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A priori probabilities of separable quantum states

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Abstract. Życzkowski, Horodecki, Sanpera and Lewenstein (ZHSL) recently proposed a 'natural measure' on the N-dimensional quantum systems, but expressed surprise when it led them to conclude that for $N = 2 \times 2$, disentangled (separable) systems are more probable (0.632 ± 0.002) in nature than entangled ones. We contend, however, that ZHSL's (rejected) intuition has, in fact, a sound theoretical basis, and that the *a priori* probability of disentangled 2×2 systems should more properly be viewed as (considerably) less than 0.5. We arrive at this conclusion in two quite distinct ways, the first based on classical and the second, quantum considerations. Both approaches, however, replace (in whole or part) the ZHSL (product) measure by ones based on the volume elements of *monotone* metrics, which in the classical case amounts to adopting the Jeffreys' prior of Bayesian theory. Only the quantum-theoretic analysis—which yields the smallest probabilities of disentanglement—uses the *minimum* number of parameters possible, that is $N^2 - 1$, as opposed to $N^2 + N - 1$ (although this 'over-parametrization', as recently indicated by Byrd, should be avoidable). However, despite substantial computation, we are not able to obtain precise estimates of these probabilities and the need for additional (possibly supercomputer) analyses is indicated—particularly so for higher-dimensional quantum systems (such as the 2×3 ones, which we also study here).

1. Introduction

In a recent paper [1], Życzkowski, Horodecki, Sanpera and Lewenstein (ZHSL) [1] sought to estimate 'how many entangled (disentangled) states exist among all quantum states'. They gave three principal reasons for their study: (1) to answer the question 'is the world *more classical* or *more quantum*?'; (2) to know, for the purposes of numerical simulation, 'to what extent entangled quantum systems may be considered as typical'; and (3) 'to investigate how frequently certain nonseparable states, 'peculiarly' admitting time reversal in one subsystem, arise'. In response to the first query, ZHSL concluded—to their 'surprise' [1, p 889]—that although the (higher-dimensional) 'world' is, in general, more quantum than classical, this is not so for the 2×2 quantum systems. We contend here, however, that alternative analyses based on the concept of *monotone* metrics on classical and quantum systems [2], lead to the elimination of this exception to their general rule.

In their investigation, ZHSL obtained a variety of both analytical and numerical bounds on the volumes of the sets of separable states for various dimensions, using what they asserted was a 'natural measure' on the space of density matrices (cf [3]). In the first analytical part of this paper (section 2), we indicate an essential degree of arbitrariness in the choice of measure by ZHSL, and its consequences for the results they have reported (cf [4]). We then argue in favour of a specific alternative—well-founded on statistical principles—which leads to a markedly *smaller* probability of encountering a disentangled (separable) state. (The numerical results we report are for the 2×2, 2×3 and 3×3 quantum systems.) Then, in section 3, we study the use of methods more fundamentally quantum-theoretic in nature—requiring us to develop a quite distinct set of procedures than those used by ZHSL and followed in section 2. (Due to the associated large computational demands, we have primarily limited our analyses to the 2×2 systems, but in section 3.6 we do, in fact, initiate a parallel investigation of the 2×3 systems.) We obtain for each of more than 30 pairs of parameters, determining the fineness of approximating square grids and three-dimensional simplicial decompositions, a set of three probabilities of disentanglement (table 1), each probability being based on a distinct form of monotone metric [6, 7]. The sets are intended to determine a range of values within which any suitable candidate (meeting underlying natural criteria of *monotonicity*) for the 'true' *a priori* probability of disentanglement must lie. Essentially all such probabilities we obtain turn out to be considerably smaller than both the result of ZHSL (0.632 ± 0.002) and the alternative to it (≈ 0.35) we promote in section 2, based on the Jeffreys' prior of Bayesian theory. However, the need for additional computational work is indicated in order to sharpen the estimates reported in sections 3.1–3.3, as well as to extend our general approach to higher-dimensional quantum systems. (We are reminded, to some degree, of the computational/combinatorial challenges of lattice gauge theory [5].) In section 3.5, we switch from the explicit enumeration approach (based on regular grids and simplicial decompositions) to a randomization methodology (such as ZHSL employed in their studies)—but also find this to be highly computationally demanding, since we must search in a high-dimensional parameter space for those particular points corresponding to density matrices.

A conservative evaluation of the accumulated evidence of the multiple quantum-theoretic analyses we report (tables 1–3) indicates that the *a priori* probability of disentanglement for the 2×2 systems should be regarded—using any of a continuum of possible acceptable standards, in particular that provided by the *minimal* monotone (Bures) metric—as *no more* than 11%. As to a *lower* bound, on the other hand, on the probability of separability, it remains an unsettled issue as to whether or not the *maximal* monotone metric should be viewed as furnishing a bound strictly greater than zero.

In our concluding remarks (section 4), we draw attention to an interesting recent analysis of M Byrd (personal communication), bearing upon the issue of whether or not the use of 'over-parametrizations' by ZHSL and (following them) by us in section 2, can be averted.

2. Semiclassical statistical analyses of 3×3, 2×3 and 2×2 quantum systems

ZHSL [1] used as a measure on the space of $N \times N$ density matrices the product of the Haar measure for the unitary group $U(N)$ and the uniform distribution on the $(N-1)$-dimensional simplex spanned by the N eigenvalues of the density matrix. Now, we see no basis (within the semiclassical framework adopted by ZHSL) for questioning the use of the Haar measure. However, the selection of the uniform distribution on the simplex appears not to be so compelling, as it lacks as convincing a rationale as the group-theoretic argument for the Haar measure (cf [8]). Also, we must point out that the analyses of ZHSL are based on 'over-parametrizations', since $N^2 + N - 1$ parameters are used, while the convex set of $N \times N$ density matrices is only $(N^2 - 1)$-dimensional in nature. Though we adhere to this over-parametrization in the analyses of this section, in section 3 we revert to the more natural and conventional form.

The uniform distribution on the $(N-1)$-dimensional simplex ($p_1 + \cdots + p_N = 1$; $p_i \geqslant 0$) can be considered to be that specific member of the (continuous) family of Dirichlet probability distributions [9, 10, section 7.7],

$$\frac{\Gamma(\nu_1 + \cdots + \nu_N)}{\Gamma(\nu_1)\ldots\Gamma(\nu_N)} p_1^{\nu_1-1} \ldots p_{N-1}^{\nu_{N-1}-1}(1 - p_1 - \cdots - p_{N-1})^{\nu_N-1} \qquad \nu_1 > 0, \ldots, \nu_N > 0 \quad (1)$$

which has all its N parameters (ν) set equal to unity. The family of Dirchlet distributions is *conjugate*, in that if one selects a *prior* distribution belonging to it, then, through the application of Bayes' rule to observations drawn from a multinomial distribution, one arrives at a *posterior* distribution which is also within the family.

2.1. *Jeffreys' prior*

Of strongest interest, however, for our purposes here, is that the principle of reparametrization invariance (based on the *Fisher information* [11, 12]) leads to the special case (Jeffreys' prior) in which (1) has all its N parameters set equal to *one-half* [13, 14, equation (3.7)] and not *unity*, as for the uniform distribution. 'The main intuitive motivation for Jeffreys' priors is *not* their invariance, which is certainly a necessary, but in general far from sufficient condition to determine a sensible reference prior; what makes Jeffreys' priors unique is that they are *uniform* measures in a particular metric which may be defended as the 'natural' choice for statistical inference' [15]. By way of illustration, Kass [14, section 2] (cf [16]), using the transformations $p_i = 2z_i^2$, demonstrates how the Jeffreys' prior for the trinomial model ($N = 3$) on the two-dimensional simplex can be (making use of spherical polar coordinates) transformed to the uniform distribution on the positive-octant portion of the two-dimensional sphere, $z_1^2 + z_2^2 + z_3^2 = 4$ of radius 2. (Braunstein and Milburn [17] show that for two-level *quantum* systems, statistical distinguishability is just the (Bures/minimal monotone) metric on the surface of the unit sphere in *four* dimensions. In contrast, the space of n-level quantum systems is 'not a space of constant curvature for $n > 2$ and not even a locally symmetric space. The physical meaning of this fact seems to be an interesting open question' [18] (cf [19, 20]).)

Clarke and Barron [21, 22] (cf [23]) have established that Jeffreys' priors (the normalized volume elements of Fisher information metrics) asymptotically maximize Shannon's mutual information between a sample of size n and the parameter, and that Jeffreys' prior is the unique continuous prior that achieves the asymptotic minimax risk when the loss function is the Kullback–Leibler distance between the true density and the predictive density. (The possibility of extending the 'universal coding' results of Clarke and Barron to the *quantum* domain, has been investigated in [24] (cf [25]).) Clarke [26] asserts that 'Jeffreys' prior can be justified by four distinct arguments'. In addition, Balasubramanian [27] 'cast parametric model selection as a disordered statistical mechanics on the space of probability distributions' and 'derived and discussed a novel interpretation of Jeffreys' prior as the uniform prior on the probability distributions indexed by a parametric family' (cf [28]).

Now, it is of interest to note that in the limit in which the N parameters (ν) of the Dirichlet distribution (1) all go to zero, the distribution becomes totally concentrated on the pure states of the N-dimensional quantum system. Since ZHSL showed that in 'the subspace of all pure states, the measure of separable states is equal to zero' [1, p 886], we would anticipate, making use of a continuity argument, that the measure or volume of the set of separable states would increase if all N parameters of (1) were fixed at one-half (Jeffreys' prior), but still be less than if they were all taken to be equal to unity, etc. ('The purer a quantum state is, the smaller its probability of being separable' [1, p 891].)

2.2. The case of 3 × 3 quantum systems

We have, in fact, tested these last contentions regarding competing measures of separability, through numerical means, first, generating a set of 3000 random 9×9 unitary matrices ($N = 9$), following the (Hurwitz/Euler angle) prescription given in [29, equations (3.1)–(3.5)]. From it, we produced (in the manner of ZHSL [1, equation (34)]) three sets of 3000 9×9 density matrices: one set based on the selection $\nu_1 = \cdots = \nu_9 = \frac{1}{2}$; another for $\nu_1 = \cdots = \nu_9 = 1$ (as, in effect, done in [1]); and a third for $\nu_1 = \ldots = \nu_9 = \frac{3}{2}$. (Random realizations of the Dirichlet distributions were generated based on the fact that they can be considered to be joint distributions of (univariate) gamma distributions [9, 10]. The 3000 instances we obtain are obviously far fewer in number than the 'several millions' ZHSL [1] apparently employed as a general rule in their series of analyses of quantum systems of various dimensions. This is primarily due to our full reliance on `MATHEMATICA`, while ZHSL—as K Życzkowski wrote in a personal communication—employed `FORTRAN` routines for random number generation. Nevertheless, as noted immediately below, Życzkowski, using his speedier routines, has confirmed the main aspects of our analysis. Additionally, the *quantum-theoretic* analyses of section 3 require a quite different set of algorithms, and it is far from clear whether our use there of `MATHEMATICA` is in any way relatively inefficient.)

Then, we determined whether all (nine of) the eigenvalues of the *partial transpositions* of the random density matrices (viewing them as $(3 \times 3) \times (3 \times 3)$ density matrices, in the manner of [30, equation 21]) were positive (as they must be in the separable case) or not. For the $\nu = \frac{1}{2}$ (Jeffreys' prior) scenario, 83 of the 3000 density matrices had this positivity property, while considerably more (602) possessed it for $\nu = 1$ and still more (1296) for $\nu = \frac{3}{2}$. Thus, we note an approximate decrease by a factor of $\frac{83}{602} \approx 0.138$ in the upper bound on our suggested probability of encountering a separable state *vis-á-vis* the analysis of ZHSL.

2.3. The cases of 2 × 3 and 2 × 2 quantum sytems

We, then, conducted parallel analyses to those in section 2.2 for the 2×3 and 2×2 systems. (For both such systems, but not higher-dimensional ones, such as the 3×3, the positivity of the partial transposition is a sufficient, as well as necessary condition for separability [30]. So, we will be estimating probabilities themselves, rather than upper bounds on them.) In both cases, we now employed 10 000 realizations. In the 2×3 case, we found 1309 separable states, using $\nu = \frac{1}{2}$, and 4135 for $\nu = 1$, as well as 6,357 for $\nu = \frac{3}{2}$. (Our statistic of 0.4135 needs to be compared with that of 0.384 ± 0.002 of ZHSL—which, as noted, was based on a much larger sample.) For the 2×2 systems, the analogous results were 3633, 6564 and and 7946. So, we would conclude, in this analytical framework, that the proportion of separable states among the 2×2 quantum systems should be taken to be approximately 0.36—which is well *below* the demarcation point of 0.5, *above* which ZHSL found their result of 0.632 ± 0.002 (roughly comparable to ours of 0.6564) to (counterintuitively) lie.

K Życzkowski has kindly repeated the analyses reported above for the case $\nu = \frac{1}{2}$ (that is, Jeffreys' prior), using 200 000 random realizations for each of the three scenarios. The probabilities of separability he obtained were (all digits being significant, he states): 0.022 (for the 3×3 systems); 0.122 (2×3 systems); and 0.352 (2×2 systems). These should be compared with our results (based on considerably smaller samples) of 0.0277, 0.1309 and 0.3633, respectively.

These various numerical results are, thus, quite supportive of our arguments and help to fulfil the first objective of this letter of showing the dependence of estimates of the volume of the set of separable states on the particular choice of (symmetric) Dirichlet distribution on the

$(N-1)$-dimensional simplex spanned by the N eigenvalues of the $N \times N$ density matrix (ρ). We note again that ZHSL [1, p 889] expressed 'surprise that the probability that a mixed state $\rho \in H_2 \times H_2$ is separable exceeds fifty percent'. Thus, they would have apparently been not so confounded if the uniform distribution on the three-simplex of eigenvalues had been replaced by the Jeffreys' prior, since its use yields a *more modest* percentage of approximately 35%.

Let us also note that our suggested modification ($\nu = \frac{1}{2}$) of the ZHSL measure ($\nu = 1$) would appear to find some support in a recent paper concerned with a parametrization (sharing certain features with that of ZHSL) of the $N \times N$ density matrices [8]. Its authors consider the N eigenvalues to be parametrized by the 'squared components' of the $(N-1)$-sphere (rather than coordinates in the $(N-1)$-dimensional simplex, as in ZHSL). As noted above, in relation to [14], the Jeffreys' prior is simply the uniform distribution on such a *sphere*—while ZHSL used instead the uniform distribution on the *simplex*.

3. Quantum-theoretic statistical analyses of 2 × 2 and 2 × 3 systems

In [4, section II.C], we presented evidence that certain statistical features of the product measure employed by ZHSL [1] were not reproducible through the use of any of the possible (continuum of) *monotone* metrics. A similar conclusion appears to hold if one replaces the uniform distribution in the ZHSL product measure (as we have done above in section 2) by any other member of the family of Dirichlet distributions (1). Since Petz and Sudár [2] have argued that monotone metrics are the quantum analogues of the (classically unique) Fisher information metric, it would seem highly desirable to replace the product measures so far employed by ones based directly on the volume elements of such metrics. (In [31], efforts were reported to integrate the volume elements of the *minimal* and *maximal* monotone metrics over the convex sets of 3×3 and 4×4 density matrices.) In so doing, we would avoid the nonparsimonious 'over-parametrization' mentioned at the outset of section 2. (However, it will be incumbent upon us to develop a quite distinct set of computational methods than those used by ZHSL and applied in section 2.)

We have, in fact, conducted such a series of analyses for the 2×2 quantum systems, based on a MATHEMATICA program containing *two* parameters of choice, n_1 and n_2. The parameter n_1 determines the fineness of a regular decomposition of the three-dimensional simplex—the points of which correspond now to the *diagonal* entries of ρ, and not the *eigenvalues*, as in section 2 and the work of ZHSL [1] and Boya *et al* [8]. (Of course, both the eigenvalues and diagonal entries of a density matrix are non-negative and sum to unity. To compute the coordinates of the simplicial coordinates, we followed an algorithm for the next *composition* of an integer N into K parts, given in [32, chapter 5], taking $K = 4$ for our purposes, and then dividing each of the $\binom{N+3}{N}$ compositions generated by N.) The reciprocal of the parameter n_2 is the distance between adjacent points of a regular square grid—having its extreme points/corners at $(\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, -\frac{1}{2})$, $(-\frac{1}{2}, -\frac{1}{2})$ and $(-\frac{1}{2}, \frac{1}{2})$—imposed on a circle of radius one-half centred at the origin of the complex plane. (The off-diagonal entries of a density matrix cannot exceed one-half in absolute value, so they must lie within this circle.)

For specific values of n_1 and n_2, within but challenging our computational capabilities, we generated the associated three-dimensional simplicial decompositions and 12-dimensional uniform lattices (the sixfold Cartesian product of the imposed two-dimensional square grid—six, of course, corresponding to the number of pairs of off-diagonal entries). Then, we explicitly enumerated all those points in the 15-dimensional product space parametrizing the 4×4 density matrices of mixed states (that is, yielding matrices having all strictly positive eigenvalues, noting that the additional hermiticity and trace requirements are automatically satisfied by construction). We would reject any density matrices of pure states (the totality of which

Table 1. Quantum-theoretic statistical analyses based on the minimal, KMB and maximal monotone metrics. The parameters n_1 and n_2 determine the resolution of simplicial decompositions and square grids for trial diagonal and off-diagonal entries, respectively. The variable p denotes the associated probability of disentanglement and d, the averaged degree of entanglement. The only generated density matrices which have been omitted from consideration are those which correspond precisely to degenerate states, that is, det $\rho = 0$. The results are tabulated in increasing order of the total number of density matrices generated—given in the third column.

n_1	n_2	ρ	$\rho_{separable}$	p_{min}	p_{KMB}	p_{max}	d_{min}	d_{KMB}	d_{max}
23	7	1 340 928	356 096	0.111 102	0.087 3186	0.084 615 3	0.182 06	0.208 022	0.248 457
35	6	1 425 216	467 424	0.193 939	0.178 191	0.098 076 3	0.250 552	0.229 161	0.154 696
30	7	2 919 680	806 400	0.119 669	0.176 01	0.749 588	0.184 696	0.170 555	0.009 400 62
45	6	3 033 084	987 484	0.220 936	0.224 241	0.293 623	0.248 278	0.243 704	0.144 297
4	12	4 228 817	1 634 577	0.249 824	0.232 509	0.309 404	0.117 852	0.118 964	0.088 653 5
19	8	4 443 408	1 284 816	0.147 968	0.123 283	0.055 499 9	0.186 86	0.184 149	0.177 13
8	10	4 645 163	1 230 411	0.114 69	0.098 2187	0.179 838	0.189 89	0.192 975	0.143 422
35	7	4 673 024	1 286 656	0.092 7196	0.059 4478	0.152 368	0.220 529	0.266 94	0.156 327
13	9	5 540 864	1 341 440	0.075 6821	0.036 1165	0.001 737 33	0.208 862	0.252 169	0.349 782
6	11	6 161 152	1 703 808	0.114 669	0.085 9676	0.155 728	0.187 623	0.205 257	0.119 427
10	10	7 103 372	2 232 836	0.195 802	0.188 155	0.243 187	0.131 533	0.130 076	0.103 806
23	8	8 026 372	2 286 148	0.109 203	0.074 7959	0.000 112 443	0.241 79	0.260 264	0.296 032
50	7	13 522 176	3 705 472	0.101 25	0.072 653	0.687 396	0.206 883	0.230 803	0.042 287 6
19	9	16 603 136	4 096 000	0.092 0722	0.083 066	0.082 047 7	0.186 361	0.188 775	0.190 464
7	12	27 658 276	6 897 940	0.077 9479	0.055 3514	0.310 28	0.221 055	0.256 207	0.095 960 8
35	8	28 582 224	8 104 555	0.140 105	0.122 355	0.199 223	0.222 33	0.228 248	0.118 103
15	10	29 328 236	8 006 017	0.120 671	0.096 3975	0.198 144	0.194 026	0.210 798	0.134 718
11	11	36 913 664	9 049 600	0.104 142	0.089 1733	0.164 511	0.177 627	0.179 959	0.122 263
25	9	37 671 424	9 440 000	0.083 7076	0.034 3513	0.002 755 5	0.202 037	0.229 187	0.198 646
8	12	40 487 643	10 493 443	0.109 191	0.087 3665	0.168 17	0.185 359	0.201 147	0.134 193
27	9	47 381 504	11 798 016	0.090 0729	0.061 9535	0.169 748	0.197 141	0.219 559	0.124 459
6	13	47 815 680	12 558 464	0.100 372	0.071 0627	0.112 995	0.191 02	0.205 754	0.149 789
18	10	52 099 496	13 733 736	0.104 203	0.082 1789	0.083 482 8	0.205 028	0.215 253	0.198 921
29	9	58 888 704	14 645 792	0.088 6606	0.054 769	0.001 756 91	0.190 217	0.201 052	0.150 746
9	12	58 900 696	14 677 208	0.093 3132	0.072 6818	0.176 224	0.200 39	0.218 327	0.131 068
13	11	60 453 376	14 847 232	0.084 8635	0.056 9472	0.062 366	0.193 203	0.213 676	0.208 112
19	10	61 584 896	16 090 832	0.086 5202	0.052 442	0.155 109	0.226 729	0.245 587	0.127 568
30	9	65 276 416	16 252 736	0.089 2746	0.068 5755	0.083 983 5	0.202 21	0.239 333	0.095 948 5
32	9	79 412 992	19 729 792	0.085 6388	0.056 2649	0.123 084	0.200 964	0.232 005	0.141 376
21	10	83 685 188	21 982 132	0.099 3573	0.062 451	0.138 054	0.203 48	0.228 876	0.114 666
15	11	92 920 832	22 811 392	0.084 8161	0.055 0803	0.147 779	0.193 381	0.211 392	0.152 707
34	9	94 713 344	23 606 336	0.091 3722	0.063 8694	0.131 152	0.197 612	0.230 137	0.2171
22	10	96 084 402	25 272 244	0.106 789	0.080 8784	0.076 946 3	0.205 559	0.231 14	0.187 346

form a six-dimensional subspace [33]) that happened to be generated, since our measures (see immediately below) are singular on them, as well as more generally, degenerate density matrices, those density matrices not being of full rank (and hence having zero determinant). However, the possibility remains—in particular, since we will be computing (nonrobust) *averages*—that the behaviour of the measures for a relatively few *nearly* degenerate states, can strongly influence the results (cf tables 1 and 2).

By our purposeful design, the explicitly enumerated points are uniformly distributed (using the conventional parametrization) in the 15-dimensional convex set of 4×4 density matrices. We took several significant steps in our `MATHEMATICA` ('backtrack' [32, ch 27]) program to cut down on the (potentially huge) search spaces, by utilizing the requirement that all the principal

Table 2. Reanalyses of anomalous results (table 1) for $n_1 = 30$, $n_2 = 7$, using varying thresholds of degeneracy, as indexed by det ρ, below which the generated density matrices are rejected from further consideration.

Threshold on det ρ	ρ	$\rho_{separable}$	p_{min}	p_{KMB}	p_{max}	d_{min}	d_{KMB}	d_{max}
0	2 919 680	806 400	0.119 669	0.176 01	0.749 588	0.184 696	0.170 555	0.009 400 62
$\frac{1}{256} \times 10^{-4}$	2 913 536	801 792	0.102 275	0.066 4226	0.006 980 98	0.189 535	0.201 332	0.098 305 1
$\frac{1}{256} \times 10^{-3}$	2 856 704	796 672	0.123 362	0.108 123	0.386 157	0.180 807	0.191 661	0.101 308
$\frac{1}{256} \times 10^{-2}$	2 381 312	724 864	0.180 938	0.171 253	0.260 637	0.140 53	0.140 938	0.101 575

minors of a density matrix must be non-negative [34,37, theorem 7.2.5]. (A *sufficient* condition only, of possible interest, would be that the matrix is *diagonally dominant* [34].) Also, in our later, larger analyses, we exploited certain permutational symmetries.

We, then, employed an *ansatz* of ours [31], building upon a result of Dittmann [18, p 76] (pertaining to the Bures or minimal monotone metric) regarding the spectrum of the sum of the operators of left and right multiplication of matrices cf [38, p 112]. Utilizing it, we assigned as a weight to each density matrix (ρ) generated (the eigenvalues of which are denoted by λ_i), the volume elements of certain monotone metrics of particular interest. These elements we took to be of the form $[\Pi_{i,j=1}^{4} f(i,j)]^{\frac{1}{2}}$, where (the 'Morozova–Chentsov' function [2, 39, equation (3)]) $f(i,j)$ is equal to $\frac{2}{(\lambda_i+\lambda_j)}$ in the minimal monotone case, $\frac{(\lambda_i+\lambda_j)}{2\lambda_i\lambda_j}$ in the maximal monotone case, and for the Kubo–Mori/Bogoliubov (KMB) metric (associated with the relative entropy) [7, 40, 41], $\frac{\log\lambda_i - \log\lambda_j}{\lambda_i-\lambda_j}$. (In this last case, if $\lambda_i = \lambda_j$, we take $f(i,j) = \lambda_i^{-1}$. It is interesting to note that the inverses of these Morozova–Chentsov functions are simply well known indicators of *central tendency*, such as the arithmetic mean, the logarithmic mean, and the harmonic mean [42]. Choosing a particular monotone metric is, therefore, akin to selecting such an indicator.) We also checked if ρ satisfied the partial transposition condition, necessary for separability.

We now report several sets of results in this regard—but let us first make some important observations (taking into account that the determinant of a matrix is equal to the product of its eigenvalues). Using the formulae just given, one can show [43] that for an $N \times N$ density matrix (ρ), the volume element of the minimal monotone metric (and also the KMB metric) is directly proportional to $(\det \rho)^{-\frac{1}{2}}$, while for the maximal monotone metric, the volume element is directly proportional to $(\det \rho)^{\frac{1-2N}{2}}$. So, the divergence near the boundary of degenerate states ($\det \rho = 0$) of the volume element of the maximal monotone metric is much more severe than for the other two metrics under investigation. In fact, in our previous studies [6, 31], we have concluded that the integral of the volume element of the maximal monotone metric over the convex set of 2×2 density matrices does *not* converge (in contrast to those for the minimal monotone and KMB metrics). (For $N > 2$, however, the issue of convergence appears to be unsettled.) So, it would seem that—unless one chooses to remove from consideration (as was done in [6], for inferential purposes) those states the degeneracy of which exceeds some prescribed level [6] (cf section 3.4)—one cannot, in fact, define a probability distribution based on the maximal monotone metric. We have been able, however, for $N = 3$, by taking the limit of a certain ratio, to obtain associated *marginal* probability distributions using the maximal monotone metric [31].) Also, the maximal monotone metric is of substantial interest, in that it has been characterized as the most *non-informative* of the monotone metrics [6, 7].

The motivating hypothesis for pursuing the analyses immediately below is that one should be able to find values of the parameters n_1 and n_2 large enough (say, m_1 and m_2), so that the associated probabilities of disentanglement are within some ϵ of each other for *any* choices of n_1 and n_2 which *dominate* both m_1 and m_2. (It is useful to bear in mind, however, that there is a qualitative difference between analyses based on *even* or *odd* values of n_2, as will be indicated.) This would indicate a convergence of these probabilities in the continuum limit as n_1 and n_2 each become indefinitely large.

3.1. The case $n_1 = 23, n_2 = 7$

The choice of $n_2 = 7$ leads to a square grid, having 32 points—serving as trial off-diagonal entries—lying within the circle of radius one-half. (The particular arrangement of the lattice points, then, mandates that those density matrices we will be able to construct will have off-diagonal entries of modulus no less than $\frac{1}{7\sqrt{2}} \approx 0.101\,015$. This, in turn, implies that the product of any pair of diagonal entries of the density matrices will not be less than this value.) The numbers of density matrices we were, then, able to construct were 1 340 928. Of these, 356 096 passed the transposition test for separability. Applying the weights based on the three monotone metrics considered, we obtained prior probabilities of encountering separable states of

$$p_{min} = 0.111\,102 \qquad p_{KMB} = 0.087\,3186 \qquad p_{max} = 0.084\,6153. \tag{2}$$

Of course, these three values are all considerably less than both the ZHSL statistic of 0.632 ± 0.002 and the preferred one (of the three given) of section 2 based on Jeffreys' prior, that is $\approx$0.35.

We have also computed the 'degree of entanglement', $\sum_{i=1}^{4} \lambda_i' - 1$ (which must lie between zero and unity), for all the (1 340 928) density matrices and averaged the results with the same set of three weights as used to obtain (2). The outcomes were

$$d_{min} = 0.182\,06 \qquad d_{KMB} = 0.208\,022 \qquad d_{max} = 0.248\,457. \tag{3}$$

The corresponding value obtained by ZHSL for the 2×2 systems was considerably smaller, that is 0.057 [1, appendix B]. (ZHSL remarked that this quantity seemed to saturate at approximately 0.10 for large systems.)

3.2. The case $n_1 = 19, n_2 = 8$

Since the parameter n_2 is now an even integer, the origin $(0, 0)$ of the complex plane becomes, by our particular mode of construction, one of the 49 intersection points of the square grid lying within the circle of trial values for the off-diagonal entries. There are, then, no nontrivial lower bounds imposed on the moduli of these entries, as there are for odd values of n_2—such as *seven* in the immediately preceding analysis of section 3.1. We obtained 4 443 408 density matrices, of which 1 284 816 satisfied the separability criterion. Use of the volume elements of the three selected monotone metrics as weights resulted in

$$p_{min} = 0.147\,968 \qquad p_{KMB} = 0.123\,283 \qquad p_{max} = 0.055\,4999 \tag{4}$$

and

$$d_{min} = 0.186\,86 \qquad d_{KMB} = 0.184\,149 \qquad d_{max} = 0.177\,13. \tag{5}$$

3.3. Additional (nontruncated) analyses

Continuing along the same lines as sections 3.1 and 3.2, we have conducted analyses for additional choices of n_1 and n_2. (It is interesting to note that unit increases in n_2 are relatively more costly computationally than in n_1.) We report our accumulated set of results in table 1. The analyses are listed in increasing order of the total number of density matrices generated.

(During the course of conducting these analyses, we were able to undertake larger-sized studies, corresponding to those listed at the bottom of the table, by taking advantage of certain inherent permutational symmetries. An analogous assertion can be made in regard to table 4.)

As a general rule, the probability of disentanglement is greatest for the minimal monotone metric, although still markedly less than the ZHSL result (0.632 ± 0.002) or that of section 2 (≈ 0.35) based on Jeffreys' prior. The stability of the results, on the other hand, is least for the maximal monotone metric (in particular, notoriously so, for the case, $n_1 = 30$, $n_2 = 7$—but see section 3.5). This instability may be explainable by the fact that the volume element of the maximal monotone metric, as previously noted, is not normalizable (to form a probability distribution) over the convex sets of $N \times N$ density matrices (in particular, for $N = 4$), being highly singular near the degenerate states (while the volume elements of the minimal and KMB metrics, though, still singular, are markedly less so, and are apparently normalizable, extrapolating from the 2×2 case). So, one might rely upon either the minimal monotone metric or KMB-metric to provide estimates of the probabilities of disentanglement (separability)—as well as simulations of entangled systems, as ZHSL envisioned. We believe that estimates based on the minimal monotone metric should, at least for fine enough grids and simplicial decompositions, dominate estimates based on any other member of the *continuum* of monotone metrics. Following the arguments of Petz and Sudar [2], we contend that any estimates not based on such metrics (such as the 'over-parametrized' results of ZHSL [1]—cf [8]—and those of section 2 here) fail to meet certain natural requirements and should, thus, be taken *cum grano salis*.

Let us also note a specific relation between the minimal monotone (Bures) metric and the results of ZHSL. The *scalar curvature* of this metric has recently been shown to attain its *minimum*, $\frac{(5N^2-4)(N^2-1)}{2}$, for the totally mixed N-dimensional (tracial) state (corresponding to the $N \times N$ diagonal density matrix having all its nonzero entries equal to $\frac{1}{N}$), and to diverge on the degenerate states, those not of full rank [19]. Now, in their analysis, ZHSL concluded both that all states in a small enough neighbourhood of the totally mixed state are separable, and that the 'purer a quantum state is, the smaller its probability of being separable' [1]. Braunstein *et al* have given 'a constructive proof that all mixed states of N qubits in a sufficiently small neighbourhood of the maximally mixed state are separable' [35], while Vidal and Tarrach have also reached the same conclusion [36].

3.4. Reanalysis of the anomalous $n_1 = 30$, $n_2 = 7$ case based on truncation of states near to degeneracy

We have also considered the possibility of introducing a third parameter of choice, that is $\det \rho$—in addition to n_1 and n_2—into our computations. It would control the level of degeneracy below which we reject for further consideration (due to the singular behaviour of the volume elements of the monotone metrics), the (nearly degenerate) density matrices our explicit enumeration method of section 3 generates. (This third parameter has been implicitly zero in section 3.) We have, in fact, conducted three additional analyses for the case $n_1 = 30$, $n_2 = 7$, for which we previously obtained results of a peculiar nature (table 1). The largest possible value the determinant of a 4×4 density matrix can possess is $(\frac{1}{4})^4 = \frac{1}{256} = 0.003\,906\,25$. In the first analysis, we rejected all those density matrices with determinants less than $\frac{1}{256} \times 10^{-4}$, in the second, $\frac{1}{256} \times 10^{-3}$ and in the third, $\frac{1}{256} \times 10^{-2}$. We report these results in table 2.

It appears then (based on the smallest nonzero threshold, that is $\frac{1}{256} \times 10^{-4}$) that the previously reported (zero-threshold) anomalous behaviour for the maximal and KMB monotone metrics was attributable to some set (the number of which we are not

Table 3. Results of *random* searches of the 15-dimensional parameter space, using differing values of the radius (r) of the circle in the complex plane centred at $(0, 0)$, from which the possible off-diagonal entries of the 4×4 density matrices are chosen.

r	Searches	ρ	$\rho_{separable}$	p_{min}	p_{KMB}	p_{max}	d_{min}	d_{KMB}	d_{max}
$\frac{1}{2}$	847 500 000	49	12	0.071 1773	0.054 8709	0.026 978 6	0.197 979	0.215 5	0.252 218
$\frac{5}{12}$	387 900 000	175	47	0.098 809	0.040 8168	0.002 182 39	0.173 6	0.180 24	0.194 678
$\frac{1}{3}$	351 700 000	2 438	619	0.085 3483	0.065 4313	0.180 815	0.201 774	0.222 59	0.147 024
$\frac{1}{4}$	74 300 000	15 701	3912	0.084 6071	0.036 407 1	0.001 489 44	0.178 73	0.202 29	0.290 831

certain) of near-degenerate states which, in fact, passed the partial transposition test for separability.

3.5. *Analyses based on* randomized *searches*

In the previous quantum-theoretic statistical analyses of this section, we employed systematic explicit enumeration methods to generate 4×4 density matrices, which we then tested for separability. We embarked on such a course after initial computations indicated that it was extremely difficult to locate the four-by-four density matrices (in the ambient 15-dimensional parameter space) using *random* search methods, in the fashion of ZHSL [1] and section 2 of this paper. Nevertheless, at a later point, we chose to intensively pursue such a strategy.

In almost 850 000 000 *ab initio* searches, we succeeded in obtaining (only) 61 density matrices—of which 12 turned out to be separable. Realizing that the 'hit rate' would be enhanced if, instead of searching for possible off-diagonal entries in the circle of radius one-half in the complex plane, we also conducted analyses (though at the risk of introducing possible biases) based on radii of one-third and one-fourth, as well (and also, in a supplementary analysis, five-twelfths). The results are reported in table 3. (As in section 2, standard deviations were *not* determined, so no specific assessment of the number of significant digits in the probabilistic results is immediately available.) They are, then, arguably, generally consistent with the sets of smaller probabilities reported in table 1, in particular, for those based on the largest number of generated density matrices (corresponding to the bottom rows of the table), in which we naturally repose the greatest confidence.

3.6. *Probabilities as a function of the participation ratio*

In figure 1, we show (using bins of width 0.05), relying upon the analysis for the 2×2 case $n_1 = 22$, $n_2 = 10$, the conditional probability (P_{sep}) of separability based on the minimal monotone metric, for a given participation ratio R (defined as the reciprocal of the trace of the square of the density matrix [1, equation (17)]). In figure 2, we show its counterpart based on the KMB metric. (These two figures—both having an unexplained 'anomalous blip' in the interval [1.65, 1.7]—are the monotone metric analogues of figure 2(b) of [1]. It is encouraging, however, that the 'blip' does not seem to appear in analogous plots for other values of n_1 and n_2. The value of R, in the $N = 2 \times 2$ case, must lie between 1 and 4. If $R \geqslant 3$, the density matrix must be separable [1, equation (18)].)

Życzkowski [44], drawing upon a long list of open problems he presents, considers one of the 'most relevant' to be the question of 'whether the dependence of the conditional probability on the participation ratio, obtained for product measures, holds also for the measures based on the monotone metrics'. He has hypothesized the existence of certain universal/metric-independent features in this regard, that is, he proposes that all 'reasonable' metrics should

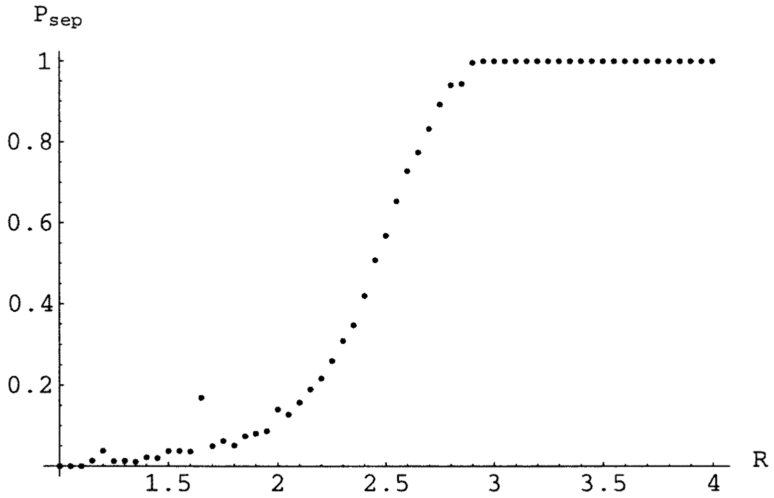

Figure 1. Conditional probability—based on the minimal monotone (Bures) metric—for $N = 2\times2$ of finding a separable state, given a certain range (of width 0.05) of the participation ratio R, for the scenario $n_1 = 22$, $n_2 = 10$.

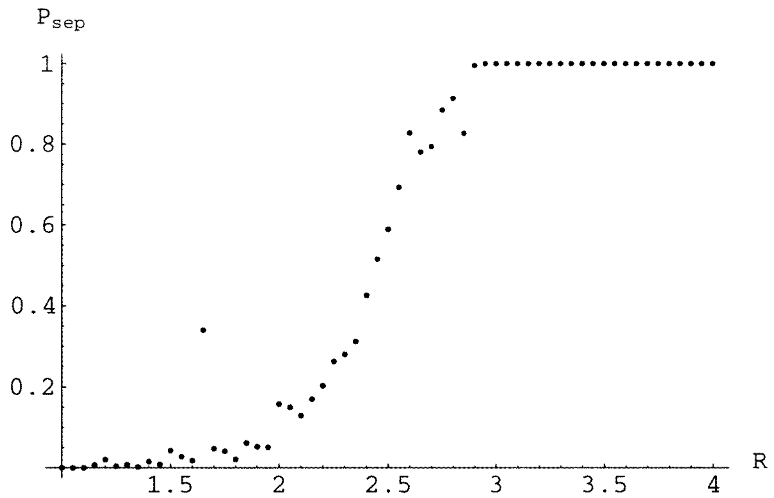

Figure 2. Conditional probability—based on the KMB metric for $N = 2 \times 2$—of finding a separable state, given a certain range (of width 0.05) of the participation ratio R, for the scenario $n_1 = 22$, $n_2 = 10$.

yield similar such plots. (He has, in fact, superimposed the figures here upon those previously generated by him, and found a strong degree of resemblance between them.)

In figures 3 and 4, we show (again for the case $n_1 = 22$, $n_2 = 10$ of table 1) the probabilities of our generating a density matrix (either separable or inseparable) based on the minimal monotone and KMB metrics, respectively. (These are the monotone metric counterparts of figure 2(*a*) of [1]. Since we find more probability concentrated at smaller values of R than did ZHSL, these two figures help us to understand why we obtain smaller *overall* probabilities of separability—in particular, less than 0.5 in the $N = 2 \times 2$ case—than their 'surprising' result of 0.632 ± 0.002.)

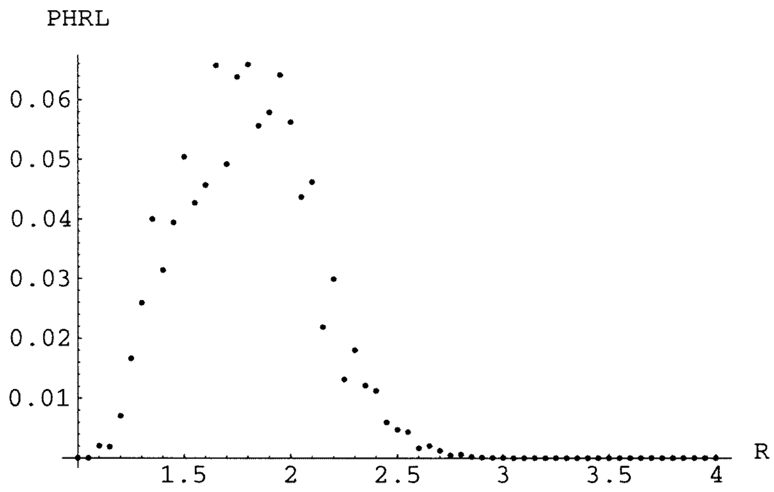

Figure 3. Probability—based on the minimal monotone (Bures) metric—for $N = 2 \times 2$ of finding a quantum state (whether separable or not), given a certain range (of width 0.05) of the participation ratio R, for the scenario $n_1 = 22, n_2 = 10$.

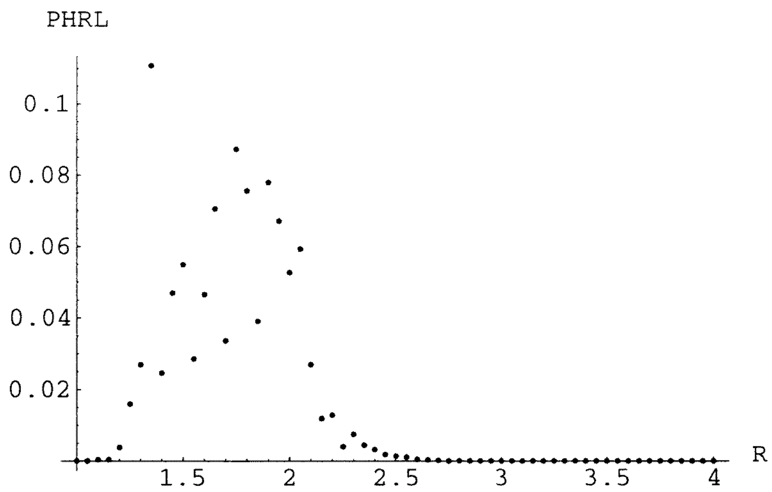

Figure 4. Probability—based on the KMB metric—for $N = 2 \times 2$ of finding a quantum state (whether separable or not), given a certain range (of width 0.05) of the participation ratio R, for the scenario $n_1 = 22, n_2 = 10$.

3.7. The case of 2×3 *systems*

In table 4, we report initial findings (of an, unfortunately, rather unstable nature) for the 2×3 systems—parallel to those given in table 1 for the 2×2 systems. (We note that the probability of separability obtained by ZHSL [1] for the 2×3 systems was 0.384 ± 0.002 and, with the alternative use of the Jeffreys' prior in section 2.3, 0.122.) There are now six diagonal entries (associated with n_1) and 15 pairs of off-diagonal entries (associated with n_2) to consider, so computational demands are substantially increased. We, of course, expect the probabilities of separability to be *less* than the corresponding ones in the 2×2 case reported in table 1, and this is certainly the case for the most extensive analysis ($n_1 = 20$, $n_2 = 8$).

Table 4. Analogues for the 2×3 systems of the results of table 1.

n_1	n_2	ρ	$\rho_{separable}$	p_{min}	p_{KMB}	p_{max}	d_{min}	d_{KMB}	d_{max}
8	8	7 581	5 205	0.643 091	0.654 085	0.678 443	0.025 4769	0.024 673	0.023 0053
11	6	35 268	9 828	0.000 171 812	0.000 192 414	0.000 212 583	0.592 094	0.592 009	0.591 929
14	6	149 607	59 727	0.368 812	0.425 491	0.461 59	0.147 718	0.118 212	0.100 94
15	6	158 522	59 185	0.147 933	0.152 787	0.128 344	0.299 006	0.281 777	0.235 139
13	9	245 760	8 448	0.034 375	0.034 375	0.034 375	0.185 994	0.185 994	0.185 994
9	8	235 616	65 840	0.234 146	0.262 858	0.266 667	0.080 3952	0.065 4659	0.063 7942
15	9	245 760	768	0.003 125	0.003 125	0.003 125	0.182 635	0.182 635	0.182 635
14	9	368 640	9 600	0.026 041 7	0.026 041 7	0.026 041 7	0.188 924	0.188 924	0.188 924
16	6	370 479	131 055	0.005 849 08	0.017 268 2	0.359 634	0.581 471	0.558 051	0.119 815
17	6	557 304	164 264	0.000 248 636	0.000 243 731	0.000 240 557	0.590 97	0.591 328	0.591 453
10	8	579 186	150 090	0.173 755	0.174 011	0.174 992	0.184 237	0.194 057	0.195 405
12	8	1 352 182	303 022	0.046 340 8	0.087 293 6	0.195 22	0.383 656	0.307 713	0.117 593
11	8	1 593 588	520 068	0.299 328	0.309 032	0.326 253	0.099 5446	0.096 8566	0.094 0759
22	6	2 875 965	974 818	0.016 003 4	0.125 932	0.072 155 8	0.562 473	0.374 128	0.259 626
24	6	3 870 989	1 360 213	0.192 395	0.199 33	0.314 609	0.292 782	0.268 782	0.140 023
13	8	4 408 872	881 397	0.055 189 2	0.065 933 3	0.256 791	0.294 217	0.259 817	0.091 5806
14	8	6 073 071	882 781	0.000 948 857	0.000 644 427	0.009 523 89	0.616 86	0.476 343	0.359 429
16	8	7 373 379	1 609 392	0.103 614	0.121 313	0.203 796	0.204 274	0.183 523	0.119 163
26	6	7 696 926	2 514 130	0.1132	0.111 881	0.099 992 4	0.368 272	0.289 389	0.229 179
15	8	15 603 746	2 109 650	0.000 899 908	0.001 623 05	0.001 146 51	0.639 42	0.599 576	0.461 553
17	8	19 413 528	3 311 159	0.054 504	0.056 265 6	0.039 816 8	0.323 892	0.298 912	0.259 056
18	8	29 075 408	5 061 131	0.081 246	0.073 791 2	0.095 851 3	0.2304	0.215 317	0.181 838
20	8	45 002 652	7 755 473	0.004 014 27	0.013 180 4	0.052 579 1	0.606 695	0.487 055	0.206 391

The somewhat counterintuitive observation that for $n_1 = 14$, the choice of $n_2 = 8$ leads to many more generated density matrices than for $n_2 = 9$, is comprehensible in that only for even values of n_2 are no nonzero lower bounds placed on the possible absolute values of off-diagonal entries. We were not able for any $n_2 = 7$ scenario—due to memory limitations—to find a large enough n_1, for which any density matrices at all were generated. We also possess no immediate explanation for the equality of the three p and d for the three cases involving $n_2 = 9$. (The relatively large probabilities for the scenario, $n_1 = 24$, $n_2 = 6$ may be attributable to a 'number-theoretic' effect, given that 24 is exactly divisible by six.)

A randomization approach, such as we pursued in section 3.5 for the 2×2 systems, would clearly yield even fewer density matrices for a given number of independent searches than there (table 3).

4. Concluding remarks

We have presented in this study, two forms of evidence (one essentially classical and the other quantum-theoretic in nature) that the specific choice of (product) measure of ZHSL [1] led them to substantially overestimate the extent to which quantum systems—in particular, for $N = 2\times2$ and 2×3—should be considered to possess, in some natural *a priori* sense, the property of separability or disentanglement. The preponderance of evidence adduced indicates that the probability of separability for the $N = 2 \times 2$ systems, based on the minimal monotone (Bures) metric is no greater than 11%—and if one views the evidence somewhat less conservatively, perhaps less than 10%. In turn, estimates founded on any other member of the continuum of monotone metrics should be lower still. For instance, for the Kubo–Mori/Bogoliubov metric [7,40,41], an estimate of 9% would seem conservatively high. Apparently, the *maximal* monotone metric—the volume element of which possesses a high degree of singularity on the degenerate states ($\det \rho = 0$), associated with its conjectured nonnormalizability over the 15-dimensional convex set of states—must, in some (perhaps limiting) sense, furnish a *lower* bound on the probability of separability. This bound would have to be strictly greater than zero, if the related arguments made in [1, 35, 36, 44], in fact, apply.

Let us also note that in continuing work, pertaining to [24], we have found a quite interesting distinguished role (that of yielding both the *minimax* and *maximin* in universal quantum coding) for a monotone metric that has not apparently previously been noted. Its associated Morozova–Chentsov function,

$$e(\lambda_i{}^{\lambda_i}/\lambda_j{}^{\lambda_j})^{\frac{1}{\lambda_j-\lambda_i}} \tag{6}$$

is simply the reciprocal of the *exponential* or *identric* mean [42] of λ_i and λ_j. The behaviour of the related monotone metric appears to be quite close to that of the minimal (Bures) monotone metric.

The need for additional computational work (possibly utilizing supercomputers) is indicated, in regard to what we contend are the theoretically superior (properly parametrized) quantum-theoretic analyses of section 3, in order to more closely pinpoint estimates. Such analyses could be based on finer simplicial decompositions for the trial diagonal entries (that is, higher values of n_1) and finer square grids for the trial off-diagonal entries (that is, higher values of n_2), than those reported in section 3, and/or possibly randomization procedures, as in section 3.5.

At several points in this paper, we have indicated that the analyses of ZHSL [1] were 'over-parametrized', in that $N^2 + N - 1$ parameters were employed, rather than $N^2 - 1$, as is clearly most natural for the $N \times N$ density matrices (which form an (N^2-1)-dimensional convex set). However, in a personal communication, M Byrd has asserted that this bothersome feature could be avoided, since $N - 1$ Euler angles (in addition to the 'phase', as is well known) can be seen to, in fact, vanish in the ZHSL-type representation [1, equation (25)] of a density matrix in the product form $U'DU$. Byrd has been able to explicitly show this in the case $N = 3$, based on the Euler angle parametrization given in [45] (the angles c and ϕ vanishing) and contends that analogous phenomena must hold for $N > 3$, as well (cf [8]). (This vanishing does not appear to occur with the particular Euler angle parametrizations (associated with Hurwitz) used by ZHSL, given in [29, 46]. Byrd suggests that this is because the 'diagonal matrices that make up the maximal torus' do not appear on the end, while if they did, they would commute with the diagonalized density matrix.) This highly interesting line of thought would suggest that the analyses of ZHSL, Życzkowski [44] and those of section 2 here (but, of course, not those 'properly parametrized' ones of section 3) should be repeated in such a more parameter-wise economical framework, and the new results compared with those previously obtained, to see whether any differences are found (cf [47]).

Acknowledgments

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