Monte-Carlo approach to the volume of etangled two-qubit systems

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26 august 2012

Is our world more "classical" or more "quantum"? What quantum states are more prevalent: separable or entangled?
It has been shown, that separability is associated with the possibility of parital time reversal, [1], [2].

We work in the finite-dimensional Hilbert space $\mathcal{H}$, more precisely, its subspace of all physically feasible states. Any quantum system of our intrest can be represented by its density matrix:

$$\mathcal{M}_d := \left\{ \rho \ : \ \rho = \rho^\dagger; \ \rho \geq 0; \ \mathrm{Tr}(\rho) = 1; \ \dim(\rho) = d \right\}, \qquad (1)$$

i.e. positive definite Hermitian matrices with unit trace. It is a convex set of dimension $d^2 - 1$.

The simplest system is *qubit* — two-level quantum system, an analogue of classical bit. It has representation:

$$\rho = \frac{1}{2}\left(1 + \alpha\sigma\right),$$

where $\alpha \in \mathbb{R}^3$,

$$\alpha = \mathrm{Tr}\left(\sigma\rho\right).$$

and σ is the set of Pauli matrices.

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

D-level quantum system [3]:

$$\rho = \frac{1}{n}\left(\mathbf{I}_n + c\ \xi\lambda\right),$$

where $\xi = \langle\lambda\rangle \in \mathbb{R}^{d^2-1}$ is $d^2 - 1$ dimenstional Bloch vector, $\lambda = (\lambda_{\mathbf{1}}, \ldots, \lambda_{\mathbf{d^2-1}})$ are elements of $su(d)$ algebra and $c \in \mathbb{R}$ is normalization factor.

Zyczkowski and Sommers' normalization [4]:

$$c = d$$

and normalizing λ_i by condition

$$\mathrm{Tr}(\lambda_i^2) = 1$$

Gerdt, Khvedelidze and Palii's normalization [3]:

$$c = \sqrt{\frac{n(n-1)}{2}}$$

$$\lambda_i \lambda_j = \frac{2}{d}\delta_{ij}\mathbb{I}_d + (d_{ijk} + i f_{ijk})\lambda_k,$$

δ_{ij} is the Kronecker symbol,

$$d_{ijk} = \frac{1}{4}\mathrm{Tr}\left(\{\lambda_i, \lambda_j\}, \lambda_k\right), \quad f_{ijk} = -\frac{i}{4}\mathrm{Tr}\left([\lambda_i, \lambda_j]\,\lambda_k]\right),$$

where

$$\{\lambda_i, \lambda_j\} = \lambda_i\lambda_j + \lambda_j\lambda_i, \quad [\lambda_i, \lambda_j] = \lambda_i\lambda_j - \lambda_j\lambda_i.$$

The metrics used (Hilbert-Schmidt metric):

$$D_{HS}(\rho_1, \rho_2) = ||\rho_1 - \rho_2||_{HS} = \sqrt{\mathrm{Tr}\left[(\rho_1 - \rho_2)^2\right]}$$

corresponding metric tensor:

$$(ds_{HS})^2 = \mathrm{Tr}\left[(d\rho)^2\right].$$

If we use the representation:

$$\rho = \frac{1}{n}\left(\mathbb{I}_n + d\ \xi\lambda\right),$$

then

$$\mathrm{D}_{HS}(\rho_{\tau_1}, \rho_{\tau_2}) = D_E(\tau_1, \tau_2).$$

In the trivial case of one qubit the phisycally feasible states is just Bloch sphere. In case of n qubits, the volume of the physical states is given by the following formula [4]:

$$\mathrm{Vol}_{HS}(\mathcal{M}_d) = \sqrt{d}(2\pi)^{d(d-1)/2}\frac{\Gamma(1)\cdots\Gamma_(d)}{\Gamma(d^2)}$$

Lepage's Vegas algorithm [5]:

$$\int_{\Omega} f(x)dx.$$

$$S^{(1)} = \frac{1}{M}\sum_{x}\frac{f(x)}{p(x)},$$

where points (x) are randomly selected. Here M is the number of points, $p(x)$ — probability distribution. It is possible to show that:

$$S^{(1)} = \frac{1}{M}\sum_{x}\frac{f(x)}{p(x)} \to I, \quad \text{as} \quad M \to \infty,$$

If M is large enough: $\sigma^2 \backsimeq \frac{S^{(2)}-(S^{(1)})^2}{M-1}$, where $S^{(2)} = \frac{1}{M}\sum_x \left(\frac{f(x)}{p(x)}\right)^2$.

The state of a quantum system is physically feasible, i.e. its density matrix is positive semi-definite, if and only if the coefficients of its characteristic equation are non-negative:

$$|\mathbb{I}_n x - \rho| = x^n - S_1 x^{n-1} + S_2 x^{n-2} - ... + (-1)^n S_n = 0.$$

$$S_i \geq 0.$$

For the system of two qubits, one can represents this condition in the terms of corresponding "Bloch" vector ξ:

$$
\begin{aligned}
S_1 &= 1, \\
S_2 &= \frac{1}{2!}\frac{n-1}{n}(1-\xi\cdot\xi), \\
S_3 &= \frac{1}{3!}\frac{(n-1)(n-2)}{n^2}(1-3\xi\cdot\xi+2(\xi\vee\xi)\cdot\xi), \\
S_4 &= \frac{1}{4!}\frac{(n-1)(n-2)(n-3)}{n^3} \\
&\quad (1-6\xi\cdot\xi+8(\xi\vee\xi)\cdot\xi+3\frac{n-1}{n-3}(\xi\cdot\xi)^2- \\
&\quad 6\frac{n-2}{n-3}(\xi\cdot\xi)\cdot(\xi\cdot\xi)),
\end{aligned} \tag{2}
$$

where $\xi\vee\xi$ is vector convolution: $(\xi\vee\xi)_k = \sqrt{\frac{d(d-1)}{2}}\frac{1}{d-1}d_{ijk}\xi_i\xi_j$.

Peres-Horodecki criterion

We will also remdind Peres-Horodecki criterion, that is used for detemining entangled states.

Let ρ be a density matrix which acts on tensor product of Hilbert spaces: $\mathcal{H}_A \otimes \mathcal{H}_B$.

$$\rho = \sum_{ijkl} p^{ij}_{kl} |i\rangle\langle j| \otimes |k\rangle\langle l|$$

Introduce partial transpose operator as following:

$$\rho^{T_B} := I \otimes T(\rho) = \sum_{ijkl} p_{kl}^{ij} |i\rangle\langle j| \otimes (|k\rangle\langle l|)^T = \sum_{ijkl} p_{kl}^{ij} |i\rangle\langle j| \otimes |l\rangle\langle k|$$

If ρ is separable then ρ^{T_B} has non-negative eigenvalues. This criterion is inconclusive if dimension is larger than 6.

There exist a more simple criterion. If we recall the representation:

$$\rho = \frac{1}{n}\left(\mathbb{I}_n + d\ \xi\lambda\right),$$

then we can formulate the separability criterion in the terms of ξ vector: ρ^{T_B} has non-negative eigenvalues if and only if its Bloch vector ξ' satisfies 2. ξ' can be easily expressed via ξ vector, corresponding to the matrix ρ:

$$\begin{aligned}
\xi'_1 &= \xi_1, & \xi'_2 &= \xi_2, & \xi'_3 &= \xi_3,\\
\xi'_4 &= \xi_4, & \xi'_5 &= -\xi_5, & \xi'_6 &= -\xi_6,\\
\xi'_7 &= \xi_7, & \xi'_8 &= -\xi_8, & \xi'_9 &= \xi_9,\\
\xi'_{10} &= \xi_{10}, & \xi'_{11} &= -\xi_{11}, & \xi'_{12} &= \xi_{12},\\
\xi'_{13} &= \xi_{13}, & \xi'_{14} &= -\xi_{14}, & \xi'_{15} &= \xi_{15},
\end{aligned}$$

To calculate numerically the volume of the all physically feasible and separable states, the program in c was written. We used `GNU GCC` compiler and Open Source `GSL` library. It was run on Intel(R) Xeon(R) CPU E5410 @ 2.33GHz.
In the table and on picutre one can see how the precision of calculations depends on amount of points:

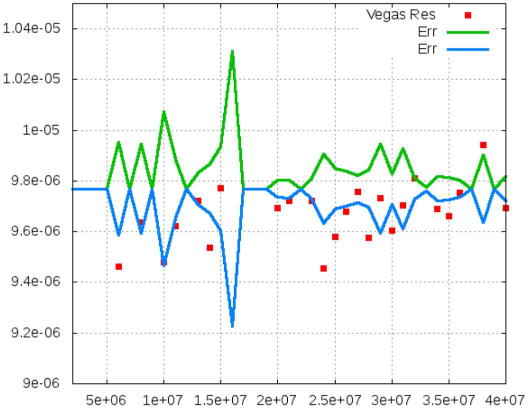

Figure: Volume of physical states

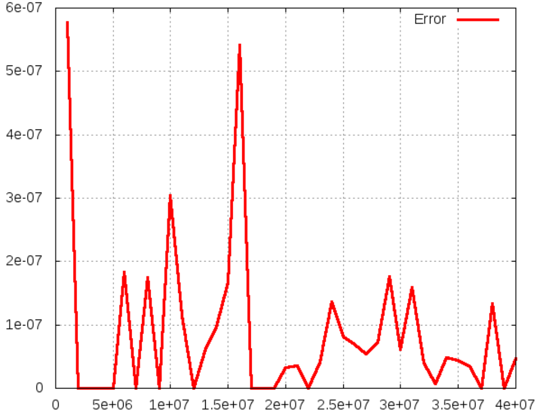

Figure: Estimated Error (σ) for the volume of physical states

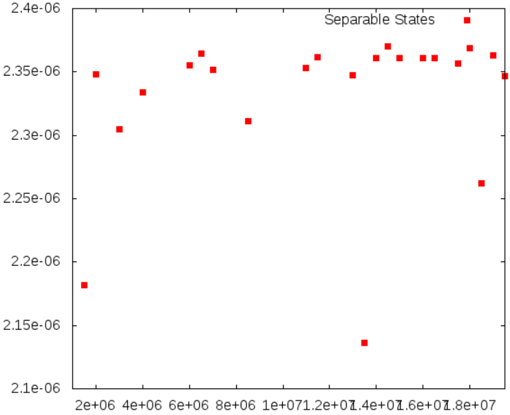

Figure: Volume of separable states

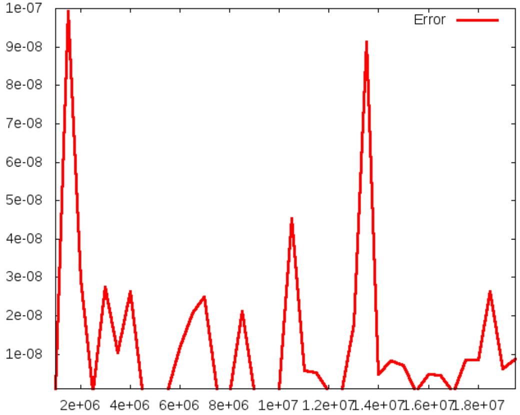

Figure: Estimated Error for the volume of separable states

N	Estimation
1000000	$(7.4 \pm 0.58) \times 10^{-6}$
2000000	$(2.5 \pm 0.4) \times 10^{-11}$
4000000	$(1.1 \pm 0.5) \times 10^{-10}$
8000000	$(9.6 \pm 0.2) \times 10^{-6}$
16000000	$(8.4 \pm 0.5) \times 10^{-6}$
24000000	$(9.6 \pm 0.1) \times 10^{-6}$
32000000	$(9.8 \pm 0.0) \times 10^{-6}$
40000000	$(9.7 \pm 0.0) \times 10^{-6}$

Figure: Estimation for the volume of physical states

N	Estimation
2000000	$(2.35 \pm 0.03) \times 10^{-6}$
4000000	$(2.33 \pm 0.03) \times 10^{-6}$
8000000	$(5.22 \pm 2) \times 10^{-10}$
8500000	$(2.31 \pm 0.02) \times 10^{-6}$
16000000	$(2.361 \pm 0.005) \times 10^{-6}$
19000000	$(2.363 \pm 0.006) \times 10^{-6}$

Figure: Estimation for the volume of separable states

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