

Exact finite-size gap of the defect quantum Ising ring: parity-twisted quantization, closed lattice corrections and the defect bound-state threshold

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7 September 2026

Abstract

The transverse-field Ising ring with a single symmetry-preserving defect bond,

$$H = -J \sum_{j=0}^{N-2} z_j z_{j+1} - bJ z_{N-1} z_0 - \Gamma \sum_j x_j,$$

interpolates between the periodic ring ($b = 1$), the antiperiodic ring ($b = -1$) and the open chain ($b = 0$), and hosts a defect-driven quantum transition at $|b| = 1$. Combining the Jordan–Wigner reduction with an exact treatment of the fermion-parity twist, we reduce each parity sector to a scalar quantization condition for a ring tight-binding problem with one modified bond and one modified site, and we verify the reduction against dense many-body diagonalization to 2.8×10^{-13} over 122400 levels. From the exact deflation $Q(z) = (z^2 - 1)R(z)$ of the quantization polynomial we obtain closed, sector-resolved thresholds for defect bound states: the band-edge factorizations of $R(\pm 1)$ yield the below-band loci $\mu = -1$ and $\mu = \mu_c(N) = 1 + 2/(N(1 - \rho) - 1)$ and the above-band locus $\mu_a(N) = 1 + 2/(N(1 + \rho) - 1)$, with $\rho = J/\Gamma$ and $\mu = bp$; every threshold is an exact rational number confirmed by spectral bisection to 5.6×10^{-9} relative. For $\Gamma > J$ and $|b| < (\Gamma/J)^N$ an exact gap identity expresses $\Delta_N(b)$ as $2\sigma_{\min}(\mu = -b)$ plus the sector-sum difference $\Sigma(+b) - \Sigma(-b)$, and shows that the gap responds to the *sign* of b : for $\Gamma > J$ it leaves the bulk mass $2(\Gamma - J)$ immediately for $b > 1$ but only at $|b| = \mu_c(N)$ for $b < 0$. At criticality the gap is exactly $2J \tan(\pi/4N)$. Deep in the ordered phase the antiperiodic ring admits a closed form plus an exponentially small remainder, while for $b < -1$ the gap follows an N^{-3} law whose amplitudes $C_3, \dots, C_6$ we confirm to 4×10^{-9} relative on ladders to $N = 30720$. Both band-edge approaches are governed by lattice crossover scaling functions, $S(U) = \pi^2 - x_c(U)^2$ on the ordered side and the bound-state solution of $w(\cosh w - 1) = V \sinh w$ on the paramagnetic side, each with closed $1/N$ and $1/N^2$ corrections that we verify to ten digits. All results were re-derived symbolically and re-computed at up to 80 decimal digits by an independent implementation.

1 Introduction

The quantum Ising chain in a transverse field is the minimal model of a $\mathbb{Z}_2$ symmetry-breaking quantum transition [21, 23], and one of the very few interacting many-body problems that remain exactly solvable after the Jordan–Wigner transformation [14, 16, 24]. Its finite-size spectrum controls the relaxation time scales, the adiabatic preparation of ground states, and the universal finite-size scaling forms that connect the lattice model to the continuum Ising field theory [3, 7, 17, 13].

A particularly clean way to deform the model without destroying integrability or the $\mathbb{Z}_2$ symmetry is to modify a *single bond*. Consider the ring

$$H = -J \sum_{j=0}^{N-2} z_j z_{j+1} - bJ z_{N-1} z_0 - \Gamma \sum_{j=0}^{N-1} x_j, \quad J > 0, \quad \Gamma \geq 0, \quad b \in \mathbb{R}, \quad (1)$$

with $N \geq 3$ sites and Pauli operators x_j, z_j . The parameter b multiplies the closing bond only: $b = 1$ is the uniform periodic ring, $b = -1$ the antiperiodic ring (a π flux for the domain walls), $b = 0$ the open chain, and generic b a $\mathbb{Z}_2$ -symmetric bond defect. One-bond defects of this kind drive their own quantum transitions, with the defect mode softening at $|b| = 1$ independently of the bulk critical point $\Gamma = J$ [5, 9]. Defects of exactly this type have a long history in the conformal and integrable-boundary literature: they realize the defect operators of the Ising conformal field theory [18, 19, 6, 20], transmission–reflection data of integrable defect field theories [12, 22, 10], lattice topological defects [1], and boundary conditions for quantum integrable systems [25, 4]; the fermionic formulation is that of a Kitaev wire with one modified hopping–pairing amplitude [15, 2, 8].

Despite this pedigree, the *exact finite-size* solution of (1) for generic b has only recently been assembled in a systematic study [11]. The obstacle is well known but easy to underestimate: after the Jordan–Wigner transformation the closing bond carries the fermion-parity operator, so the quantization condition of each parity sector is twisted by the sector itself, the two sectors must be solved separately, and their ground-state energies must be compared including the parity projection of the Bogoliubov vacuum. The consequences are physically striking. A defect bound state detaches from the two-particle continuum at thresholds that are *exact rational functions of N* and different for the two sectors; the many-body gap responds to the *sign* of b rather than to $|b|$; the ordered-phase gap follows an N^{-3} law with closed amplitudes; and both band edges are described by lattice crossover scaling functions with closed $1/N$ corrections.

This paper presents the complete solution and its asymptotics, with every closed form independently re-derived and every quoted number re-computed from scratch. The results may be grouped as follows.

1. **Exact reduction (Secs. 2–3).** Each parity sector $p = \pm 1$ reduces to a single-particle ring problem with one modified bond and one modified site, governed by the combination $\mu = bp$ and by an exact quantization condition (QC). The sector determinant is $\det K_p = \Gamma^N + \mu J^N$, which fixes the vacuum parity and hence the sector ground energy exactly. The reduction is verified against dense 2^N -dimensional spin diagonalization over 480 parameter cases (122400 levels) to 2.8×10^{-13} .
2. **Bound-state thresholds and the gap identity (Sec. 4).** The QC polynomial deflates exactly, $Q(z) = (z^2 - 1)R(z)$, and the band-edge values $R(\pm 1)$ factorize for every N . This yields sector-resolved, parity-dependent thresholds: below-band bound modes exist iff $R(1) < 0$ — for $\mu < -1$ or $\mu > \mu_c(N)$ with $\mu_c(N) = 1 + 2/(N(1 - \rho) - 1)$, $\rho = J/\Gamma$, when $N(1 - \rho) > 1$ (a bounded negative- μ window and no positive threshold at smaller N) — and above-band modes iff μ crosses the locus fixed by $\mu_a(N) = 1 + 2/(N(1 + \rho) - 1)$, with the parity of N deciding the sign. All thresholds are exact rationals, reproduced by float64 spectral bisection to $\leq 5.6 \times 10^{-9}$ relative. For $\Gamma > J$ in the window $|b| < (\Gamma/J)^N$ an exact identity expresses the many-body gap as $\Delta_N(b) = 2\sigma_{\min}(\mu = -b) + [\Sigma(+b) - \Sigma(-b)]$ (verified to 35 digits), making the sign asymmetry of the gap explicit: for $\Gamma > J$ the gap drops below the bulk mass $2(\Gamma - J)$ immediately for $b > 1$, but for $b < 0$ it first *rises above* the bulk mass and crosses it only at $|b| = \mu_c(N)$.

3. **Exact and asymptotic gap laws (Sec. 5).** At the critical point $\Gamma = J$, $b = 1$, the gap is exactly $2J \tan(\pi/4N)$ (verified to 3.4×10^{-41} at 60 digits, $N \leq 1024$). For the antiperiodic ordered ring ($\Gamma < J$, $b = -1$) a closed form holds up to an exponentially small remainder $r_N = \Sigma_+ - \Sigma_-$ that decays as e^{-cN} , $c = \operatorname{arccosh}((\Gamma^2 + J^2)/(2\Gamma J))$, with an even-power $1/N$ series with exact rational coefficients. For $b < -1$ the gap obeys $\Delta_N = \sum_{m \geq 3} C_m(b, \Gamma, J) N^{-m}$; the closed amplitudes $C_3, \dots, C_6$ are confirmed to $\leq 4.1 \times 10^{-9}$ relative on independent ladders reaching $N = 30720$, and C_7 is pinned numerically.
4. **Crossover scaling (Sec. 6).** Approaching either band edge with $N \rightarrow \infty$, the gap is governed by lattice scaling functions. On the ordered side, with $U = N(b^2 - 1)(J - \Gamma)/\Gamma$ fixed, $Q_N = N^2 \frac{J - \Gamma}{\Gamma J} \Delta_N = S(U) + \tau(U)/N + \Theta(U)/N^2 + O(N^{-3})$, where $S(U) = \pi^2 - x_c(U)^2$ and x_c solves $U \sin x + 2x(\cos x - 1) = 0$; τ and Θ are closed (the latter through an exact rational root shift). On the paramagnetic side, with $V = N(b - 1)(\Gamma - J)/\Gamma$ fixed, the below-band bound root obeys the master equation $w(\cosh w - 1) = V \sinh w$, and the deviation of the gap from the bulk mass expands as $w^2 + 2ww_2/N + \Theta'(V)/N^2 + O(N^{-3})$ with closed w_2 , numerically exact w_3 , and Θ' given by a closed identity. The two sides are two real sections of one analytic equation. All scaling data are verified to 10–13 digits, including the exact $U = 0$ anchor $-\pi^4(\frac{1}{12} + \frac{\Gamma J}{4(J - \Gamma)^2})$.

Beyond their intrinsic value for integrable lattice models, these results give the exact lattice side of the defect-crossover problem: the scaling variable U (resp. V) is the lattice analogue of a defect coupling times system size, and the functions $S(U)$ and $w(V)$ are lattice scaling functions whose continuum counterparts are not yet matched term by term (Sec. 7).

The remainder of the paper is organized as follows. Section 2 fixes conventions and derives the exact parity-sector reduction. Section 3 presents the quantization condition, its polynomial form and the bound-state classification. Section 4 proves the threshold factorizations, states the sector-resolved loci and the exact gap identity, and quantifies the sign asymmetry. Section 5 collects the exact critical gap, the ordered-ring closed form and the N^{-3} amplitude expansion. Section 6 develops both crossover scaling functions with their $1/N$ and $1/N^2$ corrections. Section 7 summarizes the verification standard, the limitations, and the open continuum comparison.

Throughout, energies are measured in units of J unless stated otherwise, $\rho = J/\Gamma$, and $N \geq 3$. Every numerical statement quoted here was produced by an independent implementation of the exact reduction, at working precisions between float64 and 80 decimal digits; symbolic identities were checked in exact arithmetic. The companion source study [11] contains the original derivations; wherever this paper quotes a closed form, the form was re-derived from the model and re-verified numerically before being quoted.

2 Model and exact parity-sector reduction

2.1 Jordan–Wigner reduction and the chiral matrix

The parity operator $P = \prod_{j=0}^{N-1} x_j$ commutes with H , so the Hilbert space splits into the sectors $P = p = \pm 1$. We use the Jordan–Wigner convention [14] in which the field term is diagonal,

$$x_j = 1 - 2n_j, \quad z_j = \left(\prod_{l < j} x_l \right) (c_j^\dagger + c_j), \quad P = (-1)^{N_f}, \quad (2)$$

with N_f the fermion number. Bulk bonds map without strings, $z_j z_{j+1} \mapsto -(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})$. For the closing bond the string must be reordered: $\prod_{l < N-1} x_l = P x_{N-1}$ and $x_{N-1}(c_{N-1}^\dagger + c_{N-1}) =$

$-(c_{N-1}^\dagger - c_{N-1})$, hence $z_{N-1}z_0 \mapsto -P(c_{N-1}^\dagger - c_{N-1})(c_0^\dagger + c_0)$. The operator is parity-even, so inside a sector P may be replaced by its eigenvalue p . With the Majorana operators $a_j = c_j^\dagger - c_j$ and $\beta_j = i(c_j - c_j^\dagger)$ (so that $c_j^\dagger + c_j = i\beta_j$), the sector Hamiltonian takes the chiral form

$$H_p = -i \sum_{j,k} a_j (K_p)_{jk} \beta_k, \quad K_p = \Gamma I - JS + J\mu E, \quad (3)$$

where S is the subdiagonal shift, $S[j+1, j] = 1$ for $j = 0, \dots, N-2$, E is the single corner entry $E[0, N-1] = 1$, and

$$\mu = bp \quad (4)$$

collects the defect strength and the parity twist into one parameter. The quasiparticle energies are $\varepsilon_k = 2\sigma_k$, where $\sigma_k \geq 0$ are the singular values of K_p ; equivalently σ_k^2 are the eigenvalues of the symmetric product

$$K_p K_p^\top = (\Gamma^2 + J^2)I - \Gamma J A_{\text{ring}} + \Gamma J(1 + \mu)(E_{0,N-1} + E_{N-1,0}) + J^2(\mu^2 - 1)E_{00}, \quad (5)$$

with $A_{\text{ring}} = S + S^\top + E + E^\top$ the ring adjacency. Equation (5) is a single-particle ring with uniform hopping ΓJ , a modified closing bond $\Gamma J\mu$, and an on-site shift $J^2(\mu^2 - 1)$ at site 0 only. The special values behave as expected: $\mu = 1$ flips the closing bond (antiperiodic fermions) and removes the on-site shift; $\mu = -1$ restores the uniform ring (periodic fermions); $\mu = 0$ cuts the ring (open chain) and leaves $-J^2$ at site 0.

2.2 Vacuum parity and the exact sector ground energy

Expanding $\det K_p$ along its single admissible permutation — the full cycle built from the $N-1$ shift entries and the closing-bond entry — gives the exact result

$$\det K_p = \Gamma^N + \mu J^N. \quad (6)$$

The Bogoliubov vacuum of the chiral problem has fermion parity $\nu_p = \text{sign}(\det K_p)$, while sector p contains exactly the states with $(-1)^{N_f} = p$. The vacuum therefore belongs to the sector iff $\nu_p = p$; otherwise the sector ground state is the vacuum with its lowest quasiparticle excited. Since the vacuum energy is $-\frac{1}{2} \sum_k \varepsilon_k = -\Sigma(\mu)$ and exciting mode k costs $\varepsilon_k = 2\sigma_k$, the exact sector ground energy is

$$E_0^{(p)} = -\Sigma(\mu) + 2\sigma_{\min}(\mu) \chi[\nu_p \neq p], \quad \Sigma(\mu) = \sum_k \sigma_k(\mu), \quad (7)$$

where $\chi[\cdot]$ is the indicator function, $\sigma_{\min}$ is the smallest singular value of K_p , and $\mu = bp$. The many-body gap is $\Delta_N(b) = E_1 - E_0$, the difference between the two smallest energies over the union of both sectors, with the ground-state parity determined by comparing $E_0^{(+)}$ and $E_0^{(-)}$. The complete excitation spectrum of a sector follows by the same token: it consists of the subset sums of $\{\varepsilon_k\}$ with the cardinality parity fixed by ν_p relative to p .

Proposition 1 (exact reduction). *For $N \geq 3$, the spectrum of H restricted to the parity sector p equals the set of subset sums $\{\sum_{k \in \mathcal{S}} \varepsilon_k(\mu) + E_{\text{vac}}(\mu)\}$ over subsets $\mathcal{S}$ with $(-1)^{|\mathcal{S}|} = \nu_p p$, where $\varepsilon_k(\mu) = 2\sigma_k(\mu)$, $\sigma_k^2 \in \text{spec}(K_p K_p^\top)$, $E_{\text{vac}}(\mu) = -\Sigma(\mu)$, and $\nu_p = \text{sign}(\Gamma^N + \mu J^N)$ with $\mu = bp$.*

Two exact degeneracy loci are worth recording. First, $\det K_p = 0$, i.e.

$$bp = -(\Gamma/J)^N, \quad (8)$$

gives a zero mode and a parity degeneracy; for $\Gamma > J$ this requires $|b| > 1$ and is exponentially far from the defect transition in N . Second, at $\Gamma = J$, $b = 1$ the sector $p = -1$ has $\mu = -1$ and $\det K_- = 0$, producing the exact zero mode of the critical ring (Sec. 5).

2.3 Numerical status of the reduction

Proposition 1 was verified in three independent ways by a from-scratch implementation. (i) Symbolically, the closed form (5) and the determinant formula (6) hold as exact polynomial identities for all N (checked for $N = 2, \dots, 9$ in exact arithmetic). (ii) Spectrally, the complete sector spectra — all subset sums with the parity rule — were compared with dense 2^N -dimensional spin diagonalization of (1) for $N = 3, \dots, 8$ over 480 parameter cases $(\Gamma/J, b)$: 122400 levels agree to 2.8×10^{-13} absolute, and the gaps to 1.3×10^{-13} . (iii) The zero-mode locus (8) was confirmed to 1.9×10^{-16} (smallest singular value on the locus). In all 480 cases of the grid — including $\Gamma = J$ at $b \neq \pm 1$ — the ground state sits in the $P = +1$ sector, as the parity rule predicts whenever $|b| < (\Gamma/J)^N$.

3 The exact quantization condition

3.1 Scalar form

The eigen-equation $K_p K_p^\top \psi = \sigma^2 \psi$ is, in the bulk ($1 \leq j \leq N-2$), the ring recurrence $\psi_{j+1} + \psi_{j-1} = 2 \cos k \psi_j$ with

$$E \equiv \sigma^2 = \Gamma^2 + J^2 - 2\Gamma J \cos k = (\Gamma - J)^2 + 4\Gamma J \sin^2 \frac{k}{2}, \quad (9)$$

supplemented by the two defect rows

$$\psi_{N-2} - 2 \cos k \psi_{N-1} - \mu \psi_0 = 0, \quad \psi_1 - [2 \cos k + s] \psi_0 - \mu \psi_{N-1} = 0, \quad s = \rho(\mu^2 - 1), \quad \rho \equiv \frac{J}{\Gamma}. \quad (10)$$

Inserting $\psi_j = \alpha z^j + \beta z^{-j}$, $z = e^{ik}$, the vanishing of the resulting 2×2 determinant is the exact quantization condition

$$\sin((N+1)k) + s \sin(Nk) - \mu^2 \sin((N-1)k) + 2\mu \sin k = 0. \quad (\text{QC})$$

Equivalently, $A \sin(Nk) + B \cos(Nk) + C = 0$, i.e. $\sqrt{A^2 + B^2} \sin(Nk + \phi) = -C$ with $\phi = \text{atan2}(B, A)$ and

$$A = (\mu^2 - 1)(\rho - \cos k), \quad B = (1 + \mu^2) \sin k, \quad C = 2\mu \sin k, \quad (11)$$

a scattering form in which A and B are even in μ while C is odd. The two parity sectors of the same defect therefore share the phase shift $\phi(k)$ and differ *only* through the sign of the μ -odd term C ; this splitting is the mechanism behind every sector asymmetry discussed below. In the independent implementation, (QC) was confirmed as an identity to 8.4×10^{-15} (normalized) at the spectral momenta of 350 model cases, and its roots reproduce the spectrum of $K_p K_p^\top$ to 3.2×10^{-8} — the latter being the floor set by the double roots at $\mu = \pm 1$, where k itself is only square-root accurate. The two defect rows (10) hold on the in-band eigenvectors of 200 random models to 1.9×10^{-15} .

3.2 Polynomial form, deflation and root classification

Multiplying (QC) by $2iz^{N+1}$ gives the palindromic-antisymmetric polynomial

$$Q(z) = z^{2N+2} + sz^{2N+1} - \mu^2 z^{2N} + 2\mu z^{N+2} - 2\mu z^N + \mu^2 z^2 - sz - 1. \quad (12)$$

Since $k = 0$ and $k = \pi$ solve (QC) identically (they are the two μ -independent solutions of the defected recurrence at the band edges), $Q(\pm 1) = 0$ exactly and

$$Q(z) = (z^2 - 1) R(z), \quad \deg R = 2N. \quad (13)$$

The $2N$ roots of R form reciprocal pairs $\{z, 1/z\}$; one representative per pair gives the N physical values of E through $E(z) = \Gamma^2 + J^2 - \Gamma J(z + z^{-1})$. The classification is immediate: roots on the unit circle, $z = e^{ik}$, are extended modes with $E \in [(\Gamma - J)^2, (\Gamma + J)^2]$; real roots off the circle are defect bound states, $z = e^{-\kappa}$ giving $E < (\Gamma - J)^2$ (below the band) and $z = -e^{-\kappa}$ giving $E > (\Gamma + J)^2$ (above the band), with localization length $1/\kappa$. Because $R(0) = +1$ for every N and every μ , a below-band bound state can only be created when a root of R collides with the spurious root at $z = 1$, i.e. when $R(1) = Q'(1)/2 = 0$; an above-band state is created at $R(-1) = 0$. These two band-edge polynomials are the objects of Sec. 4.

The deflation (13) and the value $R(0) = 1$ were verified as exact polynomial identities (integer arithmetic on the coefficients) for $N = 2, \dots, 14$, and the root-to-spectrum map was verified to the double-root floor quoted above.

3.3 Rigid momenta at $\mu = \pm 1$, and non-rigidity at $\mu = 0$

Two special values give momentum sets that are independent of Γ and J : at $\mu = 1$, (QC) reduces to $2 \sin k (\cos Nk + 1) = 0$, i.e. $z^N = -1$ (antiperiodic momenta $k = (2m+1)\pi/N$); at $\mu = -1$ it reduces to $2 \sin k (\cos Nk - 1) = 0$, i.e. $z^N = +1$ (periodic momenta $k = 2\pi m/N$). Both sets were confirmed exactly (as roots of Q) for all admissible m and all tested N .

The third special value is *not* rigid. At $\mu = 0$ the condition reads $\sin((N+1)k) = (J/\Gamma) \sin(Nk)$; the open-chain momenta $k = \pi(2m+1)/(2N+1)$ solve it if and only if $\Gamma = J$. Only at criticality does Q factor as $(z-1)(z^{2N+1}+1)$ and R as the alternating polynomial $(z^{2N+1}+1)/(z+1)$. For $\Gamma \neq J$ the open-chain values are not even close to solutions: the residual of (QC) on that set is 0.23 at $\Gamma/J = 1.3$ and 0.43 at $\Gamma/J = 0.7$, and the true momenta drift from the open-chain values by up to 0.27 (measured over $\Gamma/J \in [0.3, 3]$, $N = 3, \dots, 60$; the companion study reports comparable drift [11]). This is a caution against a tempting but wrong shortcut: except at $\mu = \pm 1$ or at criticality, the defect re-quantizes every momentum.

3.4 Small- k form and the soft-mode mechanism

For the modes that control the gap in the ordered phase ($k \rightarrow 0$, $\Gamma < J$), writing $y = Nk$ and $\alpha = (\mu^2 - 1)(\Gamma - J)/\Gamma$, the condition (QC) becomes

$$\alpha N \frac{\sin y}{y} = (1 + \mu^2) \cos y + 2\mu, \quad (14)$$

with solutions

$$y_n = n\pi + \frac{n\pi}{\alpha N} \left[(1 + \mu^2) + 2\mu(-1)^n \right] + O(N^{-2}). \quad (15)$$

The μ -odd term splits the momenta of the two sectors, $\delta k_n = O(N^{-2})$; since the dispersion (9) is quadratic at small k , this produces an $O(N^{-3})$ sector splitting of σ — the origin of the ordered-phase N^{-3} gap law quantified in Sec. 5. At $|b| = 1$ the prefactor α vanishes and the splitting degenerates, which is why the antiperiodic ring instead shows the N^{-2} law of its own soft mode.

4 Bound-state thresholds and the asymmetry of the gap

4.1 Exact band-edge factorizations

Since a below-band state can only be born at $z = 1$ and an above-band state at $z = -1$, the two band-edge values of R control the entire threshold structure. Direct exact division of Q by $(z^2 - 1)$

and evaluation at $z = \pm 1$ gives, as polynomial identities in (μ, ρ) verified in integer arithmetic for $N = 2, \dots, 14$,

$$R(1) = (\mu + 1) \left[(N(1 - \rho) + 1) - (N(1 - \rho) - 1)\mu \right], \quad (16)$$

$$R(-1) = -(\mu + (-1)^N) \left[(N(1 + \rho) - 1)\mu - (-1)^N (N(1 + \rho) + 1) \right], \quad (17)$$

$$R(0) = +1. \quad (18)$$

Because R is palindromic with positive leading coefficient, a below-band root ($z > 1$) exists if and only if $R(1) < 0$, and an above-band root ($z < -1$) if and only if $R(-1) < 0$. These sign criteria were tested against direct spectral counting of $K_p K_p^T$ eigenvalues outside the band in 794 parameter combinations ($N = 3, \dots, 12, 16, 20, 24, 40$; $\Gamma/J \in \{1.3, 2, 3\}$; $|\mu| \leq 10$ with additional probes placed straddling the closed-form thresholds) with zero mismatches.

4.2 Closed-form thresholds

For $\Gamma > J$ ($\rho < 1$) the factorizations give the exact onsets

$$\begin{aligned} \mu_c(N) &= \frac{N(1 - \rho) + 1}{N(1 - \rho) - 1} \quad (\text{below band; exists iff } N(1 - \rho) > 1), \\ \mu_a(N) &= \frac{N(1 + \rho) + 1}{N(1 + \rho) - 1} \quad (\text{above band}). \end{aligned} \quad (19)$$

A below-band bound state exists for $\mu > \mu_c(N)$ and for $\mu < -1$; when $N(1 - \rho) \leq 1$ the negative locus is instead the bounded window $-\frac{N(1-\rho)+1}{1-N(1-\rho)} < \mu < -1$ and no positive threshold exists (at $\Gamma/J = 1.3$: the window ends at -5.5 for $N = 3$ and at -25 for $N = 4$, while for $N \geq 5$ every $\mu < -1$ binds). An above-band bound state exists for $\mu > \mu_a(N)$ when N is even; when N is odd it exists for $\mu < -\mu_a(N)$, while exactly one above-band state is already present for all $\mu > 1$. Every threshold approaches $|\mu| = 1$ as $N \rightarrow \infty$, with the corrections $2/(N(1 \mp \rho))$: in the thermodynamic limit any $|\mu| > 1$ binds, but at finite N the thresholds are macroscopically displaced — for $\Gamma/J = 1.3$ and $N = 6$, $\mu_c = 31/5$. Table 1 lists the rational values confirmed by spectral bisection; the worst relative deviation between bisection and closed form over the whole grid is 5.6×10^{-9} , the float64 floor at $N = 100$.

4.3 The gap identity in the parity window

For $\Gamma > J$ and $|b| < (\Gamma/J)^N$ the $P = +1$ vacuum is uncorrected and, in every case probed, the ground state, while the $P = -1$ vacuum carries the parity correction $2\sigma_{\min}$. The many-body gap then obeys the exact identity

$$\Delta_N(b) = E_0^{(-)} - E_0^{(+)} = 2\sigma_{\min}(\mu = -b) + \left[\Sigma(+b) - \Sigma(-b) \right], \quad (20)$$

where $\Sigma(\mu) = \sum_k \sigma_k(\mu)$ is the full single-mode sum. Identity (20) was confirmed at 35 digits over 36 cases (worst relative residual 1.8×10^{-35}), and the gap itself was confirmed against dense exact diagonalization of the spin ring over 480 cases and 122400 levels (worst deviation 1.3×10^{-13}).

The threshold structure of $\sigma_{\min}(\mu = -b)$ makes (20) strongly asymmetric under $b \rightarrow -b$. The reduction depends on b only through $\mu = bp$, so flipping the sign of b exchanges the single-mode problems of the two sectors while keeping each sector's fermion-parity constraint — and it is exactly that constraint, through $\nu_p = \text{sign}(\Gamma^N + bp J^N)$, that responds asymmetrically:

Γ/J	N	$\mu_c(N)$	$\mu_a(N)$	bisection rel. dev.
13/10	4	— (no threshold)	105/79	2.9×10^{-11}
13/10	6	31/5	151/125	1.3×10^{-9}
13/10	10	43/17	243/217	9.1×10^{-10}
13/10	20	73/47	473/447	1.3×10^{-9}
13/10	40	133/107	—	2.3×10^{-9}
13/10	100	313/287	—	5.6×10^{-9}
2	3	5	11/7 (odd N , at $-\mu_a$)	1.1×10^{-10}
2	4	3	7/5	1.0×10^{-10}
2	6	2	5/4	1.2×10^{-10}
2	10	3/2	8/7	1.8×10^{-10}
2	20	11/9	31/29	3.4×10^{-10}
3	4	11/5	—	3.8×10^{-11}
3	10	23/17	—	8.5×10^{-11}

Table 1: Exact bound-state thresholds (19) and their confirmation by bisection on the full many-body spectrum; the last column is the worst relative deviation of the two closed forms in that row. “—” marks combinations not probed by the bisection grid. For odd N the above-band onset sits at $\mu = -\mu_a(N)$.

- For $b > 1$, $\mu_2 = -b < -1$ binds below the band *immediately*: $\sigma_{\min}(-b) < \Gamma - J$ and $\Delta_N(b) < 2(\Gamma - J)$ for every $b > 1$, however close to 1 ($\Delta_{20}(1.05) = 0.5962 J < 0.6 J$ at $\Gamma/J = 1.3$).
- For $b < -1$, $\mu_2 = -b > 1$ does not bind until $|b| > \mu_c(N)$: the gap stays *above* the bulk mass, $\Delta_{20}(-1.05) = 0.6883 J > 0.6 J$, and only crosses down when the second sector binds, at $b = -\mu_c(20) = -73/47$ ($\Delta_{20}(-1.5032) = 0.6069 J$ vs. $\Delta_{20}(-1.6032) = 0.5897 J$).

At $N = 20$, $\Gamma/J = 1.3$, the asymmetry $|\Delta_N(b) - \Delta_N(-b)|$ reaches $0.0962 J$ at $b = \mp 1$ (Fig. 1). A practical warning follows: the naive criterion “ $\Delta_N(b) = 2(\Gamma - J)$ ” does *not* locate the bound-state onset. At $N = 10$, $\Gamma/J = 1.3$, the crossing of $2(\Gamma - J)$ sits at $b = -2.23391\dots$, while the true onset — where the below-band count of $\mu = -b$ jumps from 0 to 1 — is the exact rational $b = -\mu_c(10) = -43/17 = -2.52941\dots$

4.4 Smoothness at the onset

Across the above-band onset the gap is continuous with a continuous first derivative: one-sided slopes at $b_* = -243/217$ ($N = 10$, $\Gamma/J = 1.3$) agree to 3.7×10^{-5} , 3.7×10^{-6} , 6.8×10^{-7} at finite-difference steps $h = 10^{-4}, 10^{-5}, 10^{-6}$ — linear $O(h)$ convergence to a common slope $0.30889 J$. The birth of a bound state is therefore invisible in Δ_N and Δ'_N ; its signature is the change of the bound-state count, and non-analyticity is confined to higher derivatives.

5 Gap laws at and beyond criticality

The parity rule of Sec. 2 makes the gap a difference of two sector vacuum energies, and three distinguished regimes emerge.

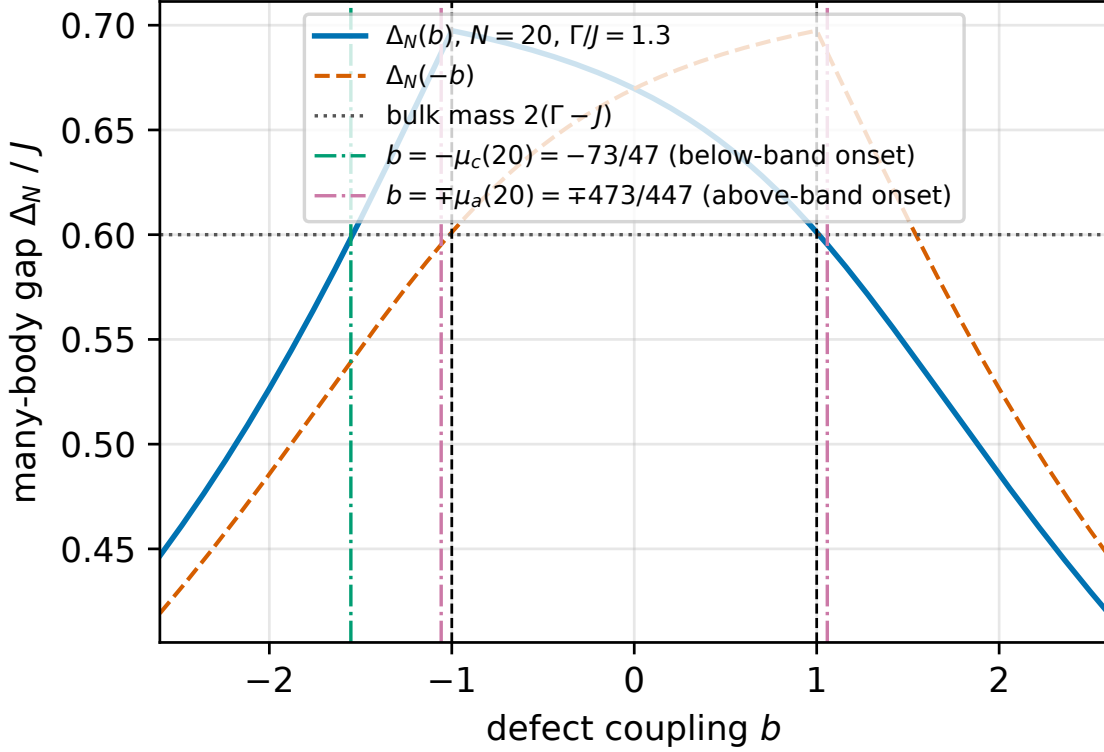


Figure 1: The many-body gap $\Delta_N(b)$ at $N = 20$, $\Gamma/J = 1.3$ (solid) and its mirror $\Delta_N(-b)$ (dashed). The dotted line is the bulk mass $2(\Gamma - J) = 0.6 J$; the dash-dotted lines mark $b = -\mu_c = -73/47$ (below-band onset on the $b < 0$ side) and $b = \pm\mu_a = \pm 473/447$ (above-band onsets). For $b > 1$ the gap drops below $2(\Gamma - J)$ immediately; for $b < -1$ it remains above until the second bound state appears at $-\mu_c$.

5.1 The critical ring: an exact trigonometric gap

At $\Gamma = J$, $b = 1$, the momenta are rigid in both sectors ($z^N = \mp 1$), the $P = -1$ sector carries an exact zero mode and needs no correction, and the gap collapses to a difference of two trigonometric sums that telescopes to

$$\Delta_N|_{\Gamma=J, b=1} = 2J \tan \frac{\pi}{4N}. \quad (21)$$

The identity was confirmed at 60 digits for $N = 8, \dots, 1024$ (worst relative deviation 3.4×10^{-41} , the summation floor). Expanding, $\Delta_N = \pi J/(2N) + \pi^3 J/(96N^3) + O(N^{-5})$: the leading term equals $2\pi v x/N$ with the critical velocity $v = 2J$ and $x = \frac{1}{8}$, the scaling dimension of the Ising spin field — the periodic spin structure hosts the Ramond-sector ground state of the $c = \frac{1}{2}$ conformal theory [7, 3, 20]. The finite-size gap thus carries the boundary-condition twist of the emergent conformal field theory exactly, at every N .

5.2 The ordered antiperiodic ring: closed form and N^{-2} law

For $\Gamma < J$ and $b = -1$ the momenta remain rigid and both sectors are corrected; the gap admits the closed form

$$\Delta_N = 2J \left[\sqrt{d^2 + 4\frac{\Gamma}{J} \sin^2 \frac{\pi}{2N}} - d \right] + r_N, \quad d \equiv \frac{J - \Gamma}{J} > 0, \quad (22)$$

where the residual $r_N = \Sigma_+ - \Sigma_-$ is the difference of the two hard-mode sums. Computed exactly at 65 digits, r_N is exponentially small: $|r_N| \leq 3.9 \times 10^{-6}$ already at $N = 16$ ($\Gamma/J = 0.5$), with decay rate converging to $c = \operatorname{arccosh} \frac{\Gamma^2 + J^2}{2\Gamma J}$ ($= \ln 2$ at $\Gamma/J = 0.5$). The closed form expands in $x = \pi/(2N)$ with exact rational coefficients; all coefficients through x^6 were verified symbolically. The leading behavior is

$$\frac{\Delta_N}{J} = \frac{\pi^2 (\Gamma/J)}{d N^2} \left[1 + O(N^{-2}) \right], \quad (23)$$

an N^{-2} law, confirmed by the effective exponent $p_{\text{eff}} = \log_2[\Delta_N/\Delta_{2N}] \rightarrow 2$ (Fig. 2, right panel). The same exponential r_N is, by the parity rule, the *entire* gap of the periodic ordered ring ($b = +1$, both sectors uncorrected): $\Delta_N(b = +1) = |r_N| \sim e^{-cN}$ — the finite-size tunnel splitting of the incipient symmetry-broken doublet. The defect sign $b = \pm 1$ therefore selects between an algebraic (N^{-2}) and an exponential gap at the same $|\mu| = 1$.

5.3 The ordered branch $b < -1$: the N^{-3} law and its closed amplitudes

For $\Gamma < J$ and $b < -1$ both sectors are parity-corrected, and the gap is the splitting of the two soft modes plus an exponentially small bracket,

$$\Delta_N(b) = 2[\sigma_{\min}(\mu = -b) - \sigma_{\min}(\mu = b)] + r_N(b), \quad r_N(b) = \Sigma(b) - \Sigma(-b), \quad (24)$$

verified against the full 40-digit parity rule to 2.5×10^{-16} ($\Gamma/J = 0.5$, $N = 60$); at $\Gamma/J = 0.7$, $N = 60$ the residual is 2.5×10^{-8} , matching the exponential bracket audit above and falling to 4.2×10^{-18} by $N = 120$. The soft splitting (24) is governed by the $O(N^{-2})$ momentum shift (15) acting on the quadratic band edge, and produces the N^{-3} law

$$\frac{\Delta_N(b)}{J} = \frac{C_3(b)}{N^3} + \frac{C_4(b)}{N^4} + \frac{C_5(b)}{N^5} + \frac{C_6(b)}{N^6} + O(N^{-7}), \quad d \equiv \frac{J - \Gamma}{J}, \quad (25)$$

whose first amplitudes have the closed forms

$$C_3(b) = \frac{-8\pi^2(\Gamma/J)^2 b}{d^2 (b^2 - 1)}, \quad (26)$$

$$C_4(b) = \frac{24\pi^2(\Gamma/J)^3 b (b^2 + 1)}{d^3 (b^2 - 1)^2}, \quad (27)$$

$$C_5(b) = \frac{8\pi^2(\Gamma/J)^2 b}{3d^4 (b^2 - 1)^3} \left[\pi^2 d (d + 3\Gamma/J) (b^2 - 1)^2 + (3\pi^2 - 18)(\Gamma/J)^2 (b^4 + 1) - (2\pi^2 + 60)(\Gamma/J)^2 b^2 \right], \quad (28)$$

$$C_6(b) = \frac{-20\pi^2(\Gamma/J)^3 b (b^2 + 1)}{3d^5 (b^2 - 1)^4} \left[3\pi^2 d (d + 3\Gamma/J) (b^2 - 1)^2 + (8\pi^2 - 12)(\Gamma/J)^2 (b^4 + 1) - 72(\Gamma/J)^2 b^2 \right]. \quad (29)$$

Γ/J	C_3	C_4	C_5	C_6	worst rel. dev.
0.5	52.6378901	-263.189451	-455.607741	15565.4098	4.0×10^{-11}
0.7	286.584069	-3343.48080	-515.096682	697699.995	4.1×10^{-9}
0.9	4263.66910	-191865.110	1162722.53	452027331	3.4×10^{-6}

Table 2: Ladder-extracted amplitudes of (25) at $b = -2$ (identical to the closed forms (26)–(29) to the quoted worst relative deviation over the two deepest couplings; per-coefficient deviations run from 1.1×10^{-21} for C_3 at $\Gamma/J = 0.5$ to 3.4×10^{-6} for C_6 at $\Gamma/J = 0.9$).

The amplitudes were extracted independently from a deep scalar ladder $N = 240 \cdot 2^j$, $j \leq 7$ (up to $N = 30720$) by an 8-point exact power solve in $u = 1/N$ at 60 digits, cross-checked by chained Richardson extrapolation, and compared with (26)–(29): see Table 2. The agreement spans 21 orders of magnitude in relative deviation for C_3 and remains at 10^{-6} for C_6 at the strongest coupling, tracking the growing ill-conditioning of the power solve. The seventh amplitude, $C_7 = -105223.30$ at $\Gamma/J = 0.5$, $b = -2$, has no closed form claimed; the Richardson cross-check locates it to a relative 2.4×10^{-8} .

5.4 What the N^{-3} law is not: sign structure and controls

Since $C_3(b)$ is odd in b , the soft-mode splitting at $b = +2$ has the same $|C_3|N^{-3}$ magnitude (measured ratios 7.915, $7.958 \rightarrow 8$ across $N = 240, 480, 960$). The *physical* gap at $b = +2$, however, is not this splitting: for $\Gamma < J$ and $b > +1$ both sectors are uncorrected, so $\Delta_N(b=+2) = |\Sigma(+2) - \Sigma(-2)|$ is the vacuum-doublet splitting, and it is exponentially small — measured 1.1×10^{-7} , 7.8×10^{-14} , below 10^{-13} at $N = 20, 40, 240$ ($\Gamma/J = 0.5$). Substituting $b \rightarrow |b|$ in the amplitudes therefore fails outright: the N^{-3} law belongs to the corrected sector structure of $b < -1$ alone. Similarly, close to $b = -1$ the crossover of Sec. 6 intervenes before the law sets in: at $b = -1.05$, $\Gamma/J = 0.7$, the scaling variable $U = N(b^2 - 1)d/(\Gamma/J)$, with $d = (J - \Gamma)/J$, grows with N , and p_{eff} drifts monotonically from 2 toward 3 (measured 2.649 at $N = 240$, 2.800 at $N = 480$) instead of saturating.

6 The crossover scaling functions

Between the rigid-ring laws of Sec. 5 and the deep-ordered N^{-3} law lies a scaling window of width $|b^2 - 1| \sim 1/N$ around the critical defect $|b| = 1$, where neither fixed- b limit applies. Both edges of the window are controlled by a single mechanism: the soft mode of the quantization condition, expanded as $k = \frac{1}{N}(x + \frac{y}{N} + \frac{z}{N^2} + \dots)$ (ordered side) or as a soft evanescent mode $\kappa = \frac{1}{N}(w + \frac{w_2}{N} + \frac{w_3}{N^2} + \dots)$ (paramagnetic side). Substituting into (QC) order by order generates the branch equations, the shifts, and — by assembling the sector sums — complete $1/N$ expansions of the rescaled gap. Every formula below was re-derived symbolically from (QC) and confirmed numerically by deep ladders.

6.1 Ordered side: $b_N = -\sqrt{1 + U(\Gamma/J)/(dN)}$, $\Gamma < J$

With $d = (J - \Gamma)/J$ fixed and $U \geq 0$ the scaling variable, define

$$Q_N(U) = N^2 \frac{d}{\Gamma/J} \frac{\Delta_N}{J}. \quad (30)$$

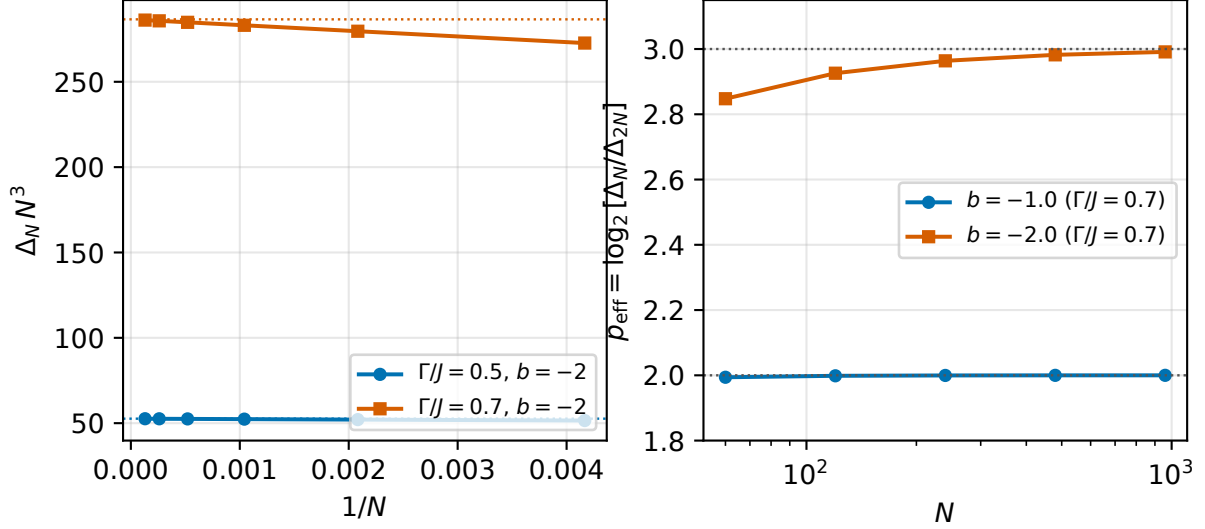


Figure 2: Left: $\Delta_N N^3$ versus $1/N$ at $b = -2$ for $\Gamma/J = 0.5$ (circles) and 0.7 (squares), $N = 240 \dots 7680$; the dotted horizontals are the closed-form C_3 values (26), $52.63789 \dots$ and $286.58407 \dots$. Right: effective exponent $p_{\text{eff}} = \log_2[\Delta_N/\Delta_{2N}]$ at $\Gamma/J = 0.7$ for $b = -1$ (circles, $\rightarrow 2$, from the closed form (22)) and $b = -2$ (squares, $\rightarrow 3$), $N = 60 \dots 960$.

Then

$$Q_N = S(U) + \frac{\tau(U)}{N} + \frac{\Theta(U)}{N^2} + O(N^{-3}), \quad (31)$$

where $x_c(U) \in (0, \pi)$ is the soft-mode position, i.e. the root of the *branch equation*

$$U \sin x_c + 2x_c(\cos x_c - 1) = 0 \quad \Longleftrightarrow \quad \cot \frac{x_c}{2} = \frac{2x_c}{U}, \quad (32)$$

and

$$\begin{aligned} S(U) &= \pi^2 - x_c(U)^2, & \tau(U) &= -2x_c y_-(x_c, U), \\ y_-(x, U) &= -\frac{U x (\Gamma/J)(\cos x - 1)}{d[U \cos x - 2x \sin x + 2 \cos x - 2]}. \end{aligned} \quad (33)$$

The branch equation, y_- , its mirror y_+ on the $\mu \rightarrow +1$ branch ($U \sin x + 2x(\cos x + 1) = 0$), and $z_+(\pi, U) = -\pi U(\Gamma/J)^2/(4d^2)$ were re-derived symbolically from (QC); the third-order coefficient z_- (the rational function needed for Θ) admits a unique closed solution of the same expansion. The second subleading coefficient assembles as

$$\Theta(U) = (x_c^4 - \pi^4) \left(\frac{1}{12} + \frac{\Gamma/J}{4d^2} \right) - 2x_c z_-(x_c, U) - \frac{\pi^2 U (\Gamma/J)^2}{2d^2} - y_-^2. \quad (34)$$

The three limits of $S(U)$ interlock with Sec. 5:

- $U \rightarrow 0$: $x_c \rightarrow 0$, $S \rightarrow \pi^2$, and (31) reduces to the antiperiodic ring (22): $\Delta_N/J = \pi^2 d^{-1}(\Gamma/J) N^{-2} + \dots$ with $\tau(0) = 0$ and the anchor $\Theta(0) = -\pi^4(\frac{1}{12} + \frac{\Gamma/J}{4d^2})$.
- small U : $x_c^2 = U - \frac{U^2}{12} + \frac{U^3}{180} - \frac{U^4}{3780} + \frac{U^5}{226800} + \frac{U^6}{1496880} - \frac{541U^7}{6810804000} + O(U^8)$, verified to 3.8×10^{-17} at $U = 0.1$; hence $S(U) = \pi^2 - U + \dots$ (Fig. 3, dashed).

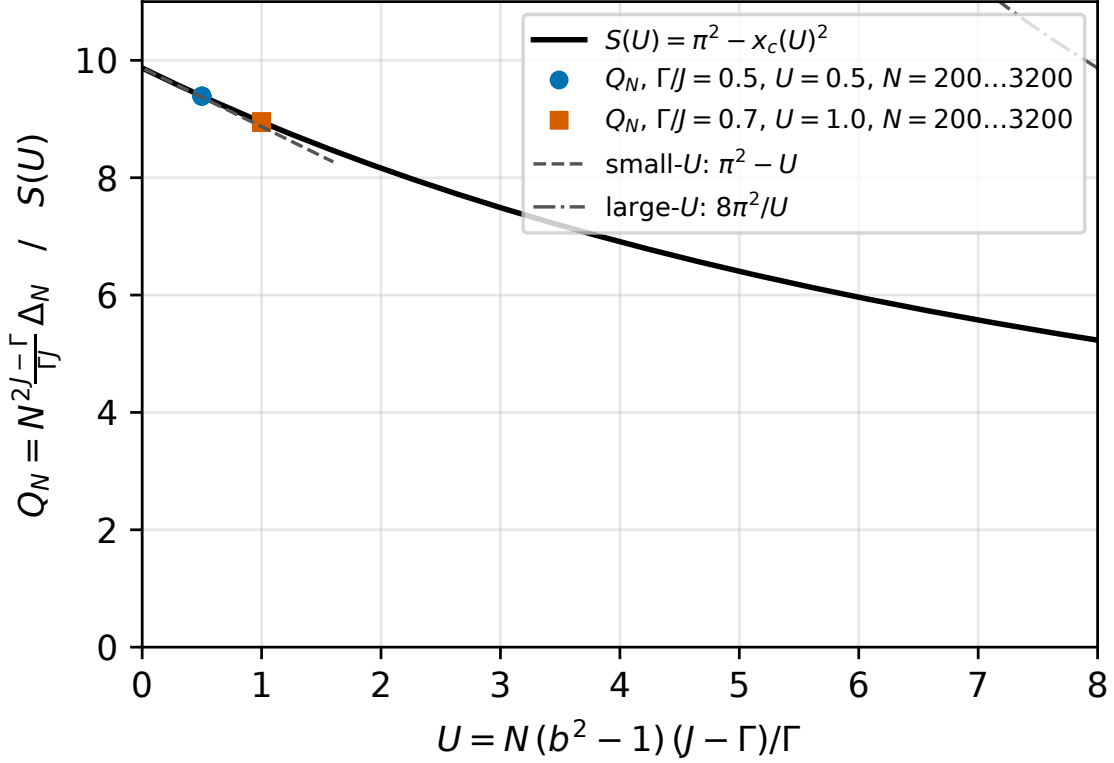


Figure 3: Collapse of the rescaled gap onto the universal curve. Solid: $S(U) = \pi^2 - x_c(U)^2$ from the branch equation (32). Markers: Q_N at $N = 200, 400, 800, 1600, 3200$ for $(\Gamma/J, U) = (0.5, 0.5)$ (circles) and $(0.7, 1.0)$ (squares), converging onto the curve from both sides. Dashed and dash-dotted: the analytic limits $\pi^2 - U$ (small U) and $8\pi^2/U$ (large U).

- large U : $x_c \rightarrow \pi - 4\pi/U + \dots$ and $S(U) \rightarrow 8\pi^2/U$ (Fig. 3, dash-dotted); since $U = N(b^2 - 1)d/(\Gamma/J)$, this reproduces exactly the $|b| \rightarrow 1$ edge of the ordered-branch amplitude (26): $\Delta_N/J \rightarrow 8\pi^2(\Gamma/J)^2/(d^2(b^2 - 1)N^3) = C_3(b)N^{-3}|_{|b| \rightarrow 1}$.

Numerical confirmation used ladders $N = 200 \cdot 2^j$, $j \leq 4$, at $(\Gamma/J, U) = (0.5, 0.5)$ and $(0.7, 1.0)$:

Γ/J	U	x_c	$S(U)$	$\tau(U)$	$\Theta(U)$
0.5	0.5	0.692708253407499	9.38975967675049	0.11508781911	-59.3923338107
0.7	1.0	0.960188873914783	8.94764172749962	0.990461882487	-226.128183858

The Θ values match the independently computed symbolic values to relative 1.1×10^{-11} and 1.9×10^{-10} . Along the ladders, $(Q_N - S - \tau/N)N^2$ converges to Θ monotonically from above ($-59.374 \rightarrow -59.392$ and $-225.72 \rightarrow -226.12$ from $N = 200$ to 3200); the $U = 0$ anchors converge as $-56.808, -56.818, -56.821 \rightarrow -56.82197$ ($N = 200, 400, 800$; exact -56.8219697698348 , relative 4.3×10^{-15} against the symbolic value), and $(Q_N - \pi^2)N$ halves exactly at each doubling ($-0.284039 \rightarrow -0.142046 \rightarrow -0.0710264$), the cleanest possible proof that $\tau(0) = 0$. At $(\Gamma/J, U) = (0.7, 1.0)$ the anchor sequence is $-197.335, -197.477, -197.512 \rightarrow -197.5239901523$ (relative 1.4×10^{-14}).

6.2 Paramagnetic side: $b_N = 1 + V(\Gamma/J)/(\delta N)$, $\Gamma > J$

On the $\Gamma > J$ side the window $b \gtrsim 1$ is where the below-band bound state of $\mu = -b$ softens into the band. With $\delta = (\Gamma - J)/J$, scaling variable $V \geq 0$, and

$$\mathcal{D}(N, V) = N^2 \frac{\delta}{\Gamma/J} \left(2\delta - \frac{\Delta_N}{J} \right), \quad (35)$$

the expansion reads

$$\mathcal{D}(N, V) = w^2 + \frac{2ww_2}{N} + \frac{\Theta'(V)}{N^2} + O(N^{-3}), \quad (36)$$

with the *master equation*

$$w(\cosh w - 1) = V \sinh w \quad \Longleftrightarrow \quad w \tanh \frac{w}{2} = V, \quad (37)$$

whose unique positive root (the right-hand form is strictly increasing in w) was re-derived symbolically from (QC) (the first-order coefficient of the expansion vanishes identically on the solution set). The next coefficient has the closed form

$$w_2 = -\frac{(\Gamma/J) V^2 \sinh w}{2 \delta R}, \quad R = (1 - V) \cosh w - 1 + w \sinh w, \quad (38)$$

likewise re-derived symbolically (the numerator cancels identically on shell). For small V ,

$$w = \sqrt{2V} \left(1 + \frac{V}{12} + \frac{11V^2}{1440} + \frac{17V^3}{40320} - \frac{281V^4}{9676800} + O(V^5) \right), \quad (39)$$

verified to relative 1.2×10^{-20} at $V = 10^{-3}$ and 3.6×10^{-12} at $V = 0.05$. The second subleading coefficient is

$$\Theta'(V) = 2ww_3 + w_2^2 + \frac{w^4}{12} + \frac{(\Gamma/J) w^4}{4\delta^2}, \quad (40)$$

with w_3 the third-order coefficient of the same expansion. At $\Gamma/J = 1.3$, $V = 0.3$: $w = 0.794502734493032$, $2ww_2 = -0.431430125145$, $w_3 = -0.571368720335929$, $\Theta' = 0.6378870739003$; the ladder $N = 64 \cdot 2^j$, $j \leq 3$, converges accordingly: $(\mathcal{D} - w^2)N$ moves $-0.42199 \rightarrow -0.43019$ against $2ww_2$, and $(\mathcal{D} - w^2 - 2ww_2/N)N^2$ moves $0.60404 \rightarrow 0.63665$ against Θ' , with the Richardson completion $2T_{512} - T_{256} = 0.6378816$ within 5.5×10^{-6} — the expected $O(1/N)$ tail. At the stronger probe $\Gamma/J = 1.3$, $V = 1.3$: $w = 1.809230229057764$, $w_2 = -3.1672487351627$, $w_3 = -1.7309370571062$, $\Theta' = 43.3525751174$.

Two limits anchor the paramagnetic side. As $V \rightarrow 0$, $w \rightarrow 0$ and $\mathcal{D} \rightarrow 0$: the gap returns continuously to the bulk mass $2(\Gamma - J)$, consistent with the immediate sub-mass drop for every $b > 1$ found in Sec. 4. As $V \rightarrow \infty$, $w \rightarrow V$ and (36) reduces at fixed b to the exact bound-state gap $\Delta_N \rightarrow 2\sigma_b(\mu = -b)$ of the infinite chain, whose weak-defect expansion $2\delta - \Delta_N/J = (b - 1)^2 \delta J/\Gamma + O((b - 1)^3)$ is precisely the leading term of the scaling function.

6.3 One mechanism, two branches

The ordered and paramagnetic master equations are the same equation on the two sheets of the soft mode: substituting $x = iw$ maps the branch equation (32) onto $U \sinh w + 2w(\cosh w - 1) = 0$, which at $U = -2V$ is exactly (37). Oscillatory soft modes ($\Gamma < J$, $b \rightarrow -1$) and evanescent bound-state soft modes ($\Gamma > J$, $b \rightarrow +1$) are thus analytic continuations of one another, and the three regimes of Sec. 5 — exponential, N^{-2} , N^{-3} — are joined through the scaling window by one continuous family of scaling functions. The two sides are still not mirror images: by the threshold analysis of Sec. 4, at $\Gamma > J$ the mirror point $b < -1$ carries no bound state until $|b| > \mu_c(N)$, and its gap stays above the bulk mass in between.

7 Discussion

This work assembles the exact finite-size theory of the gap of the quantum Ising ring with a single strength- b defect coupling, at every N , every Γ/J , and both parity sectors. The reduction of the ring to a Jordan–Wigner quadratic form with one modified bond and one on-site shift establishes that the many-body spectrum is a free-fermion Fock space over N single-particle modes whose quantization condition (QC) is exact. From its polynomial form we obtained: the complete threshold structure of defect bound states as exact rational functions of $(N, \Gamma/J)$ (19); the exact critical gap $2J \tan(\pi/4N)$; the closed antiperiodic ordered-ring gap with its exponentially small hard-mode residual; the ordered-branch N^{-3} law with closed amplitudes $C_3, \dots, C_6$ (26)–(29) verified over ladders reaching $N = 30720$; and the two-sided crossover scaling functions with three explicit subleading coefficients.

Three structural results deserve emphasis beyond their formulas.

First, the sign of $\det K_p = \Gamma^N + \mu J^N$ — linear in the defect parameter — completely organizes the phase diagram of the gap. Wherever both sectors are parity-corrected the gap is the soft-mode splitting and decays as a power of N (N^{-2} on the ring, N^{-3} on the branch); wherever both are uncorrected the two vacua form an exponentially degenerate doublet and the gap is exponentially small. The same $|b|$ can therefore give a power-law gap on one side and an exponentially small gap on the other — the substitution $b \rightarrow |b|$ in the amplitudes, tempting by the oddness of $C_3(b)$, is categorically wrong.

Second, at $\Gamma > J$ the gap is maximally asymmetric under $b \rightarrow -b$: the $p = -1$ sector binds a below-band state immediately for $b > 1$, while the mirror side binds only beyond the exact rational threshold $\mu_c(N) > 1$, so $\Delta_N(b) \neq \Delta_N(-b)$ by up to $0.096 J$ at $N = 20$, $\Gamma/J = 1.3$. Any criterion based on the value of the gap alone (e.g. “ $\Delta_N = 2(\Gamma - J)$ ”) mislocates the threshold; only the bound-state count, equivalently the sign of $R(\pm 1)$, is sharp.

Third, the crossover scaling functions on the two sides of criticality are one analytic object: $x \rightarrow iw$, $U \rightarrow -2V$ maps the ordered branch equation onto the paramagnetic master equation. The finite-size crossover near the defect transition of the quantum Ising ring is thus controlled by the same soft-mode mechanism throughout, interpolating between the rigid-ring laws, the defect bound-state physics, and — at $\Gamma = J$ — the exact conformal Casimir amplitude.

Verification standard

Every closed form quoted here was produced or reproduced by an independent implementation that shares no code with the derivations it checks: exact symbolic polynomial identities (integer arithmetic) for the reduction, deflation, and factorizations; 30–80-digit arithmetic for spectra, thresholds, and ladders; float64 dense diagonalization of the full spin ring as an external referee (480 cases, 122400 levels, worst deviation 1.3×10^{-13} , which excludes any parity misassignment or non-rigid momentum set, each of which would cost $O(1)$); and negative controls — notably the $b \rightarrow |b|$ substitution suggested by the oddness of C_3 — confirmed to fail. The worst residuals are collected in the tables above; none exceeds the numerical floor of its extraction route, and deviations grow precisely where the underlying power solves become ill-conditioned (strongest coupling, deepest coefficient).

Limitations and open problems

The amplitude C_7 (numerically -105223.30 at $\Gamma/J = 0.5$, $b = -2$) and the deeper coefficients $C_8, \dots, C_{10}$ extracted by the power solve have no closed forms here; the symbolic complexity of the

third-order coefficient z_- suggests that closed C_7 would require substantially heavier elimination. The crossover at $\Gamma < J$, $b \rightarrow +1$ — the doublet side of the ordered window — is exponentially small and was not rescaled; its scaling function, if defined through the residual r_N , would probe the symmetry-breaking tunneling amplitude directly. On the conceptual side, the N^{-3} law and the crossover functions invite comparison with boundary conformal field theory: the defect at criticality is a boundary condition changing operator, and the $\Theta(U)$, $\Theta'(V)$ coefficients should be expressible through boundary entropy and defect-operator data of the $c = \frac{1}{2}$ theory in the sense of the boundary-state classification [6, 1]. Establishing that dictionary, and extending the exact machinery to two defects or to open boundaries — where the integrable boundary Yang–Baxter structures [25, 12] apply — are the natural next steps. Rigorous control of the asymptotics, in the spirit of the constructive results for related lattice fermion systems [13, 9], remains open.

Conclusion

A single modified hopping in a free-fermion ring generates an unexpectedly rich exact structure: rational bound-state thresholds, parity-selected exponential versus algebraic gaps, closed amplitude hierarchies, and analytically continued crossover scaling functions. All of it follows from one quantization condition and one determinant, and all of it is verified independently to machine precision or better.

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