RESEARCH ARTICLE

Classical Computer Assisted Analysis of Small Multiqudit Systems

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ABSTRACT Quantum computation model is regarded as a model which can overcome barriers in calculations efficiency of problems which appear in modern science. In spite of hardware development, in particular a recent emergence of several different physical installations of the pioneering quantum machines, the contemporary and numerical analysis of problems concerning quantum computing is very important. In the first part of this article, some useful computing techniques for quantum registers processed by a quantum circuits are presented. Applied classical parallel computational techniques are utilised to shorten the whole computational time. New methods of processing state vectors for qudits and density matrices are presented, indicating which operations may be performed in parallel in the context of the implementation of local unitary operations. There is also shown, how to use the reduction operation in parallel implementation of the von Neumann measurement by performing local measurements on a system of qudits. In addition to the purely technical results as described above, the paper includes also a bunch of purely theoretical results which substitute a solid mathematical ground for the computations performed with the help of the computational routines as described in Section III. In particular, a discussion concerning general multi-qudit quantum states through the prism of Entropy and Negativity measures of entanglement included in has been presented. Additionally, the notion of the total entanglement has been introduced. For certain classes of popular multi-qudit states, the introduced deficits of entanglement defined with the use of von Neumann Entropy and Negativity have been discussed. In particular, by the use of Gram matrix technique, the corresponding deficits of entanglement in the analysed states have been computed in an explicit way. Additionally, some new results on AME states for some multiqudit systems are also included in Section V. The last part of the article presents some numerical experiments on multi-qudit entanglement and determination of total entanglement values for convex combinations of GHZ and W states. Some details concerning technical nature of results are included in the attached Appendix.

INDEX TERMS Quantum computing, quantum circuits, entanglement, entropy, Schmidt decomposition, parallel computations.

I. INTRODUCTION

Quantum computing is believed to be a source of new ideas and solutions leading to a very significant increase of computations performance, especially by shortening its duration

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in many areas of science e.g. applications to fuzzy logic [1], machine [2] and deep learning methods [3]. Unfortunately, quantum computers are still in an early stage of development what may be seen in restricted capabilities and an appearance of a high intensity of errors appearance during the computational process. Presently, there exist some physical installations of a small scale quantum computational

systems, e.g. IBM Q Experience [4], D-Wave Systems [5], Rigetti Computing [6], IonQ [7], Xanadu Quantum Technologies [8]. However, theoretical analysis – but also computation and simulation (a very actual and complete list of software simulators is available at Quantiki [9]) – in the field of quantum computing are still a basic cognitive tools, despite the expected quantum supremacy [10]–[12] with large scale quantum machines [13]. On the other hand, small quantum computers with intermediate noise scale, so-called NISQ computers, are used to perform quantum computations and simulations of quantum systems that are much larger than the NISQ machine itself [14], nowadays.

The reasons mentioned above maintain importance of developing classical simulation techniques for quantum computations. This approach has already appeared in nineties of the previous century [15] and it is still utilised what is shown in [16], [17]. For example, recent works on the topic show that even some computationally hard problems may be solved successfully with use of the real quantum computer [18], e.g. tensor networks are capable of solving high-dimensional problems [19]. Other simulations techniques of quantum programs on modern multi-GPU platforms may be crucial in validating quantum algorithms i.e. the robustness of the proposed error corrections codes against quantum noise, and designing applications for future large scale and universal quantum computers [20], [21] what is also confirmed in [22] where the constructed simulator is highly efficient.

To sum up, thanks to the computer simulations of quantum computing, it is possible e.g. to model a quantum noise and check whether analysed system is capable to successfully perform calculations. Therefore, it seems valuable to propose efficient, or at least better, approaches to performing numerical calculations. In this paper, we discuss classically based computational solutions prepared for simulation of quantum circuits what causes a need of basic concepts introduction, like quantum registers, vector states, density matrices, quantum measurement, etc. The nature of quantum computation, where parallel processing [23], [24] is present on the exponential level, obliges us to build a very demanding model – especially, in the context of restricted utilisation of additional temporary data buffers which are necessary to process a vector state or a density matrix.

This paper is organised as follows. In Section II, there are included selected basic concepts relating to simulations of quantum circuits. Next, in Section III, computational procedures are shown which serve to process quantum register in a form of vectors (our approach is also adapted to density matrices case). The notion and importance of local operations is also highlighted, and computational complexity with the possibilities of parallel processing is analysed. In Section IV, several new variants of operator decompositions for general multi-qudit quantum states are discussed. In particular, a canonical relation between the coefficients of basic Hilbert-Schmidt inner product based on Schmidt decomposition with coefficients arising from the combined spectral and Schmidt decompositions of the corresponding eigenstates

TABLE 1. Some symbols, notations, sets and functions used in the paper.

Notation	Description
$\mathbb{N}$	set of integer numbers
$\mathbb{R}$	set of real numbers
$\mathbb{C}$	set of complex numbers
$\mathfrak{U}$	set of unitary operators
$\mathcal{H}$	Hilbert space
$\alpha, \beta, \gamma, \lambda, \ldots$	real or complex numbers
$\otimes$	tensor product
$\oplus$	direct sum of matrices/operators
$\times$	multiplication or product of two scalars and/or matrices
$\mathfrak{M}$	set of matrices
$\mathrm{tr}\,(-)$	trace of operator/matrix
$\mathrm{tr}_S\,(-)$	partial trace of operator/matrix for subsystem S
$\mathbb{I}, \mathbb{I}_N$	identity matrix/operator, identity operator defined in system with N qudits
$\mathbb{I}_{d^N}$	identity operator with declared dimensionality
$u_{(i)}$	operator U applied to the i-th qubit/qudit in a quantum register
E	projection matrix
$A^\star, A^\dagger$	conjugation of matrix, hermitian adjoint of matrix
$\langle - | - \rangle$	inner product
$\partial E(\mathbb{C}^d)$	set of pure states on $\mathbb{C}^d$
$1:n$	means the sequence of $1, 2, 3, \ldots, n$
$\mathfrak{I}_n = \{1, 2, 3, \ldots, n\}$	set of $1, 2, 3, \ldots, n$
$(i_1, \ldots, i_k) \subset \mathfrak{I}_N$	elements of tuple belonging to the set $\mathfrak{I}_N$
$\mathbb{U}(d)$	group of unitary matrices acting in $\mathbb{C}^d$

is presented there for a general quantum states [25]. Some problems concerning multi-qudit entanglement anatomy are presented in Section V. In this section, von Neumann entropy, negativity, and entanglement deficit notions for some quantum states, like multi-qudit GHZ and W states, are discussed. In the last part of Section V, some numerical examples are also presented. Appendix includes mathematical description of local quantum operation introduced in Section III. Summary, acknowledgements, and bibliography end this article.

II. MATHEMATICAL PRELIMINARIES

In this part of the article, the basic mathematical concepts directly referring to quantum states processing are presented. In particular, we describe single-qubit (single-qudit) unitary operations, controlled two-qubit (two-qudit) operations, and von Neumann quantum measurement. Table 1 contains symbols, notations, sets, and functions which are used in further parts of the paper.

We denote a set of complex numbers as $\mathbb{C}$, the real values as $\mathbb{R}$, and integers by $\mathbb{N}$. The floor function for real numbers will be denoted as $\lfloor \cdot \rfloor$.

Let the space $\mathcal{H} = \mathbb{C}^{d^N} = \mathbb{C}^d \otimes \mathbb{C}^d \otimes \mathbb{C}^d \otimes \ldots \otimes \mathbb{C}^d$ be a finite d^N dimensional complex Hilbert space where d and N are integers $d \geq 2$, $N \geq 1$. The symbol $\otimes$ stands for the tensor product and it is repeated N times.

A given pure quantum state $|\Psi\rangle \in \mathcal{H}$ forms a quantum register containing N quantum information units. It should be emphasised that in the further part of the article the expression quantum register is a substitute of quantum state denoted as $|\Psi\rangle$. Naturally, the Dirac notation is applied to express so-called pure states, i.e. column vectors $|\Psi\rangle$ (additionally by $\langle\Psi|$ we denote co-vector i.e. transposed and complex conjugated component-wise row vector from $|\Psi\rangle$).

The generalised unit of quantum information is called a qudit (its application to quantum computing is discussed in paper [26]):

$$|\Psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle + \ldots + \alpha_{d-1}|d-1\rangle \quad \alpha_i, \in \mathbb{C}, \quad (1)$$

and $\sum_{i=0}^{d-1} |\alpha_i|^2 = 1$ where α_i are so-called probability amplitudes. For $d = 2$, a unit termed as a qubit (quantum bit) is obtained. Another well-known unit of quantum information is a qutrit with $d = 3$. The degree of freedom (marked as d) is an integer which points out the informational capacity of single qudit.

An arbitrary qubit vector state, which is expressed with the use of basis states, may be denoted as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}, \quad \alpha, \beta \in \mathbb{C} \text{ and}$$
$$|\alpha|^2 + |\beta|^2 = 1, \quad (2)$$

where the basis vectors $|0\rangle$, $|1\rangle$ are:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad (3)$$

and mentioned vectors are orthonormal, and are also called the standard computational basis.

For vector states with $d \geq 2$, the following basis vectors are very often marked with integers from 0 to $d - 1$ written in decimal form, but the binary number or general dit coding is also used. For example, the state $|010\rangle$ is a three qubit state where the first qubit is $|0\rangle$, the second $|1\rangle$, and the third $|0\rangle$. Of course, for qubits ($d = 2$), 010 is treated as the binary number. If there is a four qutrit state $|0221\rangle$, then 0221 is a ternary number.

Any complete factorizable state of N qudits may be put into a quantum register with the use of tensor product:

$$|\Psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle. \quad (4)$$

Remark 1: In this paper, for simplicity, all qudits $|\psi_i\rangle$, $1 \leq i \leq N$ have the same dimension. It should be emphasised that numerical routines which will be presented later in the text, can be also applied to the registers with qudits possessing different dimensions d. In this case, an additional array of used d values for the corresponding qudits is required.

States of quantum registers may be expressed also as density matrices ρ. The density matrix for the pure state $|\Psi\rangle$ is:

$$\rho = |\Psi\rangle\langle\Psi|. \quad (5)$$

It should be mentioned that in case of a density matrix ρ, we sometimes also use the name quantum register.

Remark 2: It should be also stressed that some pure quantum states cannot be presented as a tensor product states of single qudits, as in (4). These states are called entangled states [27]–[30]. As an example of entangled state, we can present one of so-called Bell states (or EPR pairs):

$$|\psi^+\rangle = \frac{1}{\sqrt{2}}\Big(|00\rangle + |11\rangle\Big). \quad (6)$$

Further definitions of important notions, in the context of quantum entanglement as von Neumann entropy and Schmidt decompositions, will be presented in Section IV and Section V.

A fundamental restriction of efficient structures processing, containing information about quantum states, is based on their dimensions. If N qubit system is taken into consideration, i.e. $d = 2$, then dimensions of vector Ψ and matrix ρ are:

$$\dim|\Psi\rangle = 2^N, \quad \dim\rho = |\Psi\rangle\langle\Psi| = 2^N \times 2^N. \quad (7)$$

For any $d \geq 2$, the dimensionality of quantum states, expressed as the vector or the matrix, is as follows:

$$\dim|\Psi\rangle = d^N, \quad \dim\rho = |\Psi\rangle\langle\Psi| = d^N \times d^N. \quad (8)$$

Taking into account Remark 2 for entangled systems, there is no possibility of expressing a quantum register as a direct tensor product of smaller subsystems.

One of the basic operations performed on a given register $|\Psi\rangle$ are unitary operations given by unitary matrices U. The second type of operation which can change a state of a quantum register is measurement. The von Neumann measurement (VNM) [31] is a basic scheme which may be presented in the context of quantum register measurements.

The unitary operation performed on the quantum register $|\Psi\rangle$ is described by the matrix U (it is naturally a unitary matrix, i.e. $UU^\dagger = \mathbb{I}$). In the context of the so-called quantum circuits, a unitary operation is called a quantum gate. Its action on the vector state $|\Psi\rangle$ and the density matrix ρ is described as follows:

$$U|\Psi\rangle = |\Psi'\rangle, \quad U\rho U^\dagger = \rho'. \quad (9)$$

In other words, the operation U transforms state $|\Psi\rangle$ (or state ρ in the case of density matrices) to the state $|\Psi'\rangle$ (or to the state ρ', respectively).

It is worth to mention that the global unitary operation can be composed from a smaller unitary operations. As an example, let us consider the following unitary operator U:

$$U = u_{(1)} \otimes \mathbb{I}_{(2)} \otimes u_{(3)} \otimes \mathbb{I}_{(4)}, \quad (10)$$

where only two of four qubits are modified, because operators $\mathbb{I}_{(2)}$, $\mathbb{I}_{(4)}$ are identity operations, and $u_{(1)}$, $u_{(3)}$ are unitary operations performed on the first and the third qubit. Let us emphasise that this product-like structure of U allows defining a computational procedure which, in spite of exponential grow of sizes of quantum state, processes the quantum register by the direct use of the parallel computing methods. Adequate solutions are shown and discussed in Section III.

In case of qubits, a basic set of Pauli operators (together with the identity operation) and Hadamard gate can be expressed with the following matrix representations:

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$
$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (11)$$

Next to single-qubit (qudit) gates, there also exist controlled quantum gates. A basic example of such a gate is the controlled negation operation – CNOT. The way it works for qubits can be written as follows:

$$
\begin{aligned}
\text{CNOT}|00\rangle &= |00\rangle, \\
\text{CNOT}|01\rangle &= |01\rangle, \\
\text{CNOT}|10\rangle &= |11\rangle, \\
\text{CNOT}|11\rangle &= |10\rangle.
\end{aligned}
\tag{12}
$$

If the state of the first qubit is $|1\rangle$, then the state changing operation is performed on the second qubit using a negation gate – NOT. The first qubit is called the controlling qubit and the second qubit is the controlled qubit. The described mode of operation can be also expressed in the form of a matrix:

$$
\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.
\tag{13}
$$

The CNOT gate works on two qubits, but there are variants with more controlling lines, e.g. Toffoli gate [36]. An important property of the CNOT gate is the possibility of introducing entanglement to the quantum register, because the introduction of entanglement is not possible using only gates operating on one qubit/qudit. The entanglement phenomenon is an important and vital quantum resource, necessary to perform teleportation protocol [37], [38].

Remark 3: It is important to notice that unitary operations, just like entangled states (Remark 2), may have a form which cannot be obtained as a result of other local unitary operations in the tensor product. These operations may be called non-primitive [39]. The basic example of such gate is the CNOT gate, i.e. controlled negation:

$$
CNOT = \mathbb{I} \oplus X,
\tag{14}
$$

where X represents the unitary negation (Pauli gate X) and $\oplus$ stands for direct sum of matrices. However, the presence of so-called controlling lines decreases by d^c the number of computational operations which have to be performed on a quantum register, where d is a freedom level and c is the number of controlling qudits.

In the context of quantum gates, the notion of a universal quantum gates set should be recalled. It can be said that a set of universal quantum gates is represented by any set of gates with following property: any other unitary operation can be expressed as a finite sequence of gates from the universal set of gates. For the case of qubits, the rotation gates build on the base of Pauli gates and CNOT gate can be regarded as the universal set of quantum gates, for more details please see [40].

The von Neumann measurement [31] is a basic scheme which may be presented in a context of quantum register measurement. The operation is described by the observable M which is a Hermitian operator acting in a subspace of a system to be measured (naturally, also the whole system may be measured not only its subspace). The spectral decomposition of observable M is:

$$
M = \sum_i \lambda_i P_i,
\tag{15}
$$

where P_i is a projector on eigenspace of M with the eigenvalue λ_i. The measurement's results are represented by the eigenvalues λ_i. The probability of obtaining the result λ_i on the state $|\psi\rangle$ is given as:

$$
p(\lambda_i) = \langle \Psi | P_i | \Psi \rangle.
\tag{16}
$$

After a measurement, the result λ_i influences the system's state in the following way:

$$
|\Psi'\rangle = \frac{P_i|\Psi\rangle}{\sqrt{p(\lambda_i)}}.
\tag{17}
$$

Remark 4: Quantum measurements may be realised in various computational bases what requires a selection of proper set of projectors. However, in case of the standard basis, a very efficient implementation of measurement can be presented, what is shown in Section III-A.

A broader introduction to quantum gates, quantum computation models, and quantum circuits is beyond the scope of this article. A solid introduction to the topics of quantum circuits can be found, for example, at [41]. Let us just mention that the Pauli X gate plays the role of a negation gate, that is, like its classical equivalent, the state $|0\rangle$ transforms into $|1\rangle$ and by analogy $|1\rangle \rightarrow |0\rangle$.

III. PROCESSING OF QUANTUM REGISTER FOR QUANTUM CIRCUITS

Processing of a quantum register [41], in the context of quantum circuits simulation, can be depict by the use of three main procedures: single unitary operators, controlled unitary operators, and a measurement operations.

Utilising the basic properties of the tensor product, which describes the whole quantum register, we can present some characteristic values for effective addressing of particular probability amplitudes in a quantum state. The applied solutions, presented in previous publications [42], and in our papers [43], [44], refer mainly to qubits. In this paper, the proposed routines are extended to the case of qudits. Parallel techniques, in a context of quantum simulators harnessing qubits, are also known [45]–[47] but routines, presented here, can be implemented directly and do not depend on other computational libraries for linear algebra. We also directly emphasise which operations can be parallelised. The procedures, shown in this section, have a characteristic feature: the operations are always grouped in several groups which contain one set of local operations which may be executed regardless of other sets of local operations. This makes possible the parallel processing of indicated local operations, and applying additional optimisation when it comes to operational memory access.

In the proposed calculation procedures, in the context of the measurement implementation, we propose the use of

a parallel reduction operation. The reduction operation itself can be described as the transformation of a sequence of data, e.g. an array of elements, into a single element/scalar. An example of this type of operation is the sum of array elements, e.g.:

$$T = [1, 3, 5, 7, 9, 11], \tag{18}$$

the result of the reduction is the following operation:

$$T_r = 1 + 3 + 5 + 7 + 9 + 11. \tag{19}$$

Naturally, the sum operation can be split into e.g. pairs of sums:

$$T_{r_1} = 1 + 3, \quad T_{r_2} = 5 + 7, \; T_{r_3} = 9 + 11. \tag{20}$$

Each of these operations can be performed independently of the others, and then the partial results can be combined together. Despite the triviality of the example, in an analogous way, it is possible to effectively implement the state's measurement of a given quantum register, what is shown in the next Section III-A.

Additionally, for a detailed mathematical description of an arbitrary local quantum operation's action on the general multi-qudit states, we refer to the paper [48] and Appendix of the present article.

A. LOCAL MEASUREMENT OPERATION AS PARALLEL REDUCTION

The von Neumann measurement [31] in the standard basis may be efficiently performed by the use of the parallel reduction. Let us consider a system composed of two qutrits being in the pure state $|\Psi\rangle = |ab\rangle = \sum_{i=0}^{8} \alpha_i |i\rangle$ and the second qutrit b is measured. If the measurement is realised as described in Section II, then three probability values have to be calculated: $p(\lambda_0^b), p(\lambda_1^b), p(\lambda_2^b)$. However, instead of vector operations, three following sums have to be computed:

$$
\begin{aligned}
p(\lambda_0^b) &= p_0 = |\alpha_{00}|^2 + |\alpha_{10}|^2 + |\alpha_{20}|^2, \\
p(\lambda_1^b) &= p_1 = |\alpha_{01}|^2 + |\alpha_{11}|^2 + |\alpha_{21}|^2, \\
p(\lambda_2^b) &= p_2 = |\alpha_{02}|^2 + |\alpha_{12}|^2 + |\alpha_{22}|^2,
\end{aligned}
\tag{21}
$$

where lower indexes are ternary numbers. All above operations may be performed in separate threads. The parallel reduction is easy to apply. The reduction process may be depict in a form of a tree what is shown in Fig. 1.

If the result of the von Neumann measurement is denoted as λ_i, then according to (16), probability is expressed as $p(\lambda_i) = \langle \Psi | P_i | \Psi \rangle$ where P_i is a projector representing the result eigenspace. Performing the measurement operation requires the modification of a vector which represents a pure state. Adopted solution is based on putting zeros in amplitudes which are not related to measurement result λ_i. In other words, if the result is e.g. λ_1^b with probability equal to $p(\lambda_1^b)$, then the amplitudes in which the second qutrit is not in state $|1\rangle$ get the zero values, and values of other amplitudes which belong to the measurement results are divided by $\sqrt{p(\lambda_1^b)}$.

Parallel reduction for gathering information about second qutrit in two qutrit quantum register
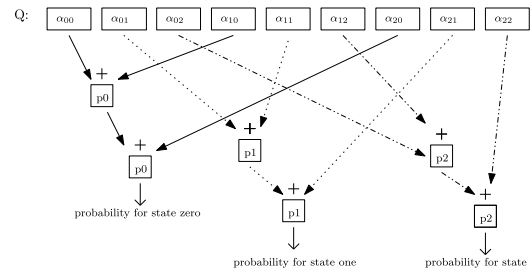

FIGURE 1. A scheme of parallel reduction for the von Neumann operation during gathering information about probability of measurement result on single qutrit (e.i. qudit with $d = 3$) in two qutrit quantum register Q. One can presume on the basis of the presented approach that the state of the second qutrit in the register is measured.

This operation may be performed independently on indicated amplitudes. Finally, the measurement process can be realised in parallel because each probability amplitude is processed independently.

Algorithm 1: The computational procedure VNM realising a special case of measurement, i.e. the von Neumann measurement in the standard basis. The first parameter $|\Psi\rangle$ represents a quantum state, α_i stands for i-th amplitude of $|\Psi\rangle$, d is qudit's freedom level, n marks the number of qudits, t stands for ordinal number of qudit, mm is a mask function which points out the qudits to be measured.

> **procedure** VNM($|\Psi\rangle$, d, N, mm)
> $p_0, p_1, \ldots p_{d-1} \leftarrow 0$
> **for** $j \leftarrow 0 \ldots (d^N - 1)$ **do in parallel**
>   **if** $mm(j, 0) = $ true **then** $p_0 \leftarrow p_0 + |\alpha_j|^2$
>   **if** $mm(j, 1) = $ true **then** $p_1 \leftarrow p_1 + |\alpha_j|^2$
> $\vdots$ $\vdots$
>   **if** $mm(j, d-1) = $ true **then** $p_{d-1} \leftarrow p_{d-1} + |\alpha_j|^2$
> **end for**
> $(r, m) \leftarrow$ uniform random select from :
> $(p_0, mm_0), \ldots, (p_{d-1}, mm_{d-1})$
> **for** $j \leftarrow 0 \ldots (d^N - 1)$ **do in parallel**
>   **if** $mm(j, \{0, 1, \ldots, d-1\}, (r, m))$ **is false then**
> $\alpha_j \leftarrow 0$
>   **else**
> $\alpha_j \leftarrow \frac{1}{\sqrt{r}} \alpha_j$
>   **end if**
> **end for**
> **end procedure**

If we use a mask, for example mm(j, 1), then we check whether j-th amplitude refers to the state result denoted as λ_1 under measurement operation and the result of measurement is given as (r, m) pair. In the case like mm_1, the outcome of the measurement is related to the result denoted as λ_1.

The estimation of computational complexity T_{VNM} of the VNM procedure directly refers to two *for* loops:

$$T_{VNM} = \left(\sum_{i=0}^{d^N - 1} T_{mm} \right) + T_{RS} + \left(\sum_{i=0}^{d^N - 1} T_{norm} \right) = O\left(d^N \right), \tag{22}$$

where T_{mm} represents complexity of operations on a mask, and T_{RS} stands for the operation of measurement selection, T_{norm} denotes the last part of the measurement operation – normalisation. However, it is easy to allocate individual operations in both loops between particular computational cores, the basic unroll optimisation for loops can be also applied in this case.

It should be added that the VMN procedure, described by Algorithm 1, may be used as measurement's simulation in a context of One-Way Quantum Computation Model (1WQC) [32]–[35]. In this model, the operation of measurement (realised in different computational bases) is a fundamental computational mechanism. The relevant modifications, concerning a measurement in basis described by a set of P_i projectors for observable M (as in (15)), are presented as Algorithm 2.

Algorithm 2: The computational procedure VNM$^{\{P_i\}}$ *realising a measurement in a basis described by the set of projectors P_i. Parameters have the same meaning as for the VNM routine*

> **procedure** VNM$^{\{P_i\}}$($|\Psi\rangle$, d, N, mm)
> $\quad p_0, p_1, \ldots p_{d-1} \leftarrow 0$
> $\quad$ **for** $j \leftarrow 0 \ldots (d^N - 1)$ **do in parallel**
> $\quad\quad$ **if** $mm(j, 0) = $ true **then** $p_0 \leftarrow p_0 + |\alpha_j^\dagger \cdot P^i_{(j/mm(j,0))0} \cdot \alpha_j|^2$
> $\quad\quad$ **if** $mm(j, 1) = $ true **then** $p_1 \leftarrow p_1 + |\alpha_j^\dagger \cdot P^i_{(j/mm(j,1))1} \cdot \alpha_j|^2$
> $\quad\quad\quad\vdots \qquad\qquad\qquad \vdots$
> $\quad\quad$ **if** $mm(j, d-1) = $ true **then**
> $\quad\quad\quad p_{d-1} \leftarrow p_{d-1} + |\alpha_j^\dagger \cdot P^i_{(j/mm(j,d-1))(d-1)} \cdot \alpha_j|^2$
> $\quad$ **end for**
> $\quad (r, m) \leftarrow$ uniform random select from :
> $\quad\quad\quad (p_0, mm_0), \ldots, (p_{d-1}, mm_{d-1})$
> $\quad$ **for** $j \leftarrow 0 \ldots (d^N - 1)$ **do in parallel**
> $\quad\quad$ **if** $mm(j, \{0, 1, \ldots, d-1\}, (r, m))$ **is false then**
> $\quad\quad\quad \alpha_j \leftarrow 0$
> $\quad\quad$ **else**
> $\quad\quad\quad \alpha_j \leftarrow \frac{1}{\sqrt{r}} P^i_{(j/mm(j,r))(\{0,1,\ldots,d-1\})}\alpha_j$
> $\quad\quad$ **end if**
> $\quad$ **end for**
> **end procedure**

The masks are used just like in the previous algorithm, e.g. $mm(i, 1)$ stands for the i-th amplitude referring to the state result denoted as λ_1.

The main modifications are, naturally, additional multiplications on probability amplitudes which include projectors P_i with their dimension d, what may be stated as:

$$p_0 \leftarrow p_0 + |\alpha_j^\dagger \cdot P^i_{(j/mm(j,0))0} \cdot \alpha_j|^2, \qquad (23)$$

and it means a fragmentary execution of the operation (16) on the j-th probability amplitude related to one of P_i operators under the measure mask ($P^i_{(j/mm(j,0))0}$) when the probability

distribution is calculated. The entry

$$\alpha_j \leftarrow \frac{1}{\sqrt{r}} P^i_{(j/mm(j,r))(\{0,1,\ldots,d-1\})}\alpha_j, \qquad (24)$$

expresses amplitude's modification according to utilised projectors for final measurement result denoted as r.

Just like in the VNM routine for measurements in the standard basis, the computational complexity of the modified procedure is still $O(d^N)$. The additional operations, connected with the computational basis, influence only parameters T_{mm} and T_{norm}.

B. LOCAL UNITARY OPERATORS

An impact of a unitary operation on one qubit, also when we deal with controlled operations, may be implemented with an effective usage of many computational cores (thanks to the way in which a unitary operator is applied to a register). Fig. 2 depicts some quantities which may be formalised in the following way:

Proposition 1: If N is the number of qudits in a quantum register, d stands for the the corresponding dimension of single qudit, and t is the number of qudit modified by a unitary operation U, then:

(I) *the number of so-called local blocks $p = d^{t-1}$,*
(II) *the space between elements in a local operation step $= d^{N-t} - 1$,*
(III) *the space between local blocks $vstep = \frac{d^N}{p} = \frac{d^N}{d^{t-1}} = d^{N-t+1}$.*

Algorithm 3: The algorithm for processing pure state vector with unitary operator u for single qudit (UPST). The parameter $|\Psi\rangle$ represents a quantum state, d is qudit's freedom level, N number of qudits, t ordinal number of a qudit, u is a unitary matrix for single qudit.

> **procedure** UPST($|\Psi\rangle$, d, N, t, u)
> $\quad step \leftarrow d^{N-t} - 1$, $p \leftarrow d^{t-1}$, $vstep \leftarrow (d^N)/p$, $irow \leftarrow 0$
> $\quad$ **for** $ip \leftarrow 0 \ldots p - 1$ **do**
> $\quad\quad$ **for** $i \leftarrow 0 \ldots step$ **do in parallel**
> $\quad\quad\quad r_1 \leftarrow irow + (1 \cdot (step + 1)) + i$,
> $\quad\quad\quad r_2 \leftarrow irow + (2 \cdot (step + 1)) + i$,
> $\quad\quad\quad \ldots,$
> $\quad\quad\quad r_k \leftarrow irow + (d \cdot (step + 1)) + i$
> $\quad\quad\quad$ LocUniOpForStateVector($|\Psi\rangle$, $[r_1, r_2, \ldots, r_k]$, u)
> $\quad\quad$ **end for**
> $\quad\quad irow \leftarrow irow + vstep$
> $\quad$ **end for**
> **end procedure**

The operation LocUniOpForStateVector($\cdot$) is a realisation of interaction between operator u and pointed out elements of state $|\Psi\rangle$:

$$\begin{bmatrix} \alpha_{r_1} \\ \alpha_{r_2} \\ \vdots \\ \alpha_{r_d} \end{bmatrix} \leftarrow \begin{bmatrix} u_{11} & \cdots & \cdots & u_{1d} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ u_{d1} & \cdots & \cdots & u_{dd} \end{bmatrix} \begin{bmatrix} \alpha_{r_1} \\ \alpha_{r_2} \\ \vdots \\ \alpha_{r_d} \end{bmatrix}. \qquad (25)$$
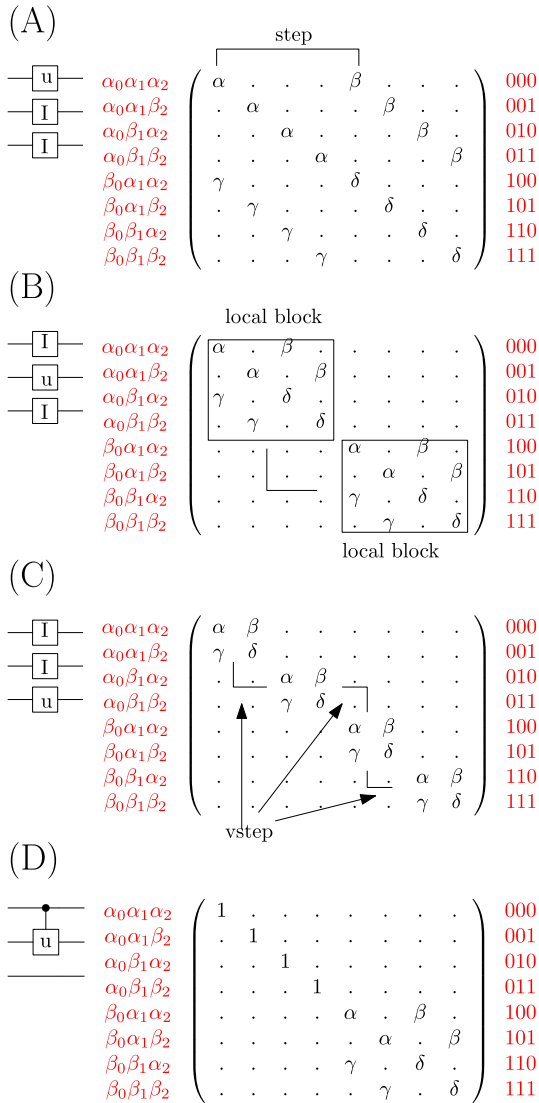
(A)

(B)

(C)

(D)

FIGURE 2. Exemplary indication of independent local operations in the process of utilising the unitary operator (A), (B), (C) (also in a case of controlled operation) on a three qubit register (D).

Additionally, the number of LocUniOpForStateVector($\cdot$) calls in Algorithm 3 is $l_{num} = d^{N-1}$.

In other words, a matrix is multiplied by a vector, but this operation concerns only d elements of a vector $|\Psi\rangle$. Each operation of this type is local and may be performed independently. Again, just like for the operation VNM, the computational complexity of procedure described as Algorithm 3 is:

$$T_{UPST} = T_{ini} + \left(\sum_{i=0}^{d^N-1} T_{LUO} \right) = O\left(d^N\right), \quad (26)$$

where T_{ini} represents initialisation operation. Main loop contains operations T_{LUO}, but complexity T_{LUO} is constant and depends only on d. Finally, d^N complexity is obtained. Owing to UPST approach, an algorithm for controlled unitary operations can be presented.

Algorithm 4: The algorithm of vector state processing for a controlled 1-qudit gate u (CUPST). Parameters are the same as in Algorithm 3, and c is an ordinal number of controlling qudit.

> **procedure** CUPST($|\Psi\rangle$, d, N, t, c, u)
> $l_c \leftarrow |c|$, $step \leftarrow d^{N-t} - 1$, $p \leftarrow d^{t-l_c-1}$;
> $vstep \leftarrow (d^{N-l_c})/p$,
>   idxMask $\leftarrow mask(c)$
>   **for** $ip \leftarrow 0$; $ip < p$; $ip++$ **do**
>   **for** $i \leftarrow 0 \ldots step$ **do in parallel**
> $r_1 \leftarrow$ idxMask$|(irow + (1 \cdot (step + 1) + i))$,
> $r_2 \leftarrow$ idxMask$|(irow + (2 \cdot (step + 1) + i))$,
> $\ldots$,
> $r_k \leftarrow$ idxMask$|(irow + (d \cdot (step + 1) + i))$
>   LocUniOpForStateVector($|\Psi\rangle$, [r_1, r_2, $\ldots$, r_k], u)
>   **end for**
> $irow \leftarrow irow + vstep$
>   **end for**
> **end procedure**

Function $mask(\cdot)$ is responsible for preparing the index number based on the information which qudits are used as controlling qudits. This information and information from Proposition 1 allows pointing out indexes of probability amplitudes and the expression:

$$\text{idxMask}|(irow + (1 \cdot (step + 1) + i))$$

means that the index which points out the given row r_i is calculated under additional dits mask which points the controlling qudit.

Remark 5: Increasing number of controlling lines decreases the number of local operations, i.e. $l_{num} = d^{N-l_c-1}$, where l_c is the number of controlling qudits. If $l_c = N - 1$, then we carry out only one local operation in the quantum register which modifies d probability amplitudes.

The computational complexity remains exponential, but it should be emphasised that the number of controlling lines may significantly decrease the number of local operations:

$$T_{CUPST} = T_{ini} + \left(\sum_{i=0}^{d^N-l_c} T_{LUO} \right) = O(d^{N-l_c}). \quad (27)$$

Also for the case when the quantum register is described by a density matrix, one can analogously formulate computational procedures in which the processing is done in-place by means of the indicated local operations which can be performed independently. In earlier work [44], the computational procedure for density matrices for qubits has been presented. However, the Proposition 1 can be used directly to construct analogous routines for density matrices containing qudits. Algorithm 5 shows how to process density matrices of N qudits with local unitary operator which acts on qudit numbered as t. The Algorithm 6 implements computational routine to process density matrix ρ where qudit t is modified

by an operator u if qudit c is in given state represented by the function $mask(\cdot)$ – similarly as in computational routines for a vector state.

Algorithm 5: The algorithm of density matrix processing for single-qubit gate (DMT). The parameter ρ represents a density matrix, n number of qudits, t ordinal number of a qudit, u is a unitary matrix for single qudit.

> **procedure** DMT(ρ, N, t, u)
> $\quad step = \mathrm{d}^{N-t} - 1 \,;\, p = \mathrm{d}^{t-1}$
> $\quad vstep = (\mathrm{d}^N)/p \,;\, sizeReg = \mathrm{d}^N$
> $\quad$ **for** $i \leftarrow 0, 1 \cdot vstep, \dots, (k \cdot vstep) < sizeReg$ **do**
> $\quad\quad$ **for** $j \leftarrow 0, 1 \cdot vstep, \dots, (k \cdot vstep) < sizeReg$
> **do**
> $\quad\quad\quad$ **for** $x \leftarrow 0 \dots step$ **do**
> $\quad\quad\quad\quad$ **for** $y \leftarrow 0 \dots step$ **do**
> $\quad\quad\quad\quad\quad$ LocUniOpForDenMatrix(ρ, t,
> $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad i + x, j +$
> $y, step, u, u^\dagger$);
> $\quad\quad\quad\quad$ **end for**
> $\quad\quad\quad$ **end for**
> $\quad\quad$ **end for**
> $\quad$ **end for**
> **end procedure**

Algorithm 6: The algorithm of density matrix processing for a controlled 1-qudit gate u (CDMT). The parameter ρ represents a quantum state, other parameters remain the same as in the previous algorithms.

> **procedure** CDMT(ρ, N, t, c, u)
> $\quad step = \mathrm{d}^{N-t} - 1 \,;\, p = \mathrm{d}^{t-l_c-1}$
> $\quad vstep = (d^N)/p \,;\, sizeReg = d^N$
> $\quad idxMask \leftarrow mask(c)$
> $\quad$ **for** $i \leftarrow 0, 1 \cdot vstep, \dots, (k \cdot vstep) < sizeReg$ **do**
> $\quad\quad$ **for** $j \leftarrow 0, 1 \cdot vstep, \dots, (k \cdot vstep) < sizeReg$
> **do**
> $\quad\quad\quad$ **for** $x \leftarrow 0 \dots step$ **do**
> $\quad\quad\quad\quad$ **for** $y \leftarrow 0 \dots step$ **do**
> $\quad\quad\quad\quad\quad$ LocUniOpForDenMatrix(ρ, t,
> $\qquad\qquad\qquad\qquad\qquad idxMask|(i + x), idxMask|(j +$
> $y), step, u, u^\dagger$);
> $\quad\quad\quad\quad$ **end for**
> $\quad\quad\quad$ **end for**
> $\quad\quad$ **end for**
> $\quad$ **end for**
> **end procedure**

The local operation LocalUnitaryOpForDenMatrix($\cdot$) performs changes in indicated elements of matrix ρ. In this case, $d \times d$ elements are modified. For example, in case of a qutrit, the local operations are (s is a shorthand of the variable step):

$$A_l \leftarrow U_l \times A_l \times U_l^\dagger, \tag{28}$$

where

$$A_l = \begin{bmatrix} dm_{x,y} & dm_{x+s+1,y} & dm_{x+s+2,y} \\ dm_{x,y+s+1} & dm_{x+s+1,y+s+1} & dm_{x+s+2,y+s+1} \\ dm_{x,y+s+2} & dm_{x+s+1,y+s+2} & dm_{x+s+2,y+s+2} \end{bmatrix},$$

$$U_l = \begin{bmatrix} u_1 & u_2 & u_3 \\ u_4 & u_5 & u_6 \\ u_7 & u_8 & u_9 \end{bmatrix}. \tag{29}$$

IV. OPERATOR DECOMPOSITIONS OF GENERAL QUANTUM STATES

Let $\langle\!\langle -|- \rangle\!\rangle$ be any factorisable inner product on the space $L(\mathcal{H}_A \otimes \mathcal{H}_B)$ of linear operations acting in the product space $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_A = \mathbb{C}^{d_A}$, $\mathcal{H}_B = \mathbb{C}^{d_B}$ with $d_A \cdot d_B < \infty$ and equipped with the standard Euclidean scalar products $\langle -|- \rangle$. This means that there are two inner products: $\langle -|- \rangle_A^{\langle\!\langle}$ on $L(\mathcal{H}_A)$, and respectively $\langle -|- \rangle_B^{\langle\!\langle}$ on $L(\mathcal{H}_B)$ and such that for any $Q^A \in L(\mathcal{H}_A)$, $Q^B \in L(\mathcal{H}_A)$ the following equality is true:

$$\langle\!\langle Q^A \otimes Q^B | Q'^A \otimes Q'^B \rangle\!\rangle = \langle Q^A | Q'^A \rangle_A^{\langle\!\langle} \cdot \langle Q^B | Q'^B \rangle_B^{\langle\!\langle}. \tag{30}$$

The following theorem generalises the well known operator Schmidt decomposition, formulated for the standard Hilbert-Schmidt products structure [41], [49] and applied in the context of quantum computations in several papers [50]–[53].

Theorem 1: For any $Q \in L(\mathcal{H}_A \otimes \mathcal{H}_B)$ there exists

- *a finite sequence $\lambda^{\langle\!\langle} = (\lambda_1^{\langle\!\langle}, \lambda_2^{\langle\!\langle}, \dots)$ of non-negative numbers called $\langle\!\langle -|- \rangle\!\rangle$-Schmidt numbers of Q and such that: $\sum_k (\lambda_k^{\langle\!\langle})^2 = \langle\!\langle Q|Q \rangle\!\rangle = ||Q||_{\langle\!\langle}^2$,*
- *a pair of $\langle\!\langle - \rangle\!\rangle$-orthonormal bases $q_k^A \in L(\mathcal{H}_A)$ and $q_l^B \in L(\mathcal{H}_B)$:*

$$\langle q_k^A | q_{k'}^A \rangle_A^{\langle\!\langle} = \delta_{kk'}, \quad \langle q_k^B | q_{k'}^B \rangle_B^{\langle\!\langle} = \delta_{kk'}, \tag{31}$$

and such that

$$Q = \sum_k \lambda_k^{\langle\!\langle} q_k^A \otimes q_k^B. \tag{32}$$

$\square$

Example 1: Let the inner product be given by the Hilbert-Schmidt's formula:

$$\langle Q|Q' \rangle_{HS} = \mathrm{tr}\left(Q^\dagger Q'\right), \tag{33}$$

where $\mathrm{tr}\,(-)$ stands for the trace of $(-)$ in the corresponding Hilbert space.

The corresponding Schmidt decomposition of Q will be called the HS-Schmidt decomposition of Q and is given by:

$$Q = \sum_k \lambda_k^{HS} E_k^{HS(A)} \otimes E_k^{HS(B)}, \tag{34}$$

where λ_k^{HS} stands for the corresponding HS-Schmidt coefficients and $E_k^{HS(A)}$, resp. $E_k^{HS(B)}$ are the corresponding orthonormal and complete systems of operators in $L(\mathcal{H}_A)$, resp. in $L(\mathcal{H}_B)$:

$$\mathrm{tr}\left(\left(E_k^{HS(A)}\right)^\dagger E_{k'}^{HS(A)}\right) = \delta_{kk'}, \tag{35}$$

and similarly for $E_k^{HS(B)}$.

The phenomenon of quantum entanglement is, by no doubts, one of the fundamental resources for the emerging

Quantum Information Processing technology. Basic information concerning entanglement can be found in widely available textbooks and several review papers [49], [50], [53]–[55]. The following result is known [51], [52], [56] for the Hilbert-Schmidt decomposition.

Theorem 2: Let $Q \in E(\mathcal{H}_A \otimes \mathcal{H}_B)$, i.e. $Q \in L(\mathcal{H}_A \otimes \mathcal{H}_B)$, $Q = Q^\dagger \geq 0$ and $\mathrm{tr}\,(Q) = 1$. If Q is separable, then $\sum_k \lambda_k^{HS} \leq 1$. □

Example 2: Let $Q \in E(\mathcal{H}_A \otimes \mathcal{H}_B)$ be such that $\mathrm{tr}\,(Q^2) = 1$. Then, there exists an unique (up to the phase coefficient) unit vector $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ such that $Q = |\Psi\rangle\langle\Psi|$.

Let

$$|\Psi\rangle = \sum_{\alpha=1}^{\min(d_A, d_B)} \tau_\alpha |\psi_\alpha\rangle \otimes |\theta_\alpha\rangle \tag{36}$$

be the Schmidt decomposition of $|\Psi\rangle$ and the Schmidt coefficients of $|\Psi\rangle$ obey $\sum_\alpha \tau_\alpha^2 = 1$. The systems of vectors $\{|\psi_\alpha\rangle, \alpha = 1 : d_A\}$, resp. $\{|\theta_\beta\rangle, \beta = 1 : d_B\}$ form complete orthonormal systems in $\mathcal{H}_A$, and resp. in $\mathcal{H}_B$.

Using (36) it follows that:

$$Q = \sum_{\alpha,\beta} \tau_\alpha \tau_\beta |\psi_\alpha\rangle\langle\psi_\beta| \otimes |\theta_\alpha\rangle\langle\theta_\beta|. \tag{37}$$

□

Corollary 1: Let $Q \in \partial E(\mathcal{H}_A \otimes \mathcal{H}_B)$, i.e. $\mathrm{tr}\,(Q^2) = 1$.

(1) Then the HS-Schmidt numbers of Q are given by

$$\lambda_{\alpha\beta}^{HS} = \tau_\alpha \tau_\beta. \tag{38}$$

(2) the state Q is separable if and only if $(\sum_\alpha \tau_\alpha)^2 = 1$ which means that the canonical Schmidt's rank of $|\Psi\rangle$ is equal to 1.

Proof: It is easy to observe:

$$\langle |\psi_\alpha\rangle\langle\psi_\beta| \, || \, |\psi_{\alpha'}\rangle\langle\psi_{\beta'}| \rangle_{HS} = \delta_{\alpha\alpha'} \cdot \delta_{\beta\beta'}, \tag{39}$$

and similarly for $|\theta_\alpha\rangle\langle\theta_\beta|$. Moreover, the system $\{|\psi_\alpha\rangle\langle\psi_\beta|\}$ forms a complete system in $HS(\mathcal{H}_A)$, and similarly $\{|\theta_\alpha\rangle\langle\theta_\beta|\}$ forms a complete system in $HS(\mathcal{H}_B)$.

The part (2) follows from the use of Theorem 2. □

For the case of a general $Q \in E(\mathcal{H}_A \otimes \mathcal{H}_B)$, the spectral decomposition of Q is considered:

$$Q = \sum_{k=1}^{(d_A \cdot d_B)^2} \lambda_k E_k, \tag{40}$$

where $\lambda_k \geq 0$, $\sum_k \lambda_k = 1$ are eigenvalues of Q, and $E_k = |\Psi_k\rangle\langle\Psi_k|$ are the orthogonal projectors onto the corresponding eigenvectors.

Let,

$$E_k = \sum_{\alpha,\beta=1}^{\min(d_A, d_B)} \tau_\alpha^k \tau_\beta^k |\psi_\alpha^k\rangle\langle\psi_\beta^k| \otimes |\theta_\alpha^k\rangle\langle\theta_\beta^k|, \tag{41}$$

be the Schmidt decomposition of the corresponding eigenvectors of $|\Psi_k\rangle$. Then, comparing the arising

expansions for Q:

$$Q = \sum_{k=1}^{(d_A \cdot d_B)^2} \lambda_k \sum_{\alpha,\beta=1}^{\min(d_A, d_B)} \tau_\alpha^k \tau_\beta^k |\psi_\alpha^k\rangle\langle\psi_\beta^k| \otimes |\theta_\alpha^k\rangle\langle\theta_\beta^k|, \tag{42}$$

with expansion (32) one can obtain:

$$\lambda_k^{\langle\!\langle} = \sum_{l=1}^{(d_A \cdot d_B)^2} \lambda_l \sum_{\alpha,\beta=1}^{\min(d_A, d_B)} \tau_\alpha^l \tau_\beta^l \langle\!\langle q_k^A || \psi_\alpha^l\rangle\langle\psi_\beta^l| \rangle\!\rangle_{\mathcal{H}_A}$$
$$\times \langle\!\langle q_k^B || \theta_\alpha^l\rangle\langle\theta_\beta^l| \rangle\!\rangle_{\mathcal{H}_B}$$
$$= \sum_{l=1}^{(d_A \cdot d_B)^2} \lambda_l \sum_{\alpha,\beta=1}^{\min(d_A, d_B)} \langle\!\langle q_k^A \otimes q_k^B |$$
$$\times |\tau_\alpha^l \psi_\alpha^l \otimes \theta_\alpha^l\rangle\langle\tau_\beta^l \psi_\beta^l \otimes \theta_\beta^l|$$
$$= \sum_{l=1}^{(d_A \cdot d_B)^2} \lambda_l \langle\!\langle q_k^A \otimes q_k^B || \Psi_l\rangle\langle\Psi_l| \rangle\!\rangle. \tag{43}$$

Let:

$$\sum{}^{\langle\!\langle} = \sum_k \lambda_k^{\langle\!\langle} = \langle\!\langle \sum_k \langle q_k^A \otimes q_k^B || Q \rangle\!\rangle. \tag{44}$$

For further use, let us define:

$$D_- = \sup_{Q^A, Q^B} ||Q^A||_{\langle\!\langle} \cdot ||Q^B||_{\langle\!\langle}, \tag{45}$$

where

$$||Q^A||_{\langle\!\langle}^2 = \langle\!\langle Q^A | Q^A \rangle\!\rangle, \quad Q^A \in E(\mathcal{H}_A), \tag{46}$$

and similarly for the part B, and let:

$$D_+ = \inf_{Q' \in E(\mathcal{H}_A \otimes \mathcal{H}_B)} \langle\!\langle Q' | \mathbb{I} \rangle\!\rangle, \tag{47}$$

where $\mathbb{I}$ is the identity matrix.

Remark 6: The finiteness of D_- and D_+ follows from the fact that the sets $E(\mathcal{H}_A)$, $E(\mathcal{H}_B)$, $\mathrm{Sep}(\mathcal{H}_A \otimes \mathcal{H}_B)$ are compact and the straightforward application of the Weierstrass theorem [57].

Theorem 3: Let $Q \in E(\mathcal{H}_A \otimes \mathcal{H}_B)$ and $\langle\!\langle -|- \rangle\!\rangle$ be any factorisable inner product on $L(\mathcal{H}_A \otimes \mathcal{H}_B)$ and such that

(1) $D_- \leq 1$,
(2) $D_+ \geq 1$.

In this case, if Q is separable the following is true:

$$\sum{}^{\langle\!\langle} = \sum_k \lambda_k^{\langle\!\langle} \leq \langle\!\langle Q | \mathbb{I} \rangle\!\rangle + (D_- - D_+). \tag{48}$$

Proof: We start the proof with assumptions: let $Q \in E(\mathcal{H}_A \otimes \mathcal{H}_B)$ be a separable state, then $Q = \sum_\alpha p_\alpha Q_\alpha^A \otimes Q_\alpha^B$, $\sum_\alpha p_\alpha = 1$ and $Q_\alpha^A \in E(\mathcal{H}_A)$ and $Q_\alpha^B \in E(\mathcal{H}_B)$.

For the complete proof, it is enough to assume (without lost of generality) that the actual Q is of the form $Q' = Q^A \otimes Q^B$.

Let us define, for any $Q \in L(\mathcal{H}_A \otimes \mathcal{H}_B)$, the following (witness-like) operator:

$$W_Q = \sum_k q_k^A \otimes q_k^B, \tag{49}$$

where q_k^A, and resp. q_k^B are given from the corresponding Schmidt decomposition (32). Then, by an easy computations

$$\langle\!\langle Q'|\mathbb{I} - W_{Q'}\rangle\!\rangle \geq D_+ - D_-, \tag{50}$$

from which it follows:

$$\sum_k \lambda_k^{\langle\!\langle} \leq \langle\!\langle Q'|\mathbb{I}\rangle\!\rangle + (D_- - D_+). \tag{51}$$

□

Remark 7: It easy to observe that in the HS-inner products Theorem 3 reproduces the well known Rudolph theorem [50], which is also called the realignment criterion. The proven by us Theorem 3 is a slight generalisation of the original realignment criterion although is of a similar nature.

V. THE ANATOMY OF MULTI-QUDIT ENTANGLEMENT PROBLEM

Let $\mathfrak{I}_N = \{1, 2, 3, \ldots, N\}$ for integer $N > 1$, and let $2 - Par(\mathfrak{I}_N)$ stand for the set of all two-partitions π of $\mathfrak{I}_N$, i.e. $\pi = (\pi_1, \pi_2)$, $\pi_1, \pi_2 \subseteq \mathfrak{I}_N$, $\pi_1 \vee \pi_2 = \mathfrak{I}_N$, and $\pi_1 \wedge \pi_2 = \emptyset$. Actually the length of the list $2 - Par(\mathfrak{I}_N)$ grows as 2^N with $N \to \infty$. Of special interest for us will be the set $2q - Par(\mathfrak{I}_N)$ consisting of these $\pi \in 2 - Par(\mathfrak{I}_N)$ such that $|\pi_1| \leq \lfloor N/2 \rfloor$, where $\lfloor N/2 \rfloor$ means the floor of $N/2$. Fixing π_1 causes that π_2 is uniquely fixed.

A. MULTI-QUDIT QUANTUM STATES

Let $d \geq 2$ be a fixed integer and let $h(N)$ be d^N-dimensional, complex euclidean Hilbert space $\mathbb{C}^{d^N} = \otimes_{i=1}^N \mathbb{C}_{(i)}^d$. The standard arithmetical orthonormal basis in $\mathbb{C}^d$ is denoted as $|i\rangle$, $i = 0, \ldots, d - 1$, and the corresponding product basis in $\mathbb{C}^{d^N}$ as $|i_1 i_2 \ldots i_N\rangle$. The set of quantum states describing the system of N qudits is defined as $E(\mathbb{C}^{d^N}) = \{Q \in L(\mathbb{C}^{d^N}) : Q = Q^\dagger \geq 0 \text{ and } \mathrm{tr}(Q) = 1\}$. Of particular interest is the topological boundary of $E(\mathbb{C}^{d^N})$, denoted as $\partial E(\mathbb{C}^{d^N})$ and defined as $\partial E(\mathbb{C}^{d^N}) = \{Q \in E(\mathbb{C}^{d^N}) : \mathrm{tr}(Q^2) = \mathrm{tr}(Q) = 1\}$. If $Q \in \partial E$, then there exists (essentially) unique normalised vector $|\Psi\rangle \in \mathbb{C}^{d^N}$ such that $Q = |\Psi\rangle\langle\Psi|$ (i.e. Q represents pure state).

B. SCHMIDT DECOMPOSITIONS

Let $\pi = \pi_1 \vee \pi_2 \in 2q - Par(\mathfrak{I}_N)$ and let $|\Psi\rangle\langle\Psi| \in \partial E(\mathbb{C}^{d^N})$. Then it follows:

(1) there exists a sequence of non-negative numbers $\tau_j^{\pi_1} \geq 0$, $j = 1 : d^{|\pi_1|}$ such that $\sum_j (\tau_j^{\pi_1})^2 = 1$,

(2) a pair of complete orthonormal systems $(|\psi_j^{\pi_1}\rangle) \subseteq \otimes_{\alpha \in \pi_1} \mathbb{C}_{(\alpha)}^d$ and $(|\theta_j^{\pi_1}\rangle) \subseteq \otimes_{\alpha \in \pi_1} \mathbb{C}_{(\alpha)}^d$ such that:

$$|\Psi\rangle = \sum_j \tau_j^{\pi_1} |\psi_j^{\pi_1}\rangle \otimes |\theta_j^{\pi_1}\rangle, \tag{52}$$

from which it follows

$$Q = |\Psi\rangle\langle\Psi| = \sum_{j_1, j_2} \tau_{j_1}^{\pi_1} \tau_{j_2}^{\pi_1} |\psi_{j_1}\theta_{j_1}\rangle\langle\psi_{j_2}\theta_{j_2}|. \tag{53}$$

C. TOTAL VON NEUMANN ENTROPY OF THE QUANTUM STATES

For a given $\pi_1 \in 2q - Par(\mathfrak{I}_N)$ and $|\Psi\rangle\langle\Psi|$, one can define:

(1) the von Neumann entropy of the decomposition $\mathfrak{I}_N \longrightarrow \pi_1 \vee \pi_2$ as

$$\mathcal{E}^{\pi_1}\left(|\Psi\rangle\right) = -\sum_j \left(\tau_j^{\pi_1}\right)^2 \ln\left(\tau_j^{\pi_1}\right)^2. \tag{54}$$

Note that:

$$\sup_{|\Psi\rangle \in \partial E(\mathbb{C}^{d^N})} \mathcal{E}^{\pi_1}\left(|\Psi\rangle\right) = \ln\left(d^{|\pi_1|}\right). \tag{55}$$

(2) the total von Neumann entropy of $|\Psi\rangle$:

$$\mathcal{E}\left(|\Psi\rangle\right) = \sum_{\pi_1 \in 2q - Par(\mathfrak{I}_N)} \mathcal{E}^{\pi_1}\left(|\Psi\rangle\right). \tag{56}$$

Note that:

$$\mathcal{E}(N, d) = \sup_{|\Psi\rangle \in \partial E(\mathbb{C}^{d^N})} \mathcal{E}\left(|\Psi\rangle\right)$$
$$\leq \sum_{k=1}^{N^\star} \binom{N}{k} \ln\left(d^k\right) = \ln\left(d^{\sum_{k=1}^{N^\star} k\binom{N}{k}}\right), \tag{57}$$

where $N^\star = \lfloor N/2 \rfloor$.

Deficit of entanglement contained in $|\Psi\rangle$ is defined as

$$\Delta\mathcal{E}\left(|\Psi\rangle\right) = \mathcal{E}(N, d) - \mathcal{E}\left(|\Psi\rangle\right). \tag{58}$$

A method of Gram matrix based computations as described in details in [58] will be used in our computations. Let

$$|\Psi\rangle = \sum_{\substack{i_1=0:(d-1) \\ i_2=0:(d-1) \\ \vdots \\ i_n=0:(d-1)}} \psi_{i_1 \ldots i_N} |i_1 \ldots i_N\rangle, \tag{59}$$

be a general N-qudit state.

For any $\pi = \pi_1 \vee \pi_2$, $\pi_1 = \{\alpha_1, \ldots \alpha_k\} \subseteq \mathfrak{I}_N$ the corresponding and consisting of d^k-elements frame $\mathfrak{F}^{\pi_1}$ is defined as

$$\mathfrak{F}^{\pi_1} = (V_{i_{\alpha_1} \ldots i_{\alpha_k}}), \tag{60}$$

where

$$V_{i_{\alpha_1} \ldots i_{\alpha_k}} = \sum_{j_{\beta_1} \ldots j_{\beta_{N-k}}} \psi_{j_{\alpha_1} \ldots j_{\alpha_k}} |j_{\beta_1} \ldots j_{\beta_{N-k}}\rangle_{N-k}, \tag{61}$$

is the vector contraction of the tensor composed of all coefficients of Ψ over the coordinates labelled by $j_{\beta_1} \ldots j_{\beta_{N-k}}$ such that $\{\beta_1, \ldots, \beta_{N-k}\} = \pi_2$.

Then the Gram matrix $\mathfrak{G}^{\pi_1}(|\Psi\rangle)$ corresponding to π_1 is defined as $k^d \times k^d$ matrix, with matrix elements given by

$$\mathfrak{G}^{\pi_1}_{i_{\alpha_1} \ldots i_{\alpha_k} | i'_{\alpha_1} \ldots i'_{\alpha_k}} = \langle V^{\pi_1}_{i_{\alpha_1} \ldots i_{\alpha_k}} | V^{\pi_2}_{i'_{\alpha_1} \ldots i'_{\alpha_k}}\rangle_{\mathbb{C}^{d^{N-k}}}. \tag{62}$$

It was proved in [58] that, in particular:

(1) $\mathfrak{G}^{\pi_1}(|\Psi\rangle) = \mathrm{tr}_{\pi_2}(|\Psi\rangle\langle\Psi|)$, where the quantum operation denoted as $\mathrm{tr}_{\pi_2}(|\Psi\rangle\langle\Psi|)$ is the partial trace operation over the degrees of freedom of qudits labelled by elements of π_2, i.e. $\mathfrak{G}^{\pi_1}(|\Psi\rangle)$ is equal to the corresponding reduced density matrix (RDM), describing qudits labelled by indices contained in π_1,

(2) the spectrum of $\mathfrak{G}^{\pi_1}(|\Psi\rangle)$ (modulo zeros values) denoted as $\sigma_0(\mathfrak{G}^{\pi_1}(|\Psi\rangle))$ coincides with the squares of the Schmidt numbers entering in the standard Schmidt decomposition of $|\Psi\rangle$, see (52), according to the (formal) decomposition:

$$\mathbb{C}^{d^N} \simeq \mathbb{C}^{d^{|\pi_1|}} \otimes \mathbb{C}^{d^{|\pi_2|}}, \qquad (63)$$

(3) if

$$\sigma_0 = (\lambda_1^{\pi_1}, \ldots, \lambda_n^{\pi_1}), \lambda_1^{\pi_1} \geq \ldots \lambda_n^{\pi_1} > 0, \quad (64)$$

then

$$\mathcal{E}^{\pi_1}(|\Psi\rangle) = -\sum_{k=1}^{n} \lambda_k^{\pi_1} \ln\left(\lambda_k^{\pi_1}\right), \qquad (65)$$

and the quantity $\mathcal{E}^{\pi_1}(|\Psi\rangle)$ is

(i) $\mathbb{U}(\mathcal{H}^{\pi_1}) \otimes \mathbb{U}(\mathcal{H}^{\pi_2})$ – invariant (where $\mathcal{H}^{\pi_\alpha}$, $\alpha = 1, 2$, corresponds to the corresponding factor in the decomposition $\mathbb{C}^{d^N} \simeq \mathbb{C}^{d^{|\pi_1|}} \otimes \mathbb{C}^{d^{|\pi_2|}}$ and $\mathbb{U}(-)$ are sets of all unitary (forming an unitary transformation groups) maps on the corresponding factors),

(ii) let Ω be any of the π-local quantum operation (with respect to the decomposition $\mathcal{H} \approx \mathcal{H}^{\pi_1} \otimes \mathcal{H}^{\pi_2}$). Then, the entropy $\mathcal{E}^{\pi_1}$, for any $|\Psi\rangle$ is not increasing under the action of Ω, i.e.,

$$\mathcal{E}^{\pi_1}\left(\Omega(|\Psi\rangle\langle\Psi|)\right) \leq \mathcal{E}^{\pi_1}\left(|\Psi\rangle\langle\Psi|\right), \quad (66)$$

(iii) for any $\otimes_{\alpha=1}^{N} \mathbb{C}_{(\alpha)}^{d}$ – local unitary operation (i.e. unitary operation of the form $U = u_{(1)} \otimes u_{(2)} \otimes \ldots \otimes u_{(N)}$), where $u_{(\alpha)}$ is unitary in $\mathbb{C}_{(\alpha)}^{d}$), the total entropy of any $\Psi \in \partial E(\mathbb{C}^{d^N})$ does not change, i.e.:

$$\mathcal{E}(|\Psi\rangle) = \mathcal{E}\left((u_{(1)} \otimes u_{(2)} \otimes \ldots \otimes u_{(N)})|\Psi\rangle\right), \qquad (67)$$

(iv) for any $\otimes_{\alpha=1}^{N} \mathbb{C}_{(\alpha)}^{d}$ – local quantum operation Ω the total entropy as defined in (58) of any pure state does not increase, i.e. for any quantum operation of the form $\Omega = \Omega_1 \otimes \ldots \otimes \Omega_N$:

$$\mathcal{E}\left(\Omega(|\Psi\rangle\langle\Psi|)\right) \leq \mathcal{E}\left(|\Psi\rangle\langle\Psi|\right). \qquad (68)$$

D. THE NEGATIVITY

For a given $|\Psi\rangle \in \mathbb{C}^{d^N}$ and $\pi_1 \in 2q - Par(\mathfrak{I}_N)$, we define negativity of Ψ and corresponding to the decomposition $\mathfrak{I}_N = \pi_1 \vee \pi_2$ as

$$\mathcal{N}^{\pi_1}(|\Psi\rangle) = \frac{1}{2}\left(\left(\sum_j \tau_j^{\pi_1}\right)^2 - 1\right). \qquad (69)$$

Note that:

$$\mathcal{N}^{\star\pi_1} = \sup_{|\Psi\rangle \in \partial E(\mathbb{C}^{d^N})} \mathcal{N}^{\pi_1}\left(|\Psi\rangle\right) = \frac{1}{2}\left(d^{|\pi_1|} - 1\right). \qquad (70)$$

The total negativity of the pure quantum state $|\Psi\rangle$ is given by

$$\mathcal{N}\left(|\Psi\rangle\right) = \sum_{\pi_1 \in 2q - Par(\mathfrak{I}_N)} \mathcal{N}^{\pi_1}\left(|\Psi\rangle\right). \qquad (71)$$

Note that:

$$\sup_{|\Psi\rangle \in \partial E(\mathbb{C}^{d^N}))} \mathcal{N}\left(|\Psi\rangle\right) = \sum_{\pi_1 \in 2q - Par(\mathfrak{I}_N)} \mathcal{N}^{\star\pi_1} \qquad (72)$$

$$= \frac{1}{2}\left(\frac{1 - d^{\lfloor N/2 \rfloor}}{1 - d} - \lfloor N/2 \rfloor\right). \qquad (73)$$

Remark 8: The defined by (69) and resp. by (71) quantities corresponding to the negativities of a given many-qudit state Ψ along given cut π_1 (see (69)) and the total negativity defined by (71) also posses most of the properties as it was listed for the von Neumann entropies in points (i)–(iv) at the end of the previous section.

The computational complexity of the evaluations of the entanglement deficit by the use the corresponding von Neumann entropy or the use of Negativity measure grows exponentially fast as the number of qudits N is increasing and this is why the suitable parallelisation has to be prepared. For example, taking $N = 10$ and $d = 2$, one has to deal with the ensemble of 31 matrices of size 1024×1024.

Remark 9: The states for which the maximal value of the total entropy (56) or the total negativity (71) are attained, are known under the name of absolutely maximally multi-partite entangled states (AME [59], [60]). The problem of their existence is strictly connected to the so-called quantum marginal problems [61] and belongs, according to [62] to one of the most important (and mathematically most complicated) problems of the quantum information theory foundations.

The new results on the existence and morphology of AME states for some special many qudit systems are presented here.

Let $\mathcal{S}$ be a system composed of N-qudits where each qudit's dimension is d_i (for $i = 1 : N$). Let us assume that there exists a value of i such that

$$d_i \geq \prod_{j \neq i} d_j. \qquad (74)$$

Then, the set AME$(d_1, \ldots, d_N)$ of all AME states in such system is given by the following construction.

Let us assume, without loss of generality, that the value of i for which the condition (74) is valid is equal to N. Let $\{e_\alpha^i, \alpha = 1 : d_i\}$ be a system of orthonormal bases, for $i = 1 : N$ in the corresponding spaces d_i. Any unit vector $|\Psi\rangle \in \partial E(\otimes_{i=1}^{N} \mathbb{C}^{d_i})$ is given by the following formula

$$|\Psi\rangle = \sum_{\alpha_1, \ldots, \alpha_N} \psi_{\alpha_1, \ldots, \alpha_N} |e_{\alpha_1}^1 \otimes \ldots \otimes e_{\alpha_N}^N\rangle$$

$$= \sum_{\alpha_1,\ldots,\alpha_{N-1}} |e^i_{\alpha_1} \otimes \ldots \otimes e^{N-1}_{\alpha_{N-1}}\rangle \otimes |\mathcal{F}_{\alpha_1,\ldots,\alpha_{N-1}}\rangle, \tag{75}$$

where

$$\mathcal{F}_{\alpha_1,\ldots,\alpha_{N-1}} = \sum_{\alpha_N=1}^{d_N} \psi_{\alpha_1,\ldots,\alpha_{N-1}\alpha_N} e^N_{\alpha_N}. \tag{76}$$

Let $Q_\Psi = |\Psi\rangle\langle\Psi|$. Then the corresponding reduced density matrix $Q^{1,\ldots,N-1}_\Psi$, given by

$$Q^{1,\ldots,N-1}_\Psi = \mathrm{tr}_{\mathbb{C}^{d_N}}(Q_\Psi), \tag{77}$$

is a $d_1 \cdot \ldots \cdot d_{N-1}$ dimensional matrix with the matrix elements

$$(Q^{1\ldots N-1}_\Psi)_{\alpha_1,\ldots,\alpha_{N-1}|\beta_1,\ldots,\beta_{N-1}} = \langle \mathcal{F}_{\beta_1,\ldots,\beta_{N-1}} | \mathcal{F}_{\alpha_1,\ldots,\alpha_{N-1}} \rangle. \tag{78}$$

If the state Q_Ψ is AME state then the following must be true:

$$\forall^{\alpha_1,\ldots,\alpha_{N-1}}_{\beta_1,\ldots,\beta_{N-1}} \langle \mathcal{F}_{\beta_1,\ldots,\beta_{N-1}} | \mathcal{F}_{\alpha_1,\ldots,\alpha_{N-1}} \rangle$$
$$= \frac{1}{D^N} \delta_{\alpha_1\beta_1} \cdot \ldots \cdot \delta_{\alpha_{N-1}\beta_{N-1}}, \tag{79}$$

where $D^N = \prod_{i=1}^N \frac{d_i}{d_N}$.

If these equalities are true, then it follows that for any $(i_1,\ldots,i_k) \subset (1,\ldots,N-1)$ the corresponding reduced density matrix $Q^{i_1\ldots i_k}_\Psi$, given by

$$Q^{i_1\ldots i_k}_\Psi = \mathrm{tr}_{i_1\ldots i_k}\left(Q^{1\ldots N-1}_\Psi\right), \tag{80}$$

where the partial trace operation $\mathrm{tr}_{i_1\ldots i_k}(\cdot)$ is performed on corresponding Hilbert spaces describing the system of qudits labelled by lists $(i_1\ldots i_k)$. Then all the appearing reduced density matrices are maximally mixed as it follows from simple handmade calculations. Therefore, the entanglement of the all $(i_1\ldots i_k)$ is maximal possible (in the sense that entropy and negativity are maximal).

Thus, we have proved the following results.

Proposition 2: Let $\underline{d} = (d_1,\ldots,d_N)$ be such that $d_N \geq \prod_{j=1}^{N-1} d_i$. Then, the set $\mathrm{AMS}(\underline{d})$ is composed exactly as an $\otimes_{j=1}^N \mathbb{U}(d_i)$ – orbit of any $|\Psi\rangle \in \otimes_{i=1}^N \mathbb{C}^{d_i}$, $\||\Psi\|| = 1$ and such that:

$$|\Psi\rangle = \sum_{i_1,\ldots,i_{N-1}} |e^1_{i_1} \ldots e^{N-1}_{i_{N-1}}\rangle \otimes |\mathcal{F}_{\alpha_1\ldots\alpha_N}\rangle, \tag{81}$$

where $(e^\alpha_{i_\alpha})$ is any complete orthonormal system in $\mathbb{C}^{d_\alpha}$, for each α, $(\mathcal{F}_{\alpha_1\ldots\alpha_{N-1}})$ is as system of orthogonal vectors in $\mathbb{C}^{d_N}$ and such that

$$\||\mathcal{F}_{\alpha_1\ldots\alpha_{N-1}}\||^2 = \frac{1}{\prod_{\alpha=1}^{N-1} d_\alpha}. \tag{82}$$

Remark 10: The introduced here notion of deficite of entanglement and the notion of the total negativity are very close to the previously used in the similar context notion of the many qudit tangle [63]–[65]. In particular, for a specific bipartite division, the notion of the corresponding negativity

is essentially equal to the widely used in the literature notion of the generalised concurrence [66], [67].

The definitions of entropy (and negativity respectively) for the partition π, and the definitions of total entropy (and respectively negativity) allow constructing the algorithm for determining these quantities:

Algorithm 7: Algorithm Bipartition Entropy and Negativity – BPEN for calculating values of entropy and negativity. Q represents the analysed quantum state, N is the number of qudits, and d is qudits' degree of freedom.

> **procedure** BPEN(Ψ, N, d)
> $\mathcal{E}_\Psi \leftarrow 0, \mathcal{N}_Q \leftarrow 0$
> $L_{2p} \leftarrow 2q - Par(\mathfrak{I}_N)$
>   **for** $\pi = \pi_1 \wedge \pi_2 \in L_{2p}$ **do in parallel**
>   calculate $\tau^{\pi_1}_j$ for $j = 1{:}d^{|\pi_1|}$ and such that $|\Psi\rangle = \sum_j \tau^{\pi_1}_j |\psi^{\pi_1}_j\rangle \otimes |\theta^{\pi_1}_j\rangle$,
> $\mathcal{E}_\Psi \leftarrow \mathcal{E}_\Psi + (-\sum_j (\tau^{\pi_1}_j)^2 \ln(\tau^{\pi_1}_j)^2)$
> $\mathcal{N}_\Psi \leftarrow \mathcal{N}_\Psi + \frac{1}{2}\left(\left(\sum_j \tau^{\pi_1}_j\right)^2 - 1\right)$
>   **end for**
>   **return** $\mathcal{E}_Q, \mathcal{N}_Q$
> **end procedure**

The 2^N-element list of partitions influences the complexity of the algorithm. The particular operations interact with data sized d^N. The algorithm's complexity is:

$$\begin{aligned} T_{BPEN} &= T_{ini} + \sum_{\pi_1 \in 2q - Par(\mathfrak{I}_N)} \left(T_{SHM}(d^N) + T_{E_Q} + T_{N_Q}\right) \\ &= T_{ini} + 2^{N/2}(\cdot T_{SHM}(d^N) + T_{E_Q} + T_{N_Q}) \\ &= O(2^{N/2} \cdot d^{N+3}), \end{aligned} \tag{83}$$

where T_{SHM} represents the Schmidt decomposition which is performed at $O(N^3)$. Therefore, the final computational complexity contains two exponential factors.

However, the analysis of particular partitions π may be performed independently, what shows the pseudo-code in Algorithm 7. It means that analysis of a each individual partition may be dispersed among available computational nodes which of course is still of exponential complexity computation as number of qudits, the number N grows.

E. ENTANGLEMENT DEFICIT FOR SOME QUANTUM STATES

Let $d = 2$ and let $N \geq 2$. The following N-qubits state:

$$\mathrm{GHZ}_N(d) = \mathrm{GHZ}_N(2) = \frac{1}{\sqrt{2}}(|000\ldots1\rangle + |1\ldots000\rangle) \tag{84}$$

is called the (generalised) Greenberger–Horne–Zeilinger state (GHZ state for shorthand). For $N = 2$, the $\mathrm{GHZ}_2(2)$ state is maximally entangled 2-qubit state in the sense that the corresponding one qubit reduced density matrices (RDM) are maximally mixed. Additionally, the $\mathrm{GHZ}_2(2)$ state is maximally entangled with respect to LOCC semi-order relation on the set $\partial E(\mathbb{C}^2 \otimes \mathbb{C}^2)$.

For $N = 3$, all the one qubit RDMs:

$$Q_{(1)} = \text{tr}_{23}\left(|\text{GHZ}_3(2)\rangle\langle\text{GHZ}_3(2)|\right) =$$
$$Q_{(2)} = \text{tr}_{13}\left(|\text{GHZ}_3(2)\rangle\langle\text{GHZ}_3(2)|\right) =$$
$$Q_{(3)} = \text{tr}_{12}\left(|\text{GHZ}_3(2)\rangle\langle\text{GHZ}_3(2)|\right) = \begin{pmatrix} \dfrac{1}{2} & 0 \\ 0 & \dfrac{1}{2} \end{pmatrix}, \quad (85)$$

are equal to each other and are maximally mixed (where $\text{tr}_{ij}(-)$ means the quantum operation of tracing out the corresponding to qubits i and j degrees of freedom).

This shows that the $\text{GHZ}_3(2)$ state has maximal total entropy (56) and maximal negativity as well. Additionally, one can show that $\text{GHZ}_3(2)$ state is maximal state with respect to LOCC semi-order relation.

In the case of $N = 4$, the situation is different as it was proved by Higuchi and Sudberry [68], and also confirmed in [69] (see also the fundamental work of Klyachko [61]) that four qubits states which have maximally mixed all two-qubits RDMs do not exist. However, the state $\text{GHZ}_4(2)$ is maximal with respect to LOCC semi-ordering relation.

Observation 1: The deficit of $\text{GHZ}_N(2)$ *state entanglement as given by (58) obeys the rule:*

$$\lim_{N\to\infty} \Delta\mathcal{E}\left(\text{GHZ}_N(2)\right) = \infty. \quad (86)$$

Proof: From the permutational symmetry of the $\text{GHZ}_N(2)$ state (see Definition 1), it follows that for any 2-partition $\pi = (\pi_1, \pi_2)$ of $\mathfrak{I}_N$, and such that $|\pi_1| = k$, it is enough to consider the partition with $\pi_1 = \{1, 2, \ldots, k\}$.

Moreover, it appears that the corresponding Schmidts ranks are equal to two and the values of non-vanishing Schmidt's numbers are $\lambda_1 = \frac{1}{\sqrt{2}}$ and $\lambda_2 = \frac{1}{\sqrt{2}}$. The corresponding to π_1 partition von Neumann entropy is equal to $\ln(2)$, for each $k = 1:N$. Therefore, the total entropy

$$\mathcal{E}\left(\text{GHZ}_N(2)\right) = \sum_{k=1}^{N^\star}\binom{N}{k}\ln(2) \quad (87)$$

comparing it with (57), concludes the proof. $\square$

Another well known, and frequently used for several purposes, is the class of the so-called W-states, defined for N-qubit system as:

$$\text{W}_N(2) = \frac{1}{\sqrt{N}}\left(|0\ldots1\rangle + |0\ldots10\rangle + \ldots + |10\ldots0\rangle\right). \quad (88)$$

Observation 2: For $\text{W}_N(2)$ *states:*

$$\lim_{N\to\infty} \Delta\mathcal{E}(\text{W}_N(2)) = \infty. \quad (89)$$

Proof: Using the permutational symmetry of $\text{W}_N(2)$ state, it follows that it is enough to compute the corresponding entropies for the one of the representative of all classes in partition groups for which $|\pi_1| = k$. So, let $k = 1:\lfloor N/2 \rfloor$, and the corresponding partitions of $\mathfrak{I}_N$ will be denoted as

$1\ldots k = \{1, 2, \ldots, k\}$. Then, some easy and handy computations show that rank of the corresponding Gram matrix (see [70], and also the Example 5 and below) is equal to $k+1$, and the corresponding spectrum has the non-zero part equal to $\left(1 - \frac{1}{N}, \underbrace{\frac{1}{N}, \ldots, \frac{1}{N}}_{k-\text{times}}\right)$. Therefore

$$\mathcal{E}^{1\ldots k}(\text{W}_N(2)) = -\left(1 - \frac{1}{N}\right)\ln\left(1 - \frac{1}{N}\right) - k\cdot\frac{1}{N}\ln\frac{1}{N}. \quad (90)$$

From (90) it follows that

$$\mathcal{E}(\text{W}_N(2)) = \sum_{k=1}^{N^\star}\binom{N}{k}\mathcal{E}^{1\ldots k}(\text{W}_N(2)). \quad (91)$$

Comparing this formula with definition (57) concludes the proof by an elementary arguments (see also below). $\square$

Definition 1: Let $T \subseteq S_N$ *be a subset of the symmetric group* S_N. *The state* $Q \in E(\mathbb{C}^{d\otimes N})$ *will be called* T-*symmetric state if and only if*

$$\forall_{\pi\in T}\ \pi(Q) = Q, \quad (92)$$

where:

$$Q = \sum_{\substack{i_1\ldots i_N=1:d, \\ j_1\ldots j_N=1:d}} Q_{i_1\ldots i_N|j_1\ldots j_N}|i_1\rangle\langle j_1| \otimes \ldots \otimes |i_N\rangle\langle j_N|, \quad (93)$$

and $|i_\alpha\rangle\langle j_\alpha|$ *is the canonical basis in the corresponding space* $L(\mathbb{C}^d)$ *(the space of* $d \times d$ *matrices), then*

$$\pi(Q) = \sum_{\substack{i_1\ldots i_N=1:d, \\ j_1\ldots j_N=1:d}} Q_{i_{\pi(1)}\ldots i_{\pi(N)}|j_{\pi(1)}\ldots j_{\pi(N)}}|i_1\rangle\langle j_1| \otimes \ldots \otimes |i_N\rangle\langle j_N|. \quad (94)$$

Remark 11: It is easy to conclude that if the state Q *is* T *invariant, then it is also invariant under the action of the subgroup, generated by the set* T *of the corresponding symmetric group. This gives the opportunity to divide the sets of* k-*th elements partitions into equivalence classes, on which the corresponding entropy is constant.*

Example 3: The states $\text{GHZ}_N(2)$ *and* $\text{W}_N(2)$ *are examples of a* S_N-*invariant states. Also their generalisations, introduced below, denoted as* $\text{GHZ}_N(d)$ *and resp.* $\text{W}_N(d)$, *are* S_N-*invariant states.*

Let $Q \in \partial E((\mathbb{C}^d)^{\otimes N})$ be a S_N – invariant state. Let $\pi \in 2 - Par(\mathfrak{I}_N)$ and $|\pi^1| = k \leq \lfloor N/2 \rfloor$. Then, for any such π the corresponding Gram matrices (of dimension d^k) have the same (modulo numbers of zeros eigenvalues) spectrum $(\lambda_1^{\pi_1}, \ldots, \lambda_{d^k}^{\pi_1})$. Therefore, for any π^1 such that $|\pi^1| = k$, the von Neumann entropy is the same. So, it is enough to compute entropy in the case when $\pi^1 = \{1, \ldots, k\}$.

Lemma 1: Let $Q \in \partial E((\mathbb{C}^d)^{\otimes N})$ *be a* S_N-*invariants a straightforward corol* N-*qudit pure state. Then, the total*

entropy of Q is given by

$$\mathcal{E}(Q) = \sum_{k=1}^{N^\star} \binom{N}{k} \mathcal{E}^{\underline{1\dots k}}(Q). \tag{95}$$

As a straightforward corollary, we have:

Corollary 2: Let $Q_N \in \partial E((\mathbb{C}^d)^{\otimes N})$ be a sequence of S_N-invariant N-qudit pure states such that

$$|\mathcal{E}^{\underline{1\dots k}}(Q_N)| \le c \cdot k, \tag{96}$$

where $c \in \mathbb{R}$, then

$$\lim_{N\to\infty} \Delta\mathcal{E}(Q_N) = \infty. \tag{97}$$

Much more stronger version of this simple observation is the following result.

Proposition 3: Let $Q_N \in \partial E((\mathbb{C}^d)^{\otimes N})$ be any sequence of qudit states, and let for any $(\pi_1, \pi_2) \in 2 - Par(\mathfrak{I}_N)$ with $|\pi_1| = k$ the following estimate be valid:

$$\mathcal{E}^{\pi_1}(|\Psi_N\rangle) \le k^d - \frac{O(1)}{k}. \tag{98}$$

Then,

$$\lim_{N\to\infty} \Delta\mathcal{E}(|\Psi_N\rangle) = \infty. \tag{99}$$

Remark 12: The very interesting class of highly entangled N-qubit states is given by the so-called cluster states [35], [71]–[73]. It appeared that for most of them the corresponding entropy deficit also grows fast with an increase of N.

Example 4 (The Generalised GHZ-States): The following family of states generalises the notion of $\mathrm{GHZ}_N(2)$ states for qudits:

$$\mathrm{GHZ}_N(d) = \frac{1}{\sqrt{d}} (|0\dots0\rangle + |1\dots1\rangle $$
$$+ \dots + |d-1\dots d-1\rangle). \tag{100}$$

This family is evidently S_N-invariant family. The corresponding to the cut $\underline{1\dots k}$ Gramian $\mathfrak{G}^{\underline{1\dots k}}(\mathrm{GHZ}_N(d))$ is spanned by the frame

$$\mathfrak{F} = \{\frac{1}{\sqrt{d}}|0\dots0\rangle_{N-k}, \dots, \frac{1}{\sqrt{d}}|(d-1)\dots(d-1)\rangle_{N-k}\}, \tag{101}$$

where $|\alpha\dots\alpha\rangle_{N-k}$ stands for state $|\alpha\rangle\otimes\dots\otimes|\alpha\rangle$ of the qudits with label $k+1$ up to N.

The Gramian (modulo the permutations of rows and cutting-off null sectors) looks like:

$$\mathfrak{G}^{\underline{1\dots k}}(\mathrm{GHZ}_N(d)) = \frac{1}{d} \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}. \tag{102}$$

The von Neumann entropy of the cut $\underline{1\dots k}$ is now easy to compute:

$$\mathcal{E}^{\underline{1\dots k}}(\mathrm{GHZ}_N(d)) = \ln(d), \tag{103}$$

and the total entropy is equal

$$\mathcal{E}(\mathrm{GHZ}_N(d)) = \sum_{k=1}^{\lfloor N/2 \rfloor} \binom{N}{k} \ln(d). \tag{104}$$

Example 5 (The Generalised $\mathrm{W}_N(d)$-States): The following family of states seems to be a natural generalisation of the standard N-qubit W-states to the case of qudits of dimensions d:

$$\mathrm{W}_N(d) = \mathcal{N}^\star \left(|0\dots0\rangle + \sum_{i=1}^{N} \left(\sum_{\alpha_i=1}^{d-1} |0\dots\alpha_i\dots\rangle \right) \right), \tag{105}$$

where α_i is putted at i-th position, and

$$\mathcal{N}^\star = \frac{1}{\sqrt{1 + N(d-1)}}. \tag{106}$$

For a given k, the corresponding Gram matrix $\mathfrak{G}^{\underline{1\dots k}}(\mathrm{W}_N(d))$ is spanned by the frame consisting of $1 + (d-1)k$ vectors:

$$\mathfrak{F} = \{V_1, V_2, \dots, V_{1+(d-1)k}\}, \tag{107}$$

where

$$V_1 = \mathcal{N}^\star (|0\dots0\rangle_{N-k} + |0\dots01\rangle_{N-k} + \dots $$
$$+ |0\dots(d-1)\rangle_{N-k} + |0\dots10\rangle_{N-k} $$
$$+ |0\dots20\rangle_{N-k} + \dots + |0\dots(d-1)0\rangle_{N-k} + \dots $$
$$+ \dots + \dots + \dots + \dots + \dots + |10\dots0\rangle_{N-k} $$
$$+ |20\dots00\rangle_{N-k} + \dots + |(d-1)0\dots0\rangle_{N-k})$$

and

$$V_2 = V_3 = \dots = V_{1+(d-1)k} = |0\dots0\rangle_{N-k}. \tag{108}$$

The corresponding Gram matrix $\mathfrak{G}^{\underline{1\dots k}}(\mathrm{W}_N(d))$ after permuting the rows and eliminating the null sectors is given by the following $(1 + (d-1)k) \times (1 + (d-1)k)$ matrix:

$$\mathfrak{G}^{\underline{1\dots k}}(\mathrm{W}_N(d))$$
$$= (\mathcal{N}^\star)^2 \left.\begin{bmatrix} ||V_1'||^2 & 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & 1 & 1 & \dots & 1 \end{bmatrix}\right\}\begin{smallmatrix}(d-1)k \\ \text{size}\end{smallmatrix} \tag{109}$$

where $||V_1'||^2 = d + (N-k-1)(d-1)$.

If $N = 4$ and $d = 3$, the form of the Gram matrix $\mathfrak{G}^{\underline{12}}(\mathrm{W}_4(3))$ is

$$\mathfrak{G}^{\underline{12}}(\mathrm{W}_4(3)) = \frac{1}{9} \begin{bmatrix} 5 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \tag{110}$$
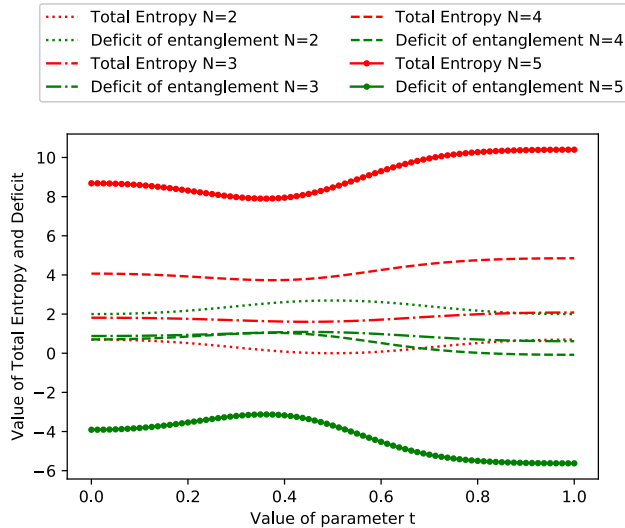
FIGURE 3. Values of Entropy and entanglement's deficit calculated by Algorithm 7 for state Q given in (112). Deficit of entanglement is calculated as $\Delta\mathcal{E}(|\Psi\rangle) = d + (\mathcal{E}(N, d) - \mathcal{E}(|\Psi\rangle))$. Entropy and deficit for state Q has been calculated for different numbers of qubits $N = 2, 3, 4, 5$.

and the corresponding entropy according to cut $\underline{12}$ is equal to:

$$\mathcal{E}(\mathfrak{G}^{\underline{12}}(W_4(3))) = \log(5) - \frac{4\log(4)}{5} \approx 0.500402,$$

$$(111)$$

where particular eigenvalues of the matrix are: $\mathfrak{G}^{\underline{12}}(W_4(3))$ this $\lambda_1 = \frac{1}{18}(9 + \sqrt{17})$, $\lambda_2 = \frac{1}{18}(9 - \sqrt{17})$, $\lambda_3 = \lambda_4 = \lambda_5 = 0$.

F. NUMERICAL EXPERIMENTS

Calculating Entropy in multi-qubit entanglement may be shown for two states families, i.e. GHZ$_N$ and W$_N$ states, where N stands for the number of qubits utilised to build the subregister. In the presented numerical example, a convex combination of these states, for $0 \leq p \leq 1$, is:

$$Q = p|GHZ_N\rangle\langle GHZ_N| + (1 - p)|W_N\rangle\langle W_N|. \quad (112)$$

Fig. 3 depicts values of Entropy for state Q, according to parameter p, and entanglement's deficit $\Delta\mathcal{E}(|Q\rangle)$ obtained after executing Algorithm 7.

Naturally, numeric computation for greater values of N shows greater values of Entropy. However, the variability of Entropy values is similar like for $N = 5$. Open source code [74] allows repeating the experiment and further calculations for greater N.

Calculating values of Entropy/Negativity with Algorithm 7, as it is pointed out by the algorithm's description, may be realised in parallel by a multiprocessor system. This approach shortens the calculations time and allows better utilisation of computing resources. It should be emphasised once more that the parallelisation is useful in calculating partial Entropy values for each partition (by creating several partition sets and performing calculations in one computational task for a specific set). Additionally, algebraic operations

TABLE 2. The worst and the best execution time for Algorithm 7, performed on a machine equipped in Intel Xeon W-2245 3.9 GHZ (base clock) processor. The shortest time was gained for two NumPy threads and eight tasks (the partition set is split into eight computational cores). The algorithm was applied to calculate Entropy values for a system, described by (112), with different number of qubits. The utilised Python distribution is dedicated for Intel One API 2022.0.22 package. The numerical experiments were performed in virtual environment WSL2 for Windows 11 (version 10.0.22000.613), Linux kernel 5.10.102.1.

Qubits	Numpy threads	Number of tasks	Time in sec.
7	1	1	5.02
7	2	8	2.58
8	1	1	13.38
8	2	8	3.88
9	1	1	47.75
9	2	8	11.67
10	1	1	235.91
10	2	8	59.6

performed on quantum states, e.g. Schmidt decomposition, may be also realised in parallel due to the NumPy package.

Values presented in Table 2 depict calculations duration for the state Q given by (112). Gathered data show that more effective usage of computational resources may be gained by properly selected number of threads and tasks (i.e. partition sets). In the testing environment, octa-core Intel Xeon W-2245 was utilised but the true number oif threads is sixteen thanks to the Hyperthreading technology. A split into eight main computational tasks – where each task has two dedicated NumPy threads – results with the quickest execution of the computation. The obtained acceleration, in systems of seven and lesser number of qubits, is about two. However, for greater number of qubits acceleration increases. The computation is performed four times quicker for a ten-qubit system in comparison to basic approach when particular steps of partition analysis are executed one after the other.

Algorithm 7 is easily scalable. Even for one node, the partition set split results with shorter calculation time. Especially, when the number of nodes is greater, the acceleration is more effective what is shown in Fig. 4. The testing environment was based on processors Intel Xeon E5420 2.50 GHZ (older solution than in the first experiment), the calculations were performed on sixteen nodes, and each node consists of two processors. This approach allows checking, if greater number of nodes results with shorter computation time.

The communication between nodes is based on the mpi4py 3.1.3 package [75]. Fig. 4 depicts that doubling the number of nodes causes proportional time shortening, what is especially visible for the ten-qubit system. It should be added that the communication between nodes is restricted only to passing partial Entropy values what means that it has no significant impact on the whole calculation process. The biggest difference between the worst and the best case is over forty-fold, if we compare cases with and without parallelisation. Naturally, this figure is lesser if we compare a node where eight compute tasks receive a split set of partitions with the cases where 2, 4, 8, and 16 compute nodes are used. For 16 nodes (10 qubit system), the acceleration is approximately
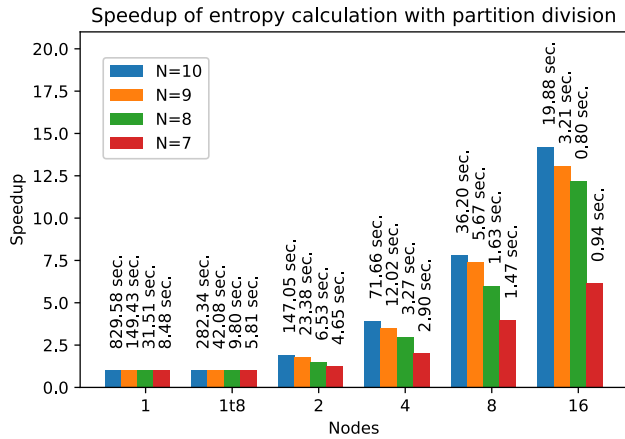
FIGURE 4. The speedup values for different sizes of quantum system given by (112), where *N* is the number of qubits. The value "1" on axis Nodes means that only one computational task was used and there was no split in partition set. Marking "1t8" stands for one node with eight computation tasks. The other values on axis Nodes point out the number of nodes, each with the eight computation tasks. Values over the bins describe duration of the experiment. The speedup is calculated between 1t8 and 2, 4, 8, 16 nodes. The computing system contains sixteen nodes and each one is built of two quad-core Intel Xeon E5420 2.50 GHZ (base clock) processors. Communication between nodes is based on MPI protocol. The numerical experiments were conducted in the operating system Debian 8.3.0-6, Linux kernel 4.19.235-1.

FIGURE 5. Entropy deficit values (in log scale) for the state $GHZ_N(dim)$ where dim = 2, dim = 3, dim = 4, for a different number of qudits *N* = 1:12. The total entropy value is defined as (58) and the entropy of state $GHZ_N(\cdot)$ is described by the formula (87).

fifteen times (or even fourteen is we compare node "1" where one computational task with the case where 16 nodes is used). For systems with lesser number of qubits, the acceleration is not so spectacular because of smaller matrix size expressing analysed quantum states.

The results of the last numerical example, presented here, are shown in Fig. 5. We calculate entropy deficit for states $GHZ_N(2)$, $GHZ_N(3)$, $GHZ_N(4)$, and in Fig. 6 for $W_N(2)$. We also present the differences between the total entropy value (58) and the entropy value for two defined states by formulas (87) and (91), respectively. Values of total entropy

FIGURE 6. Entropy deficit values (in log scale) for the state $W_N(2)$ with a different number of qubits *N* = 1:12, where the total entropy value is defined as (58) and the entropy of state $W_N(2)$ is described by the (91).

and entanglement deficit were determined for a different number of qubits, i.e. $N \in (1, \ldots, 12)$.

The source code of Python scripts, realising the shown numerical experiments, is accessible in [74].

VI. CONCLUSION

The article presents fundamental opportunities of parallelising the operations of the quantum register processing. The register may be expressed as a qudit vector state or a density matrix. The crucial element of the presented procedures is the indication of local operations that can be performed independently of one another. The approach to a very efficient implementation of the von Neumann measurement operation in the form of a parallel reduction is the contribution of this work, and it allows using many available computational units.

The problem of an entanglement's presence in the multiqubit (multi-qudit) register is also discussed and enriched by providing the necessary definitions of the entropy value and the negativity measure for a register divided into two parts. The basic technique of parallel computation for this task was also indicated and the measures for an exemplary register, which state is a convex combination of two entangled states, are shown.

Although simulations of quantum computing are burdened with the exponential size of the problems, they are subject to the possibility of parallelisation, both at the level of quantum circuit simulations or other problems, such as the presented study of multipartite entanglement (see Algorithm 7), which allows obtaining a significant reduction in the processing time of the analysed problem or simulation.

It was also shown how the problem of calculating the entanglement deficit can be effectively calculated for selected quantum states. In particular, it is shown how to use the Gramian based techniques to perform the necessary calculations. The given formulas no longer require exponential computing resources to calculate the values of total entropy or entropy at the given cuts.
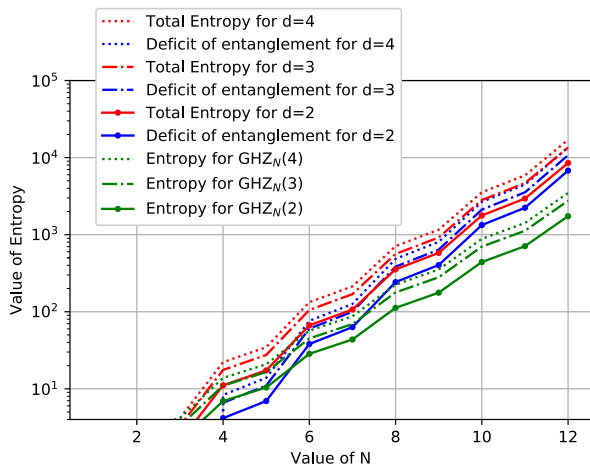
APPENDIX
LOCAL OPERATIONS ON QUANTUM COMPOSITE SYSTEMS

A compound quantum system Θ of N independent subsystems $\theta_i (i = 1:N)$ is analysed in this appendix. Let $\mathcal{H}_i$ be a adequate Hilbert space for i-th qudit (under the assumption that each space has a finite number of dimensions n_i). State space describing states of i-th qudit $\mathcal{H}_i$ is marked as $E(\mathcal{H}_i)$. Following quantum physics rules, a global Hilbert space of the composite system Θ of all qudits is defined by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_N$, and the dimensions of this space are $D = n_1 \cdot n_2 \cdot \ldots \cdot n_N$.

Let us set $\mathfrak{I}_N = \{1, 2, \ldots, N\}$, then a space of all partitions of $\mathfrak{I}_N$ is denoted by $\text{Par}(\mathfrak{I}_N)$. Elements π of $\text{Par}(\mathfrak{I}_N)$ fulfil $\pi = (\pi_1, \ldots, \pi_k)$, where $\pi_i \subset \mathfrak{I}_N$, $\pi_i \cap \pi_{i'} = \emptyset$ for $i \neq i'$ and $\bigcup_i \pi_i = \mathfrak{I}_N$. A partition $\pi = (\pi_1, \ldots, \pi_k)$ is called finer than $\pi' = (\pi'_1, \ldots, \pi'_l))$ only if for $i \in \mathfrak{I}_k$ there exists $j \in \mathfrak{I}_l$ such that $\pi_i \subseteq \pi'_j$. This allows defining the partial order α in the space $\text{Par}(\mathfrak{I}_N)$. Now, it is simple to point out the maximal element $\pi_{\max} = \{\mathfrak{I}_N\}$ and the minimal one $\pi_{\min} = \{\{1\}, \ldots, \{n\}\}$. For an arbitrary $\pi = (\pi_1, \ldots, \pi_k) \in \text{Par}(\mathfrak{I}_N)$, the space $\mathcal{H}^\pi = (\mathcal{H}_{\pi_1}, \ldots, \mathcal{H}_{\pi_k})$ may be assigned where $\mathcal{H}_{\pi_k} = \bigotimes_{i \in \pi_k} \mathcal{H}_i$. Let QP be a physical quantum operation on $E(\mathcal{H})$. The QP may be termed as an elementary π-local operation only if there exists a sequence of operations $(\text{QP}_{\pi_1}, \ldots, \text{QP}_{\pi_k})$ each transforming $E(\mathcal{H}_{\pi_i})$. Additionally, $\text{QP} = \bigotimes_{i=1:k} \hat{\mathbf{QP}}_{\pi_i}$ where $\hat{\mathbf{QP}}_{\pi_i}$ are equivalents of QP_{π_i} in the space $\text{QP}(\mathcal{H})$. Usually, a global state $\rho \in E(\mathcal{H})$ and a π-local operations are given as arithmetic bases and this raises the problem of calculating the action QP as the global operation and solving this problem is the goal of this appendix.

Another problem is that if operation QP is separable, the result of it action on entangled register may affect heavily the order of local operations performed. This problem will be not discussed here.

Let $\mathcal{M}_{n \times m}(\mathbb{C})$ stand for the space of $\mathbb{C}$-valued matrices sized $n \times m$. In this space, a family of matrices $A = A_1 \otimes \ldots \otimes A_N \in \mathcal{M}_{n_1 \cdots n_N, m_1 \cdots m_N}(\mathbb{C})$ may be defined where $A_i \in \mathcal{M}_{n_i \times m_i}(\mathbb{C})$, $i = 1:N$. Let $A(i, j)$ be an element of the matrix A. Of course, the value of $A(i, j)$ may be computed in terms of the local indices $(i_\alpha, j_\beta) \in \mathbb{I}_{n_1} \times \mathbb{I}_{m_1}$.

Proposition 4: Let $A_i \in \mathbb{M}_{n_i \times m_i}(\mathbb{C})$ for $i = 1 : N$ and let $A = A_1 \otimes \ldots \otimes A_N$. Then for any $i \in \{1, \ldots, n_1 \cdot \ldots \cdot n_N\}$, $j \in \{1, \ldots, m_1 \cdot \ldots \cdot m_N\}$ there exist unique N-element tuples

$$\underline{\alpha} = (\alpha^1, \ldots, \alpha^N), \alpha^k \in \{1, \ldots, n_k\},$$
$$\underline{\beta} = (\beta^1, \ldots, \beta^N), \beta^k \in \{1, \ldots, m_k\}, \quad (113)$$

such that

$$A(i, j) = A_1(\alpha^1, \beta^1) \cdot \ldots \cdot A_N(\alpha^N, \beta^N), \quad (114)$$

where

$$i = (\alpha^1 - 1)n_2 \cdot \ldots \cdot n_N$$
$$+ (\alpha^2 - 1)n_3 \cdot \ldots \cdot n_N$$

$$+ \ldots \quad \ldots \quad \ldots \quad \ldots$$
$$+ (\alpha^{N-1} - 1)n_N + \alpha^N, \quad (115)$$
$$j = (\beta^1 - 1)m_2 \cdot \ldots \cdot m_N$$
$$+ \beta^2 - 1)m_3 \cdot \ldots \cdot m_N$$
$$+ \ldots \quad \ldots \quad \ldots \quad \ldots$$
$$+ (\beta^{N-1} - 1)m_N + \beta^N. \quad (116)$$

Proof: The easy proof follows from the associativity of the Kronecker product and from the ancient theorem about dividing integers with remainder. The details can be found in [48]. $\square$

The above proof also determines the way how tuples $\underline{\alpha}$ and $\underline{\beta}$ have to be calculated. Some examples presenting the usage of Proposition 4 are shown below.

Example 6 (The Case of Pure States): Let $N = 2$ and $|\psi_1\rangle \in \mathcal{M}_{1 \times n_1}(\mathbb{C})$, $|\psi_2\rangle \in \mathcal{M}_{1 \times n_2}(\mathbb{C})$. Then $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{M}_{1 \times n_1 n_2}(\mathbb{C})$ has the coordinates $|\psi\rangle(i) = |\psi_1\rangle(\alpha^1) \cdot |\psi_2\rangle(\alpha^2)$ where $i = (\alpha^1 - 1)n_2 + \alpha^2$ and $\alpha^1 \in \{1, \ldots, n_1\}$, $\alpha^2 \in \{1, \ldots, n_2\}$. The coefficients α^1 and α^2 can be calculated by dividing the number i by n_2 with the remainder.

Example 7: Let $N = 3$ and $A_1 \in \mathcal{M}_{n_1 \times m_1}(\mathbb{C})$, $A_2 \in \mathcal{M}_{n_2 \times m_2}(\mathbb{C})$, $A_3 \in \mathcal{M}_{n_3 \times m_3}(\mathbb{C})$. Then $(A_1 \otimes A_2 \otimes A_3)(i, j) = A_1(\alpha^1, \beta^1)A_2(\alpha^2, \beta^2)A_3(\alpha^3, \beta^3)$ where

$$i = (\alpha^1 - 1)n_2 \cdot n_3 + (\alpha^2 - 1)n_3 + \alpha^3,$$
$$j = (\beta^1 - 1)m_2 \cdot m_3 + (\beta^2 - 1)m_3 + \beta^3, \quad (117)$$

are uniquely determined.

If $(E_{i,j})$ stands for the system of canonical unit-matrix, i.e. $(E_{i,j})(k, l) = \delta_{ki} \cdot \delta_{lj}$, then the system $(E_{\alpha_1, \beta_1} \otimes \ldots \otimes E_{\alpha_N, \beta_N})$ forms a product computational basis in the space $\bigotimes_{i=1}^N \mathcal{M}_{n_i, m_i}(\mathbb{C})$.

Any linear mapping $\text{Op} : \mathcal{M}_{n \times m}(\mathbb{C}) \to \mathcal{M}_{n \times m}(\mathbb{C})$, termed sometimes as a superoperator, can be expressed by the (super-)matrix representation in the canonical basis (E_{ij}):

$$\text{Op}(E_{ij}) = \sum_{k,l} \text{Op}[^{k,l}_{i,j}]E_{kl}, \quad (118)$$

and therefore for $A \in \mathcal{M}_{n \times m}(\mathbb{C})$:

$$\text{Op}(A)(k, l) = \sum_{i,j} A(i, j)\text{Op}[^{k,l}_{i,j}]. \quad (119)$$

For any k-element tuple $\sigma = (i_1, \ldots, i_k) \subset \mathfrak{I}_N$ exists the adequate two-element partition $\pi^\sigma = (\sigma, \sigma^c)$ where $\sigma^c = \mathfrak{I}_N \setminus \{\sigma\}$. Each partition $\pi = (\pi_1, \ldots, \pi_k) \in \text{Par}(\mathfrak{I}_N)$ can be defined by the concept of π-locality in the product $\bigotimes_{i=1}^N \mathcal{M}_{n_i, m_i}(\mathbb{C})$. A superoperator Op acting in the space $\bigotimes_{i=1}^N \mathcal{M}_{n_i, m_i}(\mathbb{C})$ is called a π-local operation only if there is a sequence of superoperators Op^{π_i}, each affecting the space $\bigotimes_{\alpha \in \pi_i} \mathcal{M}_{n_\alpha, m_\alpha}(\mathbb{C})$, such that

$$\text{Op} = \bigotimes_{i=1}^k \hat{\text{Op}}^{\pi_i}, \quad (120)$$

where $\hat{\text{Op}}^{\pi_i}$ are natural counterparts of Op^{π_i} in the space $\text{End}(\bigotimes_{i=1}^N \mathcal{M}_{n_i, m_i}(\mathbb{C}))$.

Let a π-local operation Op^π act on $\rho \in E(\mathcal{H})$. The problem is, how to compute the result of this operation on ρ, if only the local information on Op^π is available. For this purpose, the following steps have to be performed:

(1) If ρ is represented in the canonical basis $(E_{ij})_{ij}$ of the global space $\mathcal{H}$, then use Proposition (4) and pass to the corresponding representation in the product basis $(E_{\alpha_1\beta_1} \otimes \ldots \otimes E_{\alpha_n\beta_n})$:

$$\rho = \sum_{\substack{\underline{\alpha}=(\alpha_1,\ldots,\alpha_N), \\ \underline{\beta}=(\beta_1,\ldots,\beta_N)}} \tilde{\rho}(\underline{\alpha}|\underline{\beta}) E_{\underline{\alpha}\underline{\beta}}, \qquad (121)$$

where $E_{\underline{\alpha}\underline{\beta}} = \otimes_{i=1}^N E_{\alpha_i\beta_i}$.

(2) Let Op^σ be a superoperator acting in the space $\otimes_{i\in\sigma} \mathcal{H}^i$, and let Op^σ also stand for its matrix representation in the product basis $\otimes_{i\in\sigma} E_{k_i,l_i}$. Then:

$$\hat{\mathrm{Op}}^\sigma(\rho)(i,j) = \sum_{k_\sigma,l_\sigma} \mathrm{Op}^\sigma\binom{k_\sigma,l_\sigma}{i_\sigma,j_\sigma} \cdot \tilde{\rho}(k_\sigma \vee l_{\sigma^c}, i_\sigma \vee j_{\sigma^c})$$

$$(122)$$

where the multi-indices $\underline{\alpha}$ and $\underline{\beta}$ are given according to Proposition (4), and $(\alpha_\sigma \vee \alpha_{\sigma^c}) = \underline{\alpha}$, $(\beta_\sigma \vee \beta_{\sigma^c}) = \underline{\beta}$ are their decompositions.

(3) For a general $\pi = (\pi_1, \ldots, \pi_k)$-local operation $\mathrm{Op}^\pi = \hat{\mathrm{Op}}^{\pi_1} \otimes \ldots \otimes \hat{\mathrm{Op}}^{\pi_k}$ apply step (2) k-times, independently of the order, and this property allows performing step (3) in parallel.

Example 8: Let us consider three-qudit case with the following partial transposition coresponding to the decomposition of $\pi = (\{1, 3\}, \{2\})$. Let the action of $\hat{T}_2 = \mathbb{I}_{(1)} \otimes T \otimes \mathbb{I}_{(3)}$ on a given tripartite state $\rho \in \mathcal{M}_{n_1 \cdot n_2 \cdot n_3, m_1 \cdot m_2 \cdot m_3}(\mathbb{C})$ be analysed here. The locality of the operation $\hat{T}_2$ and the use of previous computations (see Proposition 4 above) allows obtaining:

$$(\hat{T}_2\rho)(i,j) = \rho(i^\star, j^\star), \qquad (123)$$

where

$$i^\star = (\alpha^1 - 1)n_2 \cdot n_3 + (\beta^2 - 1)n_3 + \beta^3,$$
$$j^\star = (\beta^1 - 1)m_2 \cdot m_3 + (\alpha^2 - 1)m_3 + \alpha^3. \qquad (124)$$

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