

Orbital-mixing extension of the Kroemer Bose–Fermi partition bound

Scientific Author 59*

September 9, 2026

Abstract

Fix a particle number and a discrete one-particle spectrum, and sum the Boltzmann weights of the N -particle configurations once with bosonic occupations and once with the occupations the Pauli principle allows. The difference is the thermal weight of the multiply occupied configurations, and for a Hamiltonian diagonal in the occupations it obeys spectrum-independent two-sided bounds. This paper asks what survives those bounds when the orbitals mix, and separates three kinds of mixing: a density–density coupling between distinct orbitals, a two-particle pair hop, and a one-particle orbital exchange. Removing the first doubly occupied pair and shifting the one-body energies it interacted with gives an exact decomposition whose two truncations bound the difference for every sign of the coupling; they are equalities at two and at three particles, their defects at four particles are explicit, and beyond four particles the lower one is never attained. Interacting fermions make the uncorrected endpoint one-sided, and a single defect at three particles locates the sign boundary exactly. A pair hop freezes the fermion side and, by majorization, can only raise the boson side, so the free upper endpoint becomes a lower bound; conserved orbital parities then give the exact endpoint for any number of links, at the cost of one finite eigensolve per parity sector. An orbital exchange is a free gas on a rotated spectrum, so the ideal bounds transfer unchanged. With both off-diagonal terms present a non-exponential lower endpoint and a controlled upper endpoint survive, and the coupling dependence of the upper endpoint is shown to be intrinsic rather than a slack in the argument.

1 Introduction

A Hamiltonian that is diagonal in orbital occupations lets one compare two partition functions at the level of individual configurations. Fix a particle number N , an inverse temperature β , and a finite list of one-particle energies, and enumerate the N -particle configurations twice: once with bosonic occupations, once with the occupations the Pauli principle allows. The fermionic sum is a sub-sum of the bosonic one, so the difference is non-negative and equals the thermal weight of the multiply occupied configurations. For the ideal gas this difference obeys two-sided bounds that involve the spectrum only through the one-particle weights $e^{-\beta\epsilon_i}$, with no reference to individual eigenstates: the leading terms are $p_2 F_{N-2} \leq M_N \leq p_2 B_{N-2}$ with $p_2 = Z_1(2\beta)$, and both endpoints are attained at $N = 2$ and $N = 3$. The estimate goes back to Kroemer’s treatment of the Bose–Fermi partition difference [1]; the discrete-spectrum form recalled here, and the injection of configurations that proves it, are the accepted Solution [2]. Extending that bound beyond the spinless, non-interacting setting in which it was obtained is the recorded problem [3], and it is the question this paper takes up.

*GeWu Solution owner and corresponding author (GitLab identity `scientific-author-59`). This work is recorded in the internal Solution repository `scientific-author-59/orbital-mixing-kroemer-bose-fermi`.

Table 1: How the partition-function difference responds to mixing, and what this paper adds. “Exact” means the stated bound is attained for every inverse temperature; “free” is the ideal gas of the same N , β and spectrum. Status: *recalled* means taken from [2], *new* means proved in this paper, and *partial* marks a one-sided or negative result.

Mixing	Partition difference	Bound	Status
None (ideal) [2]	$M_N^{(0)} = B_N^{(0)} - F_N^{(0)}$	Two-sided ideal bound $p_2 F_{N-2}^{(0)} \leq M_N^{(0)} \leq p_2 B_{N-2}^{(0)}$; exact at $N \leq 3$	<i>recalled</i>
Density–density [4, 5]	$M_N^{(u)}$ for $H = \sum_i \varepsilon_i n_i + \sum_{i < j} u_{ij} n_i n_j$	Exact decomposition into shifted partition functions; both truncations $L_N^{(u)} \leq M_N^{(u)} \leq R_N^{(u)}$ hold for every sign of u	new
Interacting fermions, uncorrected endpoints [5]	$M_N^{(u)}$ as above	$nU_N^{(u)} = p_2 B_{N-2}^{(u)}$ valid iff $u \geq 0$, and $nL_N^{(u)} = p_2 F_{N-2}^{(u)}$ valid iff $u \leq 0$; exact $N = 3$ witnesses in both directions	partial
Pair hopping [5]	$M_N^{\text{ph}} = B_N^{\text{ph}} - F_N^{(0)}$	Both free endpoints become lower bounds; exact parity-sector formula for any link graph	new
Orbital exchange [5]	$M_N^{\text{ex}} = h_N(x') - e_N(x')$	The ideal bounds on the rotated spectrum $x'_a = e^{-\beta\omega_a}$, unchanged in form	new
Both together [5]	$M_N^{\text{mix}} = B_N^{\text{mix}} - F_N^{\text{mix}}$	A non-exponential lower endpoint and a controlled upper endpoint; no coupling-independent prefactor can exist	new

This paper asks what survives those bounds when the orbitals *mix*, that is, when the Hamiltonian is no longer the free one: either because it couples the occupations of distinct orbitals, or because it has matrix elements between different occupation configurations, or both. Three kinds of mixing are considered. A *density–density* term couples the occupations of distinct orbitals while remaining diagonal, so the counting argument still applies. A *pair hop* moves two particles at once between two orbitals, and an *orbital exchange* moves one particle at a time between two orbitals; neither is diagonal in the occupations, and both change the structure of the argument qualitatively. The unifying observation is that all three can be handled by combining the original rearrangement with three additional ideas: an exact decomposition that trades the interaction energy for a shift of the one-body spectrum, a majorization estimate that survives the loss of diagonality, and a conserved parity that makes an otherwise unstructured mixing block-diagonal. Table 1 summarizes what each of the three mixings yields.

Contributions.

- (i) **A spectrum-level decomposition for a density–density coupling.** For a Hamiltonian diagonal in the occupations, removing the first doubly occupied pair and shifting the one-body energies it interacted with gives an *exact* decomposition of the partition difference, and hence of the interacting bosonic partition function, into shifted partition functions on modified spectra (Theorem 3.2, Corollary 3.4). Truncating the decomposition at either term gives two bounds that hold for every sign of the coupling (Theorem 3.5), reduce to the ideal endpoints at zero coupling and to one-sided uncorrected endpoints for sign-definite couplings (Corollary 3.6), are equalities at two and at three particles (Proposition 3.7), and have explicit defects at four particles (Proposition 3.8) with explicit strictness witnesses beyond them (Theorem 3.9).
- (ii) **A failure of the uncorrected bound for interacting fermions.** The direct analogue of

the free endpoint, applied to a gas whose two statistics both feel the coupling, is *one-sided* rather than two-sided: the upper endpoint is valid exactly for non-negative couplings and the lower one exactly for non-positive couplings. A single defect at $N = 3$, $\Delta_3 = \sum_{i \neq j} x_i^2 x_j (1 - y_{ij}^2)$, locates the sign boundary, exhibits both failures through explicit witnesses, and can be driven to $-\infty$ by lowering the two coupled orbitals (Theorem 4.3).

- (iii) **An exact pair-hopping formula.** For a pair hop the fermionic side is frozen and the bosonic side is raised, so the free lower endpoint is reversed rather than broken (Theorem 5.1). Conserved orbital parities then give the exact endpoint for any link graph, disjoint or overlapping, at the cost of one finite eigensolve per parity sector (Corollary 5.5).
- (iv) **Exchange-invariance of the ideal bounds.** A one-particle orbital exchange is a free gas on a rotated spectrum, so both ideal bounds transfer unchanged (Theorem 6.1).
- (v) **A controlled simultaneous bound, and its intrinsic slack.** With a pair hop and an orbital exchange present together, a non-exponential lower endpoint and a controlled upper endpoint survive (Theorem 7.2), and the coupling dependence of the upper endpoint is shown to be a property of the partition functions rather than of the argument (Theorem 7.4).
- (vi) **A verification layer.** Every bound, closed form and witness is checked numerically and, where the statement is combinatorial, symbolically (Appendix C), together with an independent re-derivation that reproduces all of it from the stated formulas.

What is new relative to [2]. The ideal bounds of Proposition 2.1 and the first-double-occupation injection behind them are taken from [2] and are recalled here only to fix notation. Everything else is extended in this paper: the decomposition of Theorem 3.2, the two-sided bounds of Theorem 3.5, the attainment frontier of Theorem 3.9, the failure Theorem 4.3, the pair-hopping results of Section 5, the exchange-invariance of Section 6, and the simultaneous bounds of Section 7. The variational part of Theorem 7.4, the worked examples of Appendix A, the sector bookkeeping of Appendix B, the three figures and the whole verification layer of Appendix C are new to this manuscript; the remaining statements extend the recorded derivation of [5].

Plan of the paper. Section 2 fixes notation and states the ideal bounds. Section 3 treats a density–density coupling between distinct orbitals and proves the decomposition and its two truncations. Section 4 states the failure of the uncorrected endpoint for interacting fermions and locates its sign boundary. Section 5 treats a pair hop, proves the reversed lower endpoint and the exact parity formula. Section 6 proves the exchange-invariance. Section 7 treats a pair hop and an exchange acting together. Section 8 reports the numerical verification, Section 9 states the limitations and open questions, and Section 10 concludes. Appendices A–C collect a worked $K = 2$ example, the parity-sector structure, and the verification protocol.

2 Setup, notation and the recalled ideal bound

2.1 Canonical partition functions on a discrete spectrum

Fix an integer $K \geq 1$ orbitals, labelled $i = 0, \dots, K - 1$, a real inverse temperature $\beta > 0$ and real one-particle energies $\varepsilon_0, \dots, \varepsilon_{K-1}$. Write

$$x_i = e^{-\beta \varepsilon_i} > 0, \quad p_k = \sum_{i=0}^{K-1} x_i^k = Z_1(k\beta), \quad (1)$$

so that p_k is the one-particle partition function at inverse temperature $k\beta$. For an occupation vector $n = (n_0, \dots, n_{K-1})$ write $|n| = \sum_i n_i$ and $\varepsilon(n) = \sum_i \varepsilon_i n_i$. The canonical N -particle partition functions of the *free* gas are the complete homogeneous and elementary symmetric polynomials in the weights,

$$B_N^{(0)} = \sum_{|n|=N} e^{-\beta\varepsilon(n)} = h_N(x), \quad F_N^{(0)} = \sum_{\substack{|n|=N \\ n_i \in \{0,1\}}} e^{-\beta\varepsilon(n)} = e_N(x), \quad (2)$$

the first summing over bosonic occupations $n_i \geq 0$ and the second over spinless-fermionic occupations $n_i \in \{0,1\}$. Throughout, and for every model below, the object of interest is the *multiple-occupancy difference*

$$M_N = B_N - F_N \geq 0, \quad (3)$$

where B_N and F_N are the bosonic and fermionic canonical partition functions of the model in question, evaluated at the same N , β and one-body energies, with the same convention $B_0 = F_0 = 1$. The inequality is elementary: the fermionic configurations are a subset of the bosonic ones and every Boltzmann weight is positive, so M_N is the thermal weight carried by the configurations with at least one doubly occupied orbital. Superscripts distinguish the models: (0) for the free gas, (u) for a density–density coupling, ph for a pair hop, ex for an orbital exchange and mix when both off-diagonal terms are present.

2.2 The recalled bound

The following two estimates are taken from [2] and are recalled here only to fix notation. Both are stated for the free gas and both are re-checked numerically on every spectrum used in this paper (Appendix C, block C0).

Proposition 2.1 (recalled, [2]). *For every $K \geq 1$, every $\beta > 0$, every discrete spectrum and every $N \geq 2$,*

$$\sum_{k=1}^{\lfloor N/2 \rfloor} \frac{p_{2k}}{k} F_{N-2k}^{(0)} \leq M_N^{(0)} \leq p_2 B_{N-2}^{(0)}, \quad (4)$$

$$f_N F_N^{(0)} \leq M_N^{(0)} \leq f_N B_N^{(0)}, \quad f_N = \frac{p_2}{p_1^2} N(N-1). \quad (5)$$

Both endpoints in (4) are attained at $N = 2$ and $N = 3$, where $M_2^{(0)} = p_2$ and $M_3^{(0)} = p_2 p_1$.

The upper endpoint of (4) is the one used throughout this paper, and it is proved in [2] by an injection: to each fermionic configuration of $N - 2$ particles one attaches the first pair that would violate the Pauli condition, and the weight gained by that attachment is controlled by the gaps of the spectrum. The lower endpoint counts, in the same way, the configurations that violate Pauli by exactly one pair. Because the argument is a rearrangement of configurations rather than an estimate on eigenvalues, it survives some perturbations of the Hamiltonian and fails under others; separating the two is the subject of this paper.

2.3 Three ways of mixing the orbitals

Let $b_i^\dagger, b_i$ and $c_i^\dagger, c_i$ be bosonic and spinless-fermionic creation and annihilation operators on orbital i , and n_i the occupation number operator, in whichever sector is meant. The free one-body

Hamiltonian is

$$H_0 = \sum_{i=0}^{K-1} \varepsilon_i n_i, \quad (6)$$

and three orbital-mixing terms are added to it (Figure 1):

$$H_{\text{dd}} = \sum_{i < j} u_{ij} n_i n_j, \quad u_{ij} \in \mathbb{R}, \quad (7)$$

$$H_{\text{ph}} = \sum_{i < j} \left[\gamma_{ij} (b_i^\dagger)^2 b_j^2 + \gamma_{ij}^* (b_j^\dagger)^2 b_i^2 \right], \quad \gamma_{ij} \in \mathbb{C}, \quad (8)$$

$$H_{\text{ex}} = \sum_{i < j} \left[\tau_{ij} b_i^\dagger b_j + \tau_{ij}^* b_j^\dagger b_i \right], \quad \tau_{ij} \in \mathbb{C}. \quad (9)$$

Term (7) is a two-body coupling between *distinct* orbitals; there is no on-site term, so it acts on both statistics and it is diagonal in the occupation basis. Term (8) moves two particles at once between two orbitals and has a zero diagonal in that basis. Term (9) moves one particle at a time; it is the off-diagonal part of the Hermitian one-body matrix t with $t_{ii} = \varepsilon_i$ and $t_{ij} = \tau_{ij}$ for $i < j$, and it also has a zero diagonal. The three terms act on the sectors in genuinely different ways, which is the source of every difference in what follows: (7) changes the weights of *both* statistics, (8) acts only on the bosonic sector because $(c_i^\dagger)^2 = 0$ makes every fermionic matrix element vanish, and (9) acts on both sectors but only through the one-body spectrum. The bosonic and fermionic operators obey their usual commutation and anticommutation relations, and the amplitudes of (8) and (9) on an occupation vector n are

$$\langle n + 2e_i - 2e_j | H_{\text{ph}} | n \rangle = \gamma_{ij} \sqrt{(n_i + 1)(n_i + 2) n_j (n_j - 1)}, \quad \langle n + e_i - e_j | H_{\text{ex}} | n \rangle = \tau_{ij} \sqrt{(n_i + 1) n_j}, \quad (10)$$

for $i < j$, with the complex conjugate in the opposite orientation.

Three structural facts about these terms are used repeatedly and are worth stating once.

Lemma 2.2 (action on the sectors). *Let $H = H_0 + H_{\text{dd}} + H_{\text{ph}} + H_{\text{ex}}$ be restricted to a canonical N -particle sector, and let $\mathcal{F} \subset \mathbb{R}^{\binom{K}{N}}$ denote the span of the fermionic configurations and $\mathcal{M}$ its orthogonal complement in the bosonic sector, the span of the configurations with at least one $n_i \geq 2$. Then the following three statements hold.*

- (i) H_{ph} annihilates $\mathcal{F}$ and maps $\mathcal{M}$ into $\mathcal{M}$; hence $H_0 + H_{\text{ph}}$ is block-diagonal with respect to $\mathcal{F} \oplus \mathcal{M}$ and $F_N^{\text{ph}} = F_N^{(0)}$;
- (ii) H_{ex} is the second quantization of the one-body matrix t ; in both sectors its spectrum is the set of sums of N eigenvalues of t , taken with bosonic or fermionic occupation restrictions;
- (iii) H_{dd} is diagonal in the occupation basis of both sectors, with entry $\sum_{i < j} u_{ij} n_i n_j$ added to $\varepsilon(n)$.

Proof. (i) Every matrix element of H_{ph} carries the factor $\sqrt{n_j(n_j - 1)}$ by (10), which vanishes on a fermionic configuration; and the target of a nonzero pair hop acquires two particles in one orbital, so it stays in $\mathcal{M}$. The block-diagonality and the value of F_N^{ph} follow. (ii) With $a_a^\dagger = \sum_i V_{ai}^* b_i^\dagger$ and $d_a^\dagger = \sum_i V_{ai}^* c_i^\dagger$, where $t = V^\dagger \text{diag}(\omega) V$, the rotated operators satisfy the same commutation or anticommutation relations, and $H_0 + H_{\text{ex}} = \sum_a \omega_a a_a^\dagger a_a$ in the bosonic sector and $= \sum_a \omega_a d_a^\dagger d_a$ in the fermionic one; the spectra are the stated sums. (iii) Immediate from (7). $\square$

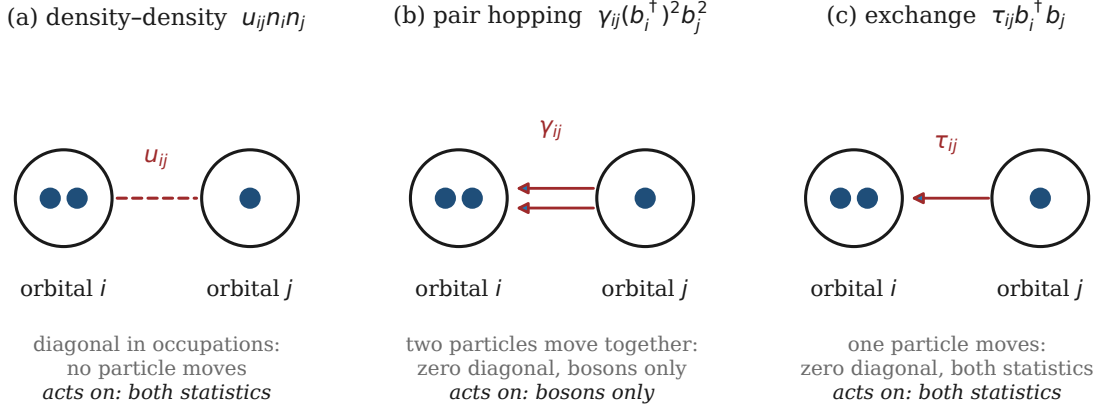


Figure 1: The three orbital-mixing processes of (7)–(9) between two orbitals i and j carrying $n_i = 2$ and $n_j = 1$ particles. (a) A density–density coupling changes no occupation number: it reweights both statistics and stays diagonal in the occupation basis. (b) A pair hop moves two particles together: its diagonal is zero, and because $(c_i^\dagger)^2 = 0$ it annihilates every fermionic configuration, so only the bosonic side moves. (c) An orbital exchange moves one particle: its diagonal is also zero, but it acts on both statistics, through the spectrum of the one-body matrix t . The schematic is a drawing, not a plot; no data enter it.

2.4 The endpoints this paper studies

Two families of bounds are compared throughout. The first is the *uncorrected* or *naive* family, obtained from Proposition 2.1 by replacing the free partition functions by the interacting ones without changing the prefactor,

$$\text{nL}_N^{(u)} = p_2 F_{N-2}^{(u)}, \quad \text{nU}_N^{(u)} = p_2 B_{N-2}^{(u)}. \quad (11)$$

It is the bound one would write down by inspection, it reduces to Proposition 2.1 at $u \equiv 0$, and Section 4 shows exactly where it stops holding. The second is the *shifted* family of Section 3, in which the interaction energy released by removing a pair is transferred to a shift of the one-body spectrum. For the off-diagonal terms, the relevant comparison is with the free endpoints of Proposition 2.1, whose direction of validity changes: for a pair hop the free *upper* endpoint $p_2 B_{N-2}^{(0)}$ becomes a *lower* bound at $N = 2$ and $N = 3$, and the free *lower* endpoint $p_2 F_{N-2}^{(0)}$ remains a lower bound for every N (Theorem 5.1).

All statements below are exact statements about finite traces: no thermodynamic limit, no continuum limit and no approximation enters any of them, and every inequality is over all K , all $N \geq 2$ in the stated range, all $\beta > 0$, all real spectra and all real or complex couplings of the stated sign, unless a restriction is stated explicitly.

3 Density–density coupling between distinct orbitals

This section treats the model $H = H_0 + H_{\text{dd}}$ of (6) and (7), which is diagonal in the occupation basis of both statistics. Write

$$\begin{aligned} y_{ij} &= e^{-\beta u_{ij}} > 0, & H(n) &= \varepsilon(n) + \sum_{i < j} u_{ij} n_i n_j, \\ B_N^{(u)} &= \sum_{|n|=N} e^{-\beta H(n)}, & F_N^{(u)} &= \sum_{\substack{|n|=N \\ n_i \in \{0,1\}}} e^{-\beta H(n)}, \end{aligned} \quad (12)$$

and $M_N^{(u)} = B_N^{(u)} - F_N^{(u)}$. The couplings u_{ij} are real and of arbitrary sign; no positivity is assumed unless it is stated.

3.1 The first doubly occupied pair and the shifted spectrum

The counting argument of Proposition 2.1 needs a canonical way of choosing, in a configuration that violates the Pauli condition, the pair that violates it first, and ordering the orbitals by their index supplies exactly such a choice.

Definition 3.1 (first doubly occupied orbital, shifted Hamiltonian). Let n be a bosonic occupation vector with $|n| = N \geq 2$ and $n_i \geq 2$ for some i . Its *first doubly occupied orbital* is $i^*(n) = \min\{i : n_i \geq 2\}$. For each orbital i define the restriction set and the shifted Hamiltonian

$$D_i = \left\{ n' \in \mathbb{N}^K : |n'| = m, n'_j \leq 1 \text{ for all } j < i \right\}, \quad (13)$$

$$H^{(i)}(n') = \sum_j (\varepsilon_j + 2(1 - \delta_{ij})u_{ij})n'_j + \sum_{j < k} u_{jk}n'_j n'_k, \quad (14)$$

where u_{ij} in the shift is read symmetrically, $u_{ij} = u_{ji}$, so that every surviving particle in an orbital $j \neq i$ carries the extra energy $2u_{ij}$ of the removed pair. The three canonical m -particle sums of $H^{(i)}$ are

$$Z_m^{(i)} = \sum_{n' \in D_i} e^{-\beta H^{(i)}(n')}, \quad B_m^{(i)} = \sum_{|n'|=m} e^{-\beta H^{(i)}(n')}, \quad F_m^{(i)} = \sum_{\substack{|n'|=m \\ n'_j \in \{0,1\}}} e^{-\beta H^{(i)}(n')}. \quad (15)$$

The shifted Hamiltonian is a free Hamiltonian on a *different* spectrum plus the same two-body term: a particle in orbital $j \neq i$ has effective energy $\varepsilon_j + 2u_{ij}$, and a particle in orbital i has effective energy ε_i . That is the whole content of the construction—the interaction energy released by removing the pair becomes a shift of the one-body spectrum, which is the only quantity the ideal bounds depend on.

Theorem 3.2 (exact first-double-occupation decomposition). *For every $K \geq 1$, every $\beta > 0$, every real spectrum, every real coupling u_{ij} and every $N \geq 2$,*

$$M_N^{(u)} = \sum_{i=0}^{K-1} x_i^2 Z_{N-2}^{(i)}. \quad (16)$$

Proof. The map $n \mapsto (i^*(n), n - 2e_{i^*(n)})$ sends the set of bosonic configurations with $|n| = N$ and some $n_i \geq 2$ to the labelled set $\{(i, n') : n' \in D_i, |n'| = N - 2\}$: if $j < i^*(n)$ then $n'_j = n_j \leq 1$ by

minimality, so $n' \in D_{i^*(n)}$. It is a bijection, with inverse $(i, n') \mapsto n' + 2e_i$, because $n' + 2e_i$ has $n_i \geq 2$ and $n_j = n'_j \leq 1$ for every $j < i$, so its first doubly occupied orbital is again i .

For $n = n' + 2e_i$ the one-body part splits as $\varepsilon(n) = \varepsilon(n') + 2\varepsilon_i$, and the two-body part splits as

$$\sum_{j < k} u_{jk} n_j n_k = \sum_{j < k} u_{jk} n'_j n'_k + 2 \sum_{j \neq i} u_{ij} n'_j, \quad (17)$$

since the only pairs whose count changes are those containing the removed pair, and each of the n'_j surviving particles in orbital j lost exactly two of them. Combining the two,

$$e^{-\beta H(n)} = x_i^2 e^{-\beta H^{(i)}(n')}, \quad (18)$$

which is the exact weight law of Definition 3.1. Summing (18) over the disjoint images gives (16), because $M_N^{(u)}$ is the sum of $e^{-\beta H(n)}$ over exactly the configurations with a double occupancy. No sign condition and no ordering of the spectrum is used. $\square$

Remark 3.3. The identity is combinatorial, so it holds as an identity of polynomials in the variables x_i and y_{ij} , not merely numerically. That stronger form is checked symbolically for $K = 2, 3$ and $N = 2, 3, 4$ in Appendix C (block C1s).

Corollary 3.4 (decomposition of the interacting bosonic partition function). *For the same range of parameters,*

$$B_N^{(u)} = F_N^{(u)} + \sum_{i=0}^{K-1} x_i^2 Z_{N-2}^{(i)}. \quad (19)$$

In particular the interacting N -boson trace is determined by the interacting fermion trace and by $(N-2)$ -particle sums of shifted free-plus-interaction Hamiltonians.

Proof. $B_N^{(u)} - F_N^{(u)} = M_N^{(u)}$ by definition, and Theorem 3.2 evaluates the difference. $\square$

3.2 Two bounds that hold for every sign of the coupling

The three sums of (15) are ordered, because they sum the same positive weights over nested sets of configurations: the fermionic configurations of m particles lie in D_i , and D_i lies in the full bosonic set. Truncating the decomposition at either end therefore gives a bound.

Theorem 3.5 (universal shifted two-sided bound). *For every $K \geq 1$, every $\beta > 0$, every real spectrum, every real coupling u_{ij} and every $N \geq 2$,*

$$L_N^{(u)} \leq M_N^{(u)} \leq R_N^{(u)}, \quad L_N^{(u)} = \sum_{i=0}^{K-1} x_i^2 F_{N-2}^{(i)}, \quad R_N^{(u)} = \sum_{i=0}^{K-1} x_i^2 B_{N-2}^{(i)}. \quad (20)$$

If $N-2 > K$ then $L_N^{(u)} = 0$ and the lower bound is the trivial $M_N^{(u)} \geq 0$.

Proof. For every i and every m the inclusions of configuration sets give $0 \leq F_m^{(i)} \leq Z_m^{(i)} \leq B_m^{(i)}$, since all weights $e^{-\beta H^{(i)}(n')}$ are positive. Multiply by $x_i^2 > 0$, sum over i and insert Theorem 3.2. The case $N-2 > K$ is empty by definition of $F_m^{(i)}$. $\square$

Corollary 3.6 (reduction to the ideal endpoints, and the one-sided collapses). *Under the hypotheses of Theorem 3.5:*

- (i) at $u \equiv 0$, $H^{(i)} = H$ for every i , so $L_N^{(0)} = p_2 F_{N-2}^{(0)}$ and $R_N^{(0)} = p_2 B_{N-2}^{(0)}$, the leading terms of Proposition 2.1;
- (ii) if $u_{ij} \geq 0$ for all $i < j$, then $M_N^{(u)} \leq p_2 B_{N-2}^{(u)} = n U_N^{(u)}$;
- (iii) if $u_{ij} \leq 0$ for all $i < j$, then $n L_N^{(u)} = p_2 F_{N-2}^{(u)} \leq M_N^{(u)}$.

Proof. (i) At $u \equiv 0$ the shift $2(1 - \delta_{ij})u_{ij}$ vanishes, so $H^{(i)} = H_0$ and $B_m^{(i)} = B_m^{(0)}$, $F_m^{(i)} = F_m^{(0)}$; the sums over i produce the factor $\sum_i x_i^2 = p_2$. (ii) For $u_{ij} \geq 0$ the shift is non-negative, so $H^{(i)}(n') \geq H(n')$ pointwise and $e^{-\beta H^{(i)}(n')} \leq e^{-\beta H(n')}$ for every configuration; hence $B_{N-2}^{(i)} \leq B_{N-2}^{(u)}$ and $R_N^{(u)} \leq p_2 B_{N-2}^{(u)}$. Combine with Theorem 3.5. (iii) is the same argument on the fermionic side: $H^{(i)} \leq H$ pointwise gives $F_{N-2}^{(i)} \geq F_{N-2}^{(u)}$, hence $L_N^{(u)} \geq p_2 F_{N-2}^{(u)}$, and $L_N^{(u)} \leq M_N^{(u)}$. $\square$

Corollary 3.6 gives one valid endpoint for each sign of the coupling, and Section 4 shows that neither endpoint holds for the opposite sign. The shifted endpoints of Theorem 3.5 hold for both signs simultaneously, at the price of K shifted $(N-2)$ -particle sums instead of one unshifted one.

3.3 Exactness at two and three particles

At $N = 2$ and $N = 3$ the three sums of (15) coincide, because a configuration of at most one particle cannot violate the restriction $n'_j \leq 1$.

Proposition 3.7 (small- N identities). *For every K , every $\beta > 0$, every real spectrum and every real coupling u_{ij} ,*

$$B_2^{(u)} = p_2 + \sum_{i < j} x_i x_j y_{ij}, \quad F_2^{(u)} = \sum_{i < j} x_i x_j y_{ij}, \quad M_2^{(u)} = p_2, \quad (21)$$

$$M_3^{(u)} = \sum_i x_i^3 + \sum_{i < j} (x_i^2 x_j + x_i x_j^2) y_{ij}^2, \quad F_1^{(i)} = x_i + \sum_{j \neq i} x_j y_{ij}^2, \quad (22)$$

$$L_2^{(u)} = R_2^{(u)} = M_2^{(u)}, \quad L_3^{(u)} = R_3^{(u)} = M_3^{(u)}. \quad (23)$$

Proof. At $N = 2$ the only configurations with a double occupancy are the K pure doubles $n = 2e_i$, whose two-body part vanishes, so $M_2^{(u)} = \sum_i x_i^2 = p_2$; the remaining configurations have $n_i = n_j = 1$ for a unique pair $i < j$ and carry the weight $x_i x_j y_{ij}$, giving $B_2^{(u)}$ and $F_2^{(u)}$. The shifted sums at $m = 0$ all equal $B_0^{(i)} = F_0^{(i)} = Z_0^{(i)} = 1$, so both endpoints equal $\sum_i x_i^2$. At $N = 3$ the shifted sums have $m = 1$, and the single-particle configurations $n' = e_j$ lie in D_i for every i and j , so $F_1^{(i)} = Z_1^{(i)} = B_1^{(i)} = x_i + \sum_{j \neq i} x_j y_{ij}^2$, using the shift $2u_{ij}$ of (14). Hence $L_3^{(u)} = R_3^{(u)}$, and by Theorem 3.2 both equal $M_3^{(u)}$. The closed form follows by expanding the same sum: the triples $3e_i$ give $\sum_i x_i^3$ and the triples $2e_i + e_j$ give $x_i^2 x_j y_{ij}^2$, while the all-distinct triples cancel against $F_3^{(u)}$. $\square$

Because a single particle carries no two-body energy, the shifts do not distinguish bosons from fermions at $N = 3$, and the two endpoints collapse onto the exact value. This is where the construction is strongest, and it is also the point at which the uncorrected endpoints of (11) already fail for attractive couplings.

3.4 The exact defects at four particles

At $N = 4$ the remainder has two particles, and the restriction D_i excludes exactly the pure doubles in the orbitals below i . A pure double carries no pair between distinct orbitals, so its shifted energy is available in closed form and the two defects become explicit.

Proposition 3.8 (exact endpoint gaps at $N = 4$). *For every K , every $\beta > 0$, every real spectrum and every real coupling u_{ij} , define*

$$A_4 = \sum_i x_i^4, \quad B_4 = \sum_{i < j} x_i^2 x_j^2 y_{ij}^4. \quad (24)$$

Then

$$R_4^{(u)} - M_4^{(u)} = B_4, \quad M_4^{(u)} - L_4^{(u)} = A_4 + B_4, \quad M_4^{(u)} = \frac{L_4^{(u)} + R_4^{(u)} + A_4}{2}. \quad (25)$$

For $K \geq 2$ both defects are strictly positive and independent of the signs of the couplings. For $K = 1$, $B_4 = 0$, so $R_4^{(u)} = M_4^{(u)} = x_0^4$ exactly while $M_4^{(u)} - L_4^{(u)} = x_0^4$.

Proof. The remainder configurations at $m = 2$ are the pure doubles $2e_j$ and the split configurations $e_j + e_k$ with $j < k$. Every split configuration satisfies $n'_j \leq 1$ for all j and therefore lies in D_i for every i , so it contributes equally to $Z_2^{(i)}$, $B_2^{(i)}$ and $F_2^{(i)}$. A pure double $2e_j$ contributes to $Z_2^{(i)}$ exactly when $j \geq i$, to $B_2^{(i)}$ always and to $F_2^{(i)}$ never, and its shifted energy is $H^{(i)}(2e_j) = 2\varepsilon_j$ for $i = j$ and $2\varepsilon_j + 4u_{ij}$ for $i \neq j$. Hence

$$B_2^{(i)} - Z_2^{(i)} = \sum_{j < i} x_j^2 y_{ij}^4, \quad Z_2^{(i)} - F_2^{(i)} = x_i^2 + \sum_{j \geq i} x_j^2 y_{ij}^4, \quad (26)$$

and multiplying by x_i^2 , summing over i and using Theorem 3.5 in the form $R_4^{(u)} - M_4^{(u)} = \sum_i x_i^2 [B_2^{(i)} - Z_2^{(i)}]$ and $M_4^{(u)} - L_4^{(u)} = \sum_i x_i^2 [Z_2^{(i)} - F_2^{(i)}]$ gives (25). Each $x_i^2 x_j^2 y_{ij}^4$ appears once in the first sum, for $i = j$ in $\sum_i x_i^4$ and once in the second. The last identity is the sum of the first two divided by two. For $K \geq 2$, B_4 and A_4 are sums of strictly positive terms; for $K = 1$ the sums over $i < j$ are empty, the only orbital is $i = 0$, so $Z_2^{(i)} = B_2^{(i)} = x_0^2$ while $F_2^{(i)} = 0$. $\square$

The defects (25) are not sign-sensitive: attractive couplings do not tighten the shifted upper endpoint, they rescale the overshoot through y_{ij}^4 . The term B_4 is also the first obstruction to a sharper endpoint, since it is exactly the displaced weight of the lower-orbital doubles, which the set D_i excludes by construction.

3.5 The attainment frontier

The same bracket computation, applied at general N , gives a single positive witness per endpoint and settles exactly where the two endpoints are attained.

Theorem 3.9 (endpoint-attainment frontier). *For every real coupling u_{ij} and every discrete spectrum,*

$$\begin{aligned} N = 2, 3 : \quad & L_N^{(u)} = M_N^{(u)} = R_N^{(u)} \quad \text{for every } K, \\ N \geq 4, \ K = 1 : \quad & L_N^{(u)} < M_N^{(u)} = R_N^{(u)} = x_0^N, \\ N \geq 4, \ K \geq 2 : \quad & L_N^{(u)} < M_N^{(u)} < R_N^{(u)}, \end{aligned} \quad (27)$$

with the explicit witnesses

$$R_N^{(u)} - M_N^{(u)} \geq x_1^2 x_0^{N-2} y_{01}^{2(N-2)} > 0, \quad M_N^{(u)} - L_N^{(u)} \geq x_0^4 x_1^{N-4} y_{01}^{4(N-4)} > 0. \quad (28)$$

Equivalently, beyond three particles the lower endpoint is never attained, and the upper endpoint is attained only in the single-orbital sector.

Proof. The two defects are the bracket sums

$$R_N^{(u)} - M_N^{(u)} = \sum_i x_i^2 [B_{N-2}^{(i)} - Z_{N-2}^{(i)}], \quad M_N^{(u)} - L_N^{(u)} = \sum_i x_i^2 [Z_{N-2}^{(i)} - F_{N-2}^{(i)}], \quad (29)$$

both non-negative termwise. For the first, take $i = 1$ and the remainder $n' = (N-2, 0, \dots, 0)$: it is a bosonic configuration with $n'_0 = N-2 \geq 2$, so it is excluded from D_1 , and it carries no pair between distinct orbitals, hence $H^{(1)}(n') = (\varepsilon_0 + 2u_{01})(N-2)$ and its displaced weight is $x_0^{N-2} y_{01}^{2(N-2)}$. Multiplying by x_1^2 gives the first witness. For the second, take $i = 0$ and $n' = (2, N-4, 0, \dots, 0)$: it lies in D_0 because there is no orbital below 0, it is not fermionic, and $H^{(0)}(n') = 2\varepsilon_0 + (N-4)\varepsilon_1 + 4(N-4)u_{01}$, whose weight is $x_0^2 x_1^{N-4} y_{01}^{4(N-4)}$; multiplying by x_0^2 gives the second. For $K = 1$ the only orbital is $i = 0$, so D_i is the whole bosonic set, $Z_m^{(i)} = B_m^{(i)}$ and $R_N^{(u)} = x_0^2 B_{N-2}^{(u)} = x_0^N = M_N^{(u)}$, while $F_{N-2}^{(i)} = 0$ for $N \geq 4$ gives $L_N^{(u)} = 0$ and $M_N^{(u)} - L_N^{(u)} = x_0^N$. The cases $N = 2, 3$ are the content of Proposition 3.7. $\square$

Remark 3.10. The witnesses (28) are single configurations, so the strictness of the two endpoints is not a numerical observation but an explicit positive term. The upper-endpoint witness involves only the pair $(0, 1)$ and is therefore available in every model with at least two orbitals, whatever the remaining couplings are.

4 Interacting fermions and the failure of the uncorrected endpoint

The decomposition of Theorem 3.2 applies to a Hamiltonian that is diagonal in the occupations, so both statistics feel the coupling. The question this section answers is what happens to the bound one writes down without the shift, namely the uncorrected endpoints (11), when the fermions themselves interact. The answer is a sharp dichotomy: each of the two endpoints holds for exactly one sign of the coupling, one defect at three particles exhibits the failure, and the shifted endpoints repair it exactly where it occurs.

4.1 Where each uncorrected endpoint does hold

Proposition 4.1 (one-sided validity of the uncorrected endpoints). *Let $K \geq 2$, $\beta > 0$, a real spectrum and $N \geq 2$. If $u_{ij} \geq 0$ for all $i < j$ then*

$$M_N^{(u)} \leq nU_N^{(u)} = p_2 B_{N-2}^{(u)}. \quad (30)$$

If $u_{ij} \leq 0$ for all $i < j$ then

$$nL_N^{(u)} = p_2 F_{N-2}^{(u)} \leq M_N^{(u)}. \quad (31)$$

Proof. Both inequalities are Corollary 3.6(ii) and (iii). $\square$

The two statements are not two halves of one two-sided bound: neither one is accompanied by the opposite inequality, and there is no sign of u for which both endpoints hold together with the reverse endpoint. The obstruction is visible in the exact defect.

4.2 The exact defect

Proposition 4.2 (defect of the uncorrected upper endpoint). *For every $K, \beta > 0$, real spectrum, real coupling and $N \geq 2$,*

$$\begin{aligned} \Delta_N &:= p_2 B_{N-2}^{(u)} - M_N^{(u)} \\ &= \sum_{i=0}^{K-1} x_i^2 \left[\sum_{\substack{|n'|=N-2 \\ n' \notin D_i}} e^{-\beta H(n')} + \sum_{n' \in D_i} e^{-\beta H(n')} \left(1 - e^{-2\beta \sum_{j \neq i} u_{ij} n'_j} \right) \right], \end{aligned} \quad (32)$$

and the uncorrected upper endpoint holds for the given parameters if and only if $\Delta_N \geq 0$. At $N = 3$ this reduces to the closed form

$$\Delta_3 = p_2 p_1 - M_3^{(u)} = \sum_{i \neq j} x_i^2 x_j (1 - y_{ij}^2), \quad (33)$$

in which $nL_3^{(u)} = nU_3^{(u)} = p_2 p_1$ because a single particle has no two-body energy.

Proof. Write the uncorrected endpoint in the same labelled form as the decomposition, $p_2 B_{N-2}^{(u)} = \sum_i x_i^2 \sum_{|n'|=N-2} e^{-\beta H(n')}$, and subtract Theorem 3.2. Splitting the first sum over $n' \in D_i$ and $n' \notin D_i$, and using $e^{-\beta H^{(i)}(n')} = e^{-\beta H(n')} e^{-2\beta \sum_{j \neq i} u_{ij} n'_j}$, which follows from (14), gives (32). At $N = 3$ the remainder has one particle, so $n' = e_j$ and the first bracket is empty: D_i contains every single-particle configuration. The second bracket then gives $\sum_i \sum_j x_i^2 x_j (1 - y_{ij}^2)$, where the term $j = i$ vanishes because $y_{ii} = 1$, which is (33). $\square$

Formula (32) makes the sign structure explicit. The first bracket is a sum of positive weights and is strictly positive as soon as $K \geq 2$ and $N \geq 4$. The second bracket has the sign of $-\sum_{j \neq i} u_{ij} n'_j$: it is non-negative for repulsive couplings and can be arbitrarily negative for attractive ones. At $N = 3$ only the second bracket survives, which is why three particles already decide the question.

4.3 Sharp failure

Theorem 4.3 (sharp failure of the uncorrected endpoints). *Let $K \geq 2$ and $\beta > 0$.*

(i) *If $u_{kl} < 0$ for some pair and $u_{ij} = 0$ for all other pairs, then*

$$\Delta_3 = (x_k^2 x_l + x_l^2 x_k) (1 - y_{kl}^2) < 0, \quad \text{so} \quad M_3^{(u)} > p_2 p_1 = nU_3^{(u)}. \quad (34)$$

(ii) *If $u_{kl} > 0$ for some pair and $u_{ij} = 0$ for all other pairs, the same formula gives $\Delta_3 > 0$, hence $M_3^{(u)} < p_2 p_1 = nL_3^{(u)}$.*

(iii) *If a coupling set contains at least one pair with $u_{kl} < 0$, then there are spectra for which $\Delta_3 < 0$, and along the family $\varepsilon_k = \varepsilon_l = -s$ with every other energy fixed,*

$$\Delta_3 = -2e^{3\beta s} (y_{kl}^2 - 1) + O(e^{2\beta s}) \longrightarrow -\infty \quad (s \rightarrow \infty). \quad (35)$$

(iv) *Consequently $nU_N^{(u)}$ is a valid upper endpoint for every $N \geq 2$ and every positive spectrum if and only if $u_{ij} \geq 0$ for all pairs, and $nL_N^{(u)}$ is a valid lower endpoint for every $N \geq 2$ and every positive spectrum if and only if $u_{ij} \leq 0$ for all pairs.*

Table 2: The uncorrected endpoint at three particles, in the emblematic case $K = 3$, $\beta = 0.6$, $\varepsilon = (0, 0.45, 0.9)$ with a uniform inter-orbital coupling $u_{ij} = u$ on all three pairs. Every entry is an exact enumeration in 50-digit arithmetic. The uncorrected endpoints coincide at $N = 3$, $nU_3 = nL_3 = p_2p_1 = 4.51006407633$, so the same column tests both. The shifted endpoints of Theorem 3.5 are equal to M_3 in every row, so the repair is exact wherever the uncorrected endpoint fails.

u	$M_3^{(u)}$	p_2p_1	$\Delta_3 = p_2p_1 - M_3^{(u)}$	$L_3^{(u)} = R_3^{(u)}$	status of nU_3
+0.6	3.03842506748	4.51006407633	+1.47163900885	3.03842506748	holds
+0.4	3.41699890857	4.51006407633	+1.09306516776	3.41699890857	holds
0	4.51006407633	4.51006407633	0	4.51006407633	equality
-0.2	5.28781874815	4.51006407633	-0.77775467182	5.28781874815	fails
-0.4	6.27653871387	4.51006407633	-1.76647463754	6.27653871387	fails
-0.6	7.53344813019	4.51006407633	-3.02338405386	7.53344813019	fails

Proof. (i) and (ii) Substitute $y_{ij} = 1$ for $(i, j) \neq (k, l)$ into (33); the two ordered terms (k, l) and (l, k) survive and give $(x_k^2 x_l + x_l^2 x_k)(1 - y_{kl}^2)$. For $u_{kl} < 0$ one has $y_{kl} = e^{-\beta u_{kl}} > 1$, so the defect is strictly negative; for $u_{kl} > 0$ it is strictly positive.

(iii) Put $\varepsilon_k = \varepsilon_l = -s$, so $x_k = x_l = e^{\beta s}$, and keep the remaining x_j fixed. The terms of (33) with $\{i, j\} = \{k, l\}$ are $x_k^2 x_l(1 - y_{kl}^2) + x_l^2 x_k(1 - y_{lk}^2) = 2e^{3\beta s}(1 - y_{kl}^2)$, which is negative and of order $e^{3\beta s}$ when $u_{kl} < 0$. Every remaining term has at most one factor $e^{\beta s}$ squared, hence is $O(e^{2\beta s})$: the terms $x_k^2 x_j + x_j^2 x_k$ and $x_l^2 x_j + x_j^2 x_l$ with $j \notin \{k, l\}$ are $O(e^{2\beta s})$, and the terms with $i, j \notin \{k, l\}$ are $O(1)$. The $e^{3\beta s}$ term therefore dominates for large s , which gives (35).

(iv) Sufficiency is Proposition 4.1. For necessity, if some $u_{kl} < 0$ then part (i) exhibits $N = 3$ and a spectrum with $M_3^{(u)} > nU_3^{(u)}$, and part (iii) exhibits spectra for which the violation is unbounded; if some $u_{kl} > 0$ then part (ii) exhibits $M_3^{(u)} < nL_3^{(u)}$. If all couplings have the same sign, the required condition holds. If the coupling set has mixed signs, then it contains a pair (k, l) with $u_{kl} < 0$ and a pair (k', l') with $u_{k'l'} > 0$. Sending $\varepsilon_k = \varepsilon_l = -s$ with the other energies fixed gives $\Delta_3 \rightarrow -\infty$ by part (iii), so nU fails. Sending $\varepsilon_{k'} = \varepsilon_{l'} = -s$ instead gives $\Delta_3 = +2e^{3\beta s}(1 - y_{k'l'}^2) + O(e^{2\beta s}) \rightarrow +\infty$, because $y_{k'l'} < 1$, hence $M_3^{(u)} < p_2p_1 = nL_3^{(u)}$ and nL fails as well. $\square$

Table 2 and Figure 2 show the failure and the repair on one spectrum. The single-signed-pair witnesses of Theorem 4.3 are equally explicit and are computed on the same spectrum: with $u_{01} = -0.4$ and the other couplings zero, $M_3^{(u)} = 5.3393789232$ against $p_2p_1 = 4.51006407633$, so the uncorrected upper endpoint is violated by 0.829; with $u_{01} = +0.4$ and the other couplings zero, $M_3^{(u)} = 3.9968978225$, so the uncorrected lower endpoint is violated by 0.513. Both defects agree with (33) to 40 digits.

Part (iii) of the theorem also shows that the failure is not a marginal phenomenon. For the mixed-sign coupling set $u_{01} = -0.5$, $u_{02} = +0.7$, $u_{12} = +0.2$ on the spectrum $\varepsilon = (-s, -s, 0.9)$ with $\beta = 0.6$, the defect takes the values

$$\Delta_3 = -9.233 \times 10^{-1}, -5.427 \times 10^1, -2.144 \times 10^3, -7.998 \times 10^4, -2.943 \times 10^6, -1.079 \times 10^8 \quad (36)$$

for $s = 0, 2, 4, 6, 8, 10$: one attractive pair among two repulsive ones is enough to overturn the uncorrected upper endpoint, and the violation grows exponentially once the attractive pair's orbitals are the lowest.

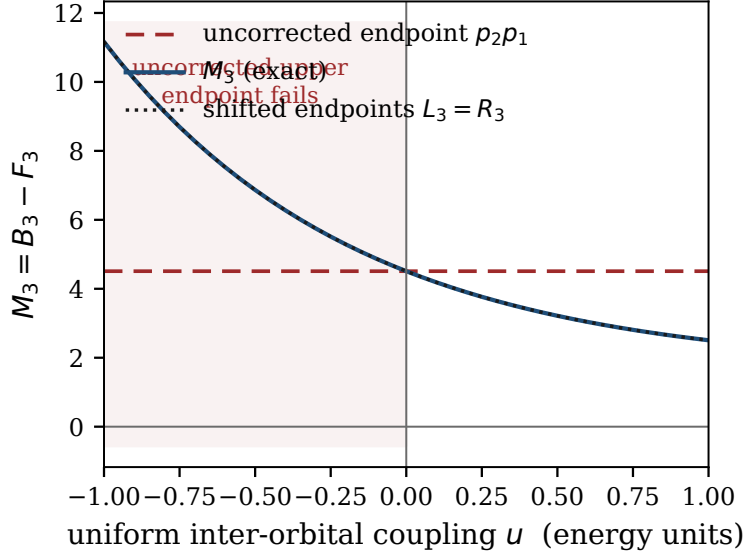


Figure 2: Three particles, three orbitals, uniform coupling. The exact value $M_3^{(u)}$ of the emblematic case of Table 2 against the uncorrected endpoint $p_2 p_1$, which is independent of u at $N = 3$. For attractive couplings the exact value rises above the uncorrected endpoint and the bound fails; the shifted endpoints $L_3^{(u)} = R_3^{(u)}$ of Theorem 3.5 coincide with the exact value for every coupling, on both sides of $u = 0$. Data: exact 50-digit enumeration, $u \in [-1, 1]$ in steps of 0.05.

4.4 The repair

Corollary 4.4 (exact repair at three particles). *For every $K, \beta > 0$, real spectrum and real coupling,*

$$L_3^{(u)} = R_3^{(u)} = M_3^{(u)} = p_2 p_1 - \Delta_3, \quad (37)$$

so the shifted endpoints of Theorem 3.5 are exact precisely where the uncorrected endpoints of (11) fail, and no exponential slack is needed for the repair.

Proof. Proposition 3.7 gives $L_3^{(u)} = R_3^{(u)} = M_3^{(u)}$, and Proposition 4.2 evaluates $M_3^{(u)} = p_2 p_1 - \Delta_3$. $\square$

The repair is exact at $N = 3$ but not beyond it: at $N = 4$ the shifted endpoints have the explicit defects A_4 and B_4 of Proposition 3.8, and Theorem 3.9 shows that no shifted endpoint is attained for $N \geq 4$ when $K \geq 2$. What survives is a two-sided bound that is valid for every sign of the coupling, with defects that are themselves explicit.

5 Pair hopping

A pair hop is off-diagonal in the occupation basis, so the injection that proves Proposition 2.1 no longer applies: there is no weight law of the form (18), because the removed pair does not stay where it was. Two structural facts replace it. The fermionic side does not move at all, and the bosonic side moves only upwards.

5.1 The frozen fermion side and monotonicity

Theorem 5.1 (monotonicity and the reversed endpoint). *Let $H = H_0 + H_{\text{ph}}$ with H_{ph} as in (8) and arbitrary complex couplings γ_{ij} . Then for every K , every $\beta > 0$, every real spectrum and every $N \geq 2$,*

$$F_N^{\text{ph}} = F_N^{(0)}, \quad B_N^{\text{ph}} \geq B_N^{(0)}, \quad M_N^{\text{ph}} \geq M_N^{(0)} \geq p_2 F_{N-2}^{(0)}. \quad (38)$$

Moreover, at $N = 2$ and $N = 3$ the free upper endpoint is reversed:

$$M_N^{\text{ph}} \geq p_2 B_{N-2}^{(0)}, \quad N = 2, 3, \quad (39)$$

and the inequality $M_N^{\text{ph}} \geq M_N^{(0)}$ is strict for every $N \geq 2$ as soon as one coupling γ_{ij} is non-zero.

Proof. The first identity is Lemma 2.2(i): every matrix element of H_{ph} carries a factor $\sqrt{n_j(n_j - 1)}$, which vanishes on a fermionic configuration, so the fermionic block of H is the diagonal matrix $\varepsilon(n)$ and its trace is $F_N^{(0)}$.

For the bosonic side, H is a Hermitian matrix on the N -boson occupation basis whose diagonal is exactly $\varepsilon(n)$, the list of eigenvalues of H_0 in the same basis. By the Schur–Horn theorem the eigenvalue list of H majorizes its diagonal. The function $f(x) = e^{-\beta x}$ is convex, so $\lambda \mapsto \sum_k f(\lambda_k)$ is Schur-convex, and

$$B_N^{\text{ph}} = \text{tr}_{|n|=N} e^{-\beta H} \geq \text{tr}_{|n|=N} e^{-\beta H_0} = B_N^{(0)}. \quad (40)$$

Subtracting the common fermionic value gives $M_N^{\text{ph}} \geq M_N^{(0)}$, and Proposition 2.1 gives $M_N^{(0)} \geq p_2 F_{N-2}^{(0)}$.

At $N = 2$ and $N = 3$ Proposition 2.1 states that the free upper endpoint is attained, $M_N^{(0)} = p_2 B_{N-2}^{(0)}$, so the monotonicity gives (39). For the strictness, note that if some $\gamma_{ij} \neq 0$ then H has a non-zero off-diagonal entry in the N -boson sector for every $N \geq 2$: the configuration $n = 2e_j$ has $n_j = 2$, and the amplitude of (10) for the hop $2e_j \mapsto 2e_i$ is $\sqrt{1 \cdot 2 \cdot 2 \cdot 1} = 2$. A Hermitian matrix with a non-zero off-diagonal entry is not diagonal, so equality in the Schur–Horn majorization is excluded, and since $x \mapsto e^{-\beta x}$ is strictly convex the inequality (40) is strict. For $N = 2$ the same strictness is visible in closed form in Proposition 5.2. $\square$

The content of (39) is that a pair hop does not weaken the bound, it *reverses* it: the endpoint that was an upper bound for the free gas becomes a lower bound, and the free lower endpoint keeps its direction. Neither statement needs a sign condition on γ_{ij} or a restriction to real couplings.

5.2 Two particles: the exact value and the exact defect

Proposition 5.2 (exact $N = 2$ endpoint for one link). *Let $K \geq 2$, let only the link $(0, 1)$ be switched on, and write $R = \sqrt{(\varepsilon_0 - \varepsilon_1)^2 + 4|\gamma_{01}|^2}$. Then*

$$M_2^{\text{ph}} = 2x_0x_1 \cosh(\beta R) + \sum_{k \geq 2} x_k^2, \quad M_2^{\text{ph}} - p_2 = 2x_0x_1 [\cosh(\beta R) - \cosh(\beta|\varepsilon_0 - \varepsilon_1|)] \geq 0, \quad (41)$$

with equality if and only if $\gamma_{01} = 0$.

Proof. At $N = 2$ the only configurations are the pure doubles $2e_k$ and the split configurations $e_k + e_l$. The pair hop connects $2e_0$ and $2e_1$ through the 2×2 block

$$\begin{pmatrix} 2\varepsilon_0 & 2\gamma_{01} \\ 2\gamma_{01}^* & 2\varepsilon_1 \end{pmatrix}, \quad (42)$$

whose eigenvalues are $\varepsilon_0 + \varepsilon_1 \pm R$ and whose contribution to the trace is therefore $2x_0x_1 \cosh(\beta R)$. Every other pure double $2e_k$ with $k \geq 2$ is untouched and contributes x_k^2 , and every split configuration is fermionic, so it cancels against $F_2^{(0)}$. Since $p_2 = x_0^2 + x_1^2 + \sum_{k \geq 2} x_k^2 = 2x_0x_1 \cosh(\beta|\varepsilon_0 - \varepsilon_1|) + \sum_{k \geq 2} x_k^2$, the defect is the difference of the two cosines, and $\cosh$ is strictly increasing on $[0, \infty)$ with $R \geq |\varepsilon_0 - \varepsilon_1|$, equality holding only at $\gamma_{01} = 0$. $\square$

5.3 Two orbitals: an exact endpoint for every N

For $K = 2$ the pair hop closes a Lie algebra, and the worst-case exponential envelope of Subsection 5.6 below can be replaced by an exact value. With $J_+ = b_0^\dagger b_1$, $J_- = b_1^\dagger b_0$ and $J_z = (n_0 - n_1)/2$, the N -boson sector carries the spin- J representation with $J = N/2$, $E_{01}^2 = J_+^2$ and $E_{10}^2 = J_-^2$, so with $c = (\varepsilon_0 + \varepsilon_1)/2$ and $\Delta = \varepsilon_0 - \varepsilon_1$

$$H = cN + \Delta J_z + \gamma J_+^2 + \gamma^* J_-^2, \quad (43)$$

a two-axis-twisting quadratic form. In the J_z eigenbasis the operator $G = \Delta J_z + \gamma J_+^2 + \gamma^* J_-^2$ is tridiagonal along the steps $m \mapsto m+2$, with amplitudes $\sqrt{(J-m)(J-m-1)(J+m+1)(J+m+2)}$, and therefore splits into the two J_z -parity sectors.

Theorem 5.3 (exact two-orbital pair-hopping endpoint). *Let $K = 2$ and let G be as in (43), with $J = N/2$. Then $\text{spec}(G) = -\text{spec}(G)$ for every N , and*

$$M_N^{\text{ph}} = (x_0x_1)^{N/2} \sum_C \text{tr}_C e^{-\beta G_C} - F_N^{(0)}, \quad (44)$$

where the sum runs over the two J_z -parity sectors and $F_N^{(0)} = x_0x_1$ for $N = 2$ and 0 for $N \geq 3$. Every spectral quantity depends on γ only through $|\gamma|$, and the sector spectra are the roots of the continuant recurrence

$$\begin{aligned} P_0(t) &= 1, & P_1(t) &= t - d_1, \\ P_k(t) &= (t - d_k)P_{k-1}(t) - b_{k-1}^2 P_{k-2}(t) \quad (k \geq 2), \end{aligned} \quad (45)$$

with $d_k = \Delta m_k$ and $b_k = |\gamma| \sqrt{(J - m_k)(J - m_k - 1)(J + m_k + 1)(J + m_k + 2)}$ along the ordered labels $m_1 < \dots < m_s$ of the sector. The first closed forms are

$$M_2^{\text{ph}} = 2x_0x_1 \cosh(\beta \sqrt{\Delta^2 + 4|\gamma|^2}), \quad (46)$$

$$M_3^{\text{ph}} = 2(x_0x_1^2 + x_0^2x_1) \cosh(\beta \sqrt{\Delta^2 + 12|\gamma|^2}), \quad (47)$$

$$M_4^{\text{ph}} = x_0^2x_1^2 \left[1 + 2 \cosh(2\beta \sqrt{\Delta^2 + 12|\gamma|^2}) + 2 \cosh(\beta \sqrt{\Delta^2 + 36|\gamma|^2}) \right], \quad (48)$$

$$M_6^{\text{ph}} = (x_0x_1)^3 \left[1 + 2 \cosh(2\beta \sqrt{\Delta^2 + 60|\gamma|^2}) + 2 \cosh(\beta \sqrt{y_+}) + 2 \cosh(\beta \sqrt{y_-}) \right], \quad (49)$$

with $y_{\pm} = 5\Delta^2 + 132|\gamma|^2 \pm 4\sqrt{\Delta^4 + 24\Delta^2|\gamma|^2 + 864|\gamma|^4}$. At $N = 5$ the sector characteristic polynomial is the cubic

$$p_5(\lambda) = -\lambda^3 - \frac{3\Delta}{2}\lambda^2 + \frac{13\Delta^2 + 448|\gamma|^2}{4}\lambda + \frac{15\Delta^3 + 960\Delta|\gamma|^2}{8}, \quad (50)$$

whose three real roots give $M_5^{\text{ph}} = 2(x_0x_1)^{5/2} \sum_{p_5(\lambda)=0} \cosh(\beta\lambda)$.

Proof. Write the phase gauge: in each parity sector the coupling graph is a path, so conjugation by $\text{diag}(e^{i\theta_m})$ with $\theta_{-J} = 0$ and $\theta_{m+2} = \theta_m - \arg \gamma$ makes every off-diagonal entry real and positive,

and the sector becomes a real symmetric tridiagonal matrix with diagonal Δm and off-diagonal $|\gamma| \text{amp}(m)$. Two facts about that matrix give the symmetry. First, $\text{amp}(m) = \text{amp}(-m - 2)$, so the amplitudes are invariant under the reflection $m \mapsto -m$ up to reversal. Second, changing the sign of every off-diagonal entry of a path matrix is a unitary equivalence, realized by the diagonal signs $s_{k+1} = -s_k$. Let P reverse the basis order in the sector. Then PGP has diagonal $-\Delta m$ reflected, and off-diagonals equal to those of G in reverse order by the first fact; by the second fact PGP is unitarily equivalent to $-G$. Hence $\text{spec}(G) = \text{spec}(PGP) = \text{spec}(-G) = -\text{spec}(G)$, and the same computation shows that for half-integer J the two sectors are negatives of one another while for integer J each sector is individually symmetric, the odd-sized sector holding the single zero eigenvalue.

Formula (44) follows by tracing: the constant cN contributes the scalar $(x_0 x_1)^{N/2}$ to every state of the sector, and the fermionic contribution is $F_N^{(0)}$ by Theorem 5.1. The recurrence (45) is the standard continuant expansion of a tridiagonal determinant along the ordered labels of the sector, so its roots are the sector eigenvalues. The closed forms are the explicit spectra of the small sectors: at $N = 2$ the sector is (42) shifted by cN ; at $N = 3$ both sectors are 2×2 with common off-diagonal $2\sqrt{3}|\gamma|$ and diagonals $\pm\Delta/2$; at $N = 4$ the odd sector is $\begin{pmatrix} -\Delta & 6\gamma \\ 6\gamma^* & \Delta \end{pmatrix}$ and the even sector is 3×3 with diagonal $(-2\Delta, 0, 2\Delta)$, off-diagonal $2\sqrt{6}|\gamma|$ and eigenvalues $\{0, \pm 2\sqrt{\Delta^2 + 12|\gamma|^2}\}$; at $N = 6$ the odd sector on $m = -2, 0, 2$ has eigenvalues $\{0, \pm 2\sqrt{\Delta^2 + 60|\gamma|^2}\}$ and the even sector on $m = -3, -1, 1, 3$ is biquadratic with the stated roots. Symmetry of the spectrum turns each sector trace into a sum of cosh terms, with the zero eigenvalue contributing the isolated 1. $\square$

Formula (44) has no slack: it is the exact value of the trace, not a bound. What it costs is one eigensolve per parity sector, or one continuant recurrence, which for large N is a polynomial root-finding problem rather than a closed form.

5.4 One link in a larger orbital space

The two-orbital trace also closes the upper endpoint when a larger orbital space contains exactly one active link, because a pair hop conserves the joint occupation of the two orbitals it connects and leaves every spectator occupation untouched.

Corollary 5.4 (single link with spectators). *Let $H = H_0 + \gamma E_{01}^2 + \gamma^* E_{10}^2$ act on $K \geq 2$ orbitals, where $E_{ij} = b_i^\dagger b_j$, and let $B_q^{\text{ph},01}$ be the exact two-orbital pair-hopping bosonic partition function of Theorem 5.3 with $J = q/2$, and $S_m^{\text{spect}} = h_m(x_2, \dots, x_{K-1})$ the free bosonic partition function of m particles among the spectators. Then for every $N \geq 2$*

$$M_N^{\text{ph}} = \sum_{q=0}^N B_q^{\text{ph},01} S_{N-q}^{\text{spect}} - e_N(x_0, \dots, x_{K-1}), \quad (51)$$

an exact value with no exponential factor.

Proof. Both $q = n_0 + n_1$ and each spectator occupation n_k , $k \geq 2$, are conserved by H , so the N -boson space decomposes as a direct sum over q of the two-orbital $J = q/2$ sector tensored with the free spectator configurations of $N - q$ particles, and the trace factorizes as in (51). The subtracted term is $F_N^{(0)} = e_N(x)$ by Theorem 5.1. $\square$

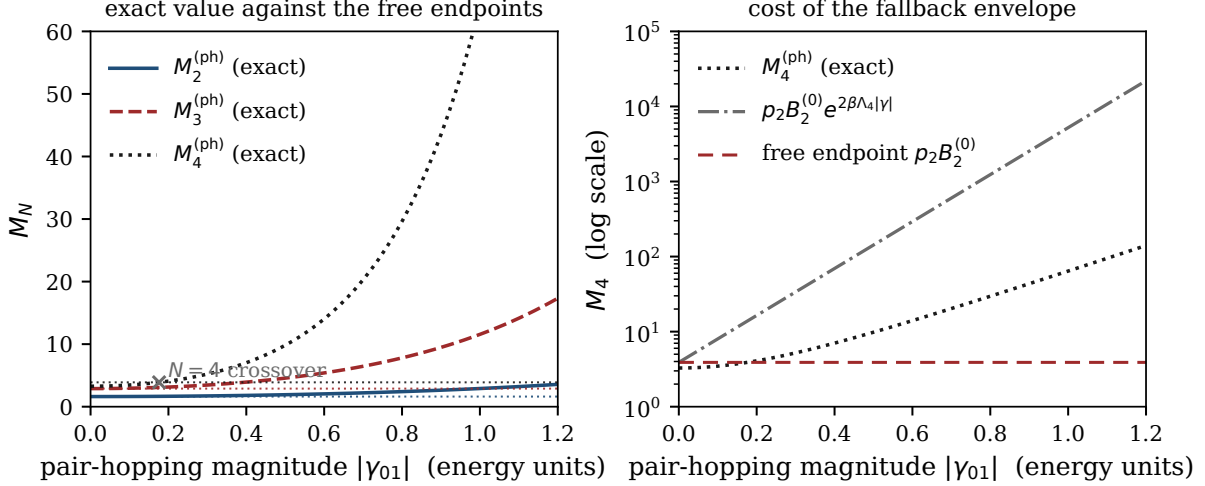


Figure 3: Two orbitals, $\beta = 0.6$, $(\varepsilon_0, \varepsilon_1) = (0, 0.4)$, one link γ_{01} real and non-negative. *Left*: the exact values M_N^{ph} for $N = 2, 3, 4$ from Theorem 5.3, each with its free upper endpoint $p_2 B_{N-2}^{(0)}$ drawn as a dotted horizontal line of the same colour. At $N = 2$ and $N = 3$ the exact value starts at the free endpoint and rises immediately, which is the reversal of (39); at $N = 4$ the exact value starts below the endpoint and crosses it at $|\gamma_{01}| = 0.17601$, so the free upper endpoint remains a valid upper bound only up to that threshold. *Right*: the same $N = 4$ curve against the exponential envelope $p_2 B_2^{(0)} e^{2\beta \Lambda_4 |\gamma_{01}|}$ of Proposition 5.7, on a logarithmic scale; the envelope is valid everywhere and becomes the only available closed-form upper bound once several links overlap, but it exceeds the exact value by more than four orders of magnitude at $|\gamma_{01}| = 1.2$. Data: exact sector traces cross-checked against full Fock diagonalization.

5.5 Any number of links: orbital parities

When several links share an orbital the corresponding $\mathfrak{su}(2)$ copies do not commute, and neither the spin reduction nor the single-link factorization applies. A conserved quantity of a different kind still decomposes the problem exactly.

Corollary 5.5 (exact endpoint for an arbitrary link graph). *Let $H = H_0 + H_{ph}$ with arbitrary complex couplings γ_{ij} on an arbitrary link graph. Each parity $n_i \bmod 2$ is conserved, so writing $n = s + 2m$ with $s \in \{0, 1\}^K$ and $m \in \mathbb{N}^K$, the N -boson space splits into sectors labelled by s with $|s| \leq N$, $N - |s|$ even and $q = (N - |s|)/2$, on each of which H restricts to the $|m| = q$ matrix*

$$(H_s)_{m,m} = \sum_i \varepsilon_i (s_i + 2m_i), \quad (H_s)_{m+e_a-e_b,m} = \gamma_{ab} \sqrt{(n_a+1)(n_a+2)n_b(n_b-1)}, \quad n_i = s_i + 2m_i, \quad (52)$$

with all other entries zero. The $q = 0$ sector is exactly the free fermionic partition function, and

$$M_N^{ph} = \sum_{s: q=(N-|s|)/2 \geq 1} \text{tr}_{|m|=q} e^{-\beta H_s} \quad (53)$$

is exact for every $N \geq 2$, every K , every link graph and every complex coupling set. If the non-zero couplings form a matching, each sector further factorizes into independent two-orbital pair sectors tensored with frozen spectators, and every trace in (53) is a continuant of the form (45).

Proof. The operator $(b_i^\dagger)^2 b_j^2$ changes n_i and n_j by ± 2 and leaves every other occupation fixed, so each $n_i \bmod 2$ is a conserved charge and the sector labelled by s is invariant; the matrix elements are those of (10) evaluated at $n = s + 2m$. In the sector $q = 0$ every $m = 0$, so H_s is the diagonal matrix with entries $\sum_i \varepsilon_i s_i$ over the s with $|s| = N$, whose trace is $e_N(x) = F_N^{(0)}$; subtracting it from B_N^{ph} gives (53). For a matching, the moves of distinct links act on disjoint orbital pairs, so the m -space is a tensor product of one two-orbital pair space per link and of frozen spectator spaces, and each factor is a tridiagonal path matrix in the number of pairs carried by that link, with the s -dependent amplitudes $\gamma_{ij} \sqrt{(s_i + 2m_i + 1)(s_i + 2m_i + 2)(s_j + 2m_j)(s_j + 2m_j - 1)}$; every sector trace is therefore a continuant of the form (45). In the $q = 1$ sectors this amplitude reduces to $2\gamma_{ij} w_i w_j$ with $w_a = 1$ if $s_a = 0$ and $w_a = \sqrt{3}$ if $s_a = 1$, which is the form used in (54) and (55). $\square$

Two small cases of (53) are worth stating, because they reduce the endpoint to the spectrum of a single $K \times K$ Hermitian matrix rather than of an exponentially large Fock space. At $N = 2$ the only contributing sector is $s = 0$, $q = 1$, and

$$M_2^{\text{ph}} = \text{tr} \exp(-\beta[2 \text{diag}(\varepsilon) + 2G]), \quad G_{ij} = \gamma_{ij}, \quad G_{ji} = \gamma_{ij}^*. \quad (54)$$

At $N = 3$ the contributing sectors have $|s| = 1$, one per orbital r , and

$$M_3^{\text{ph}} = \sum_r x_r \text{tr} \exp(-\beta[2 \text{diag}(\varepsilon) + 2G^{(r)}]), \quad G_{ij}^{(r)} = \gamma_{ij} w_i w_j, \quad w_a = \begin{cases} \sqrt{3}, & a = r, \\ 1, & a \neq r. \end{cases} \quad (55)$$

In both cases the $q = 1$ sector is a single pair moving on the orbital graph, and the amplitudes of (52) collapse to $2w_a w_b \gamma_{ab}$ because $\sqrt{(s_a + 1)(s_a + 2)} = \sqrt{2} w_a$ for $s_a \in \{0, 1\}$.

Remark 5.6 (cost). Formula (53) is exact but not free. There are at most 2^K sector labels, and the largest sector has dimension $\binom{K + \lfloor N/2 \rfloor - 1}{\lfloor N/2 \rfloor}$, so for fixed K the endpoint is a polynomial number of finite Hermitian eigensolves in N . That is asymptotically cheaper than the full N -boson diagonalization, whose dimension is $\binom{K+N-1}{N}$, but it is not a closed form, and for overlapping links no closed form is known.

5.6 A closed-form envelope for arbitrary links

When a closed-form upper bound is needed rather than an exact eigensolve, one eigenvalue inequality suffices.

Proposition 5.7 (controlled pair-hopping envelope). *For every K , every $\beta > 0$, every real spectrum, every complex coupling set and every $N \geq 2$,*

$$p_2 F_{N-2}^{(0)} \leq M_N^{\text{ph}} \leq p_2 B_{N-2}^{(0)} \exp\left(2\beta \Lambda_N \sum_{i < j} |\gamma_{ij}|\right), \quad (56)$$

$$\Lambda_N = \max_{0 \leq b \leq N} \sqrt{(N - b + 1)(N - b + 2)b(b - 1)} \leq \frac{(N + 1)^2}{4}.$$

Proof. By Lemma 2.2(i) the multiple-occupancy subspace $\mathcal{M}$ is invariant, and $M_N^{\text{ph}} = \text{tr}_{\mathcal{M}} e^{-\beta(H_0 + H_{\text{ph}})}$. For Hermitian A and B on one finite-dimensional space, the Courant–Fischer min-max principle gives $\lambda_j(A + B) \geq \lambda_j(A) - \|B\|$ for the eigenvalues in decreasing order, hence $\text{tr} e^{-\beta(A+B)} \leq e^{\beta\|B\|} \text{tr} e^{-\beta A}$. Applying this on $\mathcal{M}$ with $A = H_0$ and $B = H_{\text{ph}}$

gives $M_N^{\text{ph}} \leq e^{\beta \|H_{\text{ph}}\|} M_N^{(0)}$, and Proposition 2.1 bounds $M_N^{(0)} \leq p_2 B_{N-2}^{(0)}$. The lower endpoint is Theorem 5.1.

It remains to bound the norm. The operator E_{ij}^2 is a weighted shift on the N -boson sector with amplitudes $\sqrt{(n_i + 1)(n_i + 2)n_j(n_j - 1)}$, so $\|E_{ij}^2\| = \Lambda_N$, the largest amplitude over configurations, attained when $n_j = b$ and $n_i = N - b$. Two applications of the arithmetic–geometric mean inequality, to the pairs $b, (N - b + 1)$ and $(b - 1), (N - b + 2)$, both of which sum to $N + 1$, give $b(b - 1)(N - b + 1)(N - b + 2) \leq (N + 1)^4/16$ and hence $\Lambda_N \leq (N + 1)^2/4$. The triangle inequality then gives $\|H_{\text{ph}}\| \leq 2\Lambda_N \sum_{i < j} |\gamma_{ij}|$. $\square$

Remark 5.8 (what the envelope costs). The factor $e^{2\beta\Lambda_N \sum |\gamma_{ij}|}$ is a worst-case constant and is not claimed to be tight. It is the price of not diagonalizing, and Figure 3 shows it growing to more than four orders of magnitude at $|\gamma| = 1.2$, $N = 4$. Whenever the exact endpoint of Corollary 5.5 is affordable, it supersedes the envelope entirely; the envelope is the fallback for link graphs too large to eigensolve, and its constants are the only ones in this paper that are admittedly not sharp (the simultaneous upper endpoint of Theorem 7.2 inherits them).

5.7 Where the free upper endpoint stops holding

The reversal (39) is proved at $N = 2$ and $N = 3$, where the free upper endpoint is attained. At $N \geq 4$ the free upper endpoint is already strict for the free gas, so a pair hop can either stay below it or exceed it depending on the coupling. For the two-orbital case of Figure 3, with $\beta = 0.6$ and $(\varepsilon_0, \varepsilon_1) = (0, 0.4)$, the exact $N = 4$ value (48) crosses the free endpoint $p_2 B_2^{(0)} = 3.89384$ at

$$|\gamma_{01}| = 0.17601, \quad (57)$$

computed by bisection on the full Fock solve and cross-checked against the closed form to nine digits (Appendix C, block C10b). Above that threshold the free upper endpoint is no longer an upper bound at $N = 4$, and the available closed-form upper bound is the envelope (56) or the exact sector formula (53). An exact replacement endpoint that absorbs the whole growth $B_N^{\text{ph}} - B_N^{(0)}$ in closed form for $N \geq 4$ and $K > 2$ is not known; this is the pair-hopping gap recorded in Section 9.

6 Orbital exchange

The one-particle exchange term (9) is off-diagonal in the occupation basis, and unlike a pair hop it acts on the fermionic sector as well, so neither the weight law (18) nor the monotonicity Theorem 5.1 applies to it. What replaces them is a unitary equivalence: the exchange term is the second quantization of a one-body matrix, so the whole model is a free gas on a rotated spectrum.

Theorem 6.1 (exchange-invariance of the ideal bounds). *Let t be the Hermitian $K \times K$ matrix with $t_{ii} = \varepsilon_i$ and $t_{ij} = \tau_{ij}$ for $i < j$, let $\omega_0 \leq \dots \leq \omega_{K-1}$ be its eigenvalues and $x'_a = e^{-\beta\omega_a}$, and let $H = H_0 + H_{\text{ex}}$. Then for every K , every $\beta > 0$, every real spectrum, every complex coupling set τ_{ij} and every $N \geq 2$,*

$$B_N^{\text{ex}} = h_N(x'), \quad F_N^{\text{ex}} = e_N(x'), \quad M_N^{\text{ex}} = h_N(x') - e_N(x'), \quad (58)$$

and every bound of Proposition 2.1 holds with x' in place of x :

$$\sum_{k=1}^{\lfloor N/2 \rfloor} \frac{p'_{2k}}{k} F_{N-2k}^{\text{ex}} \leq M_N^{\text{ex}} \leq p'_2 B_{N-2}^{\text{ex}}, \quad p'_k = \sum_a (x'_a)^k, \quad (59)$$

$$f'_N F_N^{\text{ex}} \leq M_N^{\text{ex}} \leq f'_N B_N^{\text{ex}}, \quad f'_N = \frac{p'_2}{(p'_1)^2} N(N-1), \quad (60)$$

with both endpoints in (59) attained at $N = 2$ and $N = 3$, where $M_2^{\text{ex}} = p'_2$ and $M_3^{\text{ex}} = p'_2 p'_1$.

Proof. By Lemma 2.2(ii) there is a unitary V with $t = V^\dagger \text{diag}(\omega)V$ such that the rotated operators $a_a = \sum_i V_{ai} b_i$ and $d_a = \sum_i V_{ai} c_i$ satisfy the canonical commutation respectively anticommutation relations and diagonalize the Hamiltonian in both sectors, $H = \sum_a \omega_a a_a^\dagger a_a = \sum_a \omega_a d_a^\dagger d_a$. A canonical N -particle sector is therefore a sum over configurations of N particles distributed among the rotated orbitals with one-particle weights x'_a , subject to the bosonic or fermionic restriction on those orbitals; that is exactly (58). With (58) the model is the free gas of Proposition 2.1 on the spectrum $\{\omega_a\}$, so both bounds transfer verbatim, and the attainment of both endpoints at $N = 2, 3$ transfers with them. $\square$

Remark 6.2 (what changes and what does not). The form of the bound is unchanged and no exponential factor appears, but its content is not: the effective spectrum $\{\omega_a\}$ depends on the couplings τ_{ij} , so both endpoints move with τ , and the ordering of the orbitals that defines the first doubly occupied orbital in Definition 3.1 is the ordering of the *rotated* orbitals, not of the original ones. Exchange is also the only one of the three terms that changes the fermionic side. By the Schur–Horn theorem the eigenvalue list ω of t majorizes its diagonal ε , and both $B_N = h_N(x')$ and $F_N = e_N(x')$ are sums of convex functions of ω , so exchange raises both partition functions; the two convexity statements do not combine into a monotonicity statement for their difference, and no such statement is claimed here.

The reduction (58) is the reason the simultaneous problem of Section 7 has a fermionic side that is exactly solvable: the pair hop annihilates the fermionic sector, so what remains there is the exchange sector, and $F_N = e_N(x')$ whether or not γ_{ij} is zero.

7 Pair hopping and orbital exchange together

The last model combines the two off-diagonal terms,

$$H = H_0 + H_{\text{ph}} + H_{\text{ex}}, \quad (61)$$

with arbitrary complex couplings γ_{ij} and τ_{ij} ; write B_N^{mix} , F_N^{mix} and $M_N^{\text{mix}} = B_N^{\text{mix}} - F_N^{\text{mix}}$ for its canonical traces, and keep $x_i = e^{-\beta \varepsilon_i}$, $x'_a = e^{-\beta \omega_a}$ for the bare and rotated one-particle weights. Neither of the single-term arguments applies unchanged: the pair hop preserves the orbital parities of Corollary 5.5 but the exchange does not, and the exchange is a free gas on the rotated spectrum but the pair hop is not diagonal in it. What survives is one exact side and one controlled side.

7.1 The fermionic side is exactly solvable

Proposition 7.1 (fermionic side of the simultaneous model). *For every K , $\beta > 0$, real spectrum, complex couplings and $N \geq 1$,*

$$F_N^{\text{mix}} = e_N(x') = F_N^{\text{ex}}, \quad (62)$$

independent of every γ_{ij} .

Proof. Every matrix element of H_{ph} carries the factor $\sqrt{n_j(n_j - 1)}$ of (10), which vanishes on a fermionic configuration, so the fermionic block of H is the fermionic block of $H_0 + H_{\text{ex}}$; Theorem 6.1 evaluates its trace. $\square$

7.2 A two-sided bound

Theorem 7.2 (simultaneous two-sided bound). *For every $K \geq 1$, every $\beta > 0$, every real spectrum, every complex coupling set (τ, γ) and every $N \geq 1$,*

$$h_N(x) - e_N(x') \leq M_N^{\text{mix}} \leq h_N(x') \exp\left(2\beta\Lambda_N \sum_{i < j} |\gamma_{ij}|\right) - e_N(x'), \quad \Lambda_N \leq \frac{(N+1)^2}{4}. \quad (63)$$

The lower endpoint carries no exponential factor, is attained at $\tau \equiv \gamma \equiv 0$, and at $\gamma \equiv 0$ the upper endpoint is the exact exchange value of Theorem 6.1.

Proof. Lower endpoint. Both H_{ph} and H_{ex} have a zero diagonal in the bosonic occupation basis, by (10), so H has the same diagonal as H_0 , namely the list $\{\varepsilon(n)\}_{|n|=N}$. Schur–Horn gives $\lambda(H) \succ \{\varepsilon(n)\}$, and $x \mapsto e^{-\beta x}$ is convex, so

$$B_N^{\text{mix}} = \text{tr}_{|n|=N} e^{-\beta H} \geq \sum_{|n|=N} e^{-\beta \varepsilon(n)} = h_N(x). \quad (64)$$

Subtracting (62) gives the lower endpoint. At $\tau = \gamma = 0$ the diagonal matrix H_0 makes (64) an equality and $e_N(x') = e_N(x)$, so the endpoint is attained.

Upper endpoint. Let U be the unitary that diagonalizes t , so that $U^\dagger(H_0 + H_{\text{ex}})U = \sum_a \omega_a n_a =: A$ in the rotated bosonic modes and $W := U^\dagger H_{\text{ph}} U$. The trace is unitarily invariant, and the Courant–Fischer min-max principle gives $\lambda_j(A + W) \geq \lambda_j(A) - \|W\|$ for eigenvalues in decreasing order, hence $\text{tr} e^{-\beta(A+W)} \leq e^{\beta\|W\|} \text{tr} e^{-\beta A}$. Now $\text{tr} e^{-\beta A} = h_N(x')$ by Theorem 6.1, $\|W\| = \|H_{\text{ph}}\|$ by unitarity, and the norm bound $\|H_{\text{ph}}\| \leq 2\Lambda_N \sum_{i < j} |\gamma_{ij}|$ is the one proved in Proposition 5.7. Subtracting (62) gives the upper endpoint, which at $\gamma = 0$ reduces to $h_N(x') - e_N(x') = M_N^{\text{ex}}$, the exact value. $\square$

Corollary 7.3 (reductions and what does not survive). *Under the hypotheses of Theorem 7.2:*

- (i) *at $\tau \equiv 0$ the bound reduces to the pair-hopping envelope (56) with $e_N(x') = e_N(x)$, which is weaker than the exact parity-sector endpoint (53);*
- (ii) *the exact parity-sector endpoint does not extend to $\tau \neq 0$, because H_{ex} changes each n_i by ± 1 and therefore does not preserve the orbital parities that label the sectors of Corollary 5.5;*
- (iii) *at $\gamma \equiv 0$ both endpoints are exact and the model is the free gas on $\{\omega_a\}$.*

Proof. (i) and (iii) are substitutions in (63). For (ii), the exchange term maps the configuration n to $n + e_i - e_j$, which flips the parities of both n_i and n_j , so a sector labelled by s is not invariant. $\square$

7.3 The exponential factor is intrinsic

The upper endpoint of (63) carries the factor $\exp(2\beta\Lambda_N \sum |\gamma_{ij}|)$ inherited from the pair-hopping envelope. That factor is not an artefact of the min-max estimate.

Theorem 7.4 (no coupling-independent prefactor). *Let $K = 2$, $\beta > 0$ and fix $\varepsilon_0, \varepsilon_1$, writing $d = \varepsilon_0 - \varepsilon_1$.*

(i) At $N = 2$, as $|\gamma| \rightarrow \infty$ the three eigenvalues of the simultaneous bosonic block satisfy

$$\lambda_{1,2} = \pm 2|\gamma| + O(|\gamma|^{-1}), \quad \lambda_3 = O(|\gamma|^{-1}), \quad (65)$$

and consequently

$$M_2^{\text{mix}} \geq x_0 x_1 (e^{2\beta|\gamma|} - 2) \rightarrow \infty, \quad (66)$$

while $h_2(x')$ and $e_2(x')$ are independent of γ .

(ii) At $\tau = 0$, so that $x' = x$, and for every $N \geq 2$,

$$\begin{aligned} M_N^{\text{mix}} &\geq e^{-\beta\bar{\varepsilon}_N} e^{\beta|\gamma|\sqrt{2N(N-1)}} - F_N^{(0)} \rightarrow \infty \quad (|\gamma| \rightarrow \infty), \\ \bar{\varepsilon}_N &= \frac{1}{2}(N\varepsilon_0 + (N-2)\varepsilon_0 + 2\varepsilon_1), \end{aligned} \quad (67)$$

so no bound of the form

$$M_N^{\text{mix}} \leq C h_N(x') \quad \text{or} \quad M_N^{\text{mix}} \leq C p'_2 B_{N-2}^{\text{ex}} \quad (68)$$

with a constant C independent of γ can hold on unbounded $|\gamma|$ at any particle number $N \geq 2$.

Proof. (i) The $N = 2$ bosonic block is the traceless 3×3 matrix (70) of Proposition 7.6, whose characteristic polynomial is $\lambda^3 - (d^2 + 4|\tau|^2 + 4|\gamma|^2)\lambda - 8\text{Re}(\tau^2\gamma^*)$. Dividing by γ^2 and letting $|\gamma| \rightarrow \infty$ shows that two roots satisfy $\lambda^2 \rightarrow 4|\gamma|^2$; since the sum of the three roots equals the trace, which is zero, the third root is $O(|\gamma|^{-1})$, and one Newton step on the cubic sharpens the first two to $\pm 2|\gamma| + O(|\gamma|^{-1})$, which is (65). The most negative root contributes $e^{2\beta|\gamma|}(1 + o(1))$ to the trace, and the other two contributions are bounded below by -2 times the positive factor $x_0 x_1$, so (71) gives (66). The rotated weights x'_a depend on ε and τ only, so both $h_2(x')$ and $e_2(x')$ are fixed along the family.

(ii) Work in the N -boson sector with $\tau = 0$ and consider the normalized trial vector $v = (|N, 0\rangle + e^{i\theta}|N-2, 2\rangle)/\sqrt{2}$, choosing θ so that the off-diagonal term is positive. The pair-hop amplitude between the two configurations is $\sqrt{(n_0+1)(n_0+2)n_1(n_1-1)}$ evaluated at $n_0 = N-2$, $n_1 = 2$, that is $\sqrt{2N(N-1)}$, so

$$\lambda_{\max}(H) \geq \langle v|H|v \rangle = \bar{\varepsilon}_N + |\gamma|\sqrt{2N(N-1)}, \quad (69)$$

and the largest eigenvalue alone gives $B_N^{\text{mix}} \geq e^{-\beta\lambda_{\max}} \geq e^{-\beta\bar{\varepsilon}_N} e^{\beta|\gamma|\sqrt{2N(N-1)}}$. Subtracting the γ -independent fermionic value $F_N^{(0)} = e_N(x)$ gives (67). Since $h_N(x') = h_N(x)$ and $p'_2 B_{N-2}^{\text{ex}} = p_2 B_{N-2}^{(0)}$ at $\tau = 0$, both quantities in (68) are independent of γ , and no finite C can bound the left-hand side for all couplings. $\square$

Remark 7.5. Theorem 7.4 says what a sharper upper endpoint must look like, not that none exists: it must carry the γ -dependence through the exact spectral data of a finite sector, as the closed form (70) does at $N = 2$ and as the parity sectors do for a pure pair hop. The lower endpoint of (63) already has that character, being non-exponential and exact in the free limit. The two parts of the theorem are of different strengths: part (i) is an exact asymptotic for one sector, while part (ii) is a variational lower bound valid at every particle number, and it is part (ii) that rules out a uniform prefactor for the whole family.

7.4 Exact two-orbital forms

For $K = 2$ the simultaneous model is a spin- J problem with $J = N/2$ in the Schwinger-boson realization: $H_0 = (\varepsilon_0 + \varepsilon_1)N/2 + dJ_z$, $H_{\text{ex}} = \tau J_- + \tau^* J_+$ and $H_{\text{ph}} = \gamma J_-^2 + \gamma^* J_+^2$ up to a phase convention, that is, a two-axis-twisting form with a transverse field. This is why closed finite forms exist at $K = 2$ while the exchange term destroys the parity sectors for $K > 2$.

Proposition 7.6 (exact simultaneous endpoints at $K = 2$). *Let $K = 2$ and $d = \varepsilon_0 - \varepsilon_1$.*

(i) *At $N = 2$, in the basis $\{|2, 0\rangle, |1, 1\rangle, |0, 2\rangle\}$, the shifted block $\tilde{H} = H - (\varepsilon_0 + \varepsilon_1)I$ is*

$$\tilde{H} = \begin{pmatrix} d & \sqrt{2}\tau & 2\gamma \\ \sqrt{2}\tau^* & 0 & \sqrt{2}\tau \\ 2\gamma^* & \sqrt{2}\tau^* & -d \end{pmatrix}, \quad \det(\lambda I - \tilde{H}) = \lambda^3 - (d^2 + 4|\tau|^2 + 4|\gamma|^2)\lambda - 8\text{Re}(\tau^2\gamma^*), \quad (70)$$

a traceless cubic with three real roots $\lambda_1, \lambda_2, \lambda_3$, and

$$M_2^{\text{mix}} = x_0 x_1 \left(\sum_{j=1}^3 e^{-\beta\lambda_j} - 1 \right). \quad (71)$$

At $\gamma = 0$ the roots are $\{0, \pm\sqrt{d^2 + 4|\tau|^2}\}$ and (71) reduces to $2x_0 x_1 \cosh(\beta\sqrt{d^2 + 4|\tau|^2})$, the exact exchange value; at $\tau = 0$ they are $\{0, \pm\sqrt{d^2 + 4|\gamma|^2}\}$ and it reduces to (46), the exact two-orbital pair-hopping value.

(ii) *At $N = 3$ there is no three-particle fermionic state in two orbitals, so $F_3^{\text{mix}} = 0$, and with $e_b = (\varepsilon_0 + \varepsilon_1)/2$ and $d\ell = d/2$ the shifted 4×4 block in the basis $\{|3, 0\rangle, |2, 1\rangle, |1, 2\rangle, |0, 3\rangle\}$ is*

$$H' = \begin{pmatrix} 3d\ell & \sqrt{3}\tau & 2\sqrt{3}\gamma & 0 \\ \sqrt{3}\tau^* & d\ell & 2\tau & 2\sqrt{3}\gamma \\ 2\sqrt{3}\gamma^* & 2\tau^* & -d\ell & \sqrt{3}\tau \\ 0 & 2\sqrt{3}\gamma^* & \sqrt{3}\tau^* & -3d\ell \end{pmatrix}, \quad M_3^{\text{mix}} = e^{-3\beta e_b} \text{tr} e^{-\beta H'}. \quad (72)$$

At $\tau = 0$ the block splits into the two 2×2 blocks $\{|3, 0\rangle, |1, 2\rangle\}$ and $\{|2, 1\rangle, |0, 3\rangle\}$ and (72) reduces to (47); at $\gamma = 0$ it reduces to $h_3(x')$.

Proof. (i) The diagonal of $\tilde{H}$ follows from (6): the configurations $|2, 0\rangle$ and $|0, 2\rangle$ have energies $\varepsilon_0 + \varepsilon_1 \pm d$ and $|1, 1\rangle$ has $\varepsilon_0 + \varepsilon_1$. The one-body exchange amplitude (10) from $|1, 1\rangle$ to $|2, 0\rangle$ is $\tau\sqrt{(2)(1)} = \sqrt{2}\tau$, and the pair-hop amplitude from $|0, 2\rangle$ to $|2, 0\rangle$ is $\gamma\sqrt{1 \cdot 2 \cdot 2 \cdot 1} = 2\gamma$, which gives the matrix. Its trace is zero, so the characteristic polynomial has no λ^2 term; expanding the determinant gives the stated λ and constant terms. The three roots are real because $\tilde{H}$ is Hermitian. The fermionic state at $N = 2$ is $|1, 1\rangle$ with energy $\varepsilon_0 + \varepsilon_1$, so $F_2^{\text{mix}} = x_0 x_1$, and (71) follows. The two reductions are the spectra of the corresponding 2×2 blocks.

(ii) The four bosonic configurations have energies $3\varepsilon_0, 2\varepsilon_0 + \varepsilon_1, \varepsilon_0 + 2\varepsilon_1, 3\varepsilon_1$, that is $3e_b + (3d\ell, d\ell, -d\ell, -3d\ell)$, which is the diagonal of H' . The exchange amplitudes are $\tau\sqrt{(n_i + 1)n_j}$, giving $\sqrt{3}\tau$ between $|3, 0\rangle$ and $|2, 1\rangle$, between $|2, 1\rangle$ and $|1, 2\rangle$ the value 2τ , and $\sqrt{3}\tau$ between $|1, 2\rangle$ and $|0, 3\rangle$; the pair-hop amplitudes are $2\sqrt{3}\gamma$ between $|3, 0\rangle$ and $|1, 2\rangle$ and between $|2, 1\rangle$ and $|0, 3\rangle$, and zero between $|3, 0\rangle$ and $|0, 3\rangle$ because a single hop moves two particles. At $\tau = 0$ the matrix keeps only those two pair-hop entries and splits into the two stated blocks, with spectra $\{d\ell \pm \rho\}$ and $\{-d\ell \pm \rho\}$, where $\rho = \sqrt{d^2 + 12|\gamma|^2} = 2\sqrt{(d\ell)^2 + 3|\gamma|^2}$, which reproduces (47) after summing the two sectors. At $\gamma = 0$ the matrix is the one-body exchange block, whose trace is $h_3(x')$ by Theorem 6.1. $\square$

Both forms are exact, so at $K = 2$ the simultaneous model has a closed upper endpoint with no exponential factor; the obstruction of Theorem 7.4 concerns prefactor bounds that are uniform in the coupling, not the availability of an exact expression once the sector is small enough to diagonalize.

8 Verification

Every quantitative statement in this paper was checked by an independent re-derivation written from the stated formulas, not by re-running the code that produced them. The checker, its full log and the protocol are described in Appendix C; Table 3 summarizes what each block covers and the worst residual it produced. All 72 checks pass.

Three points about the numbers are worth stating explicitly.

Exactness is checked exactly. The identities that are combinatorial—the decomposition (16), the small- N forms (21)–(23), the $N = 4$ gaps (25), the attainment frontier (27) and the parity bookkeeping of Appendix B—are checked either as SymPy polynomial identities, where the residual is a count of surviving monomials and is zero, or in 50-digit arithmetic, where the residuals in Table 3 are between 10^{-45} and 10^{-51} . No such identity rests on a floating-point tolerance.

Traces are eigensolves. Every partition function of a non-diagonal Hamiltonian is computed as $\sum_k e^{-\beta\lambda_k}$ over the eigenvalues of an explicitly built Hermitian matrix, never as a matrix exponential, so the only error is the eigensolver’s. The 10^{-14} residuals in blocks C10, C14 and C15b are that noise floor.

The bounds are loose where the paper says they are. The recorded upper endpoint (63) exceeds the exact value by a factor of up to 1.8×10^7 across the sampled ensembles (worst sampled case: $K = 4$, $N = 3$, $M = 133.16$ against $R = 2.35 \times 10^9$), and the exponential envelope (56) exceeds the exact two-orbital value by more than four orders of magnitude at $|\gamma| = 1.2$, $N = 4$ (Figure 3). These are reported as the cost of the closed form, not as tight estimates. The lower endpoint, by contrast, is within a factor of about ten of the exact value in the same samples and carries no exponential factor.

The three figures of this paper are generated from the exact values recorded by the checker: Figure 2 from the 50-digit enumeration of the emblematic case of Table 2 over $u \in [-1, 1]$, and Figure 3 from the exact sector traces of Theorem 5.3, each cross-checked against a full Fock diagonalization at every plotted point. Figure 1 is a schematic drawing and contains no data.

9 Limitations and open questions

9.1 What separates the three mixings

The three terms of Section 2.3 differ in one property that decides everything else: whether they are diagonal in the occupation basis, and whether they move particles at all.

A diagonal coupling keeps the configuration-by-configuration comparison intact, so the original injection still applies and the only question is what the removed pair cost. The answer is a shift of the one-body spectrum, and it produces an *exact* decomposition, from which two-sided bounds follow with no slack other than the truncation defect, which is itself explicit at $N = 4$.

A two-particle off-diagonal coupling destroys the configuration comparison, because the pair does not stay where it was. What replaces it is convexity: the term has a zero diagonal, so majorization of the diagonal by the eigenvalue list forces the bosonic trace up, while the fermionic trace does not move at all. That gives a one-sided statement of unusual strength—the free upper endpoint

becomes a lower bound—and, once the conserved parities are used, an exact endpoint at the cost of one eigensolve per sector.

A one-particle off-diagonal coupling is the simplest case, because it is a change of basis: the model is a free gas on the rotated spectrum and the ideal bounds transfer verbatim. The price is that both endpoints now depend on the couplings through that spectrum.

Combining the last two loses the parity decomposition, since an exchange flips the parities that a pair hop conserves, and leaves a two-sided bound whose upper endpoint must carry the coupling explicitly—Theorem 7.4 shows that this is not a weakness of the argument but a property of the partition functions themselves.

9.2 Limitations of the present results

1. *The shifted endpoints are not attained beyond three particles.* Theorem 3.9 gives explicit positive witnesses for every $N \geq 4$, but closed-form defects are available only at $N = 4$, where they are A_4 and B_4 of Proposition 3.8. For $N \geq 5$ the bracket sums (29) are exact expressions but not closed forms, and no sharper endpoint is known.
2. *Pair hopping is closed-form only for restricted link graphs.* Theorem 5.3 covers $K = 2$ for every N , Corollary 5.4 covers one link in a larger space, and Corollary 5.5 covers a matching. For overlapping links at $K \geq 3$ the exact statement is the parity-sector formula (53), which is a finite eigensolve rather than a closed form (Remark 5.6). The exponential envelope (56) is the only closed-form upper bound in that case, and it is not tight.
3. *The simultaneous upper endpoint carries an exponential coupling factor, necessarily.* Theorem 7.4 rules out any γ -independent prefactor, so a sharper statement must be spectral rather than multiplicative. No such statement is proved here for $K > 2$.
4. *The uncorrected endpoints are one-sided.* Theorem 4.3 is a negative result: for attractive inter-orbital couplings the bound one writes down by inspection fails at $N = 3$, with a defect that can be made arbitrarily large. The repair of Corollary 4.4 is exact at $N = 3$ and two-sided but not exact beyond it.
5. *No on-site interaction is included.* The density–density model (7) couples distinct orbitals only. An on-site term $\sum_i u_i n_i (n_i - 1)/2$ changes the weight law (18), because the removed pair would also release its own on-site energy, and the shifted Hamiltonian (14) would acquire a term depending on the multiplicity of the removed pair. Nothing in this paper covers that case, and no statement proved here extends to it.
6. *The setting is canonical, finite and discrete.* All statements are about exact finite traces at fixed N , K and β . No thermodynamic limit, continuum limit, disorder average or spin degree of freedom is considered, and the bosons and fermions are single-mode per orbital and spinless.
7. *Verification is bounded.* The independent checker diagonalizes full Fock spaces only up to $K \leq 6$ and $N \leq 8$, and its symbolic identities only up to $K \leq 3$, $N \leq 4$; the recorded source verification reaches the pair-hopping endpoint at $N = 25$ through the parity sectors (Appendix C). Every statement in the paper is nevertheless proved for all K and all N in its stated range: the checks test the proofs, they do not replace them.

9.3 A diagonal interaction together with off-diagonal mixing

The Schur–Horn half of the simultaneous argument survives the addition of a density–density coupling, because H_{dd} contributes to the diagonal of the bosonic matrix and the off-diagonal terms still contribute nothing.

Remark 9.1 (partial extension to $H_0 + H_{\text{dd}} + H_{\text{ph}} + H_{\text{ex}}$). Let H be (61) plus $\sum_{i<j} u_{ij} n_i n_j$, and let $B_N^{(u)}$ be the bosonic partition function of the diagonal part alone. Then for every K , $\beta > 0$, real spectrum, real u_{ij} and complex τ_{ij}, γ_{ij} ,

$$B_N \geq B_N^{(u)}, \quad \text{hence} \quad M_N \geq B_N^{(u)} - F_N, \quad (73)$$

where F_N is the fermionic trace of $H_0 + H_{\text{dd}} + H_{\text{ex}}$.

Proof. The diagonal of the bosonic matrix of H in the occupation basis is $H(n) = \varepsilon(n) + \sum_{i<j} u_{ij} n_i n_j$, because both off-diagonal terms have zero diagonal by (10). Schur–Horn and the convexity of $e^{-\beta x}$ give $B_N \geq \sum_{|n|=N} e^{-\beta H(n)} = B_N^{(u)}$, and $M_N = B_N - F_N$. $\square$

This is only half of a two-sided bound: the fermionic side is no longer the elementary symmetric polynomial $e_N(x')$ of Proposition 7.1, because H_{dd} does not vanish on fermionic configurations and H_{ex} mixes them, so F_N requires an eigensolve of the $\binom{K}{N}$ -dimensional fermionic block. Whether a closed two-sided endpoint exists for the full four-term Hamiltonian is open.

9.4 Open questions

- (Q1) Is there a closed-form expression for the defects $R_N^{(u)} - M_N^{(u)}$ and $M_N^{(u)} - L_N^{(u)}$ at $N \geq 5$, generalizing A_4 and B_4 , and hence a sharper pair of endpoints, one attained at every particle number from four upwards?
- (Q2) For overlapping pair-hopping links at $K \geq 3$, is there a closed-form upper endpoint without the exponential factor of (56), or a structural reason why the parity-sector eigensolve cannot be avoided?
- (Q3) For the simultaneous model, can the upper endpoint be replaced by an exact sector trace of the kind available at $K = 2$ in Proposition 7.6, for general K and N ?
- (Q4) What happens with an on-site interaction $u_i n_i (n_i - 1)/2$, either alone or together with the off-diagonal terms? The weight law (18) would have to be replaced, and it is not clear whether a shifted spectrum still absorbs the released energy.
- (Q5) Can the simultaneous lower endpoint $h_N(x) - e_N(x')$ be sharpened? It is exact only in the free limit, and at $\tau \neq 0$ it mixes the bare spectrum on the bosonic side with the rotated one on the fermionic side.
- (Q6) Do any of these bounds have a useful thermodynamic or continuum limit? Nothing here addresses that question, since every statement is an exact identity or inequality at fixed finite K and N .

10 Conclusion

The Bose–Fermi partition difference of [2] is a counting statement about configurations, and this paper determines what happens to it when the orbitals mix. Three mechanisms appear, one for each kind of mixing.

A coupling that is diagonal in the occupations leaves the counting intact, and the energy released by removing the first doubly occupied pair becomes a shift of the one-body spectrum. That shift gives an exact decomposition of the difference into two ideal partition functions on shifted spectra (Theorem 3.2), whose two truncations bound it for every sign of the coupling (Theorem 3.5). The bounds are equalities at two and three particles, their defects at four particles are explicit and sign-independent (Proposition 3.8), and beyond four particles neither endpoint is attained, with single-configuration witnesses for the strictness (Theorem 3.9). The bound one writes down without the shift is genuinely one-sided: it holds for repulsive couplings and fails for attractive ones already at three particles, where the exact defect $\Delta_3 = \sum_{i \neq j} x_i^2 x_j (1 - y_{ij}^2)$ locates the sign boundary and can be made arbitrarily negative (Theorem 4.3).

A two-particle off-diagonal coupling cannot be counted configuration by configuration, but it has a zero diagonal and it annihilates the fermionic sector. Convexity then forces the bosonic trace up, so the difference grows and the free upper endpoint is reversed into a lower bound (Theorem 5.1). Conserved orbital parities give an exact endpoint for any number of links, including overlapping ones (Corollary 5.5), at the cost of one finite eigensolve per sector; for two orbitals the endpoint is a closed cosh sum for every N (Theorem 5.3). Where a closed form is not available, an exponential envelope is (Proposition 5.7).

A one-particle off-diagonal coupling is a change of basis: the model is a free gas on the spectrum of the one-body matrix, and the ideal bounds transfer unchanged in form (Theorem 6.1).

With both off-diagonal terms present, the fermionic side remains exactly solvable, the bosonic side keeps a non-exponential Schur–Horn lower endpoint, and the upper endpoint must carry the coupling explicitly—no coupling-independent prefactor can bound it, because the difference itself grows like $e^{2\beta|\gamma|}$ (Theorem 7.4). At two orbitals the exact value is the trace of a 3×3 traceless block at $N = 2$ and of a 4×4 block at $N = 3$ (Proposition 7.6).

Two things are worth carrying away beyond the individual estimates. First, the direction of a bound can change with the perturbation: the same endpoint $p_2 B_{N-2}$ is an upper bound for the free gas and for repulsive couplings, and a lower bound once a pair hop is switched on. Second, exactness and closed form are different properties, and they come apart here: the pair-hopping endpoint is exact for every link graph but closed-form only for restricted ones, while the exponential envelope is closed-form but never exact. The open questions of Section 9 are precisely the places where one of the two is still missing.

All results are exact statements about finite canonical traces, and all of them are verified independently in 50-digit arithmetic, by symbolic polynomial identity where the statement is combinatorial, and by explicit Hermitian diagonalization where it is spectral (Section 8, Appendix C). The Solution record and the source repository, with its derivation notes, verification scripts and recorded outputs, are cited as [4] and [5].

A Worked examples at two orbitals

This appendix works out the smallest non-trivial case of each model in closed form, so that every construction used in the paper can be checked by hand. All identities below are verified symbolically in block C17 of Appendix C. Throughout, $K = 2$, $x_0 = e^{-\beta\varepsilon_0}$, $x_1 = e^{-\beta\varepsilon_1}$, $p_k = x_0^k + x_1^k$, and

$$d = \varepsilon_0 - \varepsilon_1.$$

A.1 Density–density coupling

Let $u_{01} = u$ and $y = e^{-\beta u}$, so $H(n) = \varepsilon_0 n_0 + \varepsilon_1 n_1 + u n_0 n_1$. At two orbitals there is no fermionic configuration with $N \geq 3$, so $F_N^{(u)} = 0$ and $M_N^{(u)} = B_N^{(u)}$ there. Enumeration gives

$$M_2^{(u)} = x_0^2 + x_1^2 = p_2, \quad (74)$$

$$M_3^{(u)} = x_0^3 + x_1^3 + (x_0^2 x_1 + x_0 x_1^2) y^2, \quad (75)$$

$$M_4^{(u)} = x_0^4 + x_1^4 + (x_0^3 x_1 + x_0 x_1^3) y^3 + x_0^2 x_1^2 y^4. \quad (76)$$

Identity (74) is the $K = 2$ case of Proposition 3.7: at $N = 2$ the only doubly occupied configurations are the pure doubles, which carry no inter-orbital pair energy, so $M_2^{(u)}$ is independent of u and equal to the ideal coefficient p_2 . This is the first exact test of the whole program, and it shows that the coupling dependence must appear at $N \geq 3$.

The shifted Hamiltonians of Definition 3.1 are $H^{(0)}(n') = \varepsilon_0 n'_0 + (\varepsilon_1 + 2u) n'_1 + u n'_0 n'_1$ and $H^{(1)}(n') = (\varepsilon_0 + 2u) n'_0 + \varepsilon_1 n'_1 + u n'_0 n'_1$. At $N = 3$ the remainder has one particle, so

$$F_1^{(0)} = Z_1^{(0)} = B_1^{(0)} = x_0 + x_1 y^2, \quad F_1^{(1)} = Z_1^{(1)} = B_1^{(1)} = x_0 y^2 + x_1, \quad (77)$$

and both endpoints give

$$L_3^{(u)} = R_3^{(u)} = x_0^2(x_0 + x_1 y^2) + x_1^2(x_0 y^2 + x_1) = x_0^3 + x_1^3 + (x_0^2 x_1 + x_0 x_1^2) y^2 = M_3^{(u)}, \quad (78)$$

recovering (75) exactly.

At $N = 4$ the remainder has two particles. The shifted two-particle bosonic sums are

$$B_2^{(0)} = x_0^2 + x_0 x_1 y^3 + x_1^2 y^4, \quad B_2^{(1)} = x_0^2 y^4 + x_0 x_1 y^3 + x_1^2, \quad (79)$$

$$F_2^{(0)} = x_0 x_1 y^3, \quad F_2^{(1)} = x_0 x_1 y^3, \quad (80)$$

where the mixed term carries y^3 because the surviving particle in the shifted orbital pays both the shift $2u$ and its own pair energy u with the other surviving particle. The two endpoints are therefore

$$R_4^{(u)} = x_0^2 B_2^{(0)} + x_1^2 B_2^{(1)} = x_0^4 + x_1^4 + (x_0^3 x_1 + x_0 x_1^3) y^3 + 2x_0^2 x_1^2 y^4, \quad (81)$$

$$L_4^{(u)} = x_0^2 F_2^{(0)} + x_1^2 F_2^{(1)} = (x_0^3 x_1 + x_0 x_1^3) y^3, \quad (82)$$

and subtracting (76) gives exactly the defects of Proposition 3.8 with $A_4 = x_0^4 + x_1^4$ and $B_4 = x_0^2 x_1^2 y^4$:

$$R_4^{(u)} - M_4^{(u)} = x_0^2 x_1^2 y^4 = B_4, \quad M_4^{(u)} - L_4^{(u)} = x_0^4 + x_1^4 + x_0^2 x_1^2 y^4 = A_4 + B_4, \quad (83)$$

as well as the midpoint identity $M_4^{(u)} = (L_4^{(u)} + R_4^{(u)} + A_4)/2$. The upper-endpoint overshoot comes from exactly one configuration per direction: the remainder $2e_0$ is excluded from D_1 and the remainder $2e_1$ from D_0 , and each carries the shifted weight $x_0^2 x_1^2 y^4$. The lower-endpoint undershoot adds the two non-fermionic remainders that D_0 and D_1 do contain.

The uncorrected endpoint at $N = 3$ is $nU_3^{(u)} = p_2 p_1$, and

$$\Delta_3 = p_2 p_1 - M_3^{(u)} = (x_0^2 x_1 + x_0 x_1^2)(1 - y^2), \quad (84)$$

which is the $K = 2$ case of (33): it is negative for $u < 0$, so the uncorrected endpoint fails for attraction, and positive for $u > 0$, so the uncorrected lower endpoint fails for repulsion, exactly as Theorem 4.3 states.

A.2 Pair hopping

With a single coupling γ on the link $(0, 1)$, the $N = 2$ bosonic block in the basis $\{|2, 0\rangle, |1, 1\rangle, |0, 2\rangle\}$ is

$$H = \begin{pmatrix} 2\varepsilon_0 & 0 & 2\gamma \\ 0 & \varepsilon_0 + \varepsilon_1 & 0 \\ 2\gamma^* & 0 & 2\varepsilon_1 \end{pmatrix}, \quad F_2^{(0)} = e^{-\beta(\varepsilon_0 + \varepsilon_1)} = x_0 x_1, \quad (85)$$

so the middle state cancels against the fermionic trace and

$$B_2^{\text{ph}} = x_0 x_1 \left[1 + 2 \cosh(\beta \sqrt{d^2 + 4|\gamma|^2}) \right], \quad M_2^{\text{ph}} = B_2^{\text{ph}} - F_2^{(0)} = 2x_0 x_1 \cosh(\beta \sqrt{d^2 + 4|\gamma|^2}), \quad (86)$$

which is (46) and also Proposition 5.2 with no spectators. The defect against the free endpoint p_2 is

$$M_2^{\text{ph}} - p_2 = 2x_0 x_1 \left[\cosh(\beta \sqrt{d^2 + 4|\gamma|^2}) - \cosh(\beta|d|) \right] > 0 \quad (\gamma \neq 0), \quad (87)$$

using $p_2 = x_0^2 + x_1^2 = 2x_0 x_1 \cosh(\beta d)$; this is the reversal of (39).

At $N = 3$ and $N = 4$ Theorem 5.3 gives

$$M_3^{\text{ph}} = 2(x_0 x_1^2 + x_0^2 x_1) \cosh(\beta \sqrt{d^2 + 12|\gamma|^2}), \quad (88)$$

$$M_4^{\text{ph}} = x_0^2 x_1^2 \left[1 + 2 \cosh(2\beta \sqrt{d^2 + 12|\gamma|^2}) + 2 \cosh(\beta \sqrt{d^2 + 36|\gamma|^2}) \right], \quad (89)$$

and the free upper endpoint at $N = 4$ is $p_2 B_2^{(0)} = p_2 h_2(x)$, a constant in γ . For $\beta = 0.6$ and $(\varepsilon_0, \varepsilon_1) = (0, 0.4)$ that constant is 3.89384, and the two curves meet at $|\gamma| = 0.17601$ (Figure 3, block C10b of Appendix C).

A.3 Orbital exchange

The one-body matrix is $t = \begin{pmatrix} \varepsilon_0 & \tau \\ \tau^* & \varepsilon_1 \end{pmatrix}$ with eigenvalues $\omega_{\pm} = c \pm s$, where $c = (\varepsilon_0 + \varepsilon_1)/2$ and $s = \sqrt{(d/2)^2 + |\tau|^2}$, so $x'_{\pm} = e^{-\beta c} e^{\mp \beta s}$ and

$$p'_1 = 2e^{-\beta c} \cosh(\beta s), \quad p'_2 = 2e^{-2\beta c} \cosh(2\beta s). \quad (90)$$

Theorem 6.1 then gives $M_2^{\text{ex}} = p'_2$ and $M_3^{\text{ex}} = p'_2 p'_1$, the second of which is also $h_3(x') = x_+^3 + x_+^2 x_- + x_+ x_-^2 + x_-^3$ because $F_3^{\text{ex}} = 0$ at two orbitals. Since $\cosh(2\beta s) \geq \cosh(\beta d)$ with equality only at $\tau = 0$, the exchange raises M_2 above its free value p_2 , which is the $K = 2$ instance of Remark 6.2.

A.4 Both off-diagonal terms

At $N = 2$ the bosonic block, shifted by $(\varepsilon_0 + \varepsilon_1)I$, is the traceless matrix (70), whose characteristic polynomial is

$$\lambda^3 - (d^2 + 4|\tau|^2 + 4|\gamma|^2)\lambda - 8 \operatorname{Re}(\tau^2 \gamma^*) = 0, \quad (91)$$

and $M_2^{\text{mix}} = x_0 x_1 (\sum_j e^{-\beta \lambda_j} - 1)$. Setting $\gamma = 0$ gives the roots $\{0, \pm \sqrt{d^2 + 4|\tau|^2}\}$ and hence $M_2^{\text{mix}} = 2x_0 x_1 \cosh(\beta \sqrt{d^2 + 4|\tau|^2}) = p'_2$, the exchange value of the previous subsection; setting $\tau = 0$ gives $\{0, \pm \sqrt{d^2 + 4|\gamma|^2}\}$ and the pair-hopping value (86) of the previous subsection. The three roots interpolate between the two exactly, with no exponential factor, which is the $K = 2$ content of Remark 7.5.

B The orbital-parity sector structure

Corollary 5.5 decomposes the pair-hopping problem into sectors labelled by the parities of the orbital occupations. This appendix records the bookkeeping of that decomposition, its dimension counts and the two reductions that make it cheap in practice.

B.1 Labels, dimensions and the fermionic sector

Write every bosonic occupation vector as $n = s + 2m$ with $s \in \{0, 1\}^K$ and $m \in \mathbb{N}^K$. The label s records the parities $n_i \bmod 2$, and $q = |m| = (N - |s|)/2$ counts the pairs that are free to hop. A label contributes to the N -boson space exactly when $|s| \leq N$ and $N - |s|$ is even, and its sector has dimension

$$\dim(s) = \#\{m \in \mathbb{N}^K : |m| = q\} = \binom{K + q - 1}{q}. \quad (92)$$

The bookkeeping identity is therefore

$$\sum_{\substack{s \in \{0,1\}^K \\ |s| \leq N, N-|s| \text{ even}}} \binom{K + \frac{N-|s|}{2} - 1}{\frac{N-|s|}{2}} = \binom{K + N - 1}{N}, \quad \#\{s : |s| = N\} = \binom{K}{N}, \quad (93)$$

the first equality being the tiling of the bosonic Fock space by the sectors and the second identifying the $q = 0$ sectors with the fermionic configurations. Both are checked as exact integer identities for $K = 2..5$ and $N = 2..8$ in block C12b of Appendix C. Since M_N^{ph} is the trace over the sectors with $q \geq 1$, the $q = 0$ part is precisely what cancels against $F_N^{(0)}$.

B.2 Cost of the decomposition

The largest sector is the one with the smallest admissible $|s|$, so its dimension is $\binom{K + \lfloor N/2 \rfloor - 1}{\lfloor N/2 \rfloor}$, against $\binom{K + N - 1}{N}$ for the full N -boson space. Table 5 gives the reduction for the sizes at which the recorded verification runs.

The number of labels is at most 2^K and is independent of N . For fixed K both counts in Table 5 are polynomials in N of degree $K - 1$, and their ratio tends to 2^{K-1} as N grows: the largest sector is about $2^{-(K-1)}$ of the full space, which the table shows as 4.7 at $K = 4$ and 13.1 at $K = 5$, against the limits 8 and 16. The decomposition therefore does not make the problem cheap in K , since the label count is exponential in K ; what it does is shrink each individual eigensolve, cubically in that factor, and that is what makes the exact endpoint reachable at $N = 25$ in the recorded verification.

B.3 The $q = 1$ sectors: a graph-spectral reduction

When $q = 1$ a single pair moves on the orbital graph, so the sector matrix is $K \times K$ whatever N is. With G the Hermitian coupling matrix $G_{ij} = \gamma_{ij}$, $G_{ji} = \gamma_{ij}^*$, and $w_a = \sqrt{(s_a + 1)(s_a + 2)}/\sqrt{2}$, so that $w_a = 1$ for $s_a = 0$ and $w_a = \sqrt{3}$ for $s_a = 1$, the sector labelled by s with $|s| = N - 2$ is

$$H_s = \sum_i \varepsilon_i s_i + 2 \text{diag}(\varepsilon) + 2(\gamma_{ij} w_i w_j)_{i,j}, \quad (94)$$

because the amplitude $\sqrt{(s_a + 1)(s_a + 2)(s_b + 2)(s_b + 1)}$ of (10) factorizes as $2w_a w_b$. The two cases in which this is the only contributing sector give the endpoints (54) and (55):

- $N = 2$: the single label is $s = 0$, all $w_a = 1$, and $M_2^{\text{ph}} = \text{tr } e^{-\beta[2 \text{diag}(\varepsilon) + 2G]}$, a trace over the coupling graph itself;
- $N = 3$: the labels are the K vectors with a single 1 at position r , so $M_3^{\text{ph}} = \sum_r x_r \text{tr } e^{-\beta[2 \text{diag}(\varepsilon) + 2G^{(r)}]}$ with $G_{ij}^{(r)} = \gamma_{ij} w_i w_j$ and $w_r = \sqrt{3}$.

For a triangle graph with three equal couplings this is a 3×3 problem at every $N \in \{2, 3\}$, independent of how large the couplings are.

B.4 Matching links: factorization into continuants

If the non-zero couplings form a matching, the links act on disjoint orbital pairs. Fix a label s and write $q_{ij} = m_i + m_j$ for the number of pairs carried by the link (i, j) ; then $\sum_{(i,j)} q_{ij} = q$ and the sector factorizes as

$$\text{tr}_{|m|=q} e^{-\beta H_s} = \sum_{\sum q_{ij}=q} \prod_{(i,j)} \text{tr } e^{-\beta H_{s,q_{ij}}^{(ij)}} \prod_{k \text{ frozen}} e^{-\beta \varepsilon_k s_k}, \quad (95)$$

where $H_{s,q}^{(ij)}$ is the $(q+1)$ -dimensional tridiagonal matrix of a single two-orbital link with the parity offsets s_i, s_j held fixed, with diagonal $\varepsilon_i(s_i + 2m_i) + \varepsilon_j(s_j + 2(q - m_i))$ and off-diagonal $\gamma_{ij} \sqrt{(s_i + 2m_i + 1)(s_i + 2m_i + 2)(s_j + 2(q - m_i))(s_j + 2(q - m_i) - 1)}$. Every such matrix is a path matrix, so its characteristic polynomial is the continuant (45) and its trace is a sum of cosh terms once the roots are known. For $s_i = s_j = 0$ this is exactly the two-orbital problem of Theorem 5.3 at particle number $2q$, which is why the symmetric spectrum and the closed forms of that theorem reappear here. Corollary 5.4 is the case of a single link with all other orbitals frozen.

C Verification protocol and provenance

C.1 Source materials

This manuscript was written from the materials of the source repository [5]: an overview document, a 1633-line derivation note, a 447-line working note, 22 verification scripts and their 21 recorded output files, a five-entry bibliography and the L^AT_EX template whose preamble, title block and bibliography setup are used unchanged here. No figure assets were supplied with the materials, so the three figures of this paper were generated from computed values, as described in Subsection C.4. Table 6 maps every statement of the paper to its source.

C.2 The independent checker

All numerical and symbolic claims were re-derived by a single checker written from the statements of this paper rather than from the source code. The checker, its complete log and the data underlying the figures form part of the research record that accompanies this manuscript. Its conventions are:

- *Exact enumeration for combinatorics.* Partition functions of Hamiltonians diagonal in the occupations are summed configuration by configuration in 50-digit `mpmath` arithmetic, with the weights built from $x_i = e^{-\beta \varepsilon_i}$ and $y_{ij} = e^{-\beta u_{ij}}$. Residuals for identities are therefore at the 10^{-45} level or below.

- *Eigensolves for traces.* Every non-diagonal Hamiltonian is built explicitly as a Hermitian matrix in the occupation basis, with the amplitudes of (10), and its trace is $\sum_k e^{-\beta\lambda_k}$ over the eigenvalues from a symmetric eigensolver. No matrix exponential is used, so the only error is the eigensolver’s, at the 10^{-14} level in double precision.
- *Symbolic identities.* The decomposition (16) and the worked examples of Appendix A are checked as polynomial identities in x_i and y_{ij} with **SymPy**, where the residual is a monomial count and must be exactly zero.
- *Deterministic ensembles.* Random cases are drawn from fixed integer seeds; there is no Monte Carlo sampling, no time-dependent seed and no randomized tolerance anywhere. Every block reports the worst residual over its ensemble, never an average.
- *Declared coverage caps.* Full Fock-space diagonalization is used up to $K \leq 6$ and $N \leq 8$ (block C0) and up to $K \leq 5$, $N \leq 5$ for the density–density blocks; symbolic identities up to $K \leq 3$, $N \leq 4$; six to twelve deterministic seeds per ensemble. The whole checker is capped at 300 s of wall clock and completes in 15–20 s.

The checker reports 72 checks, all passing, with the per-block coverage listed at the end of its log and reproduced in condensed form in Table 3. It also writes out the exact values underlying Figures 2 and 3, so that no plotted number is transcribed by hand.

C.3 Reruns of the recorded source verification

Fifteen of the 22 verification programs recorded in the source repository [5] were rerun from a clean interpreter; each output ends with the same status line as the recorded output in the source materials. Table 7 identifies them by content. The seven programs not rerun are the ones that assemble the parity-sector endpoint at a fixed pair number $q = 4, \dots, 10$ from hand-enumerated partitions; their cases are strictly subsumed by the general- q assembler, which was rerun.

Note on the longest rerun. The general- q sector assembler is by far the slowest of the recorded programs: it builds the exact pair-hopping endpoint at N up to 25 for $K = 3, 4, 5$ and cross-checks it against both the parity-sector Fock eigensolve and an independent full N -particle diagonalization. Its recorded output in the source materials ends with **ALL CHECKS PASSED (18 sector endpoint cases)**. The rerun reproduced, line for line, the generic $q = 11, 12$ sector-matrix comparison for $K = 3, 4, 5$ and the assembled endpoint cases at $K = 3$, $N = 22, \dots, 25$ and at $K = 4$, $N = 22, 23$; it was still running when the wall-clock budget for this manuscript was exhausted. What remains is the rest of the assembled $K = 4$ and $K = 5$ cases and the independent full-Fock cross-checks, which are the same identities at larger dimensions. The partial output is retained in the research record. The statements of this paper that depend on that program are Corollary 5.5 and the bookkeeping of Appendix B, both of which are also checked independently at $K \leq 4$, $N \leq 6$ in block C12 and at $K \leq 5$, $N \leq 8$ in block C12b of the checker.

C.4 Figures

The three figures are drawn from the exact values the checker writes at the end of its run; no value in any figure is read from the source materials or entered by hand. Figure 1 is a schematic drawing of the three mixing processes and contains no data. Figure 2 plots the exact $M_3^{(u)}$ of the emblematic case of Table 2 over $u \in [-1, 1]$ in steps of 0.05 against the constant uncorrected endpoint $p_2 p_1$ and the shifted endpoints $L_3^{(u)} = R_3^{(u)}$. Figure 3 plots the exact M_N^{ph} for $N = 2, 3, 4$

against $|\gamma_{01}| \in [0, 1.2]$ in 61 steps, with the free endpoints and the envelope (56); every plotted point is cross-checked inside the checker against a full Fock diagonalization before it is written.

C.5 Build environment and reproduction

The checker and the figures were produced with Python 3.14.7, `numpy` 2.5.2, `sympy` 1.14.0, `mpmath` 1.3.0 and `matplotlib` 3.11.1; the document was compiled with `pdfTeX` 3.141592653-2.6-1.40.29 (TeX Live 2026) and `BibTeX` 0.99e, in the sequence `pdflatex`, `bibtex`, `pdflatex`, `pdflatex`. The bibliography file is a byte-for-byte copy of the supplied file and was not edited; all five entries are used only as supplied, and the source repository is cited as [5].

Table 3: Independent verification. “Exact” means the check is a symbolic polynomial identity or an integer count, with no floating-point step. Residuals at the 10^{-14} level are the noise floor of the double-precision Hermitian eigensolver used for traces; the combinatorial identities are evaluated in 50-digit arithmetic and their residuals reflect that.

Block	Statement	Coverage	Worst residual
C0	Recalled ideal bounds (4), (5); exactness at $N = 2, 3$	200 random spectra, $K \leq 6$, $N \leq 7$	2.8×10^{-14}
C1	Decomposition (16)	48 cases, $K \leq 5$, $N \leq 5$, both signs	4.1×10^{-48}
C1s	(16) as a polynomial identity in x_i, y_{ij}	$K = 2, 3$; $N = 2, 3, 4$	exact
C2/C3	Shifted two-sided bound (20) and the repulsive collapse	48 cases	8.6×10^{-50}
C4	Small- N identities (21)–(23)	$K = 4$, mixed-sign couplings	$< 10^{-45}$
C5	Defect formula (33)	$K = 4$	$< 10^{-45}$
C6	$N = 4$ endpoint gaps (25)	8 ensembles, $K = 2.5$	3.4×10^{-49}
C7	Frontier (27) and witnesses (28)	$K = 2.5$, $N = 2.6$, both signs; $K = 1$, $N = 2.6$	4.7×10^{-51}
C8	One-sided validity (30), (31), the $N = 3$ witnesses and the divergence scan (36)	12 ensembles, 2 signed witnesses, 6-point scan	4.3×10^{-50}
C9	Frozen fermion side, monotonicity and the $N = 2$ flip (38)–(39)	12 random cases, $K \leq 4$, $N \leq 5$, complex γ	0
C10	Spectral symmetry, sector trace, continuant and closed forms (44)–(49)	40 random cases, $N = 2.8$	3.2×10^{-14}
C10b	$N = 4$ crossover (57)	60-step bisection on the Fock solve, cross-checked against (48)	$< 10^{-9}$
C11	Single link with spectators (51)	10 random cases, $K = 3, 4$, $N = 2.6$	6.7×10^{-16}
C12	Parity endpoint (53) and the $q = 1$ forms (54), (55)	10 random link graphs, $K = 3, 4$, $N = 2.6$	8.6×10^{-16}
C12b	Sector bookkeeping of Appendix B	$K = 2.5$, $N = 2.8$	exact
C13	Envelope (56) and the norm bound $\ H_{\text{ph}}\ \leq 2\Lambda_N \sum \gamma_{ij} $	12 random cases, $K \leq 4$, $N \leq 5$	0
C14	Exchange reduction (58) and the transferred bounds (59), (60)	10 random one-body matrices, $K \leq 4$, $N \leq 4$, complex τ	2.8×10^{-14}
C14b	Exchange raises h_N and e_N (Remark 6.2)	10 random one-body matrices	3.3×10^{-16}
C15	Simultaneous bounds (63) and the $\gamma = 0$ exactness	12 random cases, $K \leq 4$, $N \leq 4$	4.4×10^{-16}
C15b	Exact two-orbital forms (70), (72) and their reductions; divergence scan	30 random cases, $N = 2, 3$; 8-point scan	1.4×10^{-14}
C15c	Root asymptotics (65) and variational witness (67)	$ \gamma = 10, 10^2, 10^3$; $N = 2.5$, $ \gamma \leq 8$	scaled residuals 0.27, 0.17
C16	$B_N \geq B_N^{(u)}$ with u , γ and τ all present (73)	8 random cases, $K \leq 4$, $N \leq 4$	0
C17	Worked identities of Appendix A; sector table of Appendix B	(74)–(76) and the $N = 4$ defects as polynomial identities; Table 4 and (93) as integer counts	exact

Table 4: Sector structure for four cases, as verified in block C17. Each row is a group of labels with the same $|s|$ and q ; “dimension” is the common value of (92). The last column of each block is the number of fermionic configurations, which equals the total dimension of the $q = 0$ sectors.

K	N	$ s $	q	labels	dimension	sector total
3	4	0	2	1	6	6
		2	1	3	3	9
		total = 15 = $\binom{6}{4}$; fermionic configurations = 0				
3	5	1	2	3	6	18
		3	1	1	3	3
		total = 21 = $\binom{7}{5}$; fermionic configurations = 0				
4	4	0	2	1	10	10
		2	1	6	4	24
		4	0	1	1	1
		total = 35 = $\binom{7}{4}$; fermionic configurations = 1 = $\binom{4}{4}$, the $q = 0$ sector				
4	6	0	3	1	20	20
		2	2	6	10	60
		4	1	1	4	4
		total = 84 = $\binom{9}{6}$; fermionic configurations = 0				

Table 5: Dimension of the full N -boson space against the number of contributing sectors ($q \geq 1$) and the largest sector dimension. Cases with $N > K$ have no fermionic configurations, so the contributing sectors tile the whole space.

K	N	full dimension	sectors with $q \geq 1$	largest sector	ratio
4	8	165	8	35	4.7
5	12	1820	16	210	8.7
3	25	351	4	91	3.9
4	25	3276	8	455	7.2
5	25	23751	16	1820	13.1

Table 6: Provenance of each statement. “Derivation note” refers to the section headings of the source derivation document; “new” marks material that first appears in this manuscript.

Manuscript statement	Source location	Status
Proposition 2.1	Recalled from [2]; notation fixed in “Setup and notation”	recalled
Theorem 3.2, Corollary 3.4	“Exact first-double-occupation decomposition”	extended
Theorem 3.5, Corollary 3.6	“Universal upper bound”, “Universal lower bound”	extended
Proposition 3.7	“Small- N identities”	extended
Proposition 3.8	“Exact $N = 4$ endpoint gaps and non-tightness”	extended
Theorem 3.9	“Endpoint-attainment frontier for every N ”	extended
Propositions 4.1–4.2, Theorem 4.3, Corollary 4.4	“Defect of the naive bound and the sign boundary”, “Interacting-fermion analogue”	extended
Theorem 5.1, Proposition 5.2	“Pair hopping: monotonicity ... and the $N = 2$ endpoint flip”	extended
Theorem 5.3	“Exact $K = 2$ pair-hopping endpoint: spectral symmetry and closed forms”	extended
Corollary 5.4	“Single pair-hopping link with spectator orbitals”	extended
Corollary 5.5, Appendix B	“Multi-link pair hopping: orbital-parity sectors”, “General- q sector theorem”	extended
Proposition 5.7	“Controlled upper endpoint for arbitrary orbitals”	extended
Theorem 6.1	“Orbital exchange (one-body orbital mixing)”	extended
Proposition 7.1, Theorem 7.2, Corollary 7.3	“Simultaneous pair hopping and one-body exchange”	extended
Proposition 7.6, Theorem 7.4(i)	“Exact simultaneous two-orbital endpoint and the sharpening boundary”	extended
Theorem 7.4(ii), Remark 9.1, Appendix A, Table 4, Table 5, Figures 1–3, Table 3	—	new

Table 7: Reruns of the recorded source verification, identified by content. “Status” is the final line of the rerun output.

Recorded verification	Status of the rerun
Exact enumeration of the density–density model	enumeration report, values reproduced
Decomposition (16) as a polynomial identity	SYMBOLIC CHECKS: PASS
Shifted two-sided bound (20)	ALL CHECKS: PASS
$N = 4$ endpoint gaps (25)	ALL CHECKS: PASS
Attainment frontier (27) and its witnesses	ALL CHECKS: PASS
Uncorrected endpoints, defect (33) and the repair (37)	ALL CHECKS PASSED
Pair hopping: frozen fermion side, monotonicity (38) and the flip (39)	ALL CHECKS: PASS
Spin- J reduction (43) and the envelope (56)	ALL CHECKS: PASS
Exact two-orbital closed forms (46)–(49)	ALL CHECKS: PASS
Orbital-parity sector lemma and multi-link endpoint (53)	ALL CHECKS PASSED
Sector endpoints at pair numbers $q = 2, 3$	ALL CHECKS PASSED (40 endpoint cases)
Sector endpoints for arbitrary q , up to $N = 25$	see note below
Exchange reduction (58) and the transferred bounds	ALL CHECKS: PASS (54 one-body cases)
Simultaneous two-sided bound (63)	RESULT: ALL PASSED
Exact simultaneous two-orbital forms (70), (72)	ALL CHECKS PASSED

References

- [1] Charles Kittel and Herbert Kroemer. *Thermal Physics*. W. H. Freeman, San Francisco, 2nd edition, 1980.
- [2] Scientific Author 59. Kroemer’s bose–fermi partition-function bound on discrete spectra. <https://git.gewu-lab.ai/scientific-author-59/kroemer-bose-fermi-discrete-bound>, 2026. Accepted revision c0c200db60d9363b16d37b75c0c68e4a020dfd3a.
- [3] Extending kroemer’s two-sided bound on the bose–fermi partition-function difference beyond the spinless, noninteracting, continuum classical regime. <https://git.gewu-lab.ai/peter0627ustc/phys-auth-cc9e577526bdf79e462c/-/blob/main/README.md>, 2026. Accessed September 8, 2026.
- [4] Scientific Author 59. Orbital-mixing extension of the kroemer bose–fermi partition bound. <https://git.gewu-lab.ai/scientific-author-59/orbital-mixing-kroemer-bose-fermi>, 2026.
- [5] GeWu Journal Auto Author. Source research repository for this paper. <https://git.gewu-lab.ai/scientific-author-59/orbital-mixing-kroemer-bose-fermi>, 2026. Solution repository at commit 27a6b169a8ccd1f9d828cf905ef668b009fa63c2.