

# Statistical-mechanical description of quantum entanglement

J. K. Korbicz<sup>1,2,3</sup>, F. Hulpke<sup>1</sup>, A. Osterloh<sup>1</sup>, and M. Lewenstein<sup>1,3,4</sup>

<sup>1</sup> Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

<sup>2</sup> Dept. d'Estructura i Constituents de la Matèria, Universitat de Barcelona, 647 Diagonal, 08028 Barcelona, Spain

<sup>3</sup> ICFO–Institut de Ciències Fotòniques, Mediterranean Technology Park, 08860 Castelldefels (Barcelona), Spain

<sup>4</sup> ICREA-Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain

## Abstract

We present a description of finite dimensional quantum entanglement, based on a study of the space of all convex decompositions of a given density matrix. On this space we construct a system of real polynomial equations describing separable states. We further study this system using methods of statistical mechanics. As an example, we apply finally our techniques to Werner states of two qubits and obtain a sufficient criterion for separability.

## 1 Introduction

Separability is one of the central issues in quantum information theory (see Horodecki *et al.* [1] for a review) in that in a separable density matrix all correlations are of classical origin and no real quantum information processing, as based on the presence of quantum entanglement of some kind, is impossible. The solution to the separability problem has been proved to be NP-hard [8] and hence every partial solution constitutes an important achievement. Seminal corner stones in that direction have been the Peres-Horodecki criterion [2, 7], and entanglement witnessing operators [5, 6]. The first method exploits the fact that positive operators conserve the positivity of all separable density matrices, whereas some entangled density operators are mapped to non-positive operators. The latter approach uses limits for expectation values of suitably chosen witness operators to distinguish between separable and entangled states. A systematic analysis of the so called *bound* entangled states has been initiated by means of unextendible product bases (UPB) [3] which in turn also paved the way towards a formulation of the separability problem in terms of roots of complex polynomial equations [4]. As far as we know, this route has not been pursued any further and in particular no direct test of separability via the convex roof extension of a pure state separability criterion has been probed so far. The main obstacles for such an approach have their origin in the complications involved in the minimization procedure over all decompositions of the density matrix under consideration. A proposal in this direction however has been presented by Osborne [9]. In this work we follow this route proposing a similar approach for studying the bipartite separability problem in finite dimensional Hilbert space  $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \cong \mathbb{C}^m \otimes \mathbb{C}^n$  encoding the convex roof minimization in a way familiar from statistical-mechanics.

The paper is organized as follows. After a formal definition of the separability problem and a short discussion of pure state separability criteria in the next section, we give a geometrical view on the space of  $\rho$ -ensembles and a formulation of the bipartite separability problem in terms of a set of nonlinear equations in section 3. A mechanical analogy of these equations is drawn in section 4 in terms of a Hamiltonian or cost function on a restricted “phase space” and constitutes the basis for the statistical mechanical approach presented in section 5. After

presenting a proof-of-principles calculation for two-qubit Werner states in section 6 we draw our conclusions and give a short outlook of the presented formalism.

## 2 The bipartite separability problem

In order to formulate the problem, let us recall the following Definition:

**Definition 1** *A state  $\rho$  of a bipartite system  $AB$ , described by  $\mathcal{H}_A \otimes \mathcal{H}_B$ , is called separable if there exists a convex decomposition of  $\rho$  composed entirely of product vectors:*

$$\rho = \sum_{i=1}^N p_i |x_i\rangle\langle x_i| \otimes |y_i\rangle\langle y_i|, \quad |x_i\rangle \in \mathcal{H}_A, |y_i\rangle \in \mathcal{H}_B. \quad (1)$$

A natural problem arises, known as the separability problem: *Given a state  $\rho$ , decide if it is separable or not.* This problem has been proven to be NP-hard (Gurvits [8]) and (a part of) its difficulty lies in the fact that a convex decomposition of a given mixed state  $\rho$  into pure states:

$$\rho = \sum_{i=1}^N p_i |\Psi_i\rangle\langle \Psi_i| \quad (2)$$

is highly non-unique (see e.g. Bengtsson and Życzkowski [10]). Thus, the following Definition makes sense:

**Definition 2** *Unordered collection  $\{p_i, |\Psi_i\rangle\}$ ,  $i = 1 \dots N$  of probabilities and vectors satisfying (2) is called a  $\rho$ -ensemble of length  $N$ .*

In this work we develop the following approach to the separability problem: we propose to search the space of all  $\rho$ -ensembles of a given state  $\rho$  for product  $\rho$ -ensembles ( $\rho$ -ensembles containing only product vectors), by applying one of the existing necessary and sufficient entanglement tests to each member of the ensemble. We want the test which has the simplest functional form—a polynomial. Such a test is provided by the square of generalized concurrence (see e.g. Rungta *et al.* [11], Mintert *et al.* [12], Hulpke [13]):

**Proposition 1** *For any vector  $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  one has that:*

$$c^2(\psi) := \|\psi\|^4 - \text{tr}_{\mathcal{H}_A}(\text{tr}_{\mathcal{H}_B}|\psi\rangle\langle\psi|)^2 \geq 0 \quad (3)$$

*and the equality holds if and only if  $|\psi\rangle$  is product.*

This leads to a set of real polynomial equations describing separable states. The resulting system is very complicated due to the fourth order of some equations and a large number of variables. Our idea is to study it using methods of classical statistical mechanics. The motivation is that such methods have proven to be very efficient not only within classical mechanics, but also in many other, distantly related areas (for an application to fundamental combinatorial problems see e.g. Kubasiak *et al.* [14] and references therein). Hence, we first develop a mechanical analogy for our system. Then we define a suitable cost function, or “energy”, introduce a canonical ensemble, and study the resulting partition function.

### 3 The space of $\varrho$ -ensembles and separability

Let us begin with describing the space of all  $\varrho$ -ensembles of a given state  $\varrho$ . For convenience we pass from normalized  $\varrho$ -ensemble vectors  $|\Psi_i\rangle$  to subnormalized ones:  $|\psi_i\rangle := \sqrt{p_i}|\Psi_i\rangle$ , such that  $\varrho = \sum_{i=1}^N |\psi_i\rangle\langle\psi_i|$ . Let us fix an eigenensemble  $\{|e_\alpha\rangle\}$  of  $\varrho$ , where all the vectors  $|e_\alpha\rangle$  correspond to non-zero eigenvalues  $\lambda_\alpha$  of  $\varrho$ ,  $\alpha = 1 \dots r$ , and  $r := \text{rank}(\varrho)$  is the rank of  $\varrho$ . Then, all  $\varrho$ -ensembles are characterized by the well known Theorem by Schrödinger [15] (see also [16, 17])

**Theorem 1** *Any  $\varrho$ -ensemble  $\{|\psi_i\rangle\}$  of length  $N \geq r$  can be obtained from a subnormalized eigenensemble  $\{|e_\alpha\rangle\}$  such that  $\rho = \sum_\alpha |e_\alpha\rangle\langle e_\alpha|$  through the following linear transformation:*

$$|\psi_i\rangle := \sum_{\alpha=1}^r z_{i\alpha} |e_\alpha\rangle, \quad (4)$$

where the matrix  $z_{i\alpha} \in \mathbb{C}$  is an  $N \times r$  block of a unitary  $N \times N$  matrix, and hence satisfies

$$\sum_{i=1}^N \overline{z_{i\alpha}} z_{i\beta} = \delta_{\alpha\beta}. \quad (5)$$

Theorem 1 gives us the characterization of all possible  $\varrho$ -ensembles in terms of  $N \times r$  matrices  $z$ , satisfying the condition (5). Geometrically, this condition defines the so called *Stiefel manifold*

$$V_{N,r} := U(N)/U(N-r). \quad (6)$$

It forms a principal fiber bundle over the Grassmann manifold  $G_{N,r}$  (the set of  $r$ -dimensional subspaces of  $\mathbb{C}^N$ ) with a fiber diffeomorphic to  $U(r)$  (we refer to Kobayashi and Nomizu Vol. 1 [18] for the definition and basic properties of fiber bundles and to Spivak Vol. 5 [19] for more information on the Stiefel and Grassmann manifolds).

However, note that there is some additional symmetry: from Eq. (2) we see that the order of vectors in a  $\varrho$ -ensemble does not matter, and thus two  $N \times r$  matrices  $z, z'$  satisfying Eq. (5) and differing only by a permutation of their rows define the same  $\varrho$ -ensemble. To fix this freedom, observe that a  $z$ -matrix satisfying Eq. (5) has necessarily rank  $r$ , and hence we may consider only those matrices  $z$ , for which the first  $r$  rows are linearly independent. The set of such  $z$ 's constitutes a simply connected open subset of  $V_{N,r}$  (which is nevertheless dense in  $V_{N,r}$ ) and over such a neighborhood the bundle  $V_{N,r} \xrightarrow{U(r)} G_{N,r}$  is trivial by construction. This allows us to formally write down an explicit solution of the constraints (5)

$$z = GS \begin{pmatrix} \mathbf{1}_r \\ \mathbf{v} \end{pmatrix} \cdot U, \quad (7)$$

where  $U \in U(r)$ ,  $\mathbf{1}_r$  is the  $r \times r$  unit matrix,  $\mathbf{v}$  is an arbitrary, complex  $(N-r) \times r$  matrix, and  $GS$  denotes the Gram-Schmidt orthonormalization [20] applied to the columns. There are no more symmetries, since we have defined in Definition 2  $\varrho$ -ensembles using vectors  $|\psi_i\rangle$  rather than more physical projectors  $|\psi_i\rangle\langle\psi_i|$ , as the latter are harder to work with. In case of  $\varrho$ -ensembles defined through projectors, there would be an additional symmetry of multiplying each row of  $z$  by a (different) phase. Comparing Eq. (7) and Eq. (4), one sees that an arbitrary  $\varrho$ -ensemble

of length  $N$  is obtained from the fixed eigenensemble by i) applying a unitary rotation to  $|e_\alpha\rangle$ 's and ii) subsequent increasing of the length of the ensemble along the Grassmannian  $G_{N,r}$ .

So far we have characterized  $\varrho$ -ensembles of a fixed length  $N$ . It seems that in the search for product ensemble we would have to consider all possible lengths  $N \geq r$ . However, from Caratheodory's Theorem (see e.g. Kelly and Weiss [21]) we know that a separable state can be decomposed into at most  $N = m^2 n^2$  linear independent (in  $\mathbb{R}^{m^2 n^2 - 1}$ ) product states. Hence, it is enough to consider only  $\varrho$ -ensembles of the length  $N = m^2 n^2$ . (there is a natural inclusion of space of shorter ensembles in the space of longer ones).

Let us now examine the entanglement test given by Proposition 1. First, we quote some well known facts regarding the geometry of pure product states (see e.g. Bengtsson and Życzkowski [10]). Note that the polynomial  $c^2(\psi)$ , defined in Eq. (3), is in fact a sum of modulus squared of quadratic, complex-analytical polynomials in  $|\psi\rangle$ :

$$c^2(\psi) = \frac{1}{2} \sum_{a,b=1}^{d_1, d_2} |\langle \zeta_a^{AA'} \otimes \tilde{\zeta}_b^{BB'} | \psi^{AB} \otimes \psi^{A'B'} \rangle|^2, \quad (8)$$

where  $\{|\zeta_a^{AA'}\rangle\}_{a=1, \dots, d_1}$ ,  $\{|\tilde{\zeta}_b^{BB'}\rangle\}_{b=1, \dots, d_2}$  are orthonormal bases of the skew-symmetric spaces  $\mathcal{H}_A \wedge \mathcal{H}_{A'} \cong \mathbb{C}^m \wedge \mathbb{C}^m$  and  $\mathcal{H}_B \wedge \mathcal{H}_{B'} \cong \mathbb{C}^n \wedge \mathbb{C}^n$ , respectively. Thus,  $c^2(\psi) = 0$ , and hence  $|\psi\rangle$  is product, if and only if

$$\langle \zeta_a \otimes \tilde{\zeta}_b | \psi \otimes \psi \rangle = 0 \quad \text{for all } a, b. \quad (9)$$

It is worth noticing that this is just the condition for the matrix of components of  $|\psi\rangle$  to have rank one. Geometrically, the system of homogeneous equations (9), or equivalently the single equation  $c^2(\psi) = 0$ , describes the image of the so called *Segre embedding*  $\mathbb{C}P^m \times \mathbb{C}P^n \hookrightarrow \mathbb{C}P^{mn}$  given by  $([x], [y]) \mapsto [x \otimes y]$ . As we can see from Eqs. (9), this image, i.e. the set of product vectors, is a complex-analytical manifold—as an intersection of complex quadrics—in contrast to the Stiefel manifolds  $V_{N,r}$ , which are real.

Since for all  $i = 1, \dots, N$  polynomials  $c^2(\psi_i)$  are non-negative and equal to zero if and only if  $|\psi_i\rangle$  is product, we can sum them up for a given  $\varrho$ -ensemble, and thus obtain a collective separability test for the whole  $\varrho$ -ensemble, given by a single polynomial function. Combining this with the parametrization (4) and the constraint (5), we obtain the following description of separable states:

**Proposition 2** *A states  $\varrho$  of rank  $r$  on  $\mathbb{C}^m \otimes \mathbb{C}^n$  is separable if and only if the following system of equations possesses a solution*

$$E_\varrho(z) := \sum_{i=1}^{m^2 n^2} c^2(\psi_i) = \sum_{i=1}^{m^2 n^2} \sum_{\alpha, \dots, \nu=1}^r \overline{z_{i\alpha}} \overline{z_{i\beta}} E_{\alpha\beta\mu\nu}^\varrho z_{i\mu} z_{i\nu} = 0, \quad (10)$$

$$C_{\alpha\beta}(z) := \sum_{i=1}^{m^2 n^2} \overline{z_{i\alpha}} z_{i\beta} - \delta_{\alpha\beta} = 0, \quad (11)$$

where

$$E_{\alpha\beta\mu\nu}^\varrho := \frac{1}{4} \langle e_\alpha \otimes e_\beta | \Pi_m \otimes \Pi_n e_\mu \otimes e_\nu \rangle \quad (12)$$

and  $\Pi_m, \Pi_n$  are the projectors from  $\mathbb{C}^m \otimes \mathbb{C}^m$ ,  $\mathbb{C}^n \otimes \mathbb{C}^n$  onto the skew-symmetric subspaces  $\mathbb{C}^m \wedge \mathbb{C}^m$ ,  $\mathbb{C}^n \wedge \mathbb{C}^n$  respectively.

We note that the pure state entanglement measure we use is the square of the generalized concurrence  $c(\varrho)$  (cf. Rungta *et al.* [11], Mintert *et al.* [12]), however, instead of the convex roof construction  $c(\varrho) := \inf \sum_i p_i c(\Psi_i) = \inf \sum_i c(\psi_i)$  (where  $|\Psi_i\rangle$  are normalized vectors), we analyze

$$E_\varrho(z) = \sum_i p_i^2 c^2(\Psi_i). \quad (13)$$

as a "quantifier" of entanglement. We remind the reader that no caveats are introduced by this, since we are only interested in the detection of zero entanglement rather than in the full construction of an entanglement monotone.

Note that the Eqs. (10), (11) are invariant with respect to local unitary transformations, since when  $\varrho$  is separable also  $U_A \otimes U_B \varrho U_A^\dagger \otimes U_B^\dagger$  is, for arbitrary  $U_A \in U(m)$ ,  $U_B \in U(n)$ . The latter transformation can be viewed either as a local change of basis (passive view) or as an active rotation (active view). Indeed, from Eq. (3) one immediately sees that  $c^2(U_A \otimes U_B \psi) = c^2(\psi)$ . Thus, the function  $E_\varrho$  and all quantities derived from it are constant on the whole unitary class of  $\varrho$ , i.e. on  $[\varrho] := \{U_A \otimes U_B \varrho U_A^\dagger \otimes U_B^\dagger; U_A \in U(m), U_B \in U(n)\}$ . In what follows, we refer with  $\varrho$  to its local unitary class  $[\varrho]$ .

We give a brief comparison to a previous analysis carried out by Wu *et al.* in Ref. [22], also leading to a different set of polynomial equations. These authors have used a higher order polynomial test for separability: let  $\sigma_A := \text{tr}_{\mathcal{H}_B} |\psi\rangle\langle\psi|$ , then  $|\psi\rangle$  is product if and only if  $\det(\sigma_A - \mathbf{1}) = 0$ . The relation to Eq. (3) is established by observing that  $\det(\sigma_A - \mathbf{1}) = \sum_{k=0}^m (-1)^k c_k(\sigma_A)$ , where  $c_k$ 's form a basis of  $U(m)$ -invariant polynomials (see e.g. Ref. [23]). Particularly,  $2c_2(\sigma_A) = (\text{tr}\sigma_A)^2 - \text{tr}\sigma_A^2$ , which is precisely the generalized concurrence squared (cf. Eq. (3)). For testing separability, it is sufficient to consider only  $c_2$ .

## 4 Mechanical analogy

Equations (10) and (11) form a system of real (after taking real and imaginary parts) polynomial equations. Let us denote by  $\mathcal{V}_\varrho$  the set of its solutions for a given  $\varrho$ . Then the separability problem is equivalent to the question whether  $\mathcal{V}_\varrho$  is empty or not. In principle there is a general solution to such problem, provided by the so called *Real Nullstellensatz* (see e.g. Bochnak *et al.* [24]). It says that  $\mathcal{V}_\varrho = \emptyset$  if and only if the ideal generated by the polynomials  $E_\varrho$ ,  $\{\text{Re}\mathcal{C}_{\alpha\beta}, \text{Im}\mathcal{C}_{\alpha\beta}\}$ , and by all (real) sum-of-squares (SOS) polynomials<sup>1</sup> contains the constant  $-1$ . Equivalently,  $\mathcal{V}_\varrho = \emptyset$  if and only if there exist a SOS polynomial  $s = \sum_n (w_n)^2$ , a real polynomial  $t$ , and (complex) polynomials  $u_{\alpha\beta}$  such that:

$$-1 = s(z) + E_\varrho(z)t(z) + \sum_{\alpha,\beta} \text{Re}[\mathcal{C}_{\alpha\beta}(z) \overline{u_{\alpha\beta}(z)}]. \quad (14)$$

However, finding such a certificate is computationally very difficult and inefficient, due to the fact that the degrees of polynomials  $s$ ,  $t$ , and  $u_{\alpha\beta}$  are a priori unbounded (see also Refs. [9, 25]).

Here we develop a different approach based on a statistical analysis of a classical-mechanical analogy. Namely, we treat  $z_{i\alpha}$  as a collection of complex row vectors  $\mathbf{z}_i \in \mathbb{C}^r \cong \mathbb{R}^{2r}$ ,  $i = 1 \dots N$  and treat each row  $\mathbf{z}_i$  as a complex phase-space coordinate of a fictitious particle moving in

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<sup>1</sup> Interestingly, SOS polynomials also appear in a solution to the classicality problem of states of a single mechanical system—they are enough to detect a very broad family of states through generalized squeezing conditions (Korbicz *et al.* [26]).

$r$ -dimensional space. Then the whole matrix  $z_{i\alpha}$  becomes a phase-space coordinate of a system of  $N$  such particles in their composite phase-space  $\Gamma := \mathbb{R}^{2r} \times \dots \times \mathbb{R}^{2r} \cong \mathbb{C}^{Nr}$ . Now, let  $E_\varrho(\mathbf{z}_1, \dots, \mathbf{z}_N)$  and  $\mathcal{C}_{\alpha\beta}(\mathbf{z}_1, \dots, \mathbf{z}_N)$  be defined by Eqs. (10) and (11). We emphasize that  $E_\varrho$  depends on the separability class of the analyzed state  $\varrho$  through the fixed eigenensemble  $\{|e_\alpha\rangle\}$ . From the property (3) it follows that

$$E_\varrho(\mathbf{z}_1, \dots, \mathbf{z}_N) \geq 0 \quad \text{for any } (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \mathbb{C}^{Nr}. \quad (15)$$

We will think of  $E_\varrho$  as a cost function or Hamiltonian (it is extensive in the number of fictitious particles  $N$ ), of our fictitious mechanical system. Then, we can treat  $\mathcal{C}_{\alpha\beta}$  as at the primary constraints imposed on the a priori independent phase-space coordinates  $(\mathbf{z}_1, \dots, \mathbf{z}_N)$ . We note that even if the mechanical system corresponds to free particles (if  $E_\varrho$  was diagonal) the resulting model is nevertheless interacting due to the forces of inertia induced by the non-linear constraints.

The corner stones of the mechanical interpretation of the separability problem (10), (11) can be summarized as follows: the  $\varrho$ -ensembles of density matrices with a fixed rank  $r$  form the Stiefel manifold  $V_{N,r}$ , which we can be viewed at as a constraint surface in the phase-space  $\Gamma$ . Each state  $\varrho$  defines the non-negative cost operator  $E_{\alpha\beta\mu\nu}^\varrho$  (12) which uniquely defines the cost function  $E_\varrho$  on  $\Gamma$ , which probes the separability of the ensembles. The cost function  $E_\varrho$  assumes the value zero on the constraint surface  $V_{N,r}$  (which is then its global minimum) if and only if  $\varrho$  is separable.

## 5 Statistical-mechanical approach

Although in principle one could tempt to solve the constraints explicitly by Eq. (7), the resulting parametrization of the constrained manifold is rather hard to work with due to the iterative nature of the Gram-Schmidt orthonormalization. We circumvent the complications with an explicit incorporation of the constraints by using a standard method of implicit treatment of constrained systems due to Dirac [27]. It is based on the introduction of Lagrange multipliers. To this end we define the full Hamiltonian of the systems as

$$H_{full}(\mathbf{z}_1 \dots \mathbf{z}_N) := E_\varrho + \sum_{\alpha,\beta} \omega_{\alpha\beta} \mathcal{C}_{\alpha\beta}, \quad (16)$$

where  $\omega_{\alpha\beta}$  are the Lagrange multipliers. Note that the constraints written in the matrix  $\mathcal{C}_{\alpha\beta}$  are not all independent: it is in fact a hermitian matrix and we need to employ one Lagrange multiplier for each independent constraint only. On the other hand we have considerable freedom for choosing the spurious Lagrange multipliers in the Lagrange matrix  $\omega$ . We choose  $\omega$  to be hermitian. Then,  $H_{full}$  is hermitian and has only real eigenvalues. Moreover, in order to take into account all independent constraints, we require that  $\det \omega \neq 0$ . The constraints  $\mathcal{C}_{\alpha\beta} \equiv 0$  are then realized on average by setting to zero the variation of  $H_{full}$  with respect to  $\omega_{\alpha\beta}$ :  $\partial H_{full} / \partial \omega_{\alpha\beta} = 0$ .

The number of fictitious particles  $N$  will in general be notably large—in dimension  $2 \otimes 4$  for example we have  $N \geq 64$ . Thus, the direct analytical study of our fictitious mechanical system seems rather hopeless and we proceed further using methods of statistical mechanics and numerical simulations. The most natural framework would be microcanonical ensemble, however it is also difficult to work with. Hence, we will introduce a canonical ensemble, keeping in mind that this is just a technical tool, so, for example, the inverse temperature  $\beta$  plays only a role of a parameter here, without any physical meaning.

We proceed to define the canonical partition function  $Z$  for our system. The most natural definition is perhaps the following

$$\begin{aligned} Z(\beta; \varrho) &= \int \prod_{i,\mu} d^2 z_{i\mu} \prod_{\alpha \leq \beta} \delta[\mathcal{C}_{\alpha\beta}(\mathbf{z}_1 \dots \mathbf{z}_N)] e^{-\beta E_\varrho} \\ &= \int \prod_{i,\mu} d^2 z_{i\mu} \prod_{\alpha \leq \beta} \delta \left[ \sum_{i=1}^N \overline{z_{i\alpha}} z_{i\beta} - \delta_{\alpha\beta} \right] \exp \left\{ -\beta \sum_{i=1}^N \sum_{\alpha, \dots, \nu=1}^r \overline{z_{i\alpha}} \overline{z_{i\beta}} E_{\alpha\beta\mu\nu}^{\varrho} z_{i\mu} z_{i\nu} \right\}, \end{aligned} \quad (17)$$

where the integration is explicitly restricted to the constraint surface  $V_{N,r}$  (cf. Eq. (6)) given by  $\mathcal{C}_{\alpha\beta} \equiv 0$ . The intuition behind such an approach is the following. We can formally introduce constraint “state density” function

$$\rho(\epsilon) := \int \prod_{i,\mu} d^2 z_{i\mu} \prod_{\alpha \leq \beta} \delta[\mathcal{C}_{\alpha\beta}(\mathbf{z}_1 \dots \mathbf{z}_N)] \delta(\epsilon - E_\varrho(z)). \quad (18)$$

Since  $E_\varrho(z) \geq 0$ ,  $\rho(\epsilon)$  is non-zero only for  $\epsilon \geq 0$ . Then:

$$Z(\beta; \varrho) = \int_0^\infty d\epsilon \rho(\epsilon) e^{-\beta\epsilon}. \quad (19)$$

Let us assume that the state in question is entangled. Then  $E_\varrho(z)$  is strictly positive, so there exists a constant  $a$  such that  $E_\varrho(z) \geq a > 0$ . The average “energy” is then separated from zero:

$$\langle\langle E_\varrho \rangle\rangle := \frac{1}{Z(\beta; \varrho)} \int_0^\infty d\epsilon \rho(\epsilon) \epsilon e^{-\beta\epsilon} \geq \frac{1}{Z(\beta; \varrho)} \int_a^\infty d\epsilon \rho(\epsilon) a e^{-\beta\epsilon} = a. \quad (20)$$

Now let  $\varrho$  be separable. Then, by Proposition 2  $E_\varrho(z)$  has zeros on the constraint surface  $\mathcal{C}_{\alpha\beta} = 0$  with each zero corresponding to a separable  $\varrho$ -ensemble. Since such ensembles are “rare”, we expect that the state density  $\rho(\epsilon) \rightarrow 0$  with  $\epsilon \rightarrow 0$ . Let us assume for a moment that the leading term in the actual dependence of  $\rho(\epsilon)$  was given by a power law

$$\rho(\epsilon) = A\epsilon^\delta, \quad A, \delta > 0. \quad (21)$$

Then we obtain the well established result  $Z(\beta; \varrho) = \frac{A}{\beta^{\delta+1}} \Gamma(\delta + 1)$  and

$$\langle\langle E_\varrho \rangle\rangle = \frac{\Gamma(\delta + 2)}{\Gamma(\delta + 1)} \frac{1}{\beta} = \frac{\delta + 1}{\beta}. \quad (22)$$

Thus, we put forward the following conjecture:

**Conjecture.** For the “state density” function  $\rho(\epsilon)$ , defined in Eq. (18), it holds: *i*) the mean energy (defined in Eq. (20))  $\langle\langle E_\varrho \rangle\rangle = a > 0$  if and only if  $\varrho$  is entangled; *ii*) the mean energy  $\langle\langle E_\varrho \rangle\rangle$  scales as  $1/\beta$  if and only if  $\varrho$  is separable.

We anticipate that indeed we observe such a behavior in a simple case of  $2 \otimes 2$  Werner states [28]. Note that in general the exponent  $\delta$  will depend on the state  $\delta = \delta(\varrho)$ .

The partition function defined in Eq. (17) is difficult to work with analytically (however one can still investigate it numerically, e.g. using Monte Carlo methods), so we use a different object—the partition function for the full Hamiltonian (16). We first rescale the variables:  $z_{i\alpha} \mapsto z_{i\alpha}/\sqrt{N}$  and then define:

$$Z(\beta, \omega; \varrho) := \int \prod_{i,\mu} d^2 z_{i\mu} \exp \left[ -\frac{\beta}{N^2} \left( E_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) + N \sum_i \langle \mathbf{z}_i | \omega \mathbf{z}_i \rangle - N^2 \text{tr} \omega \right) \right], \quad (23)$$

where  $\langle \cdot | \cdot \rangle$  denotes the standard scalar product in  $\mathbb{C}^r$ . Performing further rescaling:

$$\beta = N^2 \tilde{\beta}, \quad \omega = \frac{N}{\beta} \tilde{\omega}, \quad (24)$$

$Z(\beta, \omega; \varrho)$  becomes (after dropping the tildes):

$$\begin{aligned} Z(\beta, \omega; \varrho) &= \int \prod_{i,\mu} d^2 z_{i\mu} \exp \left[ -\beta E_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) - \sum_i \langle \mathbf{z}_i | \omega \mathbf{z}_i \rangle + N \text{tr} \omega \right] \\ &= \int \prod_{i,\mu} d^2 z_{i\mu} \exp \left[ -\beta \sum_i \sum_{\alpha, \dots, \nu} \overline{z_{i\alpha}} \overline{z_{i\beta}} E_{\alpha\beta\mu\nu}^\varrho z_{i\mu} z_{i\nu} - \sum_i \langle \mathbf{z}_i | \omega \mathbf{z}_i \rangle + N \text{tr} \omega \right]. \end{aligned} \quad (25)$$

Now we are able to reproduce the (rescaled) constraints (11) only on average:

$$\frac{\partial}{\partial \omega_{\alpha\beta}} \log Z(\beta, \omega; \varrho) = \langle \langle N \delta_{\alpha\beta} - \sum_i \overline{z_{i\alpha}} z_{i\beta} \rangle \rangle \quad (26)$$

where the average  $\langle \langle \cdot \rangle \rangle$  is taken with respect to the probability density defined through Eq. (25):

$$P_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N; \beta, \omega) := \frac{1}{Z(\beta, \omega; \varrho)} \exp \left[ -\beta E_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) - \sum_i \langle \mathbf{z}_i | \omega \mathbf{z}_i \rangle + N \text{tr} \omega \right]. \quad (27)$$

Thus, requiring that  $\partial / \partial \omega_{\alpha\beta} \log Z(\beta, \omega; \varrho) = 0$  amounts to:

$$N \delta_{\alpha\beta} = \langle \langle \sum_i \overline{z_{i\alpha}} z_{i\beta} \rangle \rangle. \quad (28)$$

Following the standard treatment of constrained systems, the equations (28) are treated as conditions imposed on a priori arbitrary (apart from being hermitian and non-singular) matrix of Lagrange multipliers  $\omega$ . We note that the above approach based on  $H_{full}$  is nothing else but a (formal) evaluation of the integral (17) through the saddle point method with  $N \rightarrow \infty$ .

A significant simplification of the partition function (25) comes from the form of our Hamiltonian  $E_\varrho$ —from Eq. (10) it follows that  $E_\varrho(\mathbf{z}_1 \dots \mathbf{z}_N) = \sum_i E_{1\varrho}(\mathbf{z}_i)$ , where  $E_{1\varrho}$  is just the function  $E_\varrho$  with  $N = 1$ . The situation is more subtle with the constraints (28). For the purpose of this work we will assume that the contribution to the sum from each fictitious particle is equal, i.e.  $\langle \langle \overline{z_{i\alpha}} z_{i\beta} \rangle \rangle = \delta_{\alpha\beta}$  for every  $i$ . In general, such “equipartition” of course does not have to hold and it is an additional restriction on the Lagrange multipliers. By such an assumption we however achieve a factorization of the partition function:

$$Z(\beta, \omega; \varrho) = [Z_1(\beta, \omega; \varrho)]^N, \quad (29)$$

where  $Z_1$  is a one-particle partition function:

$$\begin{aligned} Z_1(\beta, \omega; \varrho) &:= \int \prod_{\mu=1}^r d^2 z_\mu \exp \left[ -\beta E_{1\varrho}(\mathbf{z}) - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \text{tr} \omega \right] \\ &= \int \prod_{\mu=1}^r d^2 z_\mu \exp \left[ -\beta \sum_{\alpha, \dots, \nu} \overline{z_\alpha} \overline{z_\beta} E_{\alpha\beta\mu\nu}^\varrho z_\mu z_\nu - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \text{tr} \omega \right]. \end{aligned} \quad (30)$$



From now on we will consider  $Z_1$  only. The constraint equations (28) are then replaced by a one-particle version:

$$\frac{\partial}{\partial \omega_{\alpha\beta}} \log Z_1(\beta, \omega; \varrho) = \delta_{\alpha\beta} - \langle \langle \bar{z}_\alpha z_\beta \rangle \rangle = 0, \quad (31)$$

in accordance with our extra assumption made above. The average in Eq. (31) is taken with respect to the probability distribution:

$$P_{1\varrho}(\mathbf{z}; \beta, \omega) := \frac{1}{Z_1(\beta, \omega; \varrho)} \exp \left[ -\beta E_{1\varrho}(\mathbf{z}) - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \text{tr} \omega \right]. \quad (32)$$

In particular, Eq. (31) implies that  $\langle \langle |z_\alpha|^2 \rangle \rangle = 1$ .

To understand the meaning of Eq. (31), let us assume that  $\omega = \omega_0(\beta; \varrho)$  is its solution. Then Eq. (31) implies that a family of vectors  $\{ |\psi(\mathbf{z})\rangle := \sum_\alpha z_\alpha |e_\alpha\rangle; \mathbf{z} \in \mathbb{C}^r \}$  forms a continuous  $\varrho$ -ensemble with respect to the probability distribution (32), i.e.:

$$\int d^{2r} \mathbf{z} P_{1\varrho}(\mathbf{z}; \beta, \omega_0) |\psi(\mathbf{z})\rangle \langle \psi(\mathbf{z})| = \varrho \quad (33)$$

irrespectively of  $\beta$ . Since  $E_{1\varrho}(\mathbf{z}) = c^2(\psi(\mathbf{z}))$  (cf. Eqs. (3) and (10)) is the concurrence squared of each  $|\psi(\mathbf{z})\rangle$ , the average ‘‘energy’’ is just the ensemble average of the concurrence squared:

$$\langle \langle E_{1\varrho} \rangle \rangle_0(\beta) := \int d^{2r} \mathbf{z} P_{1\varrho}[\mathbf{z}; \beta, \omega_0(\beta; \varrho)] E_{1\varrho}(\mathbf{z}) = -\frac{\partial}{\partial \beta} \log Z_1 \Big|_{\omega=\omega_0(\beta; \varrho)}. \quad (34)$$

Due to the property (8) one can formally simplify the integral (30) using the Hubbard-Stratonovitch trick. Indeed, Eq. (30) can be rewritten as:

$$Z_1(\beta, \omega; \varrho) = \int \prod_{\mu=1}^r d^2 z_\mu \exp \left\{ -\beta \sum_{a,b=1}^{d_1, d_1} \left| \sum_{\alpha, \beta} h_{\alpha\beta}^{ab}(\varrho) z_\alpha z_\beta \right|^2 - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \text{tr} \omega \right\}, \quad (35)$$

where:

$$h_{\alpha\beta}^{ab}(\varrho) := \langle \zeta_a \otimes \tilde{\zeta}_b | e_\alpha \otimes e_\beta \rangle \quad (36)$$

and we have rescaled  $\beta$  by 1/4. Next, we use the Hubbard-Stratonovitch substitution:

$$\exp(-\beta |y|^2) = \int \frac{d^2 s}{\pi \beta} \exp \left( -\frac{|s|^2}{\beta} + i \bar{s} y + i s \bar{y} \right). \quad (37)$$

to obtain (after a formal interchange of the integrations):

$$\begin{aligned} Z_1(\beta, \omega; \varrho) &= \int \prod_{a,b=1}^{d_1, d_2} \frac{d^2 s_{ab}}{\pi \beta} \exp \left( -\frac{1}{\beta} \sum_{a,b} |s_{ab}|^2 + \text{tr} \omega \right) \int \frac{1}{2^r} \prod_{\mu=1}^r dz_\mu d\bar{z}_\mu \\ &\times \exp \left\{ \sum_{\alpha, \beta} \left[ -\bar{z}_\alpha \omega_{\alpha\beta} z_\beta + i \sum_{a,b} \bar{s}_{ab} h_{\alpha\beta}^{ab}(\varrho) z_\alpha z_\beta + i \sum_{a,b} s_{ab} \overline{h_{\alpha\beta}^{ab}(\varrho) z_\alpha z_\beta} \right] \right\}. \end{aligned} \quad (38)$$

The above integral is finite if and only if  $\omega > 0$  (as we said earlier we assume  $\omega$  to be non-singular in order not to loose any of the constraints, hence the strong inequality here). This puts no restriction on the amount of independent parameters in  $\omega$  and from now on we will

assume this condition to hold. Performing the Gaussian integration in the  $2r$  variables  $\mathbf{z}, \bar{\mathbf{z}}$  finally yields:

$$Z_1(\beta, \omega; \varrho) = \pi^r \int \prod_{a,b=1}^{d_1, d_2} \frac{d^2 s_{ab}}{\pi \beta} \exp\left(-\frac{1}{\beta} \sum_{a,b} |s_{ab}|^2 + \text{tr} \omega\right) \frac{1}{\sqrt{\det M_\varrho(\mathbf{s}, \omega)}}, \quad (39)$$

where  $2r \times 2r$  matrix  $M_\varrho(\mathbf{s}, \omega)$  is defined as follows:

$$M_\varrho(\mathbf{s}, \omega) := \begin{bmatrix} \omega & -2i \sum_{a,b} s_{ab} \overline{\mathbf{h}^{ab}(\varrho)} \\ -2i \sum_{a,b} \bar{s}_{ab} \mathbf{h}^{ab}(\varrho) & \bar{\omega} \end{bmatrix}, \quad (40)$$

(we used the fact that  $\bar{\omega} = \omega^T$ ) and  $\mathbf{h}^{ab}(\varrho)$  denotes the  $r \times r$  matrix whose elements are  $h_{\alpha\beta}^{ab}(\varrho)$ .

## 6 Calculation for Werner states

In this Section we apply the developed statistical method to study Werner states of a  $2 \otimes 2$  dimensional system. They are defined as follows:

$$W(p) := (1-p)|\Psi_-\rangle\langle\Psi_-| + \frac{p}{4}\mathbf{1}_2 \otimes \mathbf{1}_2, \quad (41)$$

where:

$$|\Psi_\pm\rangle := \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle), \quad |\Phi_\pm\rangle := \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle) \quad (42)$$

are the Bell basis states and  $\{|0\rangle, |1\rangle\}$  is the standard basis of  $\mathbb{C}^2$ . The states  $W(p)$  have positive partial transpose, and hence are separable (Peres and Horodecki *et al.* [2]), for  $p \geq 2/3$ . As the fixed eigenensemble  $\{|e_\alpha\rangle\}$  of  $W(p)$  we take:

$$|e_1\rangle := \sqrt{1 - \frac{3}{4}p} |\Psi_-\rangle, \quad |e_2\rangle := \frac{\sqrt{p}}{2} i |\Psi_+\rangle, \quad (43)$$

$$|e_3\rangle := \frac{\sqrt{p}}{2} i |\Phi_-\rangle, \quad |e_4\rangle := \frac{\sqrt{p}}{2} |\Phi_+\rangle. \quad (44)$$

We proceed to calculate the one-particle partition function  $Z_1(\beta, \omega; W(p)) \equiv Z_1(\beta, \omega; p)$ . In what follows we assume  $p > 0$ , for  $p = 0$  corresponds to a pure state. According to the general formula (39), we have to find the matrices  $\mathbf{h}^{ab}(W(p))$  and  $M_{W(p)}(s, \omega)$ , defined in Eqs. (36) and (40). Since in the case of  $\mathbb{C}^2 \otimes \mathbb{C}^2$  the skew-symmetric subspace  $\mathbb{C}^2 \wedge \mathbb{C}^2$  is one-dimensional—it is spanned by a single vector  $|\zeta\rangle = 1/\sqrt{2}(|01\rangle - |10\rangle)$  in each copy  $AA'$  and  $BB'$ —there is only one matrix  $\mathbf{h}^{ab}(W(p)) \equiv \mathbf{h}(p)$  and only one Hubbard-Stratonovich parameter  $s_{ab} \equiv s$ . Calculation of  $\mathbf{h}(p)$  and  $M_{W(p)}(s, \omega) \equiv M_p(s, \omega)$  yields:

$$\mathbf{h}(p) = \frac{1}{8} \begin{bmatrix} 4 - 3p & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{bmatrix} \quad (45)$$

$$M_p(s, \omega) = \begin{bmatrix} \omega & -2is\mathbf{h}(p) \\ -2i\bar{s}\mathbf{h}(p) & \bar{\omega} \end{bmatrix}, \quad (46)$$

so that:

$$E_1(\mathbf{z}; p) = \frac{1}{64} |(4 - 3p)z_1^2 + pz_2^2 + pz_3^2 + pz_4^2|^2, \quad (47)$$

and:

$$Z_1(\beta, \omega; p) = \int d^2z_1 \dots d^2z_4 \exp \left[ -\beta |(4 - 3p)z_1^2 + pz_2^2 + pz_3^2 + pz_4^2|^2 - \langle \mathbf{z} | \omega \mathbf{z} \rangle + \text{tr} \omega \right] \quad (48)$$

(we have absorbed the factor  $1/64$  into the definition of the parameter  $\beta$ ).

Next, we calculate  $\det M_p(s, \omega)$  for  $p \neq 0$ . We first perform a transformation:

$$M_p \mapsto M'_p := \begin{bmatrix} \mathbf{h}(p)^{-1/2} & 0 \\ 0 & \mathbf{h}(p)^{-1/2} \end{bmatrix} M_p \begin{bmatrix} \mathbf{h}(p)^{-1/2} & 0 \\ 0 & \mathbf{h}(p)^{-1/2} \end{bmatrix} = \begin{bmatrix} \omega' & -2is \\ -2i\bar{s} & \overline{\omega'} \end{bmatrix}, \quad (49)$$

where:

$$\omega' := \mathbf{h}(p)^{-1/2} \omega \mathbf{h}(p)^{-1/2}. \quad (50)$$

Then we multiply Eq. (49) on the left by  $\begin{bmatrix} \mathbf{1} & 0 \\ 2i\bar{s} & \omega' \end{bmatrix}$  to obtain:

$$\begin{bmatrix} \mathbf{1} & 0 \\ 2i\bar{s} & \omega' \end{bmatrix} M'_p = \begin{bmatrix} \omega' & -2is \\ 0 & 4|s|^2 + \omega' \overline{\omega'} \end{bmatrix}, \quad (51)$$

and after taking the determinants of both sides:

$$\det M_p(s, \omega) = \det \mathbf{h}(p)^2 \det (4|s|^2 + \omega' \overline{\omega'}). \quad (52)$$

We then substitute Eq. (52) into Eq. (39) and finally obtain (with  $x := 4|s|^2$ ):

$$Z_1(\beta, \omega; p) = \frac{\pi^4}{4\beta \det \mathbf{h}(p)} e^{\text{tr}[\omega' \mathbf{h}(p)]} \int_0^\infty \frac{dx e^{-\frac{x}{4\beta}}}{\sqrt{\det(x + \omega' \overline{\omega'})}}, \quad (53)$$

where  $\omega'$  is defined through Eq. (50). The above integral is well defined, since  $\det(x + \omega' \overline{\omega'}) = \det(x + \sqrt{\omega' \overline{\omega'}} \sqrt{\omega'})$  and  $\sqrt{\omega' \overline{\omega'}} \sqrt{\omega'}$  is strictly positive, as we have assumed that  $\det \omega \neq 0$ . We can explicitly calculate the derivative  $\partial \log Z_1(\beta, \omega; p) / \partial \omega'$ . For a generic  $\omega'$  it takes the following form:

$$\begin{aligned} \frac{\partial \log Z_1(\beta, \omega; p)}{\partial \omega'} &= \sqrt{\mathbf{h}(p)} \frac{\partial \log Z_1(\beta, \omega; p)}{\partial \omega} \sqrt{\mathbf{h}(p)} \\ &= \left[ \int_0^\infty \frac{dy e^{-\frac{y}{4\beta}}}{\sqrt{\det(y + \omega' \overline{\omega'})}} \right]^{-1} \int_0^\infty \frac{dx e^{-\frac{x}{4\beta}}}{\sqrt{\det(x + \omega' \overline{\omega'})}} \left[ \mathbf{h}(p) - (x + \omega' \overline{\omega'})^{-1} \omega' \right]. \end{aligned} \quad (54)$$

The special case of Eqs. (53), (54) for Bell-diagonal states is straightforward—it is enough to replace matrix  $\mathbf{h}(p)$  from Eq. (45) with the diagonal matrix  $4 \text{diag}(1 - p_1 - p_2 - p_3, p_1, p_2, p_3)$ .

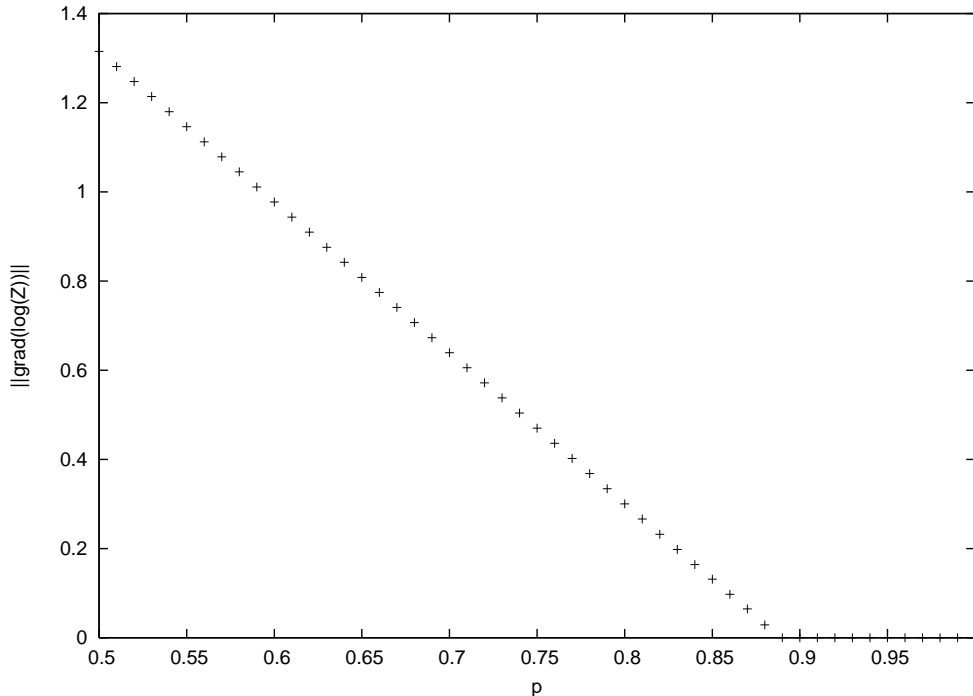


Figure 1: The plot of  $\min_{\omega'} \|\partial \log Z_1(\beta, \omega; p) / \partial \omega'\|_{HS}$  for Werner states as a function of probability  $p$  for  $\beta = 10$ .

## 7 Numerical results

Further studies of the integral (53) were performed using numerical methods. According to Eq. (31) one has to search for a saddle point of  $\log Z_1(\beta, \omega; p)$  with respect to  $\omega$  (or equivalently with respect to  $\omega'$ ; cf. Eq. (50)). The search was performed by flood-minimizing the Hilbert-Schmidt norm of  $\partial \log Z_1(\beta, \omega; p) / \partial \omega'_{\alpha\beta}$  for a range of parameters  $\beta = 10, 100, \dots$ . For simplicity we assumed a specific form of  $\omega'$ :

$$\omega' = \begin{bmatrix} \gamma & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & \lambda & 0 \\ 0 & 0 & 0 & \lambda \end{bmatrix} \quad (55)$$

and minimized the derivative (given by formula similar to to Eq. (54), but taking into account the specific symmetry of (55)) with respect to the parameters  $\gamma, \lambda > 0$ . We payed attention that the obtained minima are not on the border of the region  $\omega' > 0$  (or equivalently  $\omega > 0$ ). The specific choice (55) of  $\omega'$  was motivated by the form of the cost function (47). We also obtained some numerical evidence that in the generic case the minima of  $\|\partial \log Z_1(\beta, \omega; p) / \partial \omega'\|_{HS}$  were attained for matrices  $\omega'$  very close to (55). The results of the simulations for  $\beta = 10$  are presented in Fig. 1 (the results for higher values of  $\beta$  did not differ from those for  $\beta = 10$ ). We see that for  $p \geq 0.89$  the constraints (31) can be satisfied. We shall call the interval where it happens “equipartition region”.

Next, the dependence of the average entanglement  $\langle \langle E_{1W(p)} \rangle \rangle_0(\beta)$  (cf. Eq. (34)) of the continuous ensemble (33) on  $\beta$  within the equipartition region was examined (recall that outside this region the one-particle constraints (33) are no longer satisfied). Fig. 2 shows a sample plot

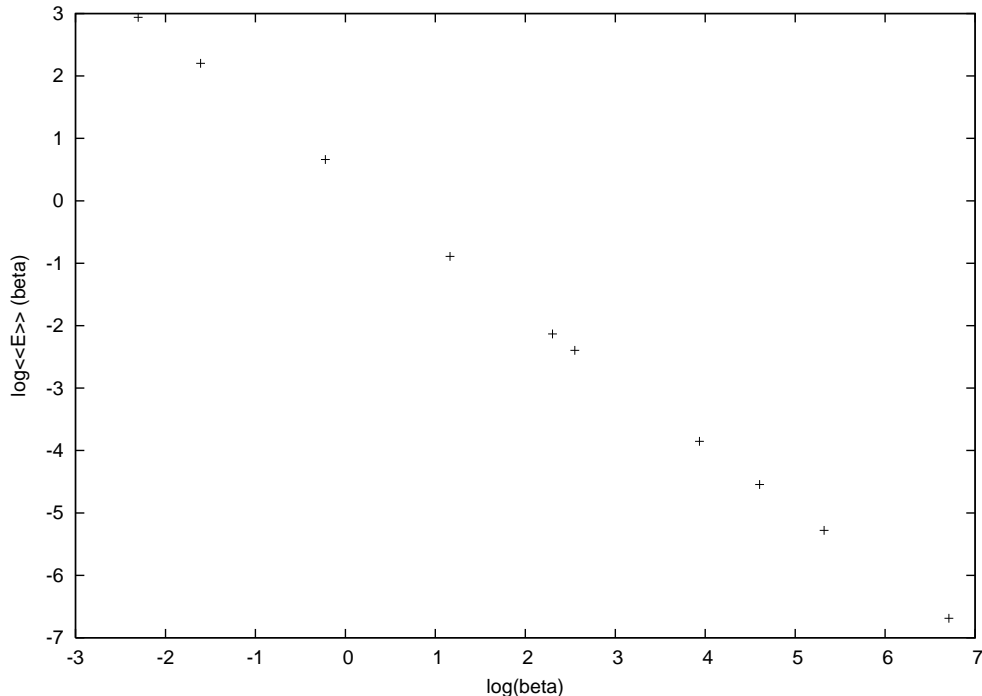


Figure 2: The plot of  $\langle\langle E_{1W(p)} \rangle\rangle_0(\beta)$  for  $p = 0.90$  on a double log scale.

for  $p = 0.9$ . One sees that the average “energy” indeed scales like  $1/\beta$ , just like predicted by the Ansatz (21) and Eq. (22). The estimated exponent  $\delta$  at this value of  $p$  is  $\delta \approx 1.75$ . We have also checked that in the limiting case  $\beta \rightarrow \infty$  the equipartition region is not altered. Hence, our procedure seems to detect separability of the Werner states (41) at least for  $p \geq 0.89$  and thus can serve only as a sufficient condition for separability. We did not check the behavior of  $\langle\langle E_{1W(p)} \rangle\rangle_0(\beta)$  outside the equipartition region  $p < 0.89$ .

## 8 Further questions and concluding remarks

The statistical mechanical approach to the separability problem as presented here differs from the more traditional techniques in that we studied the space of convex decompositions of a given state, rather than the convex set of all states. The resulting polynomial equations are real due to the constraint (11) and this real structure makes the analysis more complicated than it would be in a complex case. Hence, we applied statistical-mechanical methods to study possible zeros of this system. As an example we studied  $2 \otimes 2$  Werner states (41). However, the numerical difficulty already at this simple example was quite high and we have applied several simplifications. Nevertheless, the numerical results suggest that at least for separable states in a vicinity of the identity, the partition function and the average “energy”, related to the ensemble entanglement (cf. Eq.(13)), show some qualitative change in their behavior.

There are obviously some important questions left. First of all, we postulated rather than derived the power-law state density behavior (22) for entangled states. It would be an interesting, albeit difficult, task to try to analytically derive this law. Or at least to find some arguments in its favor.

Another thing is that in passing from the full  $N$ -particle constrains (28) to the one-particle

one (31) we have tacitly assumed a sort of “equipartition” of the constraints, i.e. that the constraints are divided equally among the particles. But it actually does not have to be like that. In particular, the shape of the curve in Fig. 1 tells us that below  $p = 0.89$  the constraints are not “equiparted”. Thus, in principle one should work with the full  $N$ -particle partition function (25) and seek regions where full constraints (28) can be satisfied. Then the scaling of the average “energy” with  $\beta$  within that regions will be able to discriminate between separability and entanglement.

As a side remark, we note that quite surprisingly, the value  $p = 0.89$  appears in Braunstein *et al.* [29] separability criterion, based on an estimation of the size of a ball of separable states around the normalized identity (see also Bengtsson and Życzkowski [10] and the references therein). It will be worth analyzing this curious coincidence in order to gain a deeper understanding of the strengths and weak points of the presented approach.

Finally, let us mention that in principle one can try to directly numerically calculate integral (17) using Monte Carlo method. The points of  $V_{N,r}$  can be generated either using Eq. (7) or, what seems more feasible, directly from definition (6). The latter method amounts to generating random unitary matrices from  $U(N)$  and discarding  $(N - r)$  of their columns (for the methods of random generation of unitary ensembles see e.g. Poźniak *et al.* [30]). However, we have not performed such simulations.

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- [20] The Gram-Schmidt orthogonalization creates an orthonormal basis of a span of a set  $\{|v_1\rangle, \dots, |v_r\rangle\}$  of a linearly independent vectors form some Hilbert space. Define:

$$|\tilde{u}_1\rangle := |v_1\rangle, \quad |\tilde{u}_i\rangle := |v_i\rangle - \sum_{j=1}^{i-1} \frac{\langle \tilde{u}_j | v_i \rangle}{\|\tilde{u}_j\|^2} |\tilde{u}_j\rangle.$$

Then  $\{|\tilde{u}_1\rangle, \dots, |\tilde{u}_r\rangle\}$  is a orthogonal system and spans the same space as  $\{|v_1\rangle, \dots, |v_r\rangle\}$ . Passing to the normalized vectors:  $|u_i\rangle := \frac{1}{\|\tilde{u}_i\|} |\tilde{u}_i\rangle$ , we obtain the desired orthonormal system.

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