Numerical Computations of Separability Probabilities

Jianjia Fe and Robert Joynt

Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA
(Dated: September 9, 2014)

We compute the probability that a bipartite quantum state is separable by Monte Carlo sampling. This is carried out for rebits, qubits and quaterbits. We sampled $5 \times 10^{11}$ points for each of these three cases. The results strongly support conjectures for certain rational values of these probabilities that have been found by other methods.

PACS numbers: 03.67 Mn, 02.30 Zz, 02.30. Gp

I. INTRODUCTION

The surprising efficacy of complex numbers in describing the physical world has led to persistent speculation that quaternions might also serve as a fruitful foundation of physical theories. Quaternions resemble the complex numbers in forming a division ring: they are the richest such number system that has the very restrictive unique division property (Frobenius). Thus there is a natural mathematical progression from the real to the complex to the quaternionic numbers. We might ask if there is a corresponding natural progression also in physical theories that use these numbers.

Real numbers are sufficient to completely describe rebits, physical objects with two degrees of freedom whose $2 \times 2$ density matrices are symmetric real matrices. Complex numbers describe the usual qubits that have been found by other methods. Two $2 \times 2$ complex Hermitian density matrices. Quaterbits are described by $2 \times 2$ density matrices with quaternionic entries. These matrices are Hermitian in the sense that the transpose is the quaternionic conjugate. The conjugate of a quaternion $h = a + ib + jc + kd$ is $\bar{h} = a - ib - jc - kd$. $a, b, c, d$ are real and Hamilton’s symbols $i, j, k$ satisfy $i^2 = j^2 = k^2 = -1$, $i j = -ji = k$, etc. The density matrices are positive and have unit trace in all cases.

Recently, there has been some interesting mathematical work that gives some indication of such a natural progression in the properties of these density matrices. This progression arises in the context of considering correlations in bipartite systems, i.e., in the $4 \times 4$ density matrices $\rho$ that describe a pair of physical objects. Two objects $A$ and $B$ are said to be separable if $\rho$ may be written as

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$$

(1)

where the real numbers $p_i$ satisfy $p_i \geq 0$ and $\sum_i p_i = 1$. $\rho_i^A$ and $\rho_i^B$ are $2 \times 2$ density matrices that refer to the two objects individually. Clearly this definition makes sense in all three number systems, as do the positivity and trace conditions.

Now there is a very fundamental question, first proposed in [1]: what proportion $P$ of bipartite systems are separable? There is an intriguing conjecture that the formula

$$P(\alpha) = \sum_{i=0}^{\infty} f(\alpha + i),$$

(2)

where

$$f(\alpha) = \frac{q(\alpha) 2^{-4\alpha-6} \Gamma (3\alpha + \frac{5}{2}) \Gamma (5\alpha + 2)}{3\Gamma (\alpha + 1) \Gamma (2\alpha + 3) \Gamma (5\alpha + \frac{7}{2})},$$

(3)

with

$$q(\alpha) = 185000\alpha^5 + 779750\alpha^4 + 1289125\alpha^3 + 1042015\alpha^2 + 410694\alpha + 63000,$$

(4)

which for simple integral and half-odd-integral values of $\alpha$ gives results that are close to rational numbers with fairly small denominators, and that the rational numbers $P(1/2)$ gives the proportion of separable 2-rebit states, and $P(1)$ gives the proportion of separable 2-qubit states. This remarkable result [2, 3] comes from the computation of moments such as $\langle |\rho|^n \rho^T \rangle$, an application of Zeilberger’s algorithm [4], and numerical evaluation of Eq. 2 to thousands of decimal places. Here the angle brackets refer to an average over all physical states (i.e., those that satisfy positivity and have unit trace), and the straight brackets denote the determinant. The average is defined using the measure induced by the Hilbert-Schmidt metric on the space of density matrices.

As we shall see, the $\alpha = 1$ and $\alpha = 1/2$ conjectures are extremely well-supported. So it is natural to ask if higher values of $\alpha$ have a physical interpretation. In this paper, we shall focus on the possibility that $\alpha = 2$ corresponds to quaterbits (quaternion-based bits), though we also present computations for qubits and rebits. Our approach is to compute $P(\alpha)$ by a Monte Carlo method.

II. QUBITS

For qubits, the conjecture based on Eq. 2 gives

$$P(1) = \frac{8}{33} = 0.24,$$
where the overbar indicates a repeating decimal.

This conjecture was also supported by numerical evidence [8], with Monte Carlo simulations yielding

\[ P_{\text{est}}(1) = 0.2424 \pm 0.0002. \]

This earlier Monte Carlo work used the condition of zero concurrence for separability [6]. This is equivalent to the Peres-Horodecki Criterion (PHC) [8, 9] which states that to be separable, it is necessary and sufficient for the partial transpose \( \rho^{PT} \) of the density matrix \( \rho \) to be positive. In the 2-qubit case, the \( 4 \times 4 \) density matrix can be written as

\[ \rho = \frac{1}{4} I + \frac{1}{4} \sum_{i,j=0}^{3} n_{ij} (\sigma_i \otimes \sigma_j), \tag{5} \]

where \( I_n \) is the \( n \times n \) identity matrix, \( \sigma_0 = I_2 \), and the \( \sigma_i \) are the Pauli matrices. The sum excludes the \( i = j = 0 \) term, and \( n_{ij} \) is thus a real 15-vector. We can use Euclidean measure to define probabilities in the space, which is equivalent to the Hilbert-Schmidt measure. The allowed values of \( n_{ij} \) form a compact and convex subset of \( \mathbb{R}^{15} \) whose boundary is set by the condition that \( \rho \) is positive. This set is the generalization of the familiar Bloch sphere for spin 1/2. Its shape has been described in at least a partial fashion [2, 10], and its volume has been computed [11]. It lies within the sphere given by \( \sum_{i,j=0}^{3} n_{ij}^2 = 3/4 \). The 15-ball of radius \( \sqrt{3/4} \) is sampled uniformly, testing both positivity and the PHC, which yields \( P(1) \). The sampling method is taken from [12]. We sampled \( 5 \times 10^{11} \) points, obtaining

\[ P_{\text{est}}(1) = 0.2424 \pm 0.0001. \]

Thus the numerical results strongly support the conjecture \( P(1) = 8/33 \).

### III. REBITS

The progression aspect of the problem arises already when we consider the same problem for rebits. Rebits are obtained by setting \( n_{02} = n_{12} = n_{32} = n_{20} = n_{21} = n_{23} = 0 \), i.e., omitting the imaginary generators. Positivity still requires that \( \sum n_{ij}^2 \leq 3/4 \) for the coefficients of the nonzero generators. The conjecture is that

\[ P(1/2) = \frac{29}{64} = 0.453125. \]

What is remarkable is that \( P(1) \) and \( P(1/2) \) are given by the same formula, changing only the parameter \( \alpha \). We have performed the Monte Carlo sampling for this case, testing positivity and the PHC for points in the 9-ball. The result is

\[ P(1/2) = 0.4531 \pm 0.0001, \quad \frac{29}{64} = 0.453125. \]

We tested \( 5 \times 10^{11} \) points. Hence the unified formula is well-confirmed by the numerical computations for both \( \alpha = 1/2 \) and \( \alpha = 1 \).

### IV. QUATERBITS

Now we consider quaterbits. It is reasonable to conjecture that \( \alpha = 2 \) formula should give the separability ratio for this 26-dimensional case. The conjecture is:

\[ P(2) = \frac{26}{323} \approx 0.080495. \]

We first note that the PHC has not been proven for this case - it is not known whether positivity of the partial transpose is equivalent to separability. Thus it is very interesting to repeat the above calculations for this case. The \( 2 \times 2 \) matrix representation of quaternions in which \( h = a + i b + j c + k d \rightarrow I_2 a + \sigma_b x + ic \sigma_y + id \sigma_z \) will be useful. \( I_n \) is the \( n \times n \) identity.

Two quaterbits are described by \( 4 \times 4 \) density matrices \( \rho \) with quaternionic entries. These matrices are self adjoint. Writing the quaternions themselves as matrices, we find

\[ \rho - \frac{I_8}{8} = \rho' = \begin{pmatrix} AI_2 & q_0 & q_1 & q_2 \\ q_0^T & BI_2 & q_3 & q_4 \\ q_1^T & q_3^T & CI_2 & q_5 \\ q_2^T & q_4^T & q_5^T & DI_2 \end{pmatrix}, \]

with

\[ q_i = \begin{pmatrix} a_i - id_i \\ ib_i - c_i \\ a_i + id_i \end{pmatrix}, \quad q_i^T = \begin{pmatrix} a_i + id_i \\ -ib_i + c_i \\ a_i - id_i \end{pmatrix}. \]

We must have that \( A + B + C + D = 0 \). Defining \( u = 2A + 2B, v = 2A + 2C, w = -2B - 2C \) and

\[ \lambda_{ijk} = \sigma_i \otimes \sigma_j \otimes \sigma_k \]

so that \( Tr \lambda_{ijk} \lambda_{i'j'k'} = 8 \delta_{ii'} \delta_{jj'} \delta_{kk'} \), we find, after a lengthy calculation:

\[ \rho' = u \lambda_{300} + v \lambda_{030} + w \lambda_{330} + \]

\[ \frac{1}{2} a_0 (\lambda_{010} + \lambda_{310}) + \frac{1}{2} b_0 (\lambda_{021} + \lambda_{321}) - \frac{1}{2} c_0 (\lambda_{022} + \lambda_{322}) \]

\[ - \frac{1}{2} d_0 (\lambda_{023} + \lambda_{323}) + \frac{1}{2} a_1 (\lambda_{100} + \lambda_{130}) - \frac{1}{2} b_1 (\lambda_{201} + \lambda_{231}) \]

\[ - \frac{1}{2} c_1 (\lambda_{202} + \lambda_{232}) - \frac{1}{2} d_1 (\lambda_{203} + \lambda_{233}) + \frac{1}{2} a_2 (\lambda_{110} - \lambda_{120}) \]

\[ - \frac{1}{2} b_2 (\lambda_{121} + \lambda_{121}) - \frac{1}{2} c_2 (\lambda_{122} + \lambda_{122}) - \frac{1}{2} d_2 (\lambda_{123} + \lambda_{123}) \]

\[ + \frac{1}{2} a_3 (\lambda_{111} + \lambda_{121}) + \frac{1}{2} b_3 (\lambda_{121} - \lambda_{121}) - \frac{1}{2} c_3 (\lambda_{122} + \lambda_{122}) \]

\[ + \frac{1}{2} d_3 (\lambda_{123} - \lambda_{123}) + \frac{1}{2} a_4 (\lambda_{100} - \lambda_{130}) - \frac{1}{2} b_4 (\lambda_{201} - \lambda_{231}) \]

\[ + \frac{1}{2} c_4 (\lambda_{202} - \lambda_{232}) - \frac{1}{2} d_4 (\lambda_{203} - \lambda_{233}) + \frac{1}{2} a_5 (\lambda_{010} - \lambda_{310}) \]

\[ - \frac{1}{2} b_5 (\lambda_{021} - \lambda_{321}) + \frac{1}{2} c_5 (\lambda_{022} - \lambda_{322}) - \frac{1}{2} d_5 (\lambda_{023} - \lambda_{323}) \]
Thus
\[ \rho' = \sum_{ijk} n_{ijk} \lambda_{ijk}, \]
where the sum \( \Sigma' \) runs only over the combinations
\[ \{ijk\} = \{300\}, \{030\}, \{330\}, \{010\}, \{310\}, \{021\}, \{321\}, \{022\}, \{322\}, \{023\}, \{323\}, \{100\}, \{130\}, \{201\}, \{231\}, \{202\}, \{232\}, \{203\}, \{233\}, \{110\}, \{220\}, \{121\}, \{211\}, \{122\}, \{212\}, \{123\}, \{213\}. \]
and positivity requires that
\[ \sum_{ijk} (n_{ijk})^2 \leq \frac{7}{64}. \]

To determine \( P(2) \) numerically, we sample the 27-ball of radius \( \sqrt{7/64} \) uniformly in the \( n_{ijk} \), which, as stated above, is also uniform in the Hilbert-Schmidt metric. We test each point for PPT and positivity, giving an estimate \( P_{\text{est}}(2) \). \( 5 \times 10^{11} \) points are sampled in the Monte Carlo simulation. We find
\[ P_{\text{est}}(2) = 0.0805 \pm 0.0001. \]

The numerical results give strong evidence in favor of the conjecture.

V. CONCLUSION

Quaternionic quantum mechanics has been investigated in detail. It can only describe the observed universe if some superselection rules are added \[13\]. Rebits do not have a rich enough mathematical structure to describe the real world - it would be very difficult to see how a rebit could display Ramsey fringes, for example, since the whole Bloch sphere is required for the dynamics. Qubits seem to be about right, of course. But it is remarkable that some mathematical structures overarch the three possibilities. The separability probability formula in Eq. 2 seems to be one of these.

Acknowledgments

We thank Dong Zhou for useful discussions. We thank P. B. Slater and K. Zyczkowski for helpful communications. We also thank the HEP, Condor, and CHTC groups at UW-Madison for computational support.

[1] K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Phys. Rev. A 58, 883 (1998).
[2] P. B. Slater and C. F. Dunkl, J. Phys. A 45, 095305 (2012).
[3] P. B. Slater, J. Phys. A 46, 445302 (2013).
[4] W. Y. C. Chen, Q.-H. Hou, and Y.-P. Mu, J. Symbolic Comput. 47, 643 (2012).
[5] D. Zhou and G.-W. Chern and J. Fei and R. Joynt, Int. J. Mod. Phys. B 26, 1250054 (2012).
[6] S. Hill and W. K. Wootters, Phys. Rev. Lett. 78, 5022 (1997).
[7] W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
[8] A. Peres, Phys. Rev. Lett. 77, 1413 (1996).
[9] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A 223, 1 (1996).
[10] M. S. Byrd and N. Khaneja, Phys. Rev. A 68, 062322 (2003).
[11] A. Andai, J. Phys. A 39, 13641 (2006).
[12] G. S. Watson, Statistics on Spheres (Wiley, New York, 1983).
[13] S. L. Adler, Quaternionic Quantum Mechanics and Quantum Fields (Oxford University Press, New York, 1995).