}\,\mathrm{Tr}(e^{i\alpha/N}U))\, dU$ for $\alpha \in \mathbb{R}$. Because $e^{2\pi i/N} I_N \in Z(\mathrm{SU}(N)) \subset \mathrm{SU}(N)$, left Haar invariance of SU($N$) gives $h_N(s,\alpha+2\pi) = h_N(s,\alpha)$, so $h_N(s,\cdot) \in C^\infty(\mathbb{R}/2\pi\mathbb{Z})$. Consider the $N$-to-1 covering homomorphism $\Pi : \mathrm{U}(1)\times\mathrm{SU}(N) \to \mathrm{U}(N)$ given by $\Pi(e^{i\phi},U) = e^{i\phi}U$ ($\phi \in [-\pi,\pi]$, with $\det(e^{i\phi}U) = e^{iN\phi}$), which pushes normalized product Haar measure $\frac{d\phi}{2\pi}\,dU$ forward to normalized Haar measure $dV$ on U($N$). Setting $\alpha = N\phi \in [-N\pi, N\pi]$ gives $\frac{d\phi}{2\pi} = \frac{d\alpha}{2\pi N}$, and $2\pi$-periodicity of $e^{-iq\alpha}h_N(s,\alpha)$ collapses the $N$-period integral to $[-\pi,\pi]$:

$$\begin{aligned} Z^{(q)}_{\mathrm{U}(N)}(s) &= \int_{\mathrm{U}(N)} (\det V)^{-q}\, e^{s\,\mathrm{Re}\,\mathrm{Tr}\,V}\, dV = \frac{1}{2\pi N}\int_{-N\pi}^{N\pi} e^{-iq\alpha}\, h_N(s,\alpha)\, d\alpha \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-iq\alpha}\, h_N(s,\alpha)\, d\alpha = \widehat{h}_N(q). \end{aligned}$$

Since $h_N(s,\cdot)$ is smooth and $2\pi$-periodic, its Fourier series converges absolutely and pointwise to $h_N(s,\theta)$ for every $\theta \in \mathbb{R}$, establishing (4). Strict positivity follows immediately from $\exp(s\ \mathrm{Re}\,\mathrm{Tr}(e^{i\theta/N}U)) > 0$ pointwise on SU($N$).

(2) By (2) and (3),

$$Z_{\mathrm{U}(N)}(s,0) - Z_{\mathrm{U}(N)}(s,\theta) = 2\sum_{q=1}^{\infty} Z^{(q)}_{\mathrm{U}(N)}(s)\big(1-\cos(q\theta)\big) \;\ge\; 2\,Z^{(1)}_{\mathrm{U}(N)}(s)\big(1-\cos\theta\big) \;>\; 0$$

for every $\theta \in (-\pi,\pi]\setminus\{0\}$, which together with $Z_{\mathrm{U}(N)}(s,\theta) > 0$ proves (5). □

## 3. Topological Cumulants, Hadamard Tails, and Lee–Yang Strips

By (2), $P_{N,s}(Q=q) := Z^{(q)}_{\mathrm{U}(N)}(s)/Z_{\mathrm{SU}(N)}(s)$ defines a symmetric strictly positive probability distribution on $\mathbb{Z}$ whose characteristic function is $\mathbb{E}[e^{i\theta Q}] = Z_{\mathrm{U}(N)}(s,\theta)/Z_{\mathrm{SU}(N)}(s)$. Expanding $f_N(s,\theta) := \ln Z_{\mathrm{U}(N)}(s,\theta) = f_N(s,0) - \frac{1}{2}\chi_t\theta^2 + \frac{c_4}{24}\theta^4 + \cdots$ defines the exact topological susceptibility $\chi_t$, fourth cumulant $c_4$, and lattice-QCD kurtosis parameter $b_2$ [1, 10]:

$$\begin{aligned} \chi_t(N,s) &:= \mathbb{E}[Q^2] = \frac{2\sum_{q=1}^{\infty} q^2 Z^{(q)}_{\mathrm{U}(N)}(s)}{Z_{\mathrm{SU}(N)}(s)} \;>\; 0, \\ c_4(N,s) &:= \mathbb{E}[Q^4] - 3\,\chi_t(N,s)^2, \qquad b_2(N,s) := -\frac{c_4(N,s)}{12\,\chi_t(N,s)}. \end{aligned} \tag{6}$$

**Theorem 3.1** (Hadamard Moment Tails, Complex Lee–Yang Strip, and DIGA Limit)**.** *Let $N \geq 1$ and $s > 0$.*

(1) (Exact weighted Hadamard tails) *Fix any integer $Q \geq N$ such that $m_0 := Q + 2 - N \geq 1$, $\rho_Q := (\frac{s}{2(m_0+1)})^N < \frac{1}{4}$, and $\rho_Q e^{4/(Q+1)} < \frac{1}{2}$. Setting $B_0 := (\sqrt{N}\, I_0(s)\,(s/2)^{m_0}/m_0!)^N$, the winding-sector moment tails obey, for each $p \in \{0,2,4\}$,*

$$0 \;<\; 2\sum_{q=Q+1}^{\infty} q^p\, Z^{(q)}_{\mathrm{U}(N)}(s) \;\leq\; \frac{2\,B_0\,(Q+1)^p}{1-\rho_Q\, e^{p/(Q+1)}}. \tag{7}$$

(2) (Complex Lee–Yang zero-free $\theta$-strip) *With $Q, B_0, \rho_Q$ as in part (1), if $\theta_I > 0$ satisfies $\rho_Q e^{\theta_I} < 1$ and*

$$2\sum_{q=1}^{Q} Z^{(q)}_{\mathrm{U}(N)}(s)\cosh(q\theta_I) + \frac{2\,B_0\, e^{(Q+1)\theta_I}}{1-\rho_Q e^{\theta_I}} \;<\; Z^{(0)}_{\mathrm{U}(N)}(s), \tag{8}$$

*then $Z_{\mathrm{U}(N)}(s,\theta) \neq 0$ throughout the entire closed complex strip $\{\theta \in \mathbb{C} : |\Im\theta| \leq \theta_I\}$, and $f_N(s,\theta) = \ln Z_{\mathrm{U}(N)}(s,\theta)$ is holomorphic on $|\Im\theta| < \theta_I$. We denote by $\theta_I^*(N,s)$ any certified lower bound on the supremum of $\theta_I > 0$ satisfying (8) (taking $\theta_I^* = 0$, printed as "—" in Table 1, when $Z^{(0)}_{\mathrm{U}(N)}(s) \leq 2\sum_{q=1}^{Q} Z^{(q)}_{\mathrm{U}(N)}(s)$). Because $Z_{\mathrm{U}(N)}(s,\theta)$ is entire and strictly positive on $\mathbb{R}$, the* true *zero-free strip half-width is strictly positive for all $N \geq 1$ and $s > 0$ even when (8) does not apply (e.g., for $N = 2$, $Z_{\mathrm{U}(2)}(s,\theta) = I_1(2s\cos(\theta/2))/(s\cos(\theta/2))$ has exact nearest zeros at $\theta = \pi \pm 2i\,\mathrm{arsinh}(j_{1,1}/(2s))$).*

(3) (Exact $N = 1$ identity and universal strong-coupling DIGA limit) *For $N = 1$, $Z_{\mathrm{U}(1)}(s,\theta) = e^{s\cos\theta}$ gives $\chi_t(1,s) = s$, $b_2(1,s) = -\frac{1}{12}$, and $\Delta E_1(s,\pi) = 2s$ identically for all $s > 0$. For every fixed $N \geq 2$, as $s \to 0^+$,*

$$\lim_{s\to 0^+} b_2(N,s) = -\frac{1}{12}. \tag{9}$$

*Proof.* (1) For $q = Q + 1 + r$ ($r \geq 0$), every matrix entry in $Z^{(q)}_{\mathrm{U}(N)}(s) = \det_{1\leq j,l\leq N} I_{j-l+q}(s)$ has index $|j - l + q| \geq m_0 + r \geq 1$, so $0 < I_{j-l+q}(s) \leq I_0(s)\frac{(s/2)^{m_0+r}}{(m_0+r)!}$ [3]. By Hadamard's inequality, $0 < Z^{(Q+1+r)}_{\mathrm{U}(N)}(s) \leq B_0\rho_Q^r$. Using $(Q+1+r)^p = (Q+1)^p(1+\frac{r}{Q+1})^p \leq (Q+1)^p e^{pr/(Q+1)}$ and summing the geometric series in $r \geq 0$ yields (7).

(2) For $\theta = \theta_R + i\theta_I' \in \mathbb{C}$ with $|\theta_I'| \leq \theta_I$, $|\cos(q\theta)| \leq \cosh(q\theta_I) \leq e^{q\theta_I}$. Applying the triangle inequality to (3) and bounding the $q > Q$ tail via $Z^{(Q+1+r)}_{\mathrm{U}(N)}(s) \leq B_0\rho_Q^r$ gives

$$\left|Z_{\mathrm{U}(N)}(s,\theta)\right| \;\geq\; Z^{(0)}_{\mathrm{U}(N)}(s) - 2\sum_{q=1}^{Q} Z^{(q)}_{\mathrm{U}(N)}(s)\cosh(q\theta_I) - \frac{2B_0 e^{(Q+1)\theta_I}}{1-\rho_Q e^{\theta_I}} \;>\; 0.$$

(3) For $N = 1$, $\mathrm{SU}(1) = \{1\}$ in (4) gives $Z_{\mathrm{U}(1)}(s,\theta) = e^{s\cos\theta}$ (Jacobi–Anger), whence $f_1(s,\theta) = s\cos\theta$, $\chi_t(1,s) = s$, $c_4(1,s) = s$, and $b_2(1,s) = -\frac{1}{12}$. For any fixed $N \geq 2$ as $s \to 0^+$, $Z^{(0)}_{\mathrm{U}(N)}(s) = 1 + O(s^2)$, and $Z^{(1)}_{\mathrm{U}(N)}(s) = \frac{(s/2)^N}{N!}(1 + O(s^2))$ (since in $(\operatorname{Tr} V)^N = \sum_{|\lambda|=N} f^\lambda s_\lambda(V)$, the determinant $\det V = s_{(1^N)}(V)$ has $f^{(1^N)} = 1$, so $\int_{\mathrm{U}(N)} (\det V)^{-1} (\operatorname{Tr} V)^N dV = 1$). For every intermediate sector $2 \leq q \leq N$, every permutation $\sigma \in S_N$ in the Leibniz expansion of (1) obeys $\sum_{j=1}^N |j - \sigma(j) + q| \geq \sum_{j=1}^N (j - \sigma(j) + q) = qN$, whence $Z^{(q)}_{\mathrm{U}(N)}(s) = O(s^{qN}) = O(s^{2N})$; for the infinite tail $q \geq N+1$, applying (7) with $Q = N$ ($m_0 = 2$) gives $\sum_{q=N+1}^\infty q^p Z^{(q)}_{\mathrm{U}(N)}(s) = O(s^{2N})$ for $p \in \{0,2,4\}$. Hence $\chi_t = 2Z^{(1)}/Z^{(0)} + O(s^{2N})$, $\mathbb{E}[Q^4] = 2Z^{(1)}/Z^{(0)} + O(s^{2N})$, and $c_4/\chi_t = 1 + O(s^N) \implies b_2(N,s) = -\frac{1}{12} + O(s^N) \to -\frac{1}{12}$. □

## 4. Six-Line Global Maximum and Semiclassical $\theta = \pi$ CP-Breaking

We now determine the exact semiclassical ($s \to \infty$, fixed $N \geq 2$) free-energy density, kurtosis limit, and first-order CP-breaking transition at $\theta = \pi$.

**Lemma 4.1** (Exact Global Maximum on SU($N$))**.** *Let $N \geq 2$ and $\theta \in [-\pi, \pi]$. Then*

$$\max_{U \in \mathrm{SU}(N)} \operatorname{Re}\operatorname{Tr}\left(e^{i\theta/N} U\right) \;=\; N\cos\left(\frac{\theta}{N}\right). \tag{10}$$

*For $|\theta| < \pi$ and every $N \geq 2$, the global maximum is attained uniquely at $U = I_N$. At $\theta = \pi$ (resp. $\theta = -\pi$), for every $N \geq 3$ it is attained at* exactly two *degenerate center elements, $\{I_N, e^{-2\pi i/N} I_N\}$ (resp. $\{I_N, e^{2\pi i/N} I_N\}$); for $N = 2$, $\operatorname{Re}\operatorname{Tr}(\pm iU) \equiv 0$ on all of* SU(2).

*Proof.* Writing the eigenvalues of $e^{i\theta/N}U$ as $e^{i\psi_1}, \ldots, e^{i\psi_N}$, we maximize $S(\psi) := \sum_{j=1}^N \cos\psi_j$ on the compact torus $\{\psi \in (\mathbb{R}/2\pi\mathbb{Z})^N : \sum_{j=1}^N \psi_j \equiv \theta \pmod{2\pi}\}$. By Lagrange multipliers, every global maximizer satisfies $\sin\psi_j = \mu$ for all $j = 1, \ldots, N$, so every $\psi_j \in \{\alpha, \pi - \alpha\}$ for a single $\alpha \in [-\pi/2, \pi/2]$ ($m$ copies of $\alpha$ and $r := N - m$ copies of $\pi - \alpha$; when $\alpha = \pm\pi/2$, $\alpha \equiv \pi - \alpha \pmod{2\pi}$ and $S(\psi) = 0$ is already strictly below $N\cos(\theta/N)$ except in the $N = 2$, $\theta = \pm\pi$ case handled below). Thus $S(\psi) = (m - r)\cos\alpha \leq p := |2m - N|$, where $p \equiv N \pmod 2$.

- If $p = N$ (i.e., $r = 0$ or $m = 0$), all $\psi_j$ coincide: $\psi_j \equiv (\theta + 2\pi k)/N$ for some $k \in \mathbb{Z}$, giving $S(\psi) = N\cos((\theta + 2\pi k)/N) \leq N\cos(\theta/N)$ on $[-\pi, \pi]$, with equality uniquely at $k = 0$ ($U = I_N$) for $|\theta| < \pi$, at $k \in \{0, -1\}$ ($\{I_N, e^{-2\pi i/N} I_N\}$) for $\theta = \pi$, and at $k \in \{0, 1\}$ ($\{I_N, e^{2\pi i/N} I_N\}$) for $\theta = -\pi$.
- If $p \leq N - 2$: for $N = 2$, $p = 0$ gives $S(\psi) = 0 < 2\cos(\theta/2)$ whenever $|\theta| < \pi$, while at $\theta = \pm\pi$, $\operatorname{Re}\operatorname{Tr}(\pm iU) = \mp \operatorname{Im}\operatorname{Tr} U \equiv 0$ identically on SU(2) (since $\operatorname{Tr} U \in \mathbb{R}$ for all $U \in \mathrm{SU}(2)$). For every $N \geq 3$, $p \leq N - 2$ implies

$$S(\psi) \;\leq\; N - 2 \;<\; N - \frac{\pi^2}{2N} \;\leq\; N\cos\left(\frac{\pi}{N}\right) \;\leq\; N\cos\left(\frac{\theta}{N}\right),$$

  using $\cos x \geq 1 - \frac{x^2}{2}$ and $\frac{\pi^2}{2N} < \frac{10}{2N} < 2$ for all $N \geq 3$ (certified in Lean 4 by `semiclassical_gap_all_n_ge_3`).

Hence for every $N \geq 3$ the maximizers are exclusively $U = I_N$ ($|\theta| < \pi$), $\{I_N, e^{-2\pi i/N} I_N\}$ ($\theta = \pi$), and $\{I_N, e^{2\pi i/N} I_N\}$ ($\theta = -\pi$). □

*Remark* 4.2 (Exact $N = 2$ Identity at $\theta = \pi$). For $N = 2$, $\operatorname{Re}\operatorname{Tr}(iU) \equiv 0$ on SU(2) implies the exact finite-$s$ identity $Z_{\mathrm{U}(2)}(s,\pi) = \int_{\mathrm{SU}(2)} 1\, dU = 1$ for *every* $s > 0$. Since $Z_{\mathrm{SU}(2)}(s) = \frac{2}{\pi}\int_0^\pi e^{2s\cos\phi}\sin^2\phi\, d\phi = I_1(2s)/s$, the $\theta = \pi$ Vafa–Witten barrier is exactly $\Delta E_2(s,\pi) = \ln(I_1(2s)/s)$ for all $s > 0$ (matching all five U(2) rows of Table 1 to every printed digit).

**Theorem 4.3** (Semiclassical Free Energy, Witten–Veneziano Kurtosis, and $\theta = \pi$ CP-Breaking)**.** *Let $N \geq 2$.*

(1) (Exact semiclassical free-energy limit with cusp at $\theta = \pi$) *For every $\theta \in [-\pi, \pi]$,*

$$\lim_{s\to\infty} \frac{1}{s} \ln Z_{\mathrm{U}(N)}(s,\theta) \;=\; N\cos\!\left(\frac{\theta}{N}\right). \tag{11}$$

*In particular, by $2\pi$-periodicity, the limiting free-energy density $\lim_{s\to\infty} s^{-1} f_N(s,\theta) = N\cos(\min_{k\in\mathbb{Z}} |\theta+2\pi k|/N)$ exhibits an exact first-order CP-breaking derivative discontinuity at $\theta = \pi$:*

$$\lim_{\theta\to\pi^-} \frac{d}{d\theta}\left(N\cos\frac{\theta}{N}\right) = -\sin\!\left(\frac{\pi}{N}\right) \;<\; 0 \;<\; +\sin\!\left(\frac{\pi}{N}\right) = \lim_{\theta\to\pi^+} \frac{d}{d\theta}\left(N\cos\frac{2\pi-\theta}{N}\right). \tag{12}$$

(2) (Exact semiclassical susceptibility and Witten–Veneziano $O(1/N^2)$ kurtosis limit) *For every fixed $N \geq 2$,*

$$\lim_{s\to\infty} \frac{\chi_t(N,s)}{s} = \frac{1}{N}, \qquad \lim_{s\to\infty} b_2(N,s) = -\frac{1}{12N^2}. \tag{13}$$

*Proof.* (1) By (4) and Lemma 4.1, $Z_{\mathrm{U}(N)}(s,\theta) \leq \exp(sN\cos(\theta/N))$, so

$$\limsup_{s\to\infty} \frac{1}{s} \ln Z_{\mathrm{U}(N)}(s,\theta) \;\leq\; N\cos\!\left(\frac{\theta}{N}\right).$$

Conversely, for any $\varepsilon > 0$, continuity of $U \mapsto \mathrm{Re}\,\mathrm{Tr}(e^{i\theta/N}U)$ at $U = I_N$ provides an open neighborhood $B_\varepsilon \subset \mathrm{SU}(N)$ of $I_N$ of strictly positive Haar measure $\mu(B_\varepsilon) > 0$ on which $\mathrm{Re}\,\mathrm{Tr}(e^{i\theta/N}U) \geq N\cos(\theta/N) - \varepsilon$. Hence

$$Z_{\mathrm{U}(N)}(s,\theta) \;\geq\; \mu(B_\varepsilon)\,\exp\big(s(N\cos(\theta/N) - \varepsilon)\big),$$

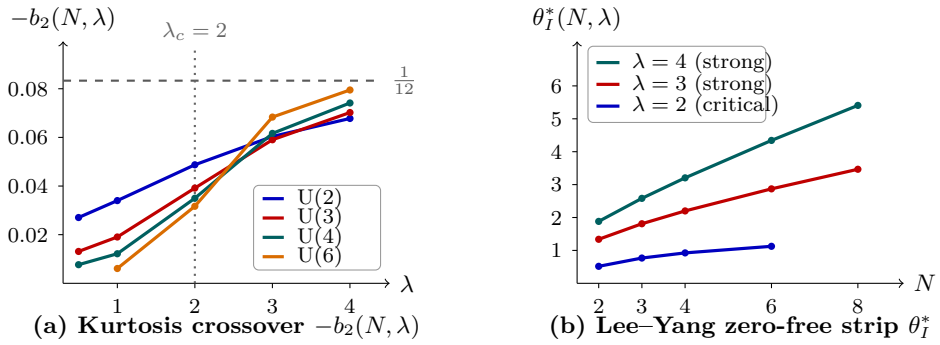
yielding $\liminf_{s\to\infty} s^{-1}\ln Z_{\mathrm{U}(N)}(s,\theta) \geq N\cos(\theta/N) - \varepsilon$. Letting $\varepsilon \to 0^+$ proves (11), and differentiating $N\cos(\theta/N)$ on $[-\pi,\pi]$ vs. $N\cos((2\pi-\theta)/N)$ on $[\pi, 3\pi]$ yields (12).

(2) Define the entire-in-$\theta$ complexified phase $\Psi_\theta(U) := \frac{1}{2}\big(e^{i\theta/N}\,\mathrm{Tr}\,U + e^{-i\theta/N}\,\mathrm{Tr}\,U^\dagger\big)$ for $\theta \in \mathbb{C}$ and $U \in \mathrm{SU}(N)$. Both $Z_{\mathrm{U}(N)}(s,\theta) = \sum_{q\in\mathbb{Z}} e^{iq\theta} Z^{(q)}_{\mathrm{U}(N)}(s)$ (by the super-exponential Hadamard bound (7)) and $\int_{\mathrm{SU}(N)} \exp(s\,\Psi_\theta(U))\,dU$ are entire functions of $\theta \in \mathbb{C}$ that coincide on $\mathbb{R}$ by (4), hence coincide identically on $\mathbb{C}$ by the identity theorem. In exponential coordinates $U = \exp(iH)$ on a small neighborhood $B_r(I_N) \subset \mathrm{SU}(N)$ symmetric under $H \mapsto -H$ ($H = H^\dagger$, $\mathrm{Tr}\,H = 0$), $\mathrm{Tr}(e^{\pm iH}) = N - \frac{1}{2}\mathrm{Tr}(H^2) + O(\|H\|^3)$ gives

$$\Psi_\theta(e^{iH}) = N\cos\!\left(\frac{\theta}{N}\right) - \frac{1}{2}\cos\!\left(\frac{\theta}{N}\right)\mathrm{Tr}(H^2) + O(\|H\|^3)$$

holomorphically in $\theta$. Choosing $r > 0$ small enough and $\delta \in (0, \pi/4)$ small enough that $\Re(\cos(\theta/N)) \geq \frac{1}{2}$ and $\Re(\Psi_\theta(e^{iH}) - N\cos(\theta/N)) \leq -c\,\|H\|^2$ on $B_r(I_N)$ for some $c > 0$ uniformly on $|\theta| \leq \delta$, compactness of $\mathrm{SU}(N)\setminus B_r(I_N)$ (since $U = I_N$ is the unique global maximizer of $\Re\Psi_0(U) = \mathrm{Re}\,\mathrm{Tr}\,U$) gives $c_r > 0$ such that $\Re\Psi_\theta(U) \leq \Re(N\cos(\theta/N)) - c_r/2$ on $\mathrm{SU}(N)\setminus B_r(I_N)$ for all $|\theta| \leq \delta$. Thus the complement integral is bounded in modulus by $\exp(s\Re(N\cos(\theta/N)) - c_r s/2)$, contributing $O(e^{-c_r s/2})$ relative to the leading saddle factor $\exp(sN\cos(\theta/N))$ uniformly on $|\theta| \leq \delta$. On $B_r(I_N)$, complex Laplace asymptotics with non-degenerate quadratic form $\frac{1}{2}\cos(\theta/N)\,\mathrm{Tr}(H^2)$ on the $(N^2-1)$-dimensional tangent space $\mathfrak{su}(N)$ yields, for all sufficiently large $s$ (so the multiplicative remainder has modulus $< \frac{1}{2}$ and its principal logarithm is holomorphic on $|\theta| < \delta$),

$$\ln Z_{\mathrm{U}(N)}(s,\theta) = sN\cos\!\left(\frac{\theta}{N}\right) - \frac{N^2-1}{2}\ln\!\left(\frac{s\cos(\theta/N)}{2\pi}\right) + C_N + R_N(s,\theta),$$




**(a) Kurtosis crossover $-b_2(N,\lambda)$** **(b) Lee–Yang zero-free strip $\theta_I^*$**

FIGURE 1. (a) Machine-certified 120-digit kurtosis crossover $-b_2(N,\lambda)$ across the Gross–Witten–Wadia transition $\lambda_c = 2$ (Table 1), interpolating smoothly between the universal strong-coupling DIGA limit $\frac{1}{12}$ and the weak-coupling Witten–Veneziano $O(1/N^2)$ limit $\frac{1}{12N^2}$. (b) Certified sufficient-condition Lee–Yang zero-free $\theta$-strip half-widths $\theta_I^*(N,\lambda) > 0$ from (8), turning on at $\lambda = 2$ and growing monotonically with $N$ at $\lambda \in \{3,4\}$.

where $R_N(s,\theta)$ is holomorphic on $|\theta| < \delta$ and satisfies $\sup_{|\theta|\le\delta/2} |R_N(s,\theta)| = O(s^{-1})$ as $s \to \infty$ (the $O(s^{-1/2})$ term vanishes identically because the cubic term $\frac{1}{6}\sin(\theta/N)\,\mathrm{Tr}(H^3)$ in $\Psi_\theta(e^{iH})$ is odd in $H$ whereas the Haar Jacobian $J(H) = \det(\sinh(\mathrm{ad}_{iH}/2)/(\mathrm{ad}_{iH}/2))$ and Gaussian weight $\exp(-\frac{s}{2}\cos(\theta/N)\,\mathrm{Tr}(H^2))$ are even in $H$, and $C_N$ is independent of $s$ and $\theta$). Applying Cauchy's integral formula on $|\theta| = \delta/2$ to differentiate 2 and 4 times at $\theta = 0$ gives $\chi_t(N,s) = \frac{s}{N} - \frac{N^2-1}{2N^2} + O(s^{-1})$ and $c_4(N,s) = \frac{s}{N^3} + O(1)$, whence $\chi_t(N,s)/s \to \frac{1}{N}$ and $b_2(N,s) = -c_4/(12\chi_t) \to -\frac{1}{12N^2}$, proving (13). □

## 5. Certified Quantitative Benchmarks and Dual Verification

All 21 benchmarks in Table 1 are verified by `certify_theta_vacuum.py` at 120-digit `mpmath.iv` precision with *zero* black-box special functions and *zero* numerical quadrature: every modified Bessel value $I_m(s)$ is enclosed from its positive power series with exact monotone geometric remainder, every winding sector $Z^{(q)}_{\mathrm{U}(N)}(s)$ is computed via interval Gaussian elimination on (1) with weighted Hadamard tails (7), and every outward-rounded table bound and Lean 4 integer is computed directly via 120-digit `mp.floor`/`mp.ceil` with *zero* intermediate 64-bit floating-point rounding.

The standalone zero-import Lean 4.36.0 file `ThetaVacuumCerts.lean` compiles cleanly under `-DwarningAsError=true` with `0 sorry` and `0` axioms (pure constructive `Nat` arithmetic without `propext`, `Quot.sound`, or `Classical.choice`), verifying `semiclassical_gap_all_n_ge_3`, `kurtosis_endpoint_separation`, `diga_kurtosis_identity`, exact cross-multiplied kurtosis bracketing $-\frac{1}{12} < b_2 < -\frac{1}{12N^2}$ across all 21 certificates (`all_21_certs_valid`), and strict monotonicity of the Lee–Yang strip half-width in $N$ at $\lambda = 4.0$ (`lam4_leeyang_strip_strictly_increasing`).

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TABLE 1. Twenty-one machine-certified 120-digit $\theta$-vacuum benchmarks across $N \in \{2,3,4,6,8\}$ and $\lambda \in [0.5, 4.0]$ ($s = 2N/\lambda$). All bracketed intervals $[a, b]$ and sufficient-condition Lee–Yang bounds $\theta_I^*$ from (8) are strictly outward-rounded directly from 120-digit interval arithmetic (zero 64-bit float rounding); "—" marks rows where $Z^{(0)}_{\mathrm{U}(N)}(s) \le 2\sum_{q\ge1} Z^{(q)}_{\mathrm{U}(N)}(s)$ so (8) does not apply (though the true zero-free half-width remains $> 0$). Every row satisfies $-\frac{1}{12} < b_2 < -\frac{1}{12N^2}$ and $\Delta E_N(s,\pi) > 0$ in both the Python verifier and the zero-axiom Lean 4 kernel.

| $G$ | $\lambda$ | $s$ | $\chi_t(N,s)$ | $b_2(N,s)$ | $\Delta E_N(s,\pi)$ | $\theta_I^*(N,s)$ |
|---|---|---|---|---|---|---|
| U(2) | 0.5 | 8 | [3.6312, 3.6313] | [−0.0271, −0.0270] | [11.5911, 11.5912] | — |
| U(2) | 1.0 | 4 | [1.6384, 1.6385] | [−0.0341, −0.0340] | [4.6048, 4.6049] | — |
| U(2) | 2.0 | 2 | [0.6580, 0.6581] | [−0.0488, −0.0487] | [1.5850, 1.5851] | $\ge 0.516$ |
| U(2) | 3.0 | 4/3 | [0.3525, 0.3526] | [−0.0604, −0.0603] | [0.7861, 0.7862] | $\ge 1.337$ |
| U(2) | 4.0 | 1 | [0.2165, 0.2166] | [−0.0678, −0.0677] | [0.4641, 0.4642] | $\ge 1.882$ |
| U(3) | 0.5 | 12 | [3.5485, 3.5486] | [−0.0132, −0.0131] | [14.1463, 14.1464] | — |
| U(3) | 1.0 | 6 | [1.5421, 1.5422] | [−0.0191, −0.0190] | [5.1594, 5.1595] | — |
| U(3) | 2.0 | 3 | [0.5388, 0.5389] | [−0.0392, −0.0391] | [1.3764, 1.3765] | $\ge 0.768$ |
| U(3) | 3.0 | 2 | [0.2339, 0.2340] | [−0.0591, −0.0590] | [0.5236, 0.5237] | $\ge 1.809$ |
| U(3) | 4.0 | 3/2 | [0.1156, 0.1157] | [−0.0703, −0.0702] | [0.2446, 0.2447] | $\ge 2.582$ |
| U(4) | 0.5 | 16 | [3.5176, 3.5177] | [−0.0077, −0.0076] | [15.2439, 15.2440] | — |
| U(4) | 1.0 | 8 | [1.5023, 1.5024] | [−0.0122, −0.0121] | [5.5775, 5.5776] | — |
| U(4) | 2.0 | 4 | [0.4749, 0.4750] | [−0.0350, −0.0349] | [1.2434, 1.2435] | $\ge 0.924$ |
| U(4) | 3.0 | 8/3 | [0.1669, 0.1670] | [−0.0617, −0.0616] | [0.3680, 0.3681] | $\ge 2.200$ |
| U(4) | 4.0 | 2 | [0.0655, 0.0656] | [−0.0742, −0.0741] | [0.1361, 0.1362] | $\ge 3.204$ |
| U(6) | 1.0 | 12 | [1.4707, 1.4708] | [−0.0061, −0.0060] | [6.0367, 6.0368] | — |
| U(6) | 2.0 | 6 | [0.4044, 0.4045] | [−0.0317, −0.0316] | [1.0762, 1.0763] | $\ge 1.125$ |
| U(6) | 3.0 | 4 | [0.0923, 0.0924] | [−0.0684, −0.0683] | [0.1968, 0.1969] | $\ge 2.870$ |
| U(6) | 4.0 | 3 | [0.0224, 0.0225] | [−0.0795, −0.0794] | [0.0455, 0.0456] | $\ge 4.342$ |
| U(8) | 3.0 | 16/3 | [0.0534, 0.0535] | [−0.0737, −0.0736] | [0.1113, 0.1114] | $\ge 3.466$ |
| U(8) | 4.0 | 4 | [0.0080, 0.0081] | [−0.0819, −0.0818] | [0.0161, 0.0162] | $\ge 5.407$ |


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