Statistical distribution of the local purity in a large quantum system

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Abstract

The local purity of large many-body quantum systems can be studied by following a statistical mechanical approach based on a random matrix model. Restricting the analysis to the case of global pure states, this method proved to be successful, and a full characterization of the statistical properties of the local purity was obtained by computing the partition function of the problem. Here we generalize these techniques to the case of global mixed states. In this context, by uniformly sampling the phase space of states with assigned global mixedness, we determine the exact expression of the first two moments of the local purity and a general expression for the moments of higher order. This generalizes previous results obtained for globally pure configurations. Furthermore, through the introduction of a partition function for a suitable canonical ensemble, we compute the approximate expression of the first moment of the marginal purity in the high-temperature regime. In the process, we establish a formal connection with the theory of quantum twirling maps that provides an alternative, possibly fruitful, way of performing the calculation.

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(Some figures may appear in colour only in the online journal)
1. Introduction

In quantum mechanics, the purity of a quantum state measures the amount of indeterminacy which originates either from lack of information on the process that led to its preparation, or from the correlations that have been established with some external party (environment). Mathematically speaking the two mechanisms are strongly interconnected, as the former can always be represented as an instance of the latter via purification [1, 2]. For a composite quantum system, one can distinguish between global purity (i.e. the purity of the system as a whole) and the local (or ‘marginal’) purities (i.e. the purities associated with the subsystems that compose it). Clarifying the connection between the global and local purities of a quantum state is an important problem of quantum information theory [3–6] which is closely related to the characterization of bipartite entanglement [7, 8]. In particular, for pure global states, the local purity of a subsystem provides a direct measure of the bipartite entanglement between the two parts: the smaller the purity, the larger the bipartite entanglement. For mixed (non-pure) global states instead, the connection between local purity and entanglement is more subtle: no direct relation between the two quantities exists and bipartite entanglement measures for the global system can be obtained only by taking proper convex-roof extensions of the local purity (the average being computed over all convex decompositions of the initial global state).

Still, studying how the global indeterminacy of a composite system affects the indeterminacy of its constituents is important on its own and raises fundamental theoretical questions which are deeply interwoven with thermodynamical issues and call for a thoughtful investigation. Specifically, here we focus on the following basic question: given a certain level of global mixedness of a many-body quantum system (say a mixture of gases at thermal equilibrium at a given temperature), which portion of such indeterminacy can be ‘accounted for’ by its constituents? (That is, how much does the local mixedness contribute to the global one?) While for classical systems global and local mixedness are strongly interconnected (e.g., the former is always greater than the latter), in quantum mechanics the relation is more ambiguous, as qualitatively different sorts of correlations can be established between the various subsystems.

In order to account for the large spectrum of possibilities, we resort to a statistical approach by exploiting tools and techniques imported from classical statistical mechanics. The distribution of the local purity of pure global states of large composite systems was studied in [9, 10] by using statistical mechanical methods. Here, we endeavor to generalize the same techniques to a system in a global mixed state. In particular, by uniformly sampling the states with a given value of the global purity, we determine the exact expression of the first two moments of the local purity and obtain a general formula, valid for arbitrary moments. These findings generalize previous results obtained for globally pure configurations by Lubkin [15], Page [17], Lloyd and Pagels [16], Scott and Caves [19] and Giraud [24, 25]. Then, through the introduction of a partition function for a suitable canonical ensemble endowed with a Lagrange multiplier that plays the role of a fictitious temperature, we compute the approximate expression of the first moment of the marginal purity in the high-temperature regime. We also establish the scaling of all these quantities with the dimension of the system, in the thermodynamic limit. Furthermore, an interesting connection appears between our problem and the theory of quantum channels. More precisely, the symmetry properties of the twirling transformations [26] can be proved to be very useful for the computation of the exact expression of the first moment of the local purity. As a final remark, let us stress the key role played by the introduction of a partition function for the system: it enables us to translate our problem, and thus the results we found, in terms of the even more general context of the theory of random matrices.

This paper is organized as follows. In section 2, we introduce the notation and set the basis of the statistical mechanical approach to the problem, starting from the simpler case of
pure states and generalizing it to the case of generic mixed states. In section 3, we consider
the high-temperature expansion of the partition function and compute the first moments of
the purity by making use of Zuber’s solution of some basic integrals over the unitary group
[11]. In section 4, we establish the connection between our problem and the properties of the
twirling maps. We conclude in section 5 by summarizing our findings and discussing them in
terms of future perspectives.

2. The statistical approach: partition function

In this section, we review the statistical approach introduced in [9] for studying the local
mixedness properties of pure states and discuss its generalization to the case of mixed states.
Consider a bipartite system \( X = AB \) made up of two subsystems \( A \) and \( B \), described by
the Hilbert space \( \mathcal{H}_X = \mathcal{H}_A \otimes \mathcal{H}_B \), with \( \dim \mathcal{H}_A = N_A \), \( \dim \mathcal{H}_B = N_B \) and \( \dim \mathcal{H}_X = N = N_A N_B \). Without loss of
generality we will assume that \( N_A \leq N_B \). The states of \( X \) are represented by
the set \( \mathfrak{S}(\mathcal{H}_X) \) of non-negative unit-trace operators (density matrices) on the Hilbert space
\( \mathcal{H}_X \). The purity of such states, defined as

\[
\pi_{AB}(\rho) := \text{Tr} \rho^2 \in [1/N, 1],
\]

for each \( \rho \in \mathfrak{S}(\mathcal{H}_X) \), provides a characterization of the global mixing of the system and induces
a partition of \( \mathfrak{S}(\mathcal{H}_X) \) into a collection of distinct subsets \( \mathcal{S}_x(\mathcal{H}_X) := \{ \rho \in \mathfrak{S}(\mathcal{H}_X) : \text{Tr} \rho^2 = x \} \).
The minimum value of \( x = 1/N \) is attained when \( X \) is in the completely mixed state \( 1/N \),
whereas the maximum \( x = 1 \) is attained over the set \( \mathcal{S}_1(\mathcal{H}_X) \) consisting of all pure states
\( |\psi\rangle_X \). For each \( \rho \in \mathfrak{S}(\mathcal{H}_X) \), we can also define its \( A \)- and \( B \)-local purity functions as

\[
\pi_A(\rho) := \text{Tr} \rho_A^2, \quad \pi_B(\rho) := \text{Tr} \rho_B^2,
\]

with \( \rho_A = \text{Tr}_B \rho \) and \( \rho_B = \text{Tr}_A \rho \) being the reduced density matrices of the subsystem \( A \) and
\( B \), respectively.

2.1. Total system in a pure state

On the special set \( \mathcal{S}_1(\mathcal{H}_X) \) of pure states \( \rho = |\psi\rangle_X \langle \psi| \) of \( X \), the \( A \)- and the \( B \)-local purities coincide,

\[
\pi(\psi) := \pi_A(\psi) = \pi_B(\psi),
\]

and provide a measure of the bipartite entanglement between \( A \) and \( B \) : the smaller \( \pi(\psi) \), the
larger the entanglement contained in \( |\psi\rangle_X \langle \psi| \). The statistical distribution of \( \pi(\psi) \) on \( \mathcal{S}_1(\mathcal{H}_X) \)
has been studied in [9, 10]. This was done by introducing the partition function

\[
Z(\beta) = \int d\mu(\psi) \ e^{-\beta \pi(\psi)},
\]

where the local purity \( \pi(\psi) \) of \( |\psi\rangle_X \) plays the role of an effective energy of the system, \( \beta \) is a
Lagrange multiplier that fixes the value of the purity/energy and selects an isopurity manifold
[12] and \( d\mu(\psi) \) is a (normalized) measure on the space of pure states \( \mathcal{S}_1(\mathcal{H}_X) \). The natural
choice for the latter is induced by the Haar (probability) measure \( d\mu_H(U) \) on the unitary group
\( U(\mathcal{H}_X) \simeq U(N) \), through the mapping

\[
|\psi\rangle_X:=U_X|\psi_0\rangle_X,
\]

with \( |\psi_0\rangle_X \) an arbitrary reference unit vector of \( \mathcal{H}_X \). Thus, the partition function becomes

\[
Z(\beta) = \int d\mu_H(U_X) \exp \left(-\beta \text{Tr} \left( U_X |\psi_0\rangle_X \langle \psi_0| U_X^\dagger \right)^2 \right).
\]
Then, by noting that for every $U_{\lambda} \in \mathcal{U}(N)$ the reduced density matrix $\rho_{A} = \text{Tr}_{B}(\hat{\psi}_{\lambda}(\hat{\psi}))$ can be written as $\rho_{A} = U_{\lambda} \Lambda_{A} U_{\lambda}^{\dagger}$, with $U_{\lambda} \in \mathcal{U}(N_{A})$ and $\Lambda_{A} = \text{diag}[\lambda_{A,1}, \lambda_{A,2}, \ldots, \lambda_{A,N_{A}}]$, expression (6) becomes

$$Z(\beta) = \int d\mu_{U}(U_{\lambda}) \int d\sigma(\Lambda_{A}) e^{-\beta \text{Tr} \lambda_{A}^{2}} = \int d\sigma(\Lambda_{A}) e^{-\beta \text{Tr} \lambda_{A}^{2}},$$

(7)

where we exploited the fact that the measure induced over the density matrices $\rho_{A}$ by $d\mu_{U}(U_{\lambda})$ factorizes into the product of a measure over the unitary group $d\mu_{U}(U_{\lambda})$ (related to the eigenvectors of $\rho_{A}$) and a measure $d\sigma(\Lambda_{A})$ over the $(N_{A} - 1)$-dimensional simplex of its eigenvalues $\lambda_{A,j}$ [13, 14]. In particular, it can be shown that $[16–18]$

$$d\sigma(\Lambda_{A}) = C_{N_{A},N_{B}} \left(1 - \sum_{1 \leq i \leq N_{A}} \frac{\lambda_{A,i}^{2}}{\lambda_{A,i}^{2}}\right) \prod_{1 \leq j \leq N_{A}} \theta(\lambda_{A,j}) \lambda_{A,j}^{N_{A,K} - N_{A}} \times \prod_{1 \leq i < m \leq N_{A}} (\lambda_{A,i} - \lambda_{A,m})^{2} d^{N_{A}} \lambda_{A},$$

(8)

with

$$C_{N_{A},N_{B}} = \frac{\Gamma(N_{A}N_{B})}{\prod_{1 \leq j \leq N_{A} - 1} \Gamma(N_{B} - j) \Gamma(N_{A} - j + 1)},$$

(9)

and $\theta(x)$ and $\Gamma$ being the unit step and the Euler gamma function, respectively. The derivatives of $Z(\beta)$, evaluated for $\beta = 0$, yield the moments of $\pi(\psi)$ with respect to the measure $d\mu(\psi)$, i.e.

$$\mathcal{M}_{n} := \left\langle \left(\text{Tr} \rho_{A}^{2}\right)^{n} \right\rangle_{\beta = 0} = \int d\mu(\psi) \pi(\psi)^{n} = (-1)^{n} \left. \frac{\partial^{n} Z(\beta)}{\partial \beta^{n}} \right|_{\beta = 0}.$$

(10)

These functions fully determine the statistical distribution of $\pi(\psi)$ on $\mathcal{S}_{1}(\mathcal{H}_{X})$ and, in the high-temperature regime, provide an expansion of $Z(\beta)$. More generally, in analogy to what is commonly done in statistical physics, one can also define the moments of $\pi(\psi)$ for $\beta \neq 0$ as

$$\mathcal{M}_{n}(\beta) := \left\langle \left(\text{Tr} \rho_{A}^{2}\right)^{n} \right\rangle_{\beta \neq 0} = \int d\mu_{\beta}(\psi) \pi(\psi)^{n} = (-1)^{n} \left. \frac{\partial^{n} Z(\beta)}{\partial \beta^{n}} \right|_{\beta = 0},$$

(11)

with $d\mu_{\beta}(\psi)$ being the canonical measure

$$d\mu_{\beta}(\psi) := d\mu(\psi) e^{-\beta \pi(\psi)} Z(\beta).$$

(12)

The latter is a deformation of the Haar measure $d\mu(\psi)$ obtained by including a non-uniform weight which explicitly depends upon the local purity, through $\beta$. In particular, as $\beta$ increases $d\mu_{\beta}(\psi)$ enhances the role of the states with lower values of $\pi(\psi)$ (i.e. larger values of bipartite entanglement) to the extent that for $\beta \to +\infty$ only the maximally entangled elements of $\mathcal{S}_{1}(\mathcal{H}_{X})$ contribute to the values (11). Since $\pi(\psi)$ is bounded above, one can also consider negative temperatures, where the role of less entangled states is enhanced, and when $\beta \to -\infty$ only the separable elements of $\mathcal{S}_{1}(\mathcal{H}_{X})$ contributes to the values (11). Consequently, across different ranges of temperatures, the moments in equation (11) characterize the statistical distribution of the local purity of $X$ computed with respect to a canonical ensemble whose constituents are selected according to an effective thermal distribution characterized by the parameter $\beta$.

In the limit of large $N$, the $\beta$-dependence of the statistics of the local purity $\pi(\psi)$ (and hence of the bipartite entanglement of the system) was characterized in [9, 10] by identifying the class of states which maximize the distributions (12), i.e. typical states with respect to the canonical measure (12). In this context, it was shown that the system undergoes two main phase transitions related to different distributions of the eigenvalues $\lambda_{A}$ of the typical states: a
second-order phase transition, mentioned above, associated with a $\mathbb{Z}_2$ symmetry breaking, and related to the vanishing of some eigenvalues of $\rho_A$, followed by a first-order phase transition, associated with the evaporation of the largest eigenvalue from the sea of the others.

2.2. Total system in a mixed state

A natural question is what happens when the global system $X$ is in a mixed state $\rho$ of purity $x < 1$, rather than in a pure state. A generalization of equation (4) is obtained by replacing $\pi(\psi)$ with (say) the $A$-local purity $\pi_A(\rho)$ of equation (2) and the measure $d\mu(\psi)$ with a proper measure $d\mu_A(\rho)$ on the set $\mathcal{S}_A(\mathcal{H}_X)$. This yields the following definition of the partition function of the $A$-local purity,

$$Z_A(x, \beta) = \int d\mu_A(\rho) \ e^{-\beta \pi_A(\rho)} = C_x \int d\mu(\rho) \ \delta(\text{Tr} \rho^2 - x) \ e^{-\beta \pi_A(\rho)}, \quad (13)$$

where $d\mu_A(\rho)$ is a probability measure on the set of mixed states (see below), and $C_x := \int \int \delta(\text{Tr} \rho^2 - x)^{-1}$ a normalization factor. An analogous expression for the $B$-local purity partition function $Z_B(x, \beta)$ is obtained by replacing $\pi_A(\rho)$ with $\pi_B(\rho)$ in equation (13): note, however, that, at variance with the case analyzed in [9, 10], for $x < 1$ the partition function $Z_B(x, \beta)$ will in general differ from $Z_A(x, \beta)$.

It is worth stressing that the function $Z_A(x, \beta)$ provides only statistical information on the local mixedness of $X$, but not directly on its bipartite entanglement properties: this is due to the fact that for generic mixed states $\rho$ of $X$ the local purities $\pi_A(\rho)$ and $\pi_B(\rho)$ are not entanglement measures. A generalization of equation (4) that retains the ability of characterizing the statistical properties of the bipartite entanglement of $X$ for $x < 1$ could in principle be constructed by replacing $\pi(\psi)$ with the convex-roof counterpart of $\pi_A(\rho)$, namely $\pi_A(\rho) = \max_{\mathcal{E} : \{p_j, |\psi_j\rangle_{XX}\}} \sum_j p_j \ \pi_A(\psi_j)$, where the maximum is taken over all ensembles $\mathcal{E} := \{p_j, |\psi_j\rangle_{XX}\}$ which yield a convex decomposition of the mixed state $\rho$ (see e.g. [20, 22]). The quantity $\pi_A(\rho)$ is a proper measure of the bipartite entanglement, but the resulting partition function does not allow for a simple analytic treatment and will not be discussed in this paper.

Finally, since there is no unique measure on mixed states [18], we need to properly specify the choice of $d\mu_A(\rho)$ which enters in equation (13)—the consistency requirement that for pure states equation (13) should reduce back to equation (4) (i.e. $Z_A(1, \beta) = Z(\beta)$) does not eliminate such ambiguity. Indeed, as previously discussed for $\rho_A$, the Hermitian matrix $\rho$ can always be diagonalized by a unitary operation, and as a consequence we can write the measure $d\mu_A(\rho)$ as the product of a measure on the $(N - 1)$-dimensional simplex of the eigenvalues and a measure on the unitary group $\mathcal{U}(N)$ related to the eigenvectors. However, if on the one hand it would be natural to take the Haar measure on $\mathcal{U}(N)$ so that $d\mu_A(\rho) = d\mu(U_N \rho U_N^\dagger)$, on the other hand the measure on the eigenvalues can be chosen in different possible ways [23]. In order to overcome this ambiguity, we will use a balanced purification strategy. Let us introduce hence the composite Hilbert space $\mathcal{H}_{XX'} = \mathcal{H}_X \otimes \mathcal{H}_X'$, where $\mathcal{H}_X \simeq \mathcal{H}_X'$ are isomorphic. In this $N^2$-dimensional Hilbert space, each $\rho$ of $X$ can be represented by those pure states $|\Psi\rangle_{XX'}$ which provide a purification for such density matrix, i.e. which satisfy the identity

$$\rho = \text{Tr}_X(|\Psi\rangle_{XX'}\langle\Psi|). \quad (14)$$

Thanks to this identification, we can now induce a measure on $\mathcal{S}(\mathcal{H}_X)$ by sampling the pure states on $\mathcal{H}_{XX'}$ according to the unique, unitarily invariant Haar measure which, as usual, is induced by the Haar measure on the unitary group $\mathcal{U}(N^2)$ through the mapping $|\Psi\rangle_{XX'} := U_{XX'}|\Psi_0\rangle_{XX'}$, where $|\Psi_0\rangle_{XX'}$ is an arbitrary reference vector and $U_{XX'} \in \mathcal{U}(N^2)$. 

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With this choice the partition function becomes

\[ Z_A(x, \beta) = C_i \int d\mu_H(U_{XX}) \delta(x - \text{Tr}(\text{Tr}_X(|\Psi\rangle_{XX}\langle\Psi|)^2)) e^{-\beta \text{Tr}(\text{Tr}_X(|\Psi\rangle_{XX}\langle\Psi|)^2)} , \]  

(15)

where we used the fact that \( \rho_A = \text{Tr}_B \rho = \text{Tr}_B (|\Psi\rangle_{XX}\langle\Psi|) \). Analogously to what we have seen for the pure case, \( x = 1 \), by writing \( \rho = U_X \Lambda_X U_X^\dagger \) with \( \Lambda_X = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N) \), we obtain

\[ Z_A(x, \beta) = C_i \int d\mu_H(U_X) \int d\sigma(\Lambda_X) \delta(x - \text{Tr} \Lambda_X^2) e^{-\beta \text{Tr}(\text{Tr}_X(U_X \Lambda_X U_X^\dagger)^2)} , \]

(16)

where \( d\mu_H(U_X) \) is the Haar measure on \( U(N) \) and

\[ d\sigma(\Lambda_X) = C_N \delta \left( 1 - \sum_{1 \leq i \leq N} \lambda_i \right) \prod_{1 \leq i \leq N} \theta(\lambda_i) \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 d^N \lambda , \]

(17)

with

\[ C_N = \frac{\Gamma(N^2)}{\Gamma(N + 1) \prod_{1 \leq i < j \leq N} \Gamma(k)^2} . \]

(18)

Therefore, we have identified the measure \( d\mu_x(\rho) \) of equation (13) with

\[ d\mu_x(\rho) = C_i d\mu_H(U_X) d\sigma(\Lambda_X) \delta(x - \text{Tr} \Lambda_X^2) . \]

(19)

Note that in the case of pure states, i.e. \( x = 1 \), the density operator of the system reduces to \( \rho = |\Psi\rangle_X \langle\Psi| \), where \( |\Psi\rangle_X = U_X |\psi_0\rangle_X \), \( |\psi_0\rangle_X \) being an arbitrary reference state (see equation (5)), and the matrix \( \Lambda_X \) becomes a rank 1 projection. Thus, expression (16) reduces to (6), namely

\[ Z_A(1, \beta) = Z(\beta) . \]

(20)

2.3. Asymptotic behavior and analysis of moments

For \( x < 1 \), the integration over the unitary group \( U(N) \) in equation (16) does not factorize, making the computation of the partition function far more complicated than for the case of a pure state (7). The only notable exception is the case of maximally mixed states (i.e. \( x = 1/N \)), when the Dirac delta in equation (16) selects a unique diagonal matrix \( \Lambda_X \) (the totally mixed state of \( X \)). This makes the exponent equal to \( e^{-\beta/N} \) for all \( U_X \) and yields the following exact expression:

\[ Z_A(1/N, \beta) = e^{-\beta/N} . \]

(21)

Otherwise, for intermediate values of the purity, \( 1/N < x < 1 \), the situation is much more complicated. Still, as we will show in the following, at small \( \beta \) the evaluation of the moments \( M_n^A(x, \beta) \) associated with \( Z_A(x, \beta) \) admits an exact analytical treatment. The latter are formally defined as

\[ M_n^A(x, \beta) := \int d\mu_{x,\beta}(\rho) \pi_n^A(\rho) = \frac{(-1)^n}{Z_A(x, \beta)} \frac{\partial^n Z_A(x, \beta)}{\partial \beta^n} \]

(22)

and represent the average value of \( \pi_n^A(\rho) \) with the canonical measure

\[ d\mu_{x,\beta}(\rho) := d\mu_x(\rho) e^{-\beta \pi_A(\rho)} Z_A(x, \beta) , \]

(23)

with \( d\mu_x(\rho) \) given by equation (19). For pure states (\( x = 1 \)), the \( M_n^A(x, \beta) \) coincide with the moments \( M_n(\beta) \) defined in equation (11): at \( \beta = 0 \), in the large \( N \) limit the expression for
such quantities has been computed in [9], while the exact expressions for first five of them can be found in [24]. In the case of a totally mixed state \((x = 1/N)\), equation (21) yields instead values which are independent of the temperature \(\beta\), namely

\[
\mathcal{M}_n^A(1/N, \beta) = \mathcal{M}_n^A(1/N, 0) = N_A^{-n}. \tag{24}
\]

For intermediate values of \(x\), by expanding equation (22) up to the first order in \(\beta\), we obtain

\[
\mathcal{M}_n^A(x, \beta) \sim \mathcal{M}_n^A(x, 0) - \beta \left[ \mathcal{M}_n^A(x, 0) - \mathcal{M}_n^A(x, 0) \right], \quad \beta \to 0. \tag{25}
\]

Incidentally, note that in agreement with equation (24), the \(\beta\)-corrections of equation (25) vanish when \(x = 1/N\). The above expression shows that, at least in the high-temperature regime, we can focus on the unbiased moments \(\mathcal{M}_n^A(x, 0)\).

3. Moments of the purity at \(\beta = 0\)

3.1. First moment

In this section, we compute the exact first moment of the purity \(\mathcal{M}_1^A(x, 0)\) by making use of Zuber’s solution of some basic integrals over the unitary group [11]. In particular, we will show that the only dependence on the spectrum of the density matrix of the global system is in terms of its purity \(x\), whose value is fixed in the partition function (13).

Let us fix the spectrum of the global density matrix \(\rho\) of the system:

\[
\Lambda_X = \text{diag}(\lambda_{N_a(a-1)+\beta}), \tag{26}
\]

with \(a = 1, \ldots, N_A\) and \(\beta = 1, \ldots, N_B\). A purification of \(\Lambda_X\) in the space \(\mathcal{H}_{XX'}\), with \(X = AB\) and \(X' = A'B'\), is

\[
|\Psi\rangle_{XX'} = \sum_{1 \leq a \leq N_A} \sum_{1 \leq \beta \leq N_B} \sqrt{\lambda_{a\beta}} \left| \alpha \beta \right\rangle_{AB} \otimes \left| \alpha \beta \right\rangle_{A'B'}, \tag{27}
\]

where we have set, for simplicity, \(\lambda_{a\beta} = \lambda_{N_a(a-1)+\beta}\) and \(|\alpha \beta\rangle_{AB} = |\alpha\rangle_A \otimes |\beta\rangle_B, \{ |\alpha\rangle_A \} \) and \(\{|\beta\rangle_B\} \) (|\alpha\rangle_A \}) and \(|\beta\rangle_B\) being the reference basis in \(\mathcal{H}_A\) and \(\mathcal{H}_B\) (\(\mathcal{H}_A\) and \(\mathcal{H}_B\)), respectively.

The set of vectors in \(\mathcal{H}_{XX'}\) with the same Schmidt coefficients is given by \(U_{XX} |\Psi\rangle_{XX'}\), where \(U_{XX} = U_X \otimes U_{X'}\), with \(U_X, U_{X'} \in \mathcal{U}(N)\), and yields the set of density matrices with the same spectrum \(\Lambda_X\), namely \(\rho = U_X \Lambda_X U_X^\dagger\). By partial tracing over subsystem \(B\) one obtains the set of reduced density matrices \(\rho_A(U) = Tr_B (Tr_X (U_{XX} |\Psi\rangle_{XX'} \langle \Psi | U_{XX}^\dagger))\). Note that this expression does not depend on \(U_{X'} \in \mathcal{U}(N)\):

\[
\rho_A = \sum_{1 \leq a \leq N_A} \sum_{1 \leq \beta \leq N_B} \lambda_{a\beta} \text{Tr}_B \left(U_{AB} |\alpha \beta\rangle_{AB} \langle \alpha \beta| U_{AB}^\dagger \right) = \sum_{1 \leq a \leq N_A} \sum_{1 \leq \beta \leq N_B} \lambda_{a\beta} \text{Tr}_B \left(U_{AB} |\alpha \beta\rangle_{AB} \langle \alpha \beta| U_{AB}^\dagger \right). \tag{28}
\]

The purity is given by

\[
\pi_A(U_X \Lambda_X U_X^\dagger) = \text{Tr} \rho_A^2 = \sum_{1 \leq a_1, a_2 \leq N_A} \sum_{1 \leq \beta_1, \beta_2 \leq N_B} \sum_{1 \leq j_1, j_2 \leq N_B} \lambda_{a_1\beta_1} \lambda_{a_2\beta_2} \times_{AB} \langle \alpha_2 \beta_2 | U_{AB}^\dagger | j_2 \rangle \langle j_1 | U_{AB} | \alpha_1 \beta_1 \rangle_{AB} \\
\times_{AB} \langle \alpha_1 \beta_1 | U_{AB}^\dagger | j_1 \rangle \langle j_2 | U_{AB} | \alpha_2 \beta_2 \rangle_{AB}, \tag{29}
\]

which, by the completeness relation for subsystem \(A\), becomes

\[
\pi_A(U_X \Lambda_X U_X^\dagger) = \sum_{1 \leq a_1, a_2 \leq N_A} \sum_{1 \leq \beta_1, \beta_2 \leq N_B} \sum_{1 \leq j_1, j_2 \leq N_B} \lambda_{a_1\beta_1} \lambda_{a_2\beta_2} \times_{AB} \langle \alpha_2 \beta_2 | U_{AB}^\dagger | j_2 \rangle \langle j_1 | U_{AB} | \alpha_1 \beta_1 \rangle_{AB} \\
\times_{AB} \langle \alpha_1 \beta_1 | U_{AB}^\dagger | j_1 \rangle \langle j_2 | U_{AB} | \alpha_2 \beta_2 \rangle_{AB}. \tag{30}
\]
Let us now compute the first moment of the purity (22) at $\beta = 0$. By recalling that $Z_A(x, 0) = 1$, $d\mu_{x,0}(\rho) = d\mu_x(\rho)$ and $d\mu_x(\rho) = C_x d\mu_H(U_X) d\sigma(\Lambda_X) \delta(x - \text{Tr} \Lambda_X^2)$, we obtain

$$\mathcal{M}_n^4(x, 0) = \int d\mu_x(\rho) \pi_n^4(\rho)$$

$$= C_x \int d\sigma(\Lambda_X) \delta(x - \text{Tr} \Lambda_X^2) \mathcal{M}_n^4(\Lambda_X) =: \langle \mathcal{M}_n^4(\Lambda_X) \rangle_x,$$

where

$$\mathcal{M}_n^4(\Lambda_X) := \int d\mu_H(U_X) \pi_n^4(U_X \Lambda_X U_X^\dagger).$$

From (30) the average over the unitary group of the first moment particularizes to

$$\mathcal{M}_1^4(\Lambda_X) = \sum_{1 \leq a_1, a_2 \leq N_A} \sum_{1 \leq b_1, b_2 \leq N_A} \lambda_{a_1 b_1} \lambda_{a_2 b_2}$$

$$\times \sum_{1 \leq i_1, i_2 \leq N_A} \sum_{1 \leq j_1, j_2 \leq N_A} \int d\mu_H(U) U_{i_1 j_1} U_{i_2 j_1} U_{i_1 j_2} U_{i_2 j_2} \delta(\pi_{(1)}),$$

where $U_{ij,\alpha\beta} = AB(i j|U|\alpha\beta)_{AB}$. This integral can be explicitly computed by using Zuber’s solution [11]:

$$\int d\mu_H(U) U_{i_1 j_1} \ldots U_{i_n j_n} U_{i_1 j_1}^\dagger \ldots U_{i_n j_n}^\dagger = \sum_{\tau, \sigma \in S_n} C[\sigma] \prod_{1 \leq a \leq n} \delta(i_a, \tau(\sigma) i_a),$$

with

$$C[\sigma] = \sum_{|Y| = 0} \frac{(\chi^k(1))^2 \chi^k(|\sigma|)}{n!^2 s_k(I)},$$

where $C[\sigma]$ is the sum over the Young diagrams $Y$ of the character $\chi^k(|\sigma|)$ of the symmetric group $S_n$ associated with $Y$, depending on the conjugacy class $[\sigma]$ of the permutation $\sigma$, $s_k(I)$ is the dimension of the representation and $\delta(a, b)$ is the Kronecker delta. Applying this solution to (33) we obtain

$$\mathcal{M}_1^4(\Lambda_X) = \sum_{1 \leq a_1, a_2 \leq N_A} \sum_{1 \leq b_1, b_2 \leq N_A} \lambda_{a_1 b_1} \lambda_{a_2 b_2}$$

$$\times \sum_{\tau, \sigma \in S_2} \sum_{\tau, \sigma \in S_2} \sum_{c \in C(S_2)} C[\sigma] f_1(\pi) \delta([\tau \sigma s], c) \lambda_{a_1(1) b_1(1)} \lambda_{a_2(2) b_2(2)},$$

where $f_1(\pi)$ depends on the permutation $\pi \in S_2$:

$$f_1(\pi) := \sum_{1 \leq i_1, i_2 \leq N_A} \delta(i_1, i_{\pi(1)}) \delta(i_2, i_{\pi(2)}) \sum_{1 \leq j_1, j_2 \leq N_A} \delta(j_1, j_{\pi(2)}) \delta(j_2, j_{\pi(1)}),$$

$s \in S_2$ is the transposition (swapping) of pairs of nearby indices ($[s] = [2]$)

$$i_{\pi(1)} = i_2 \quad \text{and} \quad i_{\pi(2)} = i_1,$$

and $C(S_2) = \{|1^2\}, [2]\}$ is the set of the conjugacy classes of the symmetric group $S_2$. From (36) it can be easily inferred that the only possible contributions of the spectrum are related to
the conjugacy classes of the symmetric group $S_2$:

$$[\tau \sigma s] = [1^2] \Rightarrow \left( \sum_{1 \leq \alpha \leq N_A} \sum_{1 \leq \beta \leq N_B} \lambda_{\alpha \beta} \right)^2 = 1.$$  

$$[\tau \sigma s] = [2] \Rightarrow \left( \sum_{1 \leq \alpha \leq N_A} \sum_{1 \leq \beta \leq N_B} \lambda_{\alpha \beta}^2 \right) = \text{Tr} \, \Lambda_X^2.$$  

By summing and by using the explicit expressions of the coefficients (35) [11]

$$C[1^2] = \frac{1}{(N - 1)(N + 1)}, \quad C[2] = -\frac{1}{(N - 1)N(N + 1)},$$

we obtain

$$\mathcal{M}_k^X(\Lambda_X) = \frac{N_A(N_B^2 - 1)}{N_A^2N_B^2 - 1} + \frac{N_B(N_A^2 - 1)}{N_A^2N_B^2 - 1} \text{Tr} \, \Lambda_X^2.$$  

The first moment of the purity of subsystem $A$ is the average of (41) over the spectrum of the system. By plugging (41) into (31), we finally obtain

$$\mathcal{M}_k^X(x, 0) = \frac{N_A(N_B^2 - 1)}{N_A^2N_B^2 - 1} + \frac{N_B(N_A^2 - 1)}{N_A^2N_B^2 - 1} x.$$  

Note that for $x = 1$, this expression reduces to the one given in [15–17, 19, 24, 25].

**Some special cases.** It is worth noting that for a balanced bipartition $N_A = N_B = \sqrt{N} \gg 1$ equation (42) yields

$$\mathcal{M}_k^X(x, 0) = \frac{\sqrt{N}(1 + x)}{N + 1} \sim \frac{1 + x}{\sqrt{N}}.$$  

At $x = 1$ (i.e. pure global states), equation (43) coincides with that obtained in [9, 15, 24].

Finally, consider the case in which $\rho$ is maximally mixed, i.e. is the density matrix $I/N$. In this case $x = 1/N$ and equation (42) gives

$$\mathcal{M}_k^X(1/N, 0) = \frac{1}{N_A}$$

in agreement with the general result (24).

### 3.2. $k$th moment

The technique shown in the previous section can be easily generalized in order to compute from (32) higher moments at $\beta = 0$. We obtain

$$\mathcal{M}_k^X(\Lambda_X) = \int \text{d}\mu_H(U_X) \, \pi_k^X(U_X \Lambda_X U_X^\dagger)$$

$$= \sum_{1 \leq a_1, \ldots, a_{2k} \leq N_A} \sum_{1 \leq \beta_1, \ldots, \beta_{2k} \leq N_B} \prod_{i \leq 2k} \lambda_{a_i \beta_i}$$

$$\times \sum_{1 \leq f_1, \ldots, f_{2k} \leq N_A} \sum_{1 \leq j_1, \ldots, j_{2k} \leq N_B} \int \text{d}\mu_H(U_X) \prod_{i \leq 2k} U_{f_i j_i a_i \beta_i}$$

$$\times \prod_{1 \leq m \leq k} U_{a_{2m-1}a_{2m-2} \ldots a_1} U_{a_{2m-1}a_{2m-2} \ldots a_1}^\dagger$$  

Equation (34) for $n = 2k$ gives

$$\mathcal{M}_k^X(\Lambda_X) = \sum_{1 \leq a_1, \ldots, a_{2k} \leq N_A} \sum_{1 \leq \beta_1, \ldots, \beta_{2k} \leq N_B} \sum_{\tau, \sigma \in S_A} \sum_{c \in C(S_A)} C[\tau \sigma s] \delta([\tau \sigma s], c) \prod_{i \leq 2k} \lambda_{a_i(\beta_i)c(i)},$$  

(46)
where \( f_k(\pi) \) depends on the permutation \( \pi \in S_{2k} 
\)
\[
f_k(\pi) := \sum_{1 \leq i_1, \ldots, i_{2k} \leq N_e} \sum_{1 \leq j_1, \ldots, j_{2k} \leq N_e} \prod_{1 \leq m \leq k} \delta(i_m, i_{\pi(m)}) \prod_{1 \leq m \leq k} \delta(j_{2m-1}, j_{\pi(2m-1)}) \quad \text{(47)}
\]
and, analogously to equation (38), \( s \) is the swapping of pairs of nearby indices
\[
i_{\ell(2\ell-1)} = i_{2\ell} \quad \text{and} \quad i_{\ell(2\ell)} = i_{2\ell-1} \quad \forall \ell = 1, \ldots, k.
\]
Observe that when \( k = 1 \) we retrieve \( M_1^X(\Lambda_X) \) (see equation (36)). The different contributions of the spectrum can be classified in terms of the conjugacy classes of the symmetric group, as shown in equation (39). However, for \( k > 1 \), they do not depend only upon the purity \( x = \text{Tr} \Lambda_X^2 \), but exhibit a more complex dependence on the spectrum, through its higher order invariants \( \text{Tr} \Lambda_X^k \), with \( k > 2 \). Thus, the integral on the spectrum (31) is in general non-trivial.

### 3.3. Second moment

Now let us fully compute the second moment of the purity for arbitrary bipartite states, with purity \( x \in [1/N, 1] \), generalizing some results found for pure states, \( x = 1 \), [9, 15, 24]. The second moment can be directly computed by setting \( k = 2 \) in equation (45). The expression for the coefficients \( C[\pi] \) in (34) when \( \pi \in S_2 \) is [11]
\[
C[1^4] = \frac{N^4 - 8N^2 + 6}{(N - 3)(N - 2)(N - 1)N^2(N + 1)(N + 2)(N + 3)}
\]
\[
C[2, 1^2] = -\frac{1}{(N - 3)(N - 1)N(N + 1)(N + 3)}
\]
\[
C[2^2] = \frac{N^2 + 6}{(N - 3)(N - 2)(N - 1)N^2(N + 1)(N + 2)(N + 3)}
\]
\[
C[3, 1] = -\frac{2N^2 - 3}{(N - 3)(N - 2)(N - 1)N^2(N + 1)(N + 2)(N + 3)}
\]
\[
C[4] = \frac{5}{(N - 3)(N - 2)(N - 1)N^2(N + 1)(N + 2)(N + 3)}.
\]

The symmetric group \( S_2 \) consists of five conjugacy classes that yield the following contributions to the integral (46) in terms of the spectrum of \( \rho \):

\[
[\tau \sigma s] = [1^4] \Rightarrow \left( \sum_{1 \leq a \leq N_e} \sum_{1 \leq \beta \leq N_e} \lambda_{a, \beta} \right)^4 = 1
\]
\[
[\tau \sigma s] = [2, 1^2] \Rightarrow \left( \sum_{1 \leq a_1 \leq N_e} \sum_{1 \leq \beta_1 \leq N_e} \lambda_{a_1, \beta_1}^2 \right) \left( \sum_{1 \leq a_2 \leq N_e} \sum_{1 \leq \beta_2 \leq N_e} \lambda_{a_2, \beta_2} \right)^2 = \text{Tr} \Lambda_X^2
\]
\[
[\tau \sigma s] = [2^2] \Rightarrow \left( \sum_{1 \leq a \leq N_e} \sum_{1 \leq \beta \leq N_e} \lambda_{a, \beta}^2 \right)^2 = (\text{Tr} \Lambda_X^2)^2
\]
\[
[\tau \sigma s] = [3, 1] \Rightarrow \left( \sum_{1 \leq a_1 \leq N_e} \sum_{1 \leq \beta_1 \leq N_e} \lambda_{a_1, \beta_1}^3 \right) \left( \sum_{1 \leq a_2 \leq N_e} \sum_{1 \leq \beta_2 \leq N_e} \lambda_{a_2, \beta_2} \right) = \text{Tr} \Lambda_X^3
\]
\[
[\tau \sigma s] = [4] \Rightarrow \sum_{1 \leq a \leq N_e} \sum_{1 \leq \beta \leq N_e} \lambda_{a, \beta}^4 = \text{Tr} \Lambda_X^4.
\]

(50)
with $\tau, \sigma \in S_4$ and $s \in S_2$ defined in (48) being $k = 2$. By gathering all we obtain
\[
\mathcal{M}_2^4(\Lambda_X) = \left[ C[1^4]N_1N_2^2N_3N_4^2 + C[2, 1^2]2N_1(N_2^2 + 2)N_2^2 + C[3, 1]8N_1N_2N_2^2
\right.
\quad + C[4]2N_1(2N_1^2 + 1)N_2^2
\quad + \text{Tr} \Lambda_X^3 \left[ C[1^4]2N_1(N_2^2 + 2)N_2^2
\right.
\quad + C[2, 1^2]2N_1N_2(N_2^2 + 3N_2^2 + 14)
\quad + C[2^2]2N_1N_2(N_2^2 + 4) + 2(N_2^2 + 1))
\quad + C[3, 1]8N_1N_2(N_2^2(N_2^2 + 2) + 2N_2^2 + 1)
\quad + C[4]4N_1(N_2^2 + 8)N_2^2)
\quad + (\text{Tr} \Lambda_X^3)^2 \left[ C[1^4]N_1(N_2^2 + 2)N_2^2
\right.
\quad + C[2, 1^2]2N_1N_2(N_2^2 - 3N_2^2 + 4)
\quad + C[3, 1]24N_1N_2^2
\quad + C[4]2N_1N_2(N_2^2 + 1) + 4N_2^2 + 1]
\quad + C[2, 1^2]8N_1N_2(N_2^2 + 2) + 2N_2^2 + 1)
\quad + C[2^2]2N_2^2N_2^2
\quad + C[3, 1]8N_1N_2(N_2^2(N_2^2 + 2) + 2N_2^2 + 1)
\quad + C[4]8N_1N_2(N_2^2(N_2^2 + 2) + 2N_2^2 + 1)
\quad + \text{Tr} \Lambda_X^3 \left[ C[1^4]2N_1(N_2^2 + 1)N_2^2 + C[2, 1^2]4N_2^2(N_2^2 + 8)N_2^2
\right.
\quad + C[2^2]2N_2N_2(N_2^2 + 1) + 4N_2^2 + 1)
\quad + C[3, 1]8N_1N_2(N_2^2(N_2^2 + 2) + 2N_2^2 + 1)
\quad + C[4]2N_1N_2(N_2^2 + 3N_2^2 + 14)]},
\]
from which it follows that
\[
\mathcal{M}_2^4(\Lambda_X) = c_{N_1,N_2} \left[ (N_2^2 - 1)(N_1N_2N_3N_4^2(N_2^2 - 1) - 2N_2^2(6N_2^2 - 7) + 22)
\right.
\quad + \text{Tr} \Lambda_X^3 \left( 2N_1N_2(N_2^2 - 1)(N_2^2 - 1)(N_2^2 - 1))
\right.
\quad + (\text{Tr} \Lambda_X^3)^2 (N_2^2 - 1)(N_2^2N_1N_2^2 + 14N_2^2N_2^2 + 6N_2^2 + 30)
\quad + \text{Tr} \Lambda_X^3 (4N_2^2 - 1)(N_2^2)
\quad + \text{Tr} \Lambda_X^3 (10N_2N_2)(N_2^2 - 1)(N_2^2 - 1)
\right.\]
\[
\]
From equations (42), (52) and (53) we can now compute the exact expression for the second cumulant of the purity at \( \beta = 0 \):

\[
\mathcal{K}_2(\Lambda_x) = \mathcal{M}_2(\Lambda_x) - \left( \mathcal{M}_1(\Lambda_x) \right)^2
= + \frac{2(N_x^2 - 1)(N_{\Lambda_1}^2 - 1)(N_\Lambda^2 N_{\Lambda_1}^2 + 11)}{(N_\Lambda N_{\Lambda_1} - 1)^2(N_\Lambda N_{\Lambda_1}^2 - 13N_\Lambda^2 N_{\Lambda_1}^2 + 36)}
+ x \frac{2(N_x^2 - 1)(N_{\Lambda_1}^2 - 1)(-2N\Lambda N_{\Lambda_1})(N_\Lambda N_{\Lambda_1}^2 + 11)}{(N_\Lambda N_{\Lambda_1} - 1)^2(N_\Lambda N_{\Lambda_1}^2 - 13N_\Lambda^2 N_{\Lambda_1}^2 + 36)}
+ x^2 \frac{2(N_x^2 - 1)(N_{\Lambda_1}^2 - 1)(N_\Lambda N_{\Lambda_1}^2 - 4N_\Lambda^2 N_{\Lambda_1}^2 + 15)}{(N_\Lambda N_{\Lambda_1} - 1)^2(N_\Lambda N_{\Lambda_1}^2 - 13N_\Lambda^2 N_{\Lambda_1}^2 + 36)}
+ \langle \text{Tr} \Lambda_x^2 \rangle_x \frac{40(N_\Lambda^2 - 1)(N_{\Lambda_1}^2 - 1)}{N_\Lambda^2 N_{\Lambda_1}^2 (N_\Lambda N_{\Lambda_1} - 7)^2 - 36}
+ \langle \text{Tr} \Lambda_x^4 \rangle_x \frac{(-10N\Lambda N_{\Lambda_1})(N_\Lambda^2 - 1)(N_{\Lambda_1}^2 - 1)}{N_\Lambda^2 N_{\Lambda_1}^2 (N_\Lambda N_{\Lambda_1} - 7)^2 - 36}. \tag{58}
\]

See [15, 24] for the case \( x = 1 \), when all the traces are 1.
3.4. High-temperature expansion of the first moment of the purity

We can now compute the approximate expression for the first moment of the purity for small $\beta$, by plugging equations (41) and (58) in equation (25), with $n = 2$:

$$\mathcal{M}_1^A(x, \beta) \sim \mathcal{M}_1^A(x, 0) + \beta \left[ (\mathcal{M}_1^A(x, 0))^2 - \mathcal{M}_2^A(x, 0) \right]$$

$$= \frac{N_B(N_A^2 - 1)}{N_A^2 N_B - 1} x + \frac{N_A(N_B^2 - 1)}{N_A^2 N_B - 1}$$

$$+ \beta \left[ - \frac{2(N_A^2 - 1)(N_B^2 - 1)(N_A^2 N_B^2 + 11)}{(N_A^2 N_B^2)(N_A^2 N_B^2 - 13N_A^2 N_B + 36)} - x \frac{2(N_A^2 - 1)(N_B^2 - 1)(-2N_A N_B)(N_A^2 N_B^2 + 11)}{(N_A^2 N_B^2 - 1)(N_A^2 N_B^2 - 13N_A^2 N_B + 36)} - x^2 \frac{2(N_A^2 - 1)(N_B^2 - 1)(N_A^2 N_B^2 - 4N_A^2 N_B^2 + 15)}{(N_A^2 N_B^2 - 1)(N_A^2 N_B^2 - 13N_A^2 N_B + 36)} - (\text{Tr} \, \lambda_3^A) \frac{40(N_A^2 - 1)(N_B^2 - 1)}{N_A^2 N_B^2(N_A^2 N_B^2 - 7)^2 - 36} - (\text{Tr} \, \lambda_4^A) \frac{(-10N_A N_B)(N_A^2 - 1)(N_B^2 - 1)}{N_A^2 N_B^2(N_A^2 N_B^2 - 7)^2 - 36} \right].$$

$$= \frac{\sqrt{N} (1 + x)}{1 + N}$$

$$+ \beta \left[ - \frac{2(N^2 + 11)}{(N + 1)^2(N^2 - 13N^2 + 36)} + x \frac{4N(N^2 + 11)}{(N + 1)^2(N^2 - 13N^2 + 36)} - x^2 \frac{2(N^2 - 4N^2 + 15)}{(N + 1)^2(N^2 - 13N^2 + 36)} - (\text{Tr} \, \lambda_3^A) \frac{40(N - 1)^2}{N^2(N^2 - 7)^2 - 36} - (\text{Tr} \, \lambda_4^A) \frac{(-10N)(N - 1)^2}{N^2(N^2 - 7)^2 - 36} \right].$$

$$= \frac{1 + x}{\sqrt{N}} - \frac{2\beta}{N^2} x^2 + \mathcal{O} \left( \frac{1}{N^{3/2}} \right)$$

For a balanced bipartition, $N_B = N_A = \sqrt{N}$, we obtain

$$\mathcal{M}_1^A(x, \beta) \sim \mathcal{M}_1^A(x, 0) + \beta \left[ (\mathcal{M}_1^A(x, 0))^2 - \mathcal{M}_2^A(x, 0) \right]$$

$$= \frac{\sqrt{N} (1 + x)}{1 + N}$$

$$+ \beta \left[ - \frac{2(N^2 + 11)}{(N + 1)^2(N^2 - 13N^2 + 36)} + x \frac{4N(N^2 + 11)}{(N + 1)^2(N^2 - 13N^2 + 36)} - x^2 \frac{2(N^2 - 4N^2 + 15)}{(N + 1)^2(N^2 - 13N^2 + 36)} - (\text{Tr} \, \lambda_3^A) \frac{40(N - 1)^2}{N^2(N^2 - 7)^2 - 36} - (\text{Tr} \, \lambda_4^A) \frac{(-10N)(N - 1)^2}{N^2(N^2 - 7)^2 - 36} \right].$$

$$\text{and in the thermodynamical limit}$$

$$\mathcal{M}_1^A(x, \beta) \sim \frac{1 + x}{\sqrt{N}} - \frac{2\beta}{N^2} x^2 + \mathcal{O} \left( \frac{1}{N^{3/2}} \right).$$

One might wonder whether higher order cumulants follow a pattern similar to (61). Note that (61) suggests a convergence radius for the high-temperature expansion $\beta_c \sim N^{3/2} (1 + x)/2x^2$, which grows indefinitely when $x \to 0$, in accordance with equation (21). See also figure 1.

Equation (61) at $x = 1$ can be compared with the results of [9] where $\beta$ was replaced by the scaled quantity $\beta' = \beta' N^{3/2}$. With this choice our expression yields

$$\mathcal{M}_1^A(1, \beta' N^{3/2}) \sim \mathcal{M}_1^A(1, 0) + \beta' N^{3/2} \left[ (\mathcal{M}_1^A(1, 0))^2 - \mathcal{M}_2^A(1, 0) \right]$$

$$\sim (1 - \beta') \frac{2}{\sqrt{N}}.$$
Figure 1. First moment of the purity as a function of $\beta$. The horizontal (red) line refers to the set of totally mixed states, with $\mathcal{M}_1^{(1/N, \beta)} = 1/N$; the (black) curve refers to pure states for $\beta > 0$; the vertical (blue) line corresponds to the first moment of the local purity at $\beta = 0$, for arbitrary mixed states; finally, the shaded (light-blue) region refers to high temperatures.

in perfect agreement with the behavior reported in figure 2 of [9]. Figure 1 yields an overview and summarizes our results.

4. An alternative approach based on twirling

In this section, we will establish an interesting connection between our problem and the theory of quantum channels. In particular, we present an alternative approach for computing the moments $\mathcal{M}_n^{(x, \beta)}$ of equation (22) which exploits the properties of twirling transformations [26–28, 20, 21].

For explanatory purposes, we start in section 4.1 by deriving a general expressions for the moments $\mathcal{M}_n^{(x = 1, \beta)}$ associated with the case in which $\rho$ is pure (i.e. the quantities $\mathcal{M}_n$ of equation (10)) and verify that it yields the exact value given by Lubkin [15] for $n = 1$. The case of mixed states is then addressed in section 4.2 showing that for $n = 1$ it reproduces the results of section 3.1.

4.1. Pure initial states

Let us consider a fixed (normalized) pure state of the global system $X = AB$, $|\psi_0\rangle_X$, and parametrize the pure states of $\mathcal{H}_X$ as in (5), i.e. $|\psi\rangle_X := U_X |\psi_0\rangle_X$, with $U_X \in \mathcal{U}(\mathcal{H}_X) \simeq \mathcal{U}(N)$ distributed according to the Haar measure $d\mu_H(U)$. Its local purity (3) can be expressed as

$$\pi(\psi) = \sum_{1 \leq \ell, \ell' \leq NB} \text{Tr} \left( |\psi\rangle\langle \psi| (U_{AB}^\dagger |\ell\rangle_B \langle \ell'|_B |\psi\rangle_{AB} (U_{AB}^\dagger |\ell'\rangle_B \langle \ell|_B |\psi\rangle_{AB}) \right).$$

where $|\psi\rangle$ is an orthonormal basis of $\mathcal{H}_B$, and the cyclicity of the trace was used. We can recast this expression into a more compact form by doubling the Hilbert space, i.e. adding two auxiliary copies $A'$ and $B'$ of $A$ and $B$, respectively. We obtain

$$\pi(\psi) = \text{Tr} \left[ (U_{AB} \otimes U_{A'B'}) |\psi\rangle_{AB} \langle \psi| \otimes |\psi_0\rangle_{A'B'} \langle \psi_0| \right] (U_{AB}^\dagger \otimes U_{A'B'}^\dagger) (S_{BB'} \otimes I_{AA'})$$

where the trace is over all degree of freedom (i.e. $AA'B'B'$), $I_{AA'}$ is the identity operator on $AA'$ and

$$S_{BB'} := \sum_{1 \leq \ell, \ell' \leq NB} |\ell\rangle_B \langle \ell'|_B \otimes |\ell'|_B \langle \ell|.$$
is the SWAP operator on $BB'$—this is the unitary, self-adjoint transformation which, for all operators $\Theta_B$ and $\Gamma_B$, gives
\[ S_{BB'} (\Theta_B \otimes \Gamma_B) S_{BB'} = \Theta_B \otimes \Gamma_B. \] (66)

Recalling that first moment $\mathcal{M}_1^x (x = 1,0) = \mathcal{M}_1$ of equation (10) is obtained by averaging over all possible $U_X$, we can then write
\[ \mathcal{M}_1 = \operatorname{Tr}(T^{(2)}(|\psi_0\rangle_X \langle \psi_0| \otimes |\psi_0\rangle_X \langle \psi_0|) (S_{BB'} \otimes I_{AA})), \] (67)
where $X = AB, X' = A'B'$, and where $T^{(2)}$ is the completely positive, trace-preserving twirling channel [26–29] which transforms the operators $\Theta_{XX}$ of $XX'$ into
\[ T^{(2)}(\Theta_{XX}) = \int d\mu_H(U) \ (U_X \otimes U_X) \Theta_{XX} \ (U_X^\dagger \otimes U_X^\dagger). \] (68)

This map plays an important role in quantum information theory where it was first introduced as a tool for characterizing the distillability of bipartite entanglement [21, 20]. It has several properties which allow us to simplify the calculation. For instance, it is known that $T^{(2)}$ maps all the states of the system into (generalized) Werner states [26, 27]. Furthermore, it is self-adjoint—i.e. its description in Heisenberg picture coincides with $T^{(2)}$. In particular, this last property can be used to rewrite (67) as
\[ \mathcal{M}_1 = \left\langle X \langle \psi_0| \otimes |X \langle \psi_0| \right\rangle T^{(2)}(S_{BB'} \otimes I_{AA}) \left( |\psi_0\rangle_X \otimes |\psi_0\rangle_X \right). \] (69)

Explicit expressions for the action of $T^{(2)}$ can be obtained by exploiting the symmetry of $d \mu_H(U)$. In particular, it is possible to show that $T^{(2)}(\Theta_{XX})$ can be decomposed as a linear combination of the projections on the symmetric and anti-symmetric subspaces of $XX' = AB A' B'$ (with respect to the bipartition $AB/A'B'$). Introducing then the SWAP operator which exchanges $X$ with $X'$ this can then be written as
\[ T^{(2)}(\Theta_{XX}) = \frac{N}{N(N^2-1)} \operatorname{Tr} \Theta_{XX} + \frac{NS_{XX'}^2 - N}{N(N^2-1)} \operatorname{Tr} (S_{XX'} \Theta_{XX'}). \] (70)

where
\[ N = N_A N_B \] is the dimension of $\mathcal{H}_{AB}$. (Here $I_{XX'}$ is the identity operator while $S_{XX'} = S_{AB/A'B'} = S_{BB'} \otimes S_{AA'}$ is the SWAP which exchanges $AB$ with $A'B'$.)

Thanks to this expression, we can now easily compute the value of $\mathcal{M}_1$, either using equation (67) or equation (69). Consider for instance the first approach. We have first to compute the quantities $\operatorname{Tr} \Theta_{XX}$ and $\operatorname{Tr} (S_{XX'} \Theta_{XX'})$ with $\Theta_{XX}$ being the operator $|\psi_0\rangle_X \langle \psi_0| \otimes |\psi_0\rangle_X \langle \psi_0|$. This is
\[ \operatorname{Tr}(|\psi_0\rangle_X \langle \psi_0| \otimes |\psi_0\rangle_X \langle \psi_0|) = 1, \]
\[ \operatorname{Tr}(S_{BB'} \otimes S_{AA'}) |\psi_0\rangle_{X} \langle \psi_0| \otimes |\psi_0\rangle_{X'} \langle \psi_0|) = 1, \] (72)
where in the second expression we used the fact that $|\psi\rangle \otimes |\psi\rangle$ is invariant under $S_{XX'}$, i.e. $(S_{BB'} \otimes S_{AA'})(|\psi\rangle \otimes |\psi\rangle) = |\psi\rangle \otimes |\psi\rangle$. Replacing all this in equation (70) we obtain
\[ T^{(2)}(|\psi_0\rangle_X \langle \psi_0| \otimes |\psi_0\rangle_X \langle \psi_0|) = \frac{I_{XX'} + S_{XX'}}{N(N+1)}. \] (73)

and thus
\[ \mathcal{M}_1 = \frac{1}{N(N+1)} \operatorname{Tr}(I_{AB/A'B'} + S_{BB'} \otimes S_{AA'}) (S_{BB'} \otimes I_{AA'})) \]
\[ = \frac{1}{N(N+1)} (\operatorname{Tr}(S_{BB'} \otimes I_{AA'}) + \operatorname{Tr}(I_{BB'} \otimes S_{AA'})) \] (74)
Let us rewrite the purification (27) of the density matrix \( \rho \).

\[
\text{Tr}(S_{BB} \otimes I_{AA}) = N_B N_A^2 \quad , \quad \text{Tr}(I_{BB} \otimes S_{AA}) = N_A N_B^2
\]

(75)

to obtain

\[
\mathcal{M}_1 = \frac{N_A + N_B}{N_A N_B + 1}
\]

(76)

which coincides with the correct value \([15, 24]\).

We mention that the same techniques can also be applied to higher moments \( \mathcal{M}_n \), the extension of equation (67) for \( n \geq 2 \) is obtained by introducing \( 2n \) copies of \( AB \) organized in the \( n \) pairs, i.e. \( A_1B_1A'_1B'_1, A_2B_2A'_2B'_2, \ldots, A_nB_nA'_nB'_n \). We then introduce the following *generalized* twirling transformation acting on \( XX' = A_1B_1A'_1B'_1, A_2B_2A'_2B'_2, \ldots, A_nB_nA'_nB'_n \), i.e.

\[
T^{(2n)}(\Theta_{XX'}) = \int d\mu_U(U) \left( U \otimes U \otimes \cdots \otimes U \right) \Theta_{XX'} \left( U^\dagger \otimes U^\dagger \otimes \cdots \otimes U^\dagger \right)
\]

(77)

with \( \Theta_{XX'} \) being a generic operator on \( \mathcal{H}_{XX'} := \mathcal{H}_{AB}^{2n} \). This channel is a proper generalization of the map \( T^{(2)} \) whose properties can be established along the lines of \([11]\). With this choice equation (10) then can be expressed as

\[
\mathcal{M}_n(x = 1, 0) = \mathcal{M}_n = \text{Tr} \left( T^{(2n)} \left( |\Psi^{(2)}_{\mu} \rangle \langle \Psi^{(2)}_{\mu} | \right) \right)
\]

(78)

where \( |\Psi^{(2)}_{\mu} \rangle \otimes \otimes |\Psi^{(2)}_{\mu} | \rangle \), \( I_A \) being the identity on the \( 2n \) copies of \( A \), \( I_B = A_1A'1 \cdots A_nA'_n \), and with \( S_{AB}^{(2n)} \) being the SWAP operator which exchanges \( B_1B'_1 \cdots B_n \) with \( B'_1B'_2 \cdots B'_n \) pairwise, i.e. \( S_{AB}^{(2n)} = \otimes_{j=1}^{2n} S_{B_jB'_j} \).

### 4.2. Mixed initial states

Consider now the case with \( x < 1 \). Following the parameterization introduced in sections 2 and 3, we split the average over the set \( \mathcal{S}_x(\mathcal{H}_X) \) of the density matrices of global purity \( x \), as an average over the unitary rotations of acting on \( \mathcal{H}_X \) followed by an average over the space of the eigenvalues \( \rho \)—see equation (16). Specifically, this is accomplished by writing \( \rho(U) = U_{AB} \Lambda_{AB} U^\dagger_{AB} \), with \( U_{AB} \) being a generic unitary transformation on \( \mathcal{H}_{AB} \), while \( \Lambda_{AB} \) represents a given arbitrary choice of the system spectrum, see equation (26). For convenience, let us rewrite the purification (27) of the density matrix \( \rho \) as

\[
|\Psi\rangle_{ABab} = \sum_{1 \leq a \leq N_A} \sum_{1 \leq b \leq N_B} \sqrt{\lambda_{ab}} \ |\alpha\rangle_a \otimes |\beta\rangle_b \otimes |\alpha\rangle_a \otimes |\beta\rangle_b
\]

(79)

where now the ancillary systems, isomorphic to \( A \) and \( B \), are labeled by \( a \) and \( b \), respectively.

The reduced density matrix \( \rho_A(U) = \text{Tr}_B \rho(U) \) can thus be written as

\[
\rho_A(U) = \text{Tr}_{Bab} (U_{AB} |\Psi\rangle_{ABab} \langle \Psi| U^\dagger_{AB}) = \sum_{1 \leq q \leq N_A^2} \langle q | U_{AB} |\Psi\rangle_{ABab} \langle \Psi| U^\dagger_{AB} q \rangle_{Bab}
\]

(80)

with \( \{|q\rangle_{Bab}\} \) being an orthonormal basis of \( Bab \). Similarly, the local A-purity of \( \rho_A(U) \) becomes

\[
\gamma_A(\rho, U) = \text{Tr} \rho_A^2(U) = \sum_{1 \leq q, q' \leq N_A^2} \text{Tr} \left( U_{AB} |\Psi\rangle_{ABab} \langle \Psi| U^\dagger_{AB} q \rangle_{Bab} \times U_{AB} |\Psi\rangle_{ABab} \langle \Psi| U^\dagger_{AB} q' \rangle_{Bab} \right)
\]

(81)
which, once more, can be casted as an expectation value on $|\Psi\rangle^\otimes 2$ by doubling the space (see equation (29)). Therefore, by integrating over $U_{AB}$ we obtain

$$
\mathcal{M}_4^A(\Lambda_X) = \text{Tr}(T(2) |\Psi\rangle_{xx} \langle \Psi| X'x' \langle \Psi| : (S_{Bab}({a'|b'}) \otimes I_{AA}) \rangle)
$$

$$
= (x_x \langle \Psi| X'x' \langle \Psi| : T(2) (S_{Bab}({a'|b'}) \otimes I_{AA}) \rangle) |\Psi\rangle_{xx} \langle \Psi| X'x',
$$

(82)

where $T(2)$ being the twirling transformation on $XX'$ of equation (68) with $X = AB, X' = AB'$, $x = ab$ and $x' = a'b'$ (here $A', a', B'$ and $b'$ are the auxiliary copies of $A, a, B$ and $b$, respectively). The above expression is the average purity of the subsystem $A$ computed for states $\rho$ having the same spectra $\Lambda_X$.

To compute the above quantity this time we use the last identity of equation (82). According to equation (71) we have to compute $\text{Tr} \Theta_{xx}$ and $\text{Tr} (S_{XX} \Theta_{XX'})$ with $\Theta_{XX}$ being the operator $S_{Bab}(a'b') \otimes I_{AA} = S_{Bab} \otimes S_{a'b'} \otimes S_{a'b'} \otimes I_{AA}$. That is

$$
\text{Tr}_{ABA'} (S_{Bab}(a'b') \otimes I_{AA}) = \text{Tr}_{ABA'} (S_{Bab} \otimes S_{a'b'} \otimes S_{a'b'} \otimes I_{AA})
$$

$$
= \text{Tr} (S_{BB'}) \text{Tr} (I_{AA}) S_{a'b'} \otimes S_{a'b'} = N_A^2 N_B S_{a'b'} \otimes S_{a'b'},
$$

(83)

$$
\text{Tr}_{ABA'} (S_{Bab}(a'b') \otimes I_{AA}) = \text{Tr}_{ABA'} (I_{BB'} \otimes S_{AA} \otimes S_{b'b'} \otimes S_{a'a'})
$$

$$
= \text{Tr} (I_{BB'}) \text{Tr} (S_{AA}) S_{b'b'} \otimes S_{a'a'} = N_B^2 N_A S_{b'b'} \otimes S_{a'a'}.
$$

(84)

Thus from equation (71) we obtain

$$
T(2) (S_{Bab}(a'b') \otimes I_{AA}) = \frac{N_B (N_A^2 - 1)}{N_A^2 N_B - 1} I_{BB'} \otimes I_{AA} \otimes S_{a'b'} \otimes S_{a'b'}
$$

$$
+ \frac{N_A (N_B^2 - 1)}{N_A^2 N_B - 1} S_{BB'} \otimes S_{AA} \otimes S_{b'b'} \otimes S_{a'a'},
$$

(85)

where we used $N = N_A N_B$. Replace now this into equation (82) and employ the identities

$$
(x_x \langle \Psi| X'x' \langle \Psi| : (I_{XX'} \otimes S_{x'x'})(|\Psi\rangle_{xx} \otimes |\Psi\rangle_{X'x'}) = \text{Tr} \Lambda_X^2,
$$

$$
(x_x \langle \Psi| X'x' \langle \Psi| : (S_{XX} \otimes S_{x'x'})(|\Psi\rangle_{xx} \otimes |\Psi\rangle_{X'x'}) = 1.
$$

(86)

The final result is thus

$$
\mathcal{M}_4^A(\Lambda_X) = \frac{N_B (N_A^2 - 1)}{N_A^2 N_B - 1} \text{Tr} \Lambda_X^2 + \frac{N_A (N_B^2 - 1)}{N_A^2 N_B - 1}
$$

(87)

which is equation (41) and depends upon the spectrum $\Lambda_X$ only through its purity. By averaging upon $\Lambda_X$ while keeping fix $x$ gives us the same result (42).

5. Conclusions

From the results obtained in the previous sections one can infer that the same phenomenon of concentration of measure that occurs for the eigenvalues of the reduced density matrices of pure states [9, 10] occurs in the present case as well. Indeed, we observe that for large $N$ the leading order of all $k$-moments equals the $k$th power of the first moment (43), that, for a balanced bipartition $N_A = N_B = \sqrt{N}$, reads

$$
\mathcal{M}_4^A(x, 0) = \frac{(1 + x)}{\sqrt{N}} + \mathcal{O} \left( \frac{1}{N^{3/2}} \right).
$$

(88)

This observation spurs from the calculation of the second moment (55):

$$
\mathcal{M}_4^A(x, 0) = \frac{(1 + x)^2}{N} + \mathcal{O} \left( \frac{1}{N^2} \right).
$$

(89)
Therefore,

\[ \mathcal{M}_2(x, 0) = \mathcal{M}_2^A(x, 0)^2 + O\left(\frac{1}{N^2}\right). \]  \hspace{0.5cm} (90)

By observing that the contributions of \(O(1/N)\) to the second moment come from the coefficients proportional to \(C[1^4]\) in (46), i.e. the identity permutation \(\sigma = 0\), and conjecturing that the leading contribution for all the \(k\)th moments comes only from \(C[1^k] \sim 1/N^k\) one obtains

\[ \mathcal{M}_n(x, 0) = \left(\frac{(1 + x)}{\sqrt{N}}\right)^k + O\left(\frac{1}{N^{k+2/2}}\right). \]  \hspace{0.5cm} (91)

Another check of the validity of (91) derives by the interpolation between maximally mixed and pure global states. See figure 1. The scaling with \(N\) is preserved, therefore allowing us to interchange the \(x \to 1\) and \(N \to \infty\) limits.

This uncovers the issue of computing the subdominant terms in the \(k\)th moments’ expansion that become instead leading-order terms in the \(k\)th cumulants. This could be possible if we had an appropriate asymptotic expansion of the combinatorics coefficients \(C\), which we do not know. We leave this as a challenge for future work.

References