

How bosonic is a pair of fermions?

Malte C. Tichy · P. Alexander Bouvrie ·
Klaus Mølmer

Received: 31 October 2013 / Accepted: 14 March 2014 / Published online: 5 June 2014
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Abstract Composite particles made of two fermions can be treated as ideal elementary bosons as long as the constituent fermions are sufficiently entangled. In that case, the Pauli principle acting on the parts does not jeopardise the bosonic behaviour of the whole. An indicator for bosonic quality is the *composite boson normalisation ratio* χ_{N+1}/χ_N of a state of N composites. This quantity is prohibitively complicated to compute exactly for realistic two-fermion wavefunctions and large composite numbers N . Here, we provide an efficient characterisation in terms of the purity P and the largest eigenvalue λ_1 of the reduced single-fermion state. We find the states that extremise χ_N for given P and λ_1 , and we provide easily evaluable, saturable upper and lower bounds for the normalisation ratio. Our results strengthen the relationship between the bosonic quality of a composite particle and the entanglement of its constituents.

1 Introduction

At all physical scales, bosons and fermions emerge as the two fundamental species for identical particles, inseparably connected to their characteristic behaviour: The Pauli principle forbids two fermions to occupy the same state, while bosonic bunching favours such multiple occupation.

We routinely treat composite particles made of an even number of fermionic constituents as bosons, which seems justified a posteriori by the success of such description: From pions composed of two quarks [1] to molecules made of a large number of electrons and nuclei [2], bosonic behaviour is truly universal. At first sight, however, the Pauli principle that acts on the fermionic parts seems to jeopardise the bosonic behaviour of the whole. Notwithstanding this apparent obstacle, a microscopic theoretical treatment of two-fermion compounds explains the emergence of ideally behaving composite bosons: A compound of two fermions exhibits bosonic behaviour as long as the constituent fermions are sufficiently entangled [3–5], such that they effectively do not compete for single-fermion states and remain undisturbed by the Pauli principle [6, 7]. This observation connects our understanding of the almost perfect bosonic behaviour at all scales ranging from sub-nuclear physics [1] to ultracold molecules [2] with the tools and concepts of quantum information [4, 8, 9].

The *composite boson normalisation ratio* χ_{N+1}/χ_N [3, 10–13] of states with $N + 1$ and N *cobosons* (composite bosons) captures the above argument quantitatively, as we discuss in more detail below. When it is close to unity, cobosons can be treated as elementary bosons [3], while deviations are observable in the statistical behaviour of the compounds [14–21]. The normalisation factor χ_N depends on the two-fermion wavefunction and answers our above question: “How bosonic is a pair of fermions?” Moreover, the argument can be taken to the realm of Cooper pairs [22] and composites made of two elementary bosons, for which a similar analysis is possible [3, 23].

The exact evaluation of χ_N becomes quickly unfeasible when the number of cobosons N and the number of relevant single-fermion states S are large, which makes approximations desirable. Simple saturable bounds to χ_N as

M. C. Tichy (✉) · K. Mølmer
Department of Physics and Astronomy, University of Aarhus,
8000, Aarhus C, Denmark
e-mail: tichy@phys.au.dk

P. A. Bouvrie
Departamento de Física Atómica, Molecular y Nuclear and
Instituto Carlos I de Física Teórica y Computacional,
Universidad de Granada, 18071 Granada, Spain

a function of the purity P of the single-fermion reduced state were derived in Refs. [12, 24], and an elegant algebraic approach to prove such bounds was put forward in [10]. For very small purities, $P \ll 1/N^2$, the upper and lower bounds converge, which yields an excellent characterisation of the emerging coboson. For moderate values of the purity $P \sim 1/N$, however, a considerable gap between the lower and the upper bound opens up [24]. In this regime, the P -dependent bounds do not characterise the coboson very well, and tighter bounds are desirable.

Here, we derive bounds for the normalisation factor χ_N and for the normalisation ratio χ_{N+1}/χ_N for two-fermion cobosons which depend on the purity P and on the largest eigenvalue λ_1 of the single-fermion density matrix $\hat{\rho}_{(a)}$, introduced below. The bounds can be evaluated efficiently for very large composite numbers N , and we show that they permit a significantly more precise characterisation of two-fermion cobosons than bounds in P alone [12, 24].

We introduce the physics of cobosons and motivate the importance of the normalisation ratio in Sect. 2. Our main result, a set of saturable bounds for the normalisation ratio, is derived in Sect. 3. Examples and a discussion of the bounds are given in Sect. 4. An outlook on possible future developments that take into account further characteristics of the wavefunction is given in Sect. 5. Technical details regarding the derivation of the bounds are given in the Appendix 1 and 2.

2 Algebraic description of cobosons

2.1 Coboson normalisation factor

We consider two distinguishable¹ fermions of species a and b prepared in a collective wavefunction of the form

$$|\Psi\rangle = \sum_{j,k=1}^{\infty} \omega_{j,k} |A_j, B_k\rangle, \quad (1)$$

where we assume that the two-fermion state can be expanded on a discrete set of single-fermion states, which is fulfilled for bound states and also incorporates possible spin coupling. The bases $\{|A_j\rangle\}$, $\{|B_k\rangle\}$ can be chosen at will, and it is convenient to use the *Schmidt decomposition* of $|\Psi\rangle$ [25], i.e. to choose two particular single-particle bases $|a_j\rangle$ and $|b_j\rangle$ with

¹ In our context, a state of two indistinguishable fermions can always be mapped formally onto distinguishable fermions [24]. Our subsequent discussion therefore applies to distinguishable and indistinguishable fermions in a similar fashion. For composites made of two bosons, however, we expect differences between distinguishable and indistinguishable bosons due to multiply populated single-boson states [23].

$$|\Psi\rangle = \sum_{j=1}^S \sqrt{\lambda_j} |a_j, b_j\rangle, \quad (2)$$

$$\lambda_1 \geq \lambda_2 \geq \dots \geq 0, \quad \sum_{j=1}^S \lambda_j = 1, \quad (3)$$

where the ordering of the S Schmidt coefficients λ_j is imposed for convenience such that λ_1 be the largest coefficient in the distribution $\Lambda = (\lambda_1, \dots, \lambda_S)$, and S is not necessarily finite. The λ_j coincide with the eigenvalues of either reduced single-fermion density matrix,

$$\hat{\rho}_{(a)} = \sum_{j=1}^S \lambda_j |a_j\rangle\langle a_j|, \quad \hat{\rho}_{(b)} = \sum_{j=1}^S \lambda_j |b_j\rangle\langle b_j|. \quad (4)$$

We treat a pair of fermions in the state $|\Psi\rangle$ as a coboson, for which we can define an approximate creation operator in second quantisation [3]

$$\hat{c}^\dagger = \sum_{j=1}^S \sqrt{\lambda_j} \hat{a}_j^\dagger \hat{b}_j^\dagger =: \sum_{j=1}^S \sqrt{\lambda_j} \hat{d}_j^\dagger, \quad (5)$$

where \hat{a}_j^\dagger (\hat{b}_j^\dagger) creates a fermion in the Schmidt mode $|a_j\rangle$ ($|b_j\rangle$). The operator \hat{d}_j^\dagger creates a *bi-fermion* in a product state, i.e. a pair of two fermions in their respective mode j . While such creation and annihilation operators commute,

$$[\hat{d}_j, \hat{d}_k] = [\hat{d}_j^\dagger, \hat{d}_k^\dagger] = 0, \quad (6)$$

bi-fermions also obey the Pauli principle, such that

$$(\hat{d}_j^\dagger)^2 = (\hat{d}_j)^2 = 0. \quad (7)$$

As a consequence, the operators \hat{c}, \hat{c}^\dagger do not fulfil the ideal bosonic commutation relation, but obey [3]

$$[\hat{c}, \hat{c}^\dagger] = 1 - \sum_{j=1}^S \lambda_j (\hat{a}_j^\dagger \hat{a}_j + \hat{b}_j^\dagger \hat{b}_j). \quad (8)$$

An N -coboson state is obtained by the N -fold application of the creation operator (5) on the vacuum [3],

$$|N\rangle = \frac{(\hat{c}^\dagger)^N}{\sqrt{\chi_N^\Lambda N!}} |0\rangle, \quad (9)$$

where $\chi_N^\Lambda \leq 1$ is the coboson *normalisation factor* [3, 11, 26], which ensures that $|N\rangle$ is normalised to unity. Inserting the definition of the coboson creation operator (5) into (9), we find

$$|N\rangle = \frac{1}{\sqrt{\chi_N^\Lambda N!}} \sum_{j_1 \neq j_2 \dots \neq j_N}^{1 \leq j_m \leq S} \prod_{k=1}^N \sqrt{\lambda_{j_k}} \hat{d}_{j_k}^\dagger, \quad (10)$$

where terms with repeated indices $j_m = j_k$ do not contribute, due to the Pauli principle ensured by Eq. (7). In other

words, the N -coboson state is a superposition of N bi-fermions that are distributed among the bi-fermion Schmidt modes. Each distribution of the bi-fermions in the modes is weighted by $N!$ coherently superposed amplitudes.

2.2 Algebraic properties of the normalisation factor

By evaluating the norm of the N -coboson state in Eq. (10), one obtains a closed expression for the coboson normalisation factor χ_N^Λ as the elementary symmetric polynomial of degree N in the Schmidt coefficients Λ [27]:

$$\chi_N^\Lambda = \Omega\{\underbrace{1 \dots 1}_N\}, \tag{11}$$

$$\Omega\{x_1 \dots x_N\} = N! \sum_{1 \leq p_1 < \dots < p_N \leq S} \prod_{k=1}^N \lambda_{p_k}^{x_k}, \tag{12}$$

where the latter can be expressed recursively

$$\Omega\{x, \underbrace{1 \dots 1}_K\} = M(x)\Omega\{\underbrace{1 \dots 1}_K\} - K\Omega\{x+1, \underbrace{1 \dots 1}_{K-1}\}, \tag{13}$$

with the help of the power sums of order 1 to N ,

$$M(k) = \sum_{j=1}^S \lambda_j^k, \quad M(2) \equiv P, \quad M(1) = 1. \tag{14}$$

Alternatively, the Newton–Girard identities [13, 27] can be used,

$$\chi_N^\Lambda = (N-1)! \sum_{m=1}^N \frac{(-1)^{1+m} \chi_{N-m}^\Lambda M(m)}{(N-m)!}, \tag{15}$$

which are more suitable in practice than Eqs. (12, 13).

The computation of χ_N becomes significantly simpler when all Schmidt coefficients in a distribution Λ are identical. In this case, all summands in Eq. (12) are equal, and counting the number of terms gives

$$\chi_N^\Lambda = \lambda^N \frac{S!}{(S-N)!} \quad \text{for } \Lambda = (\underbrace{\lambda \dots \lambda}_S), \tag{16}$$

which can be combined with [23]

$$\chi_N^{(\lambda_1 \dots \lambda_S)} = \sum_{M=0}^N \chi_M^{(\lambda_1 \dots \lambda_L)} \chi_{N-M}^{(\lambda_{L+1} \dots \lambda_S)} \binom{N}{M}, \tag{17}$$

to quickly yield χ_N^Λ for distributions Λ with large Schmidt coefficient multiplicities.

2.3 Bosonic behaviour in relation to the normalisation ratio

The *normalisation ratio* $\chi_{N+1}^\Lambda/\chi_N^\Lambda$ [3] determines the bosonic quality of a state of N cobosons. For an intuitive

picture, consider one summand in Eq. (10), in which the N bi-fermions occupy the modes j_1, \dots, j_N . In order to add an $N+1$ st coboson to the state $|N\rangle$, we need to accommodate it among the $S-N$ unoccupied Schmidt modes. The probability that the added bi-fermion successfully ends up in an unoccupied Schmidt mode is then the sum of the coefficients associated with these unoccupied modes, $\sum_{m \notin \{j_1, \dots, j_N\}} \lambda_m$. This argument can be repeated for each configuration j_1, \dots, j_N , and the success probability to add an $N+1$ st coboson to an N -coboson state becomes

$$\begin{aligned} & \frac{1}{\chi_N^\Lambda} \sum_{j_1 \neq j_2 \dots \neq j_N} \prod_{k=1}^N \lambda_{j_k} \left[\sum_{m \notin \{j_1, \dots, j_N\}} \lambda_m \right] \\ &= \frac{1}{\chi_N^\Lambda} \sum_{j_1 \neq j_2 \dots \neq j_N \neq j_{N+1}} \prod_{k=1}^{N+1} \lambda_{j_k} = \frac{\chi_{N+1}^\Lambda}{\chi_N^\Lambda}, \end{aligned} \tag{18}$$

which is reflected by the sub-normalisation of the state obtained upon application of the creation operator \hat{c}^\dagger on the N -coboson state [12]

$$\hat{c}^\dagger |N\rangle = \sqrt{\frac{\chi_{N+1}^\Lambda}{\chi_N^\Lambda}} \sqrt{N+1} |N+1\rangle. \tag{19}$$

On the other hand, the annihilation of a coboson in an N -coboson state yields a state that contains a component orthogonal to the $(N-1)$ -coboson state [3],

$$\hat{c} |N\rangle = \sqrt{\frac{\chi_N^\Lambda}{\chi_{N-1}^\Lambda}} \sqrt{N} |N-1\rangle + |\epsilon_N\rangle, \tag{20}$$

with

$$\langle \epsilon_N | \epsilon_N \rangle = 1 - N \frac{\chi_N^\Lambda}{\chi_{N-1}^\Lambda} + (N-1) \frac{\chi_{N+1}^\Lambda}{\chi_N^\Lambda}. \tag{21}$$

Combining the relations (19) and (20), one finds the expectation value of the commutator (8) on an N -coboson state [3, 10, 13],

$$\begin{aligned} \langle N | [\hat{c}, \hat{c}^\dagger] |N\rangle &= 1 - 2 \sum_{j=1}^S \lambda_j \langle N | \hat{n}_j |N\rangle \\ &= 2 \frac{\chi_{N+1}^\Lambda}{\chi_N^\Lambda} - 1, \end{aligned} \tag{22}$$

where $\hat{n}_j = \hat{d}_j^\dagger \hat{d}_j$ counts the number of bi-fermions in mode j . For an ideal boson, Eq. (22) will equate to unity. Since all observable bosonic behaviour is borne by the bosonic commutation relations, values of $\chi_{N+1}^\Lambda/\chi_N^\Lambda$ close to unity witness a statistical behaviour that is close to the ideal bosonic one, while deviations from unity come with observable consequences that are induced by the statistics of the constituent fermions [15–17, 20, 28].

3 Bounds on the normalisation factor and ratio

Given a wavefunction $|\Psi\rangle$ of two distinguishable fermions, one can, in principle, diagonalise one reduced single-fermion density matrix $\hat{\rho}_{(a/b)}$ to obtain the distribution Λ and compute χ_N with the help of the previous formulae, Eqs. (11, 12, 15, 16, 17).

In practice, however, even if the full distribution Λ or all relevant power sums $M(2) \dots M(N)$ are actually known, the evaluation of the normalisation factor χ_N is unfeasible for very large numbers of cobosons: Using Eq. (15), for example, the computation of χ_N requires the knowledge of all χ_M with $M < N$. Already for a harmonically trapped condensate of hydrogen atoms, the exact approach turns out to be unfeasible [12].

A characterisation of χ_N in terms of few, well-accessible quantities, such as the largest eigenvalue λ_1 and the purity P of the reduced single-fermion density matrix is therefore essential in practice. The largest eigenvalue can be approximated via power iteration [25], while the purity is basis-independent and fulfils $P = \text{Tr}[\rho_{(a)}^2] = \text{Tr}[\rho_{(b)}^2]$. Full diagonalisation of $\hat{\rho}_{(a/b)}$ is not necessary for either quantity, while both bear clear physical meaning as quantifier of entanglement: The *Schmidt number* [4, 29] is defined as $K = 1/P$, the *geometric measure of entanglement* [30] fulfils $E_G = 1 - \lambda_1$.

Upper and lower bounds to the normalisation factor χ_N^Λ and to the normalisation ratio $\chi_{N+1}^\Lambda/\chi_N^\Lambda$ in terms of P and λ_1 are therefore highly desirable, not only to permit the efficient evaluation of χ_N in practice, but also to provide a better physical understanding of the connection between quantum entanglement and bosonic behaviour.

Bounds as a function of the single-fermion purity $P \equiv M(2) = \text{Tr}[\rho_{(a/b)}^2]$ were put forward previously [10, 12, 13, 24]. In the regime $P \ll 1/N^2$, the bounds are efficient and tightly confine the possible values of χ_N and χ_{N+1}/χ_N [24]. For moderate values of $P \sim 1/N$, however, the upper and lower bounds differ considerably, i.e. the compounds are not well characterised by P alone, and higher-order power sums $M(m \geq 3)$ become important in the expansion in Eq. (15).

Here, we formulate bounds that depend on P and on the largest Schmidt coefficient λ_1 . Existing bounds [10, 12, 24] emerge naturally as extremal cases in the limit of the minimal and maximal value of λ_1 for a given P . The extremal distributions of Schmidt coefficients that emerge below coincide with the ones derived in Ref. [23] for two-boson composites. The alternating sign in Eq. (15), however, has no analogy for two-boson compounds, such that the approach of Ref. [23] needs to be adapted to fit the present case.

3.1 Lower bound in P and λ_1

We assume that we are given a distribution Λ with largest Schmidt coefficient λ_1 and purity P . The distribution $\Lambda_{\min}(P, \lambda_1)$ that minimises χ_N under these constraints is derived in Appendix 1.

The resulting *minimising distribution* $\Lambda_{\min}(P, \lambda_1)$ [23] contains S non-vanishing Schmidt coefficients, with $\lambda_1 \geq \lambda_2 = \lambda_3 = \dots = \lambda_{S-1} \geq \lambda_S$, and

$$S = 1 + \left\lceil \frac{(1 - \lambda_1)^2}{P - \lambda_1^2} \right\rceil. \quad (23)$$

The normalisation in Eq. (3) and the fixed purity P imply for the Schmidt coefficients λ_j

$$\begin{aligned} \lambda_1 + (S - 2)\lambda_2 + \lambda_S &= 1, \\ \lambda_1^2 + (S - 2)\lambda_2^2 + \lambda_S^2 &= P. \end{aligned} \quad (24)$$

With

$$R = \sqrt{(S - 2)(\lambda_1(2 - S\lambda_1) + (S - 1)P - 1)}, \quad (25)$$

the relevant solution to Eq. (24) is [23]

$$\begin{aligned} \lambda_{2, \dots, S-1} &= \frac{1 - \lambda_1}{S - 1} + \frac{R}{(S - 2)(S - 1)}, \\ \lambda_S &= \frac{1 - \lambda_1 - R}{S - 1}, \end{aligned} \quad (26)$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_S$ is fulfilled by construction.

Given such distribution of three distinct Schmidt coefficients $\lambda_1, \lambda_2, \lambda_S$ with multiplicities $1, S - 2, 1$, respectively, we can compute $\chi_N^{\Lambda_{\min}(P, \lambda_1)}$ using Eqs. (16, 17):

$$\begin{aligned} \chi_N^{\Lambda_{\min}(P, \lambda_1)} &= \lambda_2^{N-2} [(N - S)\lambda_2((N - S + 1)\lambda_2 \\ &\quad - N(\lambda_1 + \lambda_S)) + (N - 1)N\lambda_1\lambda_S] \frac{(S - 2)!}{(S - N)!}, \end{aligned} \quad (27)$$

where we used $1/k! = 0$ for $k < 0$. Given λ_1 and P , this expression can be readily evaluated, even for large values of N .

Consistent with the Pauli principle, it is impossible to populate S Schmidt modes with $N > S$ bi-fermions, which is ensured by the factor $1/(S - N)!$ in Eq. (27). In general, Eq. (23) imposes

$$2 + \left\lceil \frac{(1 - \lambda_1)^2}{(P - \lambda_1^2)} \right\rceil \leq N \Rightarrow \chi_N^{\Lambda_{\min}(\lambda_1, P)} = 0. \quad (28)$$

The normalisation *ratio* $\chi_{N+1}^{\Lambda_{\min}(P, \lambda_1)}/\chi_N^{\Lambda_{\min}(P, \lambda_1)}$ is a monotonically increasing function of S . We can therefore obtain a simpler, however, slightly weaker, lower bound for Eq. (27) by setting $S = 1 + (1 - \lambda_1)^2/(P - \lambda_1^2)$, i.e. we omit the ceiling function in Eq. (23):

$$\chi_N^{\Lambda_{\min}(\lambda_1, P)} \geq \frac{\Gamma\left[\frac{(1-\lambda_1)^2}{P-\lambda_1^2}\right]}{\Gamma\left[2-N+\frac{(1-\lambda_1)^2}{P-\lambda_1^2}\right]} \times (1+(N-2)\lambda_1-P(N-1))\left(\frac{P-\lambda_1^2}{1-\lambda_1}\right)^{N-2}, \tag{29}$$

which is only applicable for $1 + \left[\frac{(1-\lambda_1)^2}{(P-\lambda_1^2)}\right] \geq N$ [see Eq. (28)]. For values of P and λ_1 for which $(1-\lambda_1)^2/(P-\lambda_1^2)$ is integer, the smooth lower bound Eq. (29) exactly coincides with the exact expression, Eq. (27).

3.2 Upper bound in P and λ_1

In strict analogy to the last section, we construct the distribution $\Lambda_{\max}(\lambda_1, P)$ that *maximises* the normalisation constant χ_N for fixed λ_1 and P in Appendix 2.

In $\Lambda_{\max}(\lambda_1, P)$ [23], the multiplicity of λ_1 is chosen as large as possible, i.e. λ_1 is repeated $L-1$ times, with $L = \lceil P/\lambda_1^2 \rceil$. The L th coefficient is then maximised, while the remaining $S-L$ coefficients fulfil $\lambda_1 = \lambda_2 = \dots = \lambda_{L-1} \geq \lambda_L \geq \lambda_{L+1} = \dots = \lambda_S$. To ensure normalisation [Eq. (3)] and satisfy $M(2) = P$, we have

$$\begin{aligned} (L-1)\lambda_1 + \lambda_L + (S-L)\lambda_S &= 1, \\ (L-1)\lambda_1^2 + \lambda_L^2 + (S-L)\lambda_S^2 &= P. \end{aligned} \tag{30}$$

With

$$R' = \sqrt{(S-L)(P(S+1-L) - 1 + (L-1)\lambda_1(2-\lambda_1S))},$$

we find the relevant solution for λ_L and λ_S [23],

$$\begin{aligned} \lambda_L &= \frac{1 - (L-1)\lambda_1 + R'}{S+1-L}, \\ \lambda_S &= \frac{1 - (L-1)\lambda_1}{S+1-L} - \frac{R'}{(S-L)(S+1-L)}, \end{aligned} \tag{31}$$

where, in order to ensure $\lambda_S, \lambda_L \geq 0$, S needs to fulfill

$$S > \frac{(L-1)P + 1 - 2(L-1)\lambda_1}{P - (L-1)\lambda_1^2}. \tag{32}$$

Using Eqs. (17, 16), the normalisation factor for the maximising distribution becomes

$$\begin{aligned} \chi_N^{\Lambda_{\max}(P, \lambda_1)} &\stackrel{\text{Eq. (17)}}{=} \sum_{K=0}^N \sum_{M=0}^{N-K} \chi_M^{(\lambda_1, \dots, \lambda_1)} \chi_K^{(\lambda_L)} \chi_{N-M-K}^{(\lambda_S, \dots, \lambda_S)} \binom{N}{M, K} \\ &\stackrel{\text{Eq. (16)}}{=} \sum_{K=0}^1 \sum_{M=0}^{N-K} \frac{(L-1)!}{(L-1-M)!} \frac{(S-L)!}{(S-L-(N-K-M))!} \\ &\lambda_1^M \lambda_L^K \lambda_S^{N-M-K} \binom{N}{M, K}, \end{aligned} \tag{33}$$

where $\binom{X}{Y, Z} = \frac{X!}{Y!Z!(X-Y-Z)!}$ is the multinomial coefficient. Since this expression is an increasing function of S , we

maximise it in the limit $S \rightarrow \infty$. Defining λ_Σ as the sum of all infinitesimal coefficients λ_s in that limit, we find

$$\begin{aligned} \lambda_\Sigma &= 1 - (L-1)\lambda_1 - \sqrt{\lambda_1^2(1-L) + P}, \\ \lim_{S \rightarrow \infty} \chi_{N-M-K}^{(\lambda_S, \dots, \lambda_S)} &= \lambda_\Sigma^{N-M-K}, \end{aligned} \tag{34}$$

which gives

$$\begin{aligned} \chi_N^{\Lambda_{\max}(P, \lambda_1)} &= \sum_{K=0}^1 \sum_{M=0}^{N-K} \frac{(L-1)!}{(L-1-M)!} \lambda_1^M \lambda_L^K \lambda_\Sigma^{N-M-K} \binom{N}{M, K} \\ &= (-\lambda_1)^{L-1} \lambda_\Sigma^{N-L} \left[N \lambda_L \mathcal{U}\left(1-L, 1-L+N, -\frac{\lambda_\Sigma}{\lambda_1}\right) \right. \\ &\quad \left. + \lambda_\Sigma \mathcal{U}\left(1-L, 2-L+N, -\frac{\lambda_\Sigma}{\lambda_1}\right) \right], \end{aligned} \tag{35}$$

where $\mathcal{U}(a, b, z)$ is Tricomi's confluent hypergeometric function [31], which allows fast numerical evaluation in practice. Using $\lambda_1 \geq \lambda_L$, we find a simpler upper bound to the above expression:

$$\chi_N^{\Lambda_{\max}(P, \lambda_1)} \leq \sum_{M=0}^{\min(N, \lceil L \rceil + 1)} \frac{\Gamma(\tilde{L} + 1)}{\Gamma(\tilde{L} - M + 1)} \lambda_1^M \lambda_\Sigma^{N-M} \binom{N}{M}, \tag{36}$$

where $\tilde{L} = P/\lambda_1^2$ (note the omitted ceiling function), λ_Σ is evaluated for $L = \tilde{L}$. The last expression coincides with Eq. (35) when P/λ_1^2 is integer, since in that case $L = \tilde{L}$ and $\lambda_L = \lambda_1$.

We compare the tight saturable bounds, Eqs. (27) and (35), with their respective smooth approximations, Eqs. (29) and (36), in Fig. 1.

3.3 Bounds in P

The parameters λ_1 and P cannot be chosen independently, since, by construction [23],

$$P \leq \lambda_{1, \min}(P) \leq \lambda_1 \leq \lambda_{1, \max}(P) = \sqrt{P}, \tag{37}$$

where

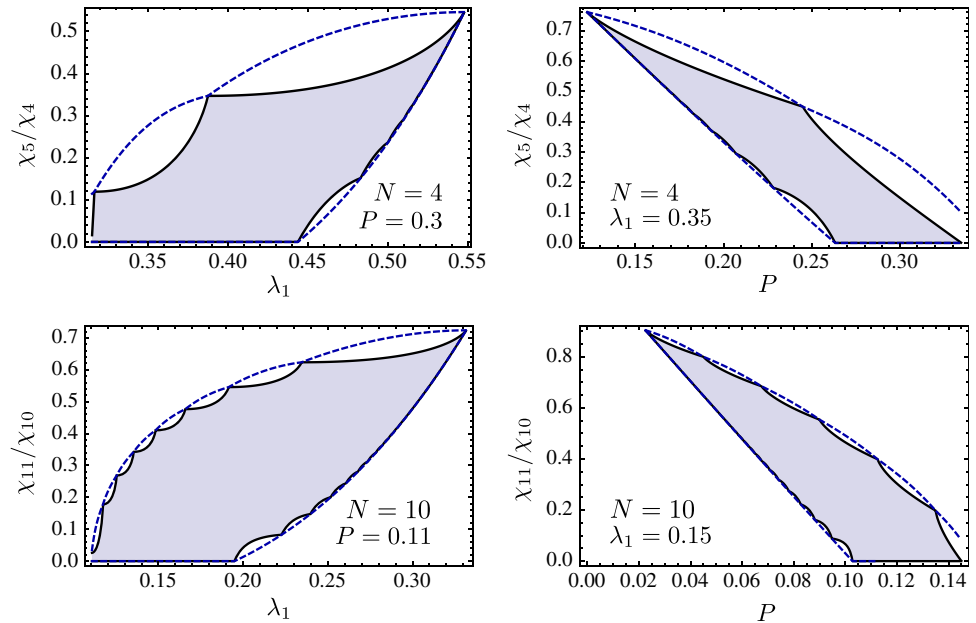
$$\lambda_{1, \min}(P) = \frac{1}{\lceil \frac{1}{P} \rceil} \left(\sqrt{\frac{P \lceil \frac{1}{P} \rceil - 1}{\lceil \frac{1}{P} \rceil - 1}} + 1 \right). \tag{38}$$

We obtain P -dependent and λ_1 -independent upper (lower) bounds to χ_N and χ_{N+1}/χ_N by fixing P and setting the largest Schmidt coefficient to its extremal value, $\lambda_{1, \max(\min)}(P)$.

3.3.1 Upper bound in P

We maximise the normalisation factor and ratio by choosing $\lambda_1 = \lambda_{1, \max}(P) = \sqrt{P}$. The minimising distribution

Fig. 1 Exact values of the normalisation ratio χ_{N+1}/χ_N for the minimising and maximising distribution [black solid lines, computed using Eqs. (27, 35)] and smooth upper and lower bounds [blue dashed lines, Eqs. (29, 36)]. Upper row $N = 4$, lower row $N = 10$. Left column Fixed purity P , the normalisation ratio is shown as a function of the largest Schmidt coefficient λ_1 . Right column Fixed λ_1 , the normalisation ratio is shown as a function of P . The normalisation ratio of any distribution $\mathbf{\Lambda}$ with P and λ_1 is restricted to the shaded range delimited by the black solid line



$\mathbf{\Lambda}_{\min}(P, \lambda_1)$ and the maximising distribution $\mathbf{\Lambda}_{\max}(P, \lambda_1)$ then both converge to the peaked distribution [24], $\bar{\mathbf{\Lambda}}_{\text{peak}}(P)$, given by the limit $S \rightarrow \infty$ of

$$\lambda_{1,\text{peak}} = \frac{1 + \sqrt{(S-1)(SP-1)}}{S}, \quad (39)$$

$$\lambda_{j \in \{2 \dots S\}, \text{peak}} = \frac{1 - \lambda_{1,\text{peak}}}{S-1}.$$

Via Eqs. (16, 17), we recover the P -dependent upper bound [24]

$$\chi_N^{\mathbf{\Lambda}_{\text{peak}}(P)} = (1 - \sqrt{P})^{N-1} \left[1 + (N-1)\sqrt{P} \right]. \quad (40)$$

3.3.2 Lower bound in P

The normalisation factor and ratio are minimised for fixed P by choosing $\lambda_1 = \lambda_{1,\min}(P)$, as given by Eq. (38). In this case, both distributions $\mathbf{\Lambda}_{\min}(P, \lambda_1)$ and $\mathbf{\Lambda}_{\max}(P, \lambda_1)$ become the uniform distribution [15], $\mathbf{\Lambda}_{\text{uni}}(P)$, with $S = L = \lceil \frac{1}{P} \rceil$ non-vanishing Schmidt coefficients given by

$$\lambda_{j \in \{1 \dots L-1\}, \text{uni}} = \lambda_{1,\min}(P), \quad (41)$$

$$\lambda_{L, \text{uni}} = 1 - \lambda_{1,\min}(P)(L-1).$$

Using Eqs. (16, 17), we recover the lower bound [24]

$$\chi_N^{\mathbf{\Lambda}_{\text{uni}}(P)} = \frac{\lambda_{1,\text{uni}}^{N-1} (L-1)!}{(L-N)!} [N - L\lambda_{1,\text{uni}}(N-1)]. \quad (42)$$

3.4 Bounds in λ_1

The constraints on λ_1 and P in Eq. (37) can be re-formulated as constraints on P :

$$\lambda_1^2 = P_{\min}(\lambda_1) \leq P \leq P_{\max}(\lambda_1) \leq \lambda_1, \quad (43)$$

where

$$P_{\max}(\lambda_1) = \lambda_1^2 \left[\frac{1}{\lambda_1} \right] + \left(1 - \lambda_1 \left[\frac{1}{\lambda_1} \right] \right)^2. \quad (44)$$

We obtain λ_1 -dependent and P -independent upper (lower) bounds to the normalisation ratio and factor by choosing $P_{\min(\max)}(\lambda_1)$.

3.4.1 Upper bound in λ_1

For $P = P_{\min}(\lambda_1)$, the distributions $\mathbf{\Lambda}_{\min/\max}(P, \lambda_1)$ become a peaked distribution, $\mathbf{\Lambda}_{\text{peak}}(P_{\min}(\lambda_1))$, with the first Schmidt coefficient λ_1 and $(S-1)$ coefficients of magnitude $(1 - \lambda_1)/(S-1)$. In the limit $S \rightarrow \infty$ the normalisation factor reads

$$\chi_N^{\mathbf{\Lambda}_{\text{peak}}(P_{\min}(\lambda_1))} = (1 - \lambda_1)^{N-1} (1 + (N-1)\lambda_1). \quad (45)$$

Since $\lambda_1 \leq \sqrt{P}$, this upper bound is always larger (i.e. weaker) than the upper bound in P given by Eq. (40):

$$\chi_N^{\mathbf{\Lambda}_{\text{peak}}(P_{\min}(\lambda_1))} \geq \chi_N^{\mathbf{\Lambda}_{\text{peak}}(P)}, \quad (46)$$

for any pair (P, λ_1) fulfilling Eq. (37).

3.4.2 Lower bound in λ_1

We find a lower bound in λ_1 by setting $P = P_{\max}(\lambda_1)$, as given by Eq. (44). The resulting distribution contains the largest possible multiplicity of λ_1 , i.e. it contains $L-1 = S-1 = \lfloor \frac{1}{\lambda_1} \rfloor$ coefficients of magnitude λ_1 and one of the magnitude $\left(1 - \lfloor \frac{1}{\lambda_1} \rfloor \lambda_1\right)$. The resulting normalisation factor fulfils

$$\chi_N^{\Lambda_{\text{uni}}(P_{\text{max}}(\lambda_1))} = \frac{\lambda_1^{N-1}(L-1)!}{(L-N)!} [N - \lambda_1 L(N-1)]. \tag{47}$$

In analogy to Eq. (46), this lower bound in λ_1 is always smaller (i.e. weaker) than the corresponding bound in P :

$$\chi_N^{\Lambda_{\text{uni}}(P_{\text{max}}(\lambda_1))} \leq \chi_N^{\Lambda_{\text{uni}}(P)}, \tag{48}$$

due to $P \leq P_{\text{max}}$.

4 Summaries of the bounds and discussion

Examples for all pertinent distributions are shown in Fig. 2: A randomly chosen distribution Λ (middle panel) with specified λ_1 and P leads to a certain normalisation factor χ_N^Λ , which is bound from below by the distributions on the left and from above by those from the right, successively. Summarising the attained values for the normalisation factor given in Eqs. (27, 35, 40, 42, 45, 47), we obtain our main result,

$$\begin{aligned} \chi_N^{\Lambda_{\text{uni}}(P_{\text{max}}(\lambda_1))} &\leq \chi_N^{\Lambda_{\text{uni}}(P)} \leq \chi_N^{\Lambda_{\text{min}}(\lambda_1, P)} \leq \chi_N^\Lambda \\ &\leq \chi_N^{\Lambda_{\text{max}}(\lambda_1, P)} \leq \chi_N^{\Lambda_{\text{peak}}(P)} \leq \chi_N^{\Lambda_{\text{peak}}(P_{\text{min}}(\lambda_1))}. \end{aligned} \tag{49}$$

This hierarchy of consecutively tighter bounds is immediately inherited by the normalisation ratio χ_{N+1}/χ_N in full analogy, which quantitatively answers our initial question, ‘‘How bosonic is a pair of fermions?’’, in terms of P and λ_1 .

In order to obtain a physical understanding of these bounds, a combinatorial approach is instructive: The normalisation factor χ_N can be interpreted as the probability that a collection of N objects that are each given a property j with probability λ_j does not contain any set of two or more objects with the same property [24] (for $S = 365$ and $\lambda_j = 1/365$, we recover the ‘‘birthday problem’’ [32]). In our physical context, no two or more bi-fermions are allowed to occupy the same Schmidt mode. The Pauli principle, enforced by Eq. (7), implies that the emerging

N -coboson state in Eq. (10) does not contain any such terms describing multiple occupation. The lack of these terms then needs to be accounted for by the normalisation factor χ_N .

4.1 Entanglement and bosonic behaviour

Combinatorially speaking, the purity P represents the probability that two randomly chosen objects possess the same property (it is therefore also called the collision entropy). Here, it reflects the probability that the wavefunction vanishes upon two bi-fermions competing for the same Schmidt mode. Therefore, the P -dependent bounds on χ_N decrease monotonically with increasing P (blue dotted lines in the right panels of Fig. 3). Larger entanglement, characterised by a smaller purity P , is therefore tantamount to a more bosonic composite [3, 12, 24].

Similarly, the λ_1 -dependent bounds decrease with increasing λ_1 (red dashed lines in the left panels of Fig. 3). Consistently, an increase in λ_1 also leads to weaker geometric entanglement, $E_G = 1 - \lambda_1$. This connection underlines, again, the relationship between quantum entanglement and the bosonic behaviour of composites.

The knowledge of λ_1 alone leaves a finite range for possible values of P [see Eq. (43)]: The remaining, unknown Schmidt coefficients $\lambda_2 \dots \lambda_S$ may be many and small, or few and large (compare the distribution $\Lambda_{\text{uni}}(P_{\text{max}}(\lambda_1))$ to $\Lambda_{\text{peak}}(P_{\text{min}}(\lambda_1))$ in Fig. 2). Indeed, the main sources of deviation from bosonic behaviour are binary ‘‘collisions’’ of bi-fermions, which is directly quantified by P . Therefore, bounds in λ_1 are always weaker than bounds in P ; in the formalism of quantum information, the purity P is more decisive than the overlap with the closest separable state, λ_1 .

The knowledge of both, λ_1 and P , yields a considerable enhancement over bounds in P alone (black solid lines in Fig. 3). In particular, the range of possible χ_N becomes narrower for extremal values of P or λ_1 , for which the

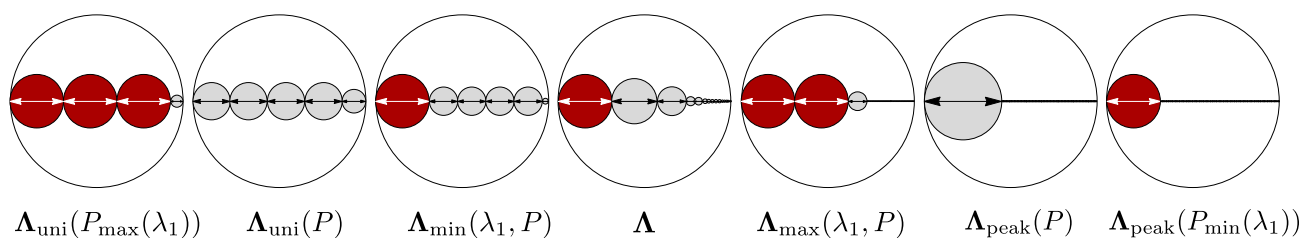


Fig. 2 Hierarchy of minimising and maximising distributions. The circle diameters correspond to the magnitude of a Schmidt coefficient λ_j , and the fraction of filled area in each large circle is the purity P of the respective distribution. A distribution Λ , with $\lambda_1 = 0.3$ and $P = 0.2$ (centre) leads to a normalisation factor χ_N that is bound from below and from above by the χ_N evaluated for the distributions on the left and on the right, respectively. The order of the distributions

reflects the hierarchy of Eq. (49). All circles that correspond to λ_1 are filled with dark red and marked with white arrows. The resulting normalisation ratios χ_{N+1}/χ_N obey the same hierarchy, as illustrated by the intersections of the vertical lines (i) with the three minimising and the three maximising limits in Fig. 3. The normalisation ratio of Λ then lies on (i) within the shaded area

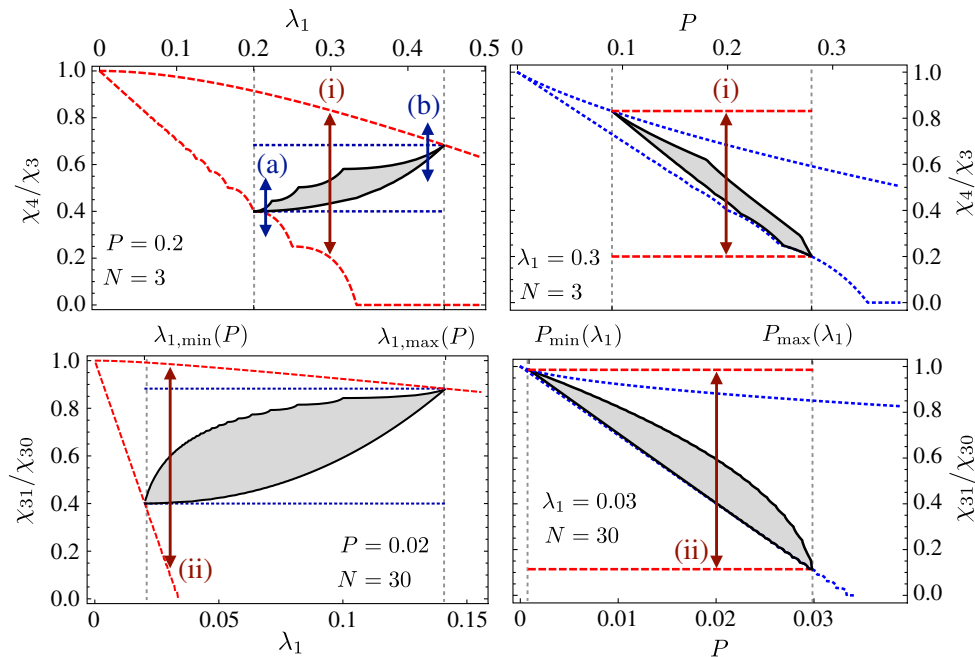


Fig. 3 Upper and lower bounds to the normalisation ratio χ_{N+1}/χ_N as a function of λ_1 (left panels) and P (right panels), for $N = 3$ (top row) and $N = 30$ (bottom row). Red dashed lines correspond to bounds in λ_1 alone, Eqs. (45, 47); blue dotted lines show the bounds in P alone, Eq. (40, 42). The combined bounds, Eqs. (27, 35), are shown as solid black lines, the shaded area is the range allowed for general distributions Λ with given λ_1 and P . The bounds in P are always superior to those in λ_1 . By setting P (left panel) or λ_1 (right panel), the

possible values of λ_1 and P , respectively, are constrained by Eqs. (37) and (43). The solid vertical lines in the upper panels indicate those values for which the maximising and minimising distributions are depicted in Fig. 2 [solid red lines (i), $\lambda_1 = 0.3, P = 0.2$] and Fig. 4 [solid dark blue lines, $P = 0.2$, (a) $\lambda_1 = 0.215$, (b) $\lambda_1 = 0.42$]. The vertical lines (ii) in the lower panel indicate corresponding values of P and λ_1

minimising and maximising distributions resemble each other, as in Fig. 4. In this case, λ_1 and P strongly constrain the remaining Schmidt coefficients.

In view of the clear dependence of χ_N on P and λ_1 , it is remarkable that the combined bound in P and λ_1 features an increase in the bosonic quality χ_N and χ_{N+1}/χ_N with λ_1 (Fig. 3). This increase, however, is due to the fixed purity P : By increasing the largest Schmidt coefficient λ_1 , all other Schmidt coefficients need to decrease in order to keep P constant, which naturally increases the total accessible number of Schmidt modes, and, consequently, χ_N . More formally speaking, χ_N actually increases with $M(3)$, as can be inferred from Eqs. (13, 15) [13].

4.2 Limit of large coboson numbers N

In Fig. 5, we show the deviation from the ideal value $\chi_{N+1}/\chi_N = 1$ as a function of the number of cobosons N . While the upper and lower bounds in P converge for small values of $N < 1/\sqrt{P}$, bounds in λ_1 do not: For small particle numbers, the coboson behaviour is essentially defined by the binary collision probability, i.e. by the purity P . The magnitude of the largest Schmidt coefficient λ_1 is secondary. For large particle numbers $N > 1/\sqrt{P}$, the

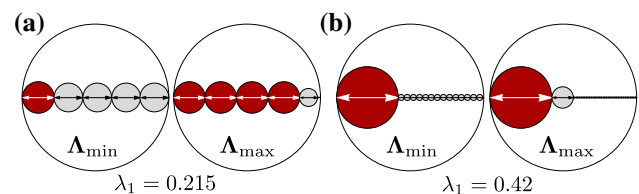


Fig. 4 Minimising and maximising distributions $\Lambda_{\min/\max}$, for close-to-extremal values of λ_1 and fixed $P = 0.2$. (a) $\lambda_1 = 0.215 \gtrsim \lambda_{1,\min}(P)$. (b) $\lambda_1 = 0.42 \lesssim \lambda_{1,\max}(P)$. The emerging bounds correspond to the black solid lines in Fig. 3 at the intersections with arrows (a) and (b), respectively. For $\lambda_1 \rightarrow \lambda_{1,\max(\min)}(P)$, the distributions converge to the peaked (uniform) distribution (compare to the corresponding sketches in Fig. 2)

knowledge of λ_1 then fixes the possible range of $M(3)$, which constrains the accessible values of the normalisation ratio. Again, very large or very small values of λ_1 lead to a tighter confinement of the range of possible χ_{N+1}/χ_N than intermediate values of λ_1 , as can be seen by comparing the panels in Fig. 5. In general, λ_1 and P determine to a wide extent up to which number of cobosons N a condensate of two-fermion composites still behaves bosonically [6, 33].

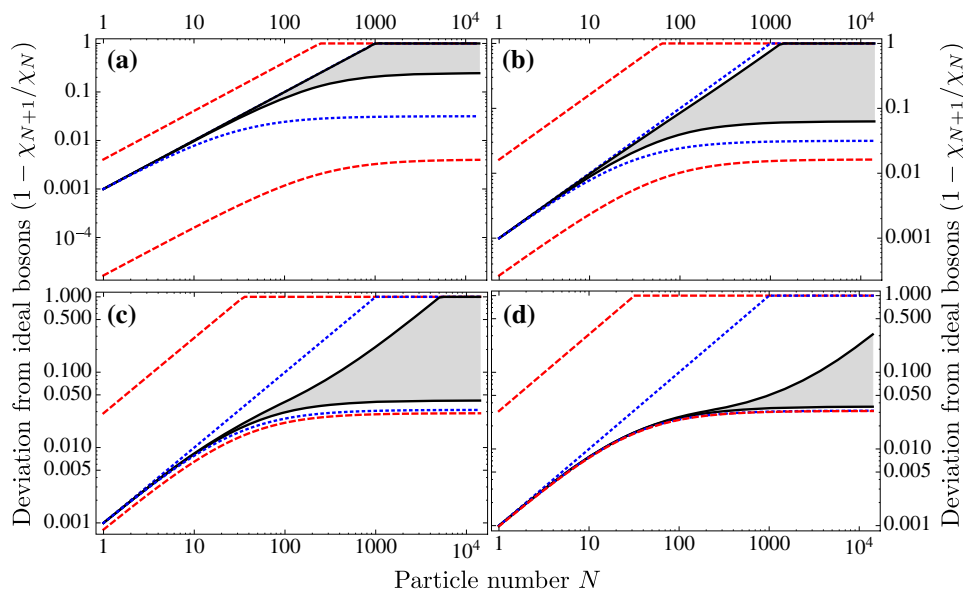


Fig. 5 Upper and lower bounds to $(1 - \chi_{N+1}/\chi_N)$, i.e. to the deviation from ideal bosonic behaviour, as a function of N . The colour code is the same as in Fig. 3. In all panels, $P = 0.001$, i.e. the bounds in P alone (blue dotted) do not change. We choose

different values of λ_1 : (a) $\lambda_1 = 0.9\lambda_{1,\min}(P) + 0.1\lambda_{1,\max}(P) \approx 0.0041$. (b) $\lambda_1 = 0.5\lambda_{1,\min}(P) + 0.5\lambda_{1,\max}(P) \approx 0.0163$. (c) $\lambda_1 = 0.1\lambda_{1,\min}(P) + 0.9\lambda_{1,\max}(P) \approx 0.0286$. (d) $\lambda_1 = 0.01\lambda_{1,\min}(P) + 0.99\lambda_{1,\max}(P) \approx 0.0313$

In comparison to the bounds on the normalisation factor for cobosons made of two elementary bosons [23], the role of the λ_1 -dependent bounds is exchanged: for two-fermion cobosons, χ_N is maximised (minimised) by choosing the smallest (largest) possible purity for a given λ_1 ; for two-boson cobosons, the normalisation factor instead *increases* with the purity. As a consequence, the clear hierarchy of bounds expressed by Eq. (49) is absent for two-boson cobosons [23]. This dependence is due to the possibility for multiple occupation of Schmidt modes by bosonic constituents, forbidden by the Pauli principle for fermionic constituents. Furthermore, when the number of cobosons N is large, $N > 1/\lambda_1$, the behaviour of two-boson bosons is very well defined by λ_1 alone, and the multiple occupation of the most prominent Schmidt mode dominates the picture, a process without analogy in the present two-fermion case.

5 Conclusions and outlook

Starting with the general description of a two-fermion composite in Eqs. (2, 5), we confined the quantitative indicator χ_{N+1}/χ_N for the bosonic behaviour of the resulting coboson. For a fixed purity P , the immediate difference between the state that minimises and the state that maximises χ_N is the magnitude of the largest Schmidt coefficient, which is of the order of P for the minimal,

uniform distribution, and \sqrt{P} for the maximal, peaked distribution [24]. Therefore, the additional constraint on λ_1 can considerably enhance P -dependent bounds [10, 12, 24].

Our bounds strengthen the relation between quantum entanglement and the bosonic quality of bi-fermion pairs, first established in Ref. [3]: Not only is the purity P a quantitative indicator for bosonic behaviour [3, 12, 13, 24], but so is the geometric measure of entanglement [30], which can be expressed here as a function of λ_1 .

Depending on the application, the single-fermion purity P , the largest eigenvalue λ_1 of the single-fermion density matrix $\hat{\rho}_{(a/b)}$, or both may be known. We can formulate a clear hierarchy: Knowledge of P is more valuable than the knowledge of λ_1 alone, whereas the combination can greatly enhance the bounds, depending on the value of the involved parameters. The effect of compositeness is observable in any physical observable that is affected by the commutation relation (22), such as, e.g. bosonic signatures in multiparticle interference [15].

Our method can be extended to formulate even stronger bounds that depend on the purity P and on the m largest Schmidt coefficients $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m$: In close analogy to the procedure in [24] (see Appendix 1 and 2), minimising and maximising distributions can be constructed, and the resulting normalisation factors can be computed. The increased accuracy will, however, come at the expense of an increased computational cost, since a larger number of distinct Schmidt coefficients (up to $m + 2$ when we fix the

m largest coefficients and the purity P) also leads to a larger number of sums when Eq. (17) is applied.

Another desideratum is the extension of the present bounds to multifermion systems in order to characterise, e.g. α -particles in extreme environments [34, 35]. The absence of the Schmidt decomposition, Eq. (2), for multipartite states [4] makes this task, however, rather challenging. In particular, a simple combinatorial interpretation of the normalisation constant seems to be excluded for such composites.

Acknowledgments The authors would like to thank Florian Mintert, Łukasz Rudnicki, Alagu Thilagam and Nikolaj Th. Zinner for stimulating discussions, and Christian K. Andersen, Durga Dasari, Jake Gulliksen, Pinja Haikka, David Petrosyan and Andrew C. J. Wade for valuable feedback on the manuscript. M.C.T. gratefully acknowledges support by the Alexander von Humboldt-Foundation through a Feodor Lynen Fellowship. K.M. gratefully acknowledges support by the Villum Foundation. P.A.B. gratefully acknowledges support by the Programa de Movilidad Internacional CEI BioTic en el marco PAP-Erasmus.

Appendix 1: Minimising distribution

For completeness, we reproduce the proofs from the Appendix of Ref. [24] in the Appendices 1 and 2, adapting the argument to our situation in which not only the purity P is fixed, but also the largest Schmidt coefficient λ_1 .

Uniforming operation

Following an analysis of the birthday problem with non-uniform birthday probabilities [32], we define a *uniforming* operation Γ^u on the distribution Λ that can modify three selected λ_j with indices $2 \leq j_1 < j_2 < j_3 \leq S$ (i.e. the operation never acts on the first Schmidt coefficient λ_1 , since its value is fixed, by assumption). We will show that this operation always decreases χ_N , and specify the distribution $\Lambda_{\min}(P, \lambda_1)$ that remains invariant under the application of Γ^u . This distribution thus minimises χ_N^Λ under the constraints (P, λ_1) .

The operation Γ^u modifies three coefficients in a distribution,

$$\Gamma^u : (\lambda_{j_1}, \lambda_{j_2}, \lambda_{j_3}) \rightarrow (\lambda_{j_1}^u, \lambda_{j_2}^u, \lambda_{j_3}^u), \tag{50}$$

such that it leaves

$$\begin{aligned} K_1 &= \lambda_{j_1} + \lambda_{j_2} + \lambda_{j_3}, \\ K_2 &= \lambda_{j_1}^2 + \lambda_{j_2}^2 + \lambda_{j_3}^2, \end{aligned} \tag{51}$$

invariant, and, consequently, also $\sum_j \lambda_j = 1$ and $\sum_j \lambda_j^2 = P$. The third power sum, $M(3) = \sum_j \lambda_j^3$, on the other hand, is changed by Γ^u . Specifically,

$$\begin{aligned} \lambda_{j_1}^u &= \lambda_{j_2}^u = \frac{1}{6} \left(2K_1 + \sqrt{6K_2 - 2K_1^2} \right), \\ \lambda_{j_3}^u &= \frac{1}{3} \left(K_1 - \sqrt{6K_2 - 2K_1^2} \right). \end{aligned} \tag{52}$$

In the case $K_1^2 < 2K_2$, in order to avoid $\lambda_{j_3}^u < 0$, we need to set

$$\begin{aligned} \lambda_{j_1/j_2}^u &= \frac{1}{2} \left(K_1 \pm \sqrt{2K_2 - K_1^2} \right), \\ \lambda_{j_3}^u &= 0. \end{aligned} \tag{53}$$

The product $\lambda_{j_1} \lambda_{j_2} \lambda_{j_3}$ decreases under Γ^u

It holds

$$\lambda_{j_1}^u \lambda_{j_2}^u \lambda_{j_3}^u \leq \lambda_{j_1} \lambda_{j_2} \lambda_{j_3}. \tag{54}$$

Proof We write the left- and right-hand side of (54) in terms of K_1, K_2 and λ_{j_1}

$$\begin{aligned} \lambda_{j_1}^u \lambda_{j_2}^u \lambda_{j_3}^u &= \begin{cases} \frac{1}{108} \left(K_1 - \sqrt{6K_2 - 2K_1^2} \right) \\ \times \left(2K_1 + \sqrt{6K_2 - 2K_1^2} \right)^2 & \text{for } K_1^2 > 2K_2 \\ 0 & \text{for } K_1^2 \leq 2K_2 \end{cases} \\ \lambda_{j_1} \lambda_{j_2} \lambda_{j_3} &= \frac{1}{2} \lambda_{j_1} \left(2\lambda_{j_1}^2 - 2\lambda_{j_1} K_1 + K_1^2 - K_2 \right) \end{aligned} \tag{55}$$

Given K_1 and K_2 , the original λ_{j_2/j_3} become functions of λ_{j_1} ,

$$\lambda_{j_2/j_3} = \frac{1}{2} \left(K_1 - \lambda_{j_1} \pm \sqrt{2\lambda_{j_1} K_1 - K_1^2 - 3\lambda_{j_1}^2 + 2K_2} \right) \tag{56}$$

The requirement $\lambda_{j_1} \geq \lambda_{j_2} \geq \lambda_{j_3} \geq 0$ imposes

$$\frac{K_1}{3} + \frac{\sqrt{3K_2 - K_1^2}}{3\sqrt{2}} \leq \lambda_{j_1} \leq \frac{K_1}{3} + \frac{\sqrt{6K_2 - 2K_1^2}}{3}. \tag{57}$$

The values of λ_{j_1} constrained to this interval then always fulfil Eq. (54). \square

χ_N^Λ decreases upon application of Γ^u

Upon application of Γ^u , the normalisation constant χ_N and the normalisation ratio χ_{N+1}/χ_N can only decrease:

$$\chi_N^{\Gamma^u(\Lambda)} \leq \chi_N^\Lambda, \tag{58}$$

$$\frac{\chi_{N+1}^{\Gamma^u(\Lambda)}}{\chi_N^{\Gamma^u(\Lambda)}} \leq \frac{\chi_{N+1}^\Lambda}{\chi_N^\Lambda}. \tag{59}$$

To ease notation in the following, we exemplarily use $j_1 = 2, j_2 = 3, j_3 = 4$, and set

$$\tilde{\chi}_N = \chi_N^{(\lambda_1, \lambda_5, \dots, \lambda_S)}, \tag{60}$$

which allows us to write χ_N as

$$\chi_N = \lambda_2 \lambda_3 \lambda_4 \cdot \tilde{\chi}_{N-3} + (\lambda_2 \lambda_3 + \lambda_4 \lambda_3 + \lambda_2 \lambda_4) \tilde{\chi}_{N-2} + (\lambda_2 + \lambda_3 + \lambda_4) \tilde{\chi}_{N-1} + \tilde{\chi}_N. \tag{61}$$

The terms

$$\lambda_2 \lambda_3 + \lambda_4 \lambda_3 + \lambda_2 \lambda_4 = \frac{1}{2} (K_1^2 - K_2), \tag{62}$$

$$\lambda_2 + \lambda_3 + \lambda_4 = K_1,$$

and $\tilde{\chi}_k \in \{N-3, \dots, N\}$ remain invariant under the application of Γ^u , whereas the product $\lambda_2 \lambda_3 \lambda_4$ decreases, due to Eq. (54). Consequently, also χ_N^Λ decreases upon the application of Γ^u .

Using $\chi_{N+1} \leq \chi_N$, one can easily show in analogy to Ref. [24] that the inequality (58) is inherited by the normalisation ratio (59). \square

Properties of the minimising distribution

The distribution $\Lambda_{\min}(P, \lambda_1)$ that minimises χ_N for fixed λ_1 and P should remain invariant under the application of Γ^u , for all choices of $2 \leq j_1, j_2, j_3 \leq S$. By the definition of Γ^u , we see that any three coefficients with $\lambda_{j_1} > \lambda_{j_2} = \lambda_{j_3}$ never constitute a fixed point of Γ^u . Therefore, the invariant distribution is of the form

$$\lambda_1 \geq \lambda_2 = \dots = \lambda_{S-1} \geq \lambda_S. \tag{63}$$

It coincides with the distribution found in Ref. [23].

Appendix 2: Maximising distribution

Peaking operation

With K_1 and K_2 defined as in Eq. (51) above, we define the *peaking* operation Γ^p as follows [24]: For $K_1 + \sqrt{6K_2 - 2K_1^2} \leq 3\lambda_1$, we set

$$\lambda_{j_1}^p = \frac{1}{3} \left(K_1 + \sqrt{6K_2 - 2K_1^2} \right), \tag{64}$$

$$\lambda_{j_2}^p = \lambda_{j_3}^p = \frac{1}{6} \left(2K_1 - \sqrt{6K_2 - 2K_1^2} \right).$$

If $K_1 + \sqrt{6K_2 - 2K_1^2} > 3\lambda_1$, the above definition leads to $\lambda_{j_1}^p > \lambda_1$, which we excluded by assumption. In this case, we define alternatively

$$\lambda_{j_1}^p = \lambda_1, \tag{65}$$

$$\lambda_{j_2}^p / j_3 = \frac{K_1 - \lambda_1 \pm \sqrt{2(K_2 - \lambda_1^2) - (K_1 - \lambda_1)^2}}{2},$$

for which $\lambda_1 = \lambda_{j_1}^p \geq \lambda_{j_2}^p \geq \lambda_{j_3}^p \geq 0$. In full analogy to the discussion in Appendix 1, one shows that

$$\chi_N^\Lambda \leq \chi_N^{\Gamma^p(\Lambda)}, \quad \frac{\chi_{N+1}^\Lambda}{\chi_N^\Lambda} \leq \frac{\chi_{N+1}^{\Gamma^p(\Lambda)}}{\chi_N^{\Gamma^p(\Lambda)}}, \tag{66}$$

i.e. the normalisation factor and ratio increase under the application of Γ^p .

Properties of the maximising distribution

The distribution $\Lambda_{\max}(P, \lambda_1)$ that maximises χ_N for fixed λ_1 and P is obtained as follows: We maximise the multiplicity of λ_1 in Λ , i.e. λ_1 is repeated $L - 1$ times, with $L = \lceil P / \lambda_1^2 \rceil$. The coefficients then need to fulfil

$$\lambda_1 = \dots = \lambda_{L-1} \geq \lambda_L \geq \lambda_{L+1} = \dots = \lambda_S, \tag{67}$$

to ensure that $\Lambda_{\max}(P, \lambda_1)$ be a fixed point of Γ^p . Again, the distribution coincides with the one found in Ref. [23].

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