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Dedicated to the memory
of Professor Vladimir Gerdt

Professor Vladimir Petrovich Gerdt
21.01.1947 – 05.01.2021

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Memorial article

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In Memory of Vladimir Gerdt

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This article is a memorial, it is dedicated to the memory of the head of the Scientific Center for Computational Methods in Applied Mathematics of RUDN, Professor V. P. Gerdt, whose passing was a great loss to the scientific center and the computer algebra community. The article provides biographical information about V. P. Gerdt, talks about his contribution to the development of computer algebra in Russia and the world. At the end there are the author's personal memories of V. P. Gerdt.

Key words and phrases: computer algebra, quantum computing, mimetic methods, polynomial computer algebra methods

1. Introduction

The name of Vladimir Gerdt is widely known among computer algebra community. Many years he was a professor at the Joint Institute for Nuclear Research (JINR), where he was the head of the Group of Algebraic and Quantum Computations (`http://compalg.jinr.ru/CAGroup`), and an organizer of many mathematical conferences. A few years ago, he was invited to head the Scientific Center for Computational Methods in Applied Mathematics founded in RUDN university. His passing was a great loss to the entire community.

2. Biography

Vladimir Gerdt was born in Engels near Saratov. He earned his M. Sc. in Theoretical Physics from Saratov State University in 1971, his Ph. D. in Theoretical and Mathematical Physics from JINR in 1976, and his D. Sc. in Mathematics and Computer Science from JINR in 1992. In 1997 he got the scientific title Professor in Mathematics and Computer Science by specialty “Application of Computer Techniques, Mathematical Modelling and Mathematical Methods to Scientific Research”.

After his M. Sc. Vladimir Gerdt worked in JINR until his death in January 5, 2021. He began as an engineer-programmer (1971–1975), then he worked as a junior researcher (1975–1977) at the JINR Department of Radiation Safety where a software for neutron spectroscopy was developed. In 1977 he moved to the JINR Laboratory of Computing Techniques and Automation renamed in 2000 as Laboratory of Information Technologies, where he worked as a researcher (1977–1980) and as a senior researcher (1980–1983), and since 1983 as the head of the research group on computer algebra. Vladimir Gerdt worked abroad for several years, in Lille and Aachen, using Russian, English, German and French in his work.

Figure 1. Vladimir Gerdt in his office. Dubna, 1998

3. Professional activities

V. Gerdt prepared 243 scientific articles, he edited 10 books. His latest researches are devoted to the construction of involutive monomial bases and to the discretizations of incompressible Navier–Stokes equations. His last huge article was published in ArXiv in September 2020.

Vladimir was the referee at journals and organizations:

— Journal of Symbolic Computation;
— Programming and Computer Software;
— Physics of Particles and Nuclei Letters;
— Russian Foundation for Basic Research;
— Russian Science Foundation.

Vladimir was a member of:

— Association for Computing Machinery (ACM);
— ACM Special Interest Group on Symbolic and Algebraic Manipulation (SIGSAM);

— Editorial Board of Journal of Symbolic Computation (Academic Press);
— Advisory Board of Computer Science Journal of Moldova;
— Special Computer Algebra Group of German Societies on Computer Science.

Vladimir took part in the coordination of the international research projects:

— he was adjoint coordinator of the INTAS-93-0030 project “Computer Algebra, Symbolic and Combinatorial Tools in Differential Algebra and Differential Equations, with impact in Fundamental Physics and Control Theory” with 10 research teams from EC countries and 7 research teams from NIS countries;
— scientific coordinator of cluster A: Computer Assisted Mathematics of the INTAS-93-0893 project “ERSIM-FSU Cooperative Network in Informatics and Applied Mathematics” with 10 research teams in EC countries and 10 research teams from NIS countries.

Vladimir Gerdt paid great attention to teaching. He gave 24 lecture courses for students and young scientists. Under his supervision 10 master theses were prepared, 9 Ph. D. theses were defended. He was the scientific consultant of Yuri Blinkov’s thesis for Doctorship of Sciences.

Figure 2. Vladimir with students. Dubna, 2002

4. Vladimir Gerdt and computer algebra

4.1. At the beginning of computer algebra

Vladimir was one of the first who started computer algebra usage in the USSR in the 70th. This activity was supported by Academic Dmitry Shirkov and Professor Nikolay Govorun.

In the early 80th the Joined Institute for Nuclear Research (JINR, Dubna) bought the computer CDC-6500. It was powerful enough for the implementation of the universal computer algebra systems. Professor Tony Hearn kindly passed the REDUCE system to the JINR during his visit to Dubna. Professor Gerdt with colleagues took a large part in its implementation in the institute and assisted in spreading the REDUCE in the scientific centers of the USSR.

Vladimir got the "First JINR Prize (1986) for the Research on Installation, Development and Application of Program Systems for Symbolic Computation on Mainframe Computers".

Vladimir was on Committees of many conferences. The main of them are:

— International Symposium on Symbolic and Algebraic Computation (ISSAC);
— Conference on Applications of Computer Algebra (ACA);
— Polynomial Computer Algebra (PCA);
— Computer Algebra in Scientific Computing (CASC), Vladimir was one of its founders. Now CASC-2021 is the 23rd conference in this series. It takes place in Sochi (Russia).

Figure 3. Foundators of the CASC Profs. Vladimir Gerdt and Ernst Mayr, Armenia, 2010

4.2. Partial differential equations

A large cycle of works by Vladimir Gerdt was devoted to the study of the compatibility of systems of partial differential equations (PDEs) by means of computer algebra. The key to solving the problem was the Cauchy-Kovalevskaya theorem, which reduces the study of the solvability of some classes of systems of partial differential equations to the study of the compatibility of a system of algebraic equations for the coefficients of the corresponding power series.

Theoretical research on the compatibility of systems of nonlinear differential equations in general form was started at the beginning of the 20th century by Riquier [1], Janet [2], and Thomas [3]. V. P. Gerdt told us about the long months he spent in the 1980s searching and studying these far from well-known works written in various European languages.

Riquier proposed a complete ordering for partial derivatives, using which he distinguished some of the derivatives, called principal ones, with respect to which the system of PDEs can be resolved. The remaining derivatives, called parametric, leave arbitrariness in the solution and affect the setting of the initial conditions. As a result, a theory was constructed containing the Cauchy–Kovalevskaya theorem as a special case. Along the way of algorithmization of these results, Janet introduced the partition of independent variables into multiplicative and non-multiplicative for the principal derivatives. Thomas generalized the Riquier–Janet approach over the case of nonlinear algebraic equations with respect to the principal derivative. He showed how to check the consistency of a system or to split it into subsystems in a finite number of steps (Thomas decomposition).

These works, at first, gave rise to a modern theory, which makes it possible to investigate the compatibility of systems of partial differential equations and carry out their decomposition into subsystems (Thomas decomposition), created by V. P. Gerdt together with D. Roberts and very elegantly inscribed in the theory of differential rings. Later, the theory was used to create the `DifferentialThomas` package, recently implemented in Maple (`https://www.maplesoft.com`). A monograph by D. Roberts is devoted to this issue [4].

4.3. Polynomial computer algebra

One of the most important achievements of algebra in the XX century was the creation of the theory of Gröbner bases, which made it possible to study problems from the theory of polynomial rings and algebraic geometry using a computer [5]. The main obstacle to the application of this technique is the cost of calculating these bases according to the Buchberger algorithm, therefore, the development of more efficient methods for finding Gröbner bases has been and remains an urgent problem of computer algebra. The key idea of the theory of Gröbner bases is the division of a polynomial into polynomials generating a certain ideal J. In the case of the ring $\mathbb{Q}[x]$ every ideal is principal and any polynomial g can be uniquely divided by the polynomial f generating the ideal (f). In the case of the ring $\mathbb{Q}[x_1, \dots, x_n]$ one can also talk about dividing the polynomial into polynomials $f_1, \dots, f_r$ generating the ideal J, but this was realized only in the middle of the XXth century. One of the very first steps in introducing the operation of division of polynomials was to define the admissible McCauley ordering [6]. In the process of such division, expressions of the form hf_i are successively subtracted from g, where $h \in \mathbb{Q}[x_1, \dots, x_n]$, so that the leading coefficients in g are canceled. As a result, instead of g, a new polynomial g' is obtained, the degree of which is less than the degree of g and $g - g' \in J$. Unfortunately, in the case of many variables, g' is uniquely determined in this way only when a special basis is chosen, the Gröbner basis, and only in this special basis it follows from $g \in J$ that $g' = 0$.

A wonderful idea proposed by V. P. Gerdt is that the division of a polynomial into polynomials generating the ideal J can be made unambiguous if we preserve an additional structure on the set of monomials M, which he called involutive division. The concept of involutive division is closely related to the partitioning of independent variables introduced by Janet (see above) in the study of the compatibility of systems of partial differential equations.

V. P. Gerdt brought ideas that arose in the theory of PDEs to polynomial algebra, which made it possible to look at old problems in a completely new light.

Involutive division allows for any monomial m choosing one of the monomials of a given finite set U and thus uniquely determine the choice of hf_i when dividing g by $(f_1, \dots, f_r)$. The remainder of the division can now be called the normal form of the polynomial g with respect to the polynomials $f_1, \dots, f_n$. However, checking $g \in (f_1, \dots, f_r)$ is reduced to checking $g' = 0$ not for every basis $f_1, \dots, f_r$, but only for an involutive basis whose principal monomials satisfy certain properties, found and described by V. P. Gerdt and his disciple Yu. A. Blinkov. The first concrete example of involutive division was described by A. Yu. Zharkov, another disciple of V. P. Gerdt [7]–[10]. Soon V. P. Gerdt and Yu. A. Blinkov constructed many other involutive divisions. This made it possible to formulate a fundamentally new algorithm for constructing Gröbner bases [11]–[19].

Under the leadership of V. P. Gerdt, his disciples Yu. A. Blinkov and D. A. Yanovich created a number of algorithms and programs for calculating involutive bases of ideals of polynomial rings, including the open-source software package GINV (`http://invo.jinr.ru`). Their algorithms for calculating involutive bases appeared to be faster than Buchberger's algorithm and able to compete with the algorithms optimized by Fougeres and his disciples. The theory of involutive bases itself has become an important branch of computer algebra, to which the participants of international conferences on computer algebra regularly devote their articles and reports.

4.4. Mimetic methods for solving partial differential equations

Power series expansions are a very poor method for finding solutions to compatible systems of differential equations, except in the rare case when the solution is interesting in a small neighborhood of a given point. The main and, by and large, the only method for solving such systems is the finite difference method, according to which the system of differential equations in $\mathbb{R}^n$ is reduced to an infinite system of algebraic equations for the values of the sought functions at the grid nodes. Research in the field of finite-difference approximations of differential equations inheriting their basic properties has more than 60 years of history. Discretizations inheriting certain properties of continuous (differential) equations are called mimetic or compatible [20]–[25]. Discussing reports at conferences, we often heard from V. P. Gerdt about the importance of this concept for the development of numerical methods of mathematical modeling, as well as about the flexibility of the concept of inheritance, allowing for different interpretations.

In the last century, the transition from differential equations to algebraic ones was done by hand. V. P. Gerdt and Yu. A. Blinkov proposed a new approach in which this transformation was performed in computer algebra systems. The studies mentioned above have stimulated interest to the question of what happens to the differential consequences of discretization. V. P. Gerdt singled out a class of strongly consistent difference schemes. The property of strong consistency means not only the approximation of the original differential equations by the finite-difference scheme, but also the approximation of any algebraic consequence of these equations by the algebraic consequence of the difference equations that make up the scheme. These consequences include, in particular, local conservation laws.

V. P. Gerdt in his recent studies, carried out together with Yu. A. Blinkov and D. Roberts, strove to show the advantages of S-compatible schemes over others. For the demonstration, they have chosen one the system of Navier–Stokes equations, one of the most complex systems of great importance for applications. For this system, an S-compatible difference scheme was constructed and numerous computer experiments were carried out. A multi-page report on this work by V. P. Gerdt was published in ArXiv [26] shortly before his death. One can only regret that the size of this study will not allow it to be published entirely as a full journal article.

4.5. Applications of polynomial computer algebra methods in generalized Hamiltonian dynamics

The use of involutive methods in applied, engineering and physical problems described by systems of underdetermined and overdetermined differential equations has become an area of special interest for V. P. Gerdt in the early 1990s. In mechanical systems, the configuration and phase spaces of which are subject to constraints and restrictions, evolution problems inevitably require involutive analysis. This is especially true for physical systems which possess a degenerate Lagrange function and are described in the framework of the generalized Dirac Hamiltonian dynamics. In a large cycle of works carried out by V. P. Gerdt together with colleagues from Bulgaria (D. Mladenov), Georgia (S. Gogilidze, A. Khvedelidze) and Moldova (Yu. Paliy), an algorithm was developed and applied for finding a complete set of constraints (of the first and second kind) for polynomial mechanical systems with a degenerate Lagrange function, which is based on the ideas of the theory of Gröbner bases and involutive division of polynomials. The efficiency of the proposed algorithm was demonstrated, in particular, when calculating the constraints in the so-called mechanical $SU(3)$ Yang–Mills model on a light cone, where, thanks to the use of computer calculations, for the first time it was possible to determine and classify the complete set of constraints inherent in the model.

4.6. Applications of polynomial computer algebra methods in quantum theory

Computational problems related to the description of quantum systems became another area of application of Gröbner bases in the studies of V. P. Gerdt. In the 21st century, quantum theory has ceased to be just a purely fundamental physical theory. It has acquired the status of the basic element of a new quantum technological design. These changes gave rise to new computationally intensive tasks. One of these problems is the problem of classifying quantum systems in terms of their quantum resource, in particular, depending on the complete set of characteristics responsible for the phenomenon of entanglement of quantum states. The joint research performed in Dubna in the period from 2006 to 2016 by V. P. Gerdt, Y. Paliya and A. Khvedelidze focused on this class of problems.

In these works, the algebraic structure of the ring of polynomial invariants of basic composite binary quantum systems, such as qubit-qubit and qubit-qutrite pairs, was studied. As these studies have shown, computer algebra methods allow performing labor-intensive computational calculations and, thereby, determine the quantum resource of low-dimensional quantum systems, which is interesting from the point of view of various applications, including the theory of quantum information.

5. Personal memories

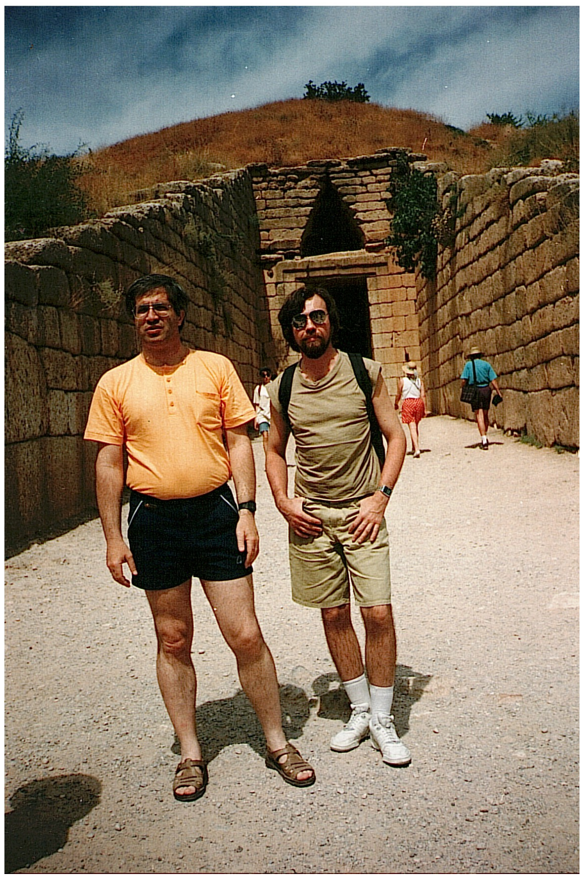

Figure 4. Vladimir Gerdt and Victor Edneral at Schliemann's excavations. Peloponnese, 1995

We met Vladimir Gerdt at the 3rd international conference on computer algebra and its applications in theoretical physics, which took place in September 1985 in Dubna. Later, we met at a couple of dozen conferences, at seminars, at defenses. I soon noticed that he took great care of those who were with him. Vladimir never spoke badly about anyone. He criticized, of course, but only in specific cases. A distinctive feature of Vladimir was great respect for people, for each person. And people felt it. It should be added, that Vladimir was a believer and observed orthodox church fasts and rituals. Without advertising it in any way.

Vladimir had wide erudition and organized very interesting excursions for conference participants in amazing places. We were with him in Peloponnese, in Germany, in France, in Japan, in Spain, in Israel, in China e.t.c.

I do not remember who said “Where the captain is, there is the captain’s bridge”. This is about Vladimir. He was quickly becoming the soul of any company, he saw any task in every detail and imagined the roles of everybody.

A clear mind allowed him to ask wonderful questions during conference reports. Always to the point. Without any self-promotion. He was very humble.

Figure 5. Alexandr Myllari and Vladimir Gerdt. Jordan river. 2017

6. Dedication

Professor Gerdt made numerous contributions to the fields of symbolic computation, differential algebra, and applications in physics. He was an excellent scientist and a kind-hearted and considerate man. Thank you very much, Vladimir!

7. List of the published works of Vladimir Gerdt

7.1. Articles

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8. Additional materials

8.1. Last video of Vladimir Gerdt

1. Compact involutive monomial bases. Joint scientific seminar of the Institute of Applied Mathematics & Communications Technology, 18 Nov. 2020. URL: `https://events.rudn.ru/event/102`.
2. Computer algebra based discretizations of incompressible Navier–Stokes equations. Joint scientific seminar of the Institute of Applied Mathematics & Communications Technology, 25 Nov. 2020. URL: `https://events.rudn.ru/event/103`.

8.2. Memorial photo galleries of Vladimir Gerdt

1. Collection of Yu. A. Blinkov.
   URL: `https://disk.yandex.ru/d/dTxdWyb2_TBAYg`
2. Collection of V. F. Edneral.
   URL: `https://yadi.sk/d/tdFNE877AzQAcw`

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Памяти Владимира Гердта

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Настоящая статья — мемориальная, она посвящена памяти руководителя научного центра вычислительных методов в прикладной математике РУДН, профессора В. П. Гердта, чей уход стал невосполнимой потерей для научного центра и всего сообщества компьютерной алгебры. В статье приведены биографические сведения о В. П. Гердте, рассказано о его вкладе в развитие компьютерной алгебры в России и мире. В конце приведены личные воспоминания автора о В. П. Гердте.

Ключевые слова: компьютерная алгебра, квантовые вычисления, миметические методы, методы полиномиальной компьютерной алгебры

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Calculation of integrals in MathPartner

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We present the possibilities provided by the MathPartner service of calculating definite and indefinite integrals. MathPartner contains software implementation of the Risch algorithm and provides users with the ability to compute antiderivatives for elementary functions. Certain integrals, including improper integrals, can be calculated using numerical algorithms. In this case, every user has the ability to indicate the required accuracy with which he needs to know the numerical value of the integral. We highlight special functions allowing us to calculate complete elliptic integrals. These include functions for calculating the arithmetic-geometric mean and the geometric-harmonic mean, which allow us to calculate the complete elliptic integrals of the first kind. The set also includes the modified arithmetic-geometric mean, proposed by Semjon Adlaj, which allows us to calculate the complete elliptic integrals of the second kind as well as the circumference of an ellipse. The Lagutinski algorithm is of particular interest. For given differentiation in the field of bivariate rational functions, one can decide whether there exists a rational integral. The algorithm is based on calculating the Lagutinski determinant. This year we are celebrating 150th anniversary of Mikhail Lagutinski.

Key words and phrases: computer algebra system, MathPartner, integral, arithmetic-geometric mean, modified arithmetic-geometric mean, Lagutinski determinant

1. Introduction

The development of computer algebra systems and cloud computing makes it possible to solve many computational problems. Vladimir Petrovich Gerdt was at the forefront of the development of computer algebra. As a professional physicist, he developed new algorithms for solving problems in mathematical physics and implemented them in many well-known systems of computer algebra. He has worked on systems such as REDUCE, Mathematica, Maple, and Singular.

Today, many useful programs and cloud services are available. A new generation of computer algebra systems is actively developing. They are cloud-based systems freely available on the Internet. The MathPartner service is a nice example of this [1]–[4]. Free access to the MathPartner service is possible at `http://mathpar.ukma.edu.ua/` as well as `http://mathpar.com/`.

In this review, we consider only a small area of MathPartner application, namely the calculation of definite and indefinite integrals. Symbolic computations and estimates of the computational complexity are of the greatest interest [5]–[9]. However, in some cases, symbolic computations need to be supplemented with numerical methods. In particular, this is true when calculating special functions [10], [11]. For example, elliptic integrals are used to calculate the period of the simple pendulum [12] as well as some properties of porous materials [13], [14].

Robert Henry Risch proposed a method to integrate elementary functions [15], [16]. The method was later improved by Manuel Bronstein [17]. In 2010–2019, an algorithm based on the Liouville–Risch–Davenport–Trager–Bronstein theory was developed at the Laboratory of Algebraic Computations of Derzhavin Tambov State University. A series of papers on symbolic integration algorithms was published by Svetlana Mikhailovna Tararova [18] and Vyacheslav Alekseevich Korabelnikov [19], [20]. The procedures were developed using object-oriented programming in Java. Their description is given in cited publications. Since the symbolic integration theory has not yet been completed, this algorithm can be considered as a good basis for further theoretical and practical development in this important area.

Historically, the first major symbolic integration project was the IBM Scratchpad project led by Richard Dimick Jenks. The development of this project as a commercial one was later stopped by the company. However, he played an important role in the development of the theory of symbolic integration and attracting interest in it.

Many general computer algebra systems today support symbolic integration of elementary functions. However, they all have a common drawback that is the incompleteness of solving the problem of symbolic integration. Another drawback is the lack of a detailed description of the procedural implementation and the technical possibility of further development of the package of procedures. The most famous example is the cloud-based SAGE system, which provides access to old open source packages that have long been discontinued. On the other hand, commercial systems do not give users access to their packages of procedures, and they do not have specialists who can complete the theory of calculating the antiderivative for the composition of simple elementary functions.

Experiments with integration problems from mathematical analysis textbooks show that many problems can be solved using any of the systems such as Mathematica, Maple, and MathPartner. Nevertheless, for each of them, one can find functions that have an antiderivative, but it is not calculated by this system. The MathPartner symbolic integration package is one of the newest packages in this area. It is developed in Java and is the most promising for further development.

In a series of important works, Mikhail Nikolaevich Lagutinski (1871–1915) developed a method for determining integrals of polynomial ordinary differential equations in finite terms. He also developed the theory of integrability in finite terms of such systems of equations [21]–[23]. Lagutinski was an outstanding mathematician. He had worked at Kharkiv and died during the First World War. In this article, we also consider the Lagutinski method.

Note that he published his papers as Lagoutinsky using the French spelling [24], [25]. The authors are grateful to Mikhail Malykh for comments and historical notes about M. N. Lagutinski.

2. Integrals of some functions

2.1. Indefinite integrals

To calculate the indefinite integral of an elementary function $f(x)$ one can run the command $\mathbf{int}(f)dx$, where x is declared in the environment SPACE. Five number sets $\mathbb{Q}$, $\mathbb{R}$, $\mathbb{R}64$, $\mathbb{C}$, and $\mathbb{C}64$ can be used. Over the field $\mathbb{Q}$, pure symbolic computations are done. For example, let us calculate $\int 2x\sin(x^2)\,dx$:

```
SPACE = Q[x];
f = 2*x*\sin(x^2);
\int(f) d x;
```

The output is equal to $(-1)\cos(x^2)$.

Next, let us calculate $\int (3x^2+2)^2\,dx$:

```
SPACE = Q[x];
\int((3x^2+2)^2) d x;
```

The output is equal to $(9/5)x^5 + 4x^3 + 4x$.

2.2. Definite integrals (the numerical algorithm)

A definite integral $\int_a^b f(x)\,dx$ can be calculated by means of the command $\mathbf{Nint}(f, a, b, \varepsilon, N)$, where ε means the approximation to ε decimals and N denotes the number of points in the Gaussian formula (optional). These parameters can be omitted.

For example, let us calculate 42 decimal places of the integral $\int_0^\pi \sin x\,dx$:

```
SPACE = R[x]; MachineEpsilonR = 42; FLOATPOS = 42;
\Nint(\sin(x), 0, \pi);
```

The output is equal to 2.000000000000000000000000000000000000000000.
Next, let us approximate π:

```
SPACE = R[x]; MachineEpsilonR = 43; FLOATPOS = 42;
2*\Nint(\sqrt(1-x^2), -1,1);
```

The output is equal to 3.141592653589793238462643383279502884197169. All 42 decimal places are accurate.

Let us consider improper integrals of the first kind $\int_a^b f(t)\,dt$, where a or b can be equal to $\pm\infty$. The integral can be calculated by means of the command $\mathbf{Nint}(f, a, b, [q_1, \cdots, q_m], \varepsilon, N)$, where $[q_1, \cdots, q_m]$ denotes the set of extreme points of the function f inside the interval of integration (a, b), the answer is the approximation to ε decimals, and N denotes the number of points in the Gaussian formula (optional). In fact, three parameters $[q_1, \cdots, q_m]$, ε, and N can be omitted. If the extreme points are not indicated, then the correctness of the output is ensured when the integrand is monotonic on the interval of integration.

For example, let us calculate $\int_{-\infty}^{+\infty} \exp\left\{-(x-5)^2\right\}\,dx$:

```
SPACE = R64[x];
f = \exp\{-(x-5)^2\};
\Nint(f, -\infty, \infty);
```

The output is equal to 1.77.

Next, let us calculate $\int_0^{\infty} \exp\{-x\}\,dx$:

```
SPACE = R[x];
MachineEpsilonR = 45; FLOATPOS = 45;
\Nint(\exp(-x), 0, \infty);
```

The output is equal to 1.000000000000000000000000000000000000000000000, where all 45 decimal places are accurate.

2.3. The complete elliptic integrals

For some improper integrals, more efficient calculation methods are known. Let us consider complete elliptic integrals [10], [12]. For positive numbers $a > 0$ and $b > 0$, the complete elliptic integral of the first kind can be calculated by means of the arithmetic-geometric mean

$$I(a,b) = \int_0^{\pi/2} \frac{d\varphi}{\sqrt{a^2\cos^2\varphi + b^2\sin^2\varphi}} = \frac{\pi}{2\mathbf{AGM}(a,b)},$$

where $\mathbf{AGM}(a,b)$ denotes the arithmetic-geometric mean of a and b. It is equal to the limit of both sequences a_n and b_n, where $a_0 = a$, $b_0 = b$, $a_{n+1} = \frac{1}{2}(a_n + b_n)$, and $b_{n+1} = \sqrt{a_n b_n}$. The proof is based on the equality $I(a,b) = I\left((a+b)/2, \sqrt{ab}\right)$. Of course, if $a = b$, then $I(a,a) = \pi/2a$.

On the other hand, the geometric-harmonic mean $\mathbf{GHM}(a,b)$ is equal to the limit of both sequences a_n and b_n, where $a_0 = a$, $b_0 = b$, $a_{n+1} = \sqrt{a_n b_n}$, and $b_{n+1} = \dfrac{2a_n b_n}{a_n + b_n}$. Note that $\mathbf{AGM}(a,b)\mathbf{GHM}(a,b) = ab$.

Both $\mathbf{AGM}(a,b)$ and $\mathbf{GHM}(a,b)$ can be calculated in the MathPartner service. For example, let us run the commands, where FLOATPOS denotes the number of decimal places:

```
SPACE = R64[];
FLOATPOS = 3;
a= \AGM(1, 5);
g= \GHM(1, 5);
\print(a, g);
```

The output is $a = 2.604$ and $g = 1.920$.

The complete elliptic integral of the second kind can be calculated by means of **MAGM**(). It is also implemented in the MathPartner service. The modified arithmetic-geometric mean $\mathbf{MAGM}(a, b)$ is equal to the limit of the sequence a_n, where $a_0 = a$, $b_0 = b$, $c_0 = 0$, $a_{n+1} = a_n + b_n/2$, $b_{n+1} = c_n + \sqrt{(a_n - c_n)(b_n - c_n)}$, and $c_{n+1} = c_n - \sqrt{(a_n - c_n)(b_n - c_n)}$,

$$\int_0^{\pi/2} \sqrt{a^2 \cos^2 \varphi + b^2 \sin^2 \varphi}\, d\varphi = \frac{\pi}{2} \cdot \frac{\mathrm{MAGM}(a^2, b^2)}{\mathrm{AGM}(a, b)}.$$

So, the circumference of an ellipse is equal to $2\pi \dfrac{\mathbf{MAGM}(a^2, b^2)}{\mathbf{AGM}(a, b)}$, where a and b denote the semi-major and semi-minor axes.

2.4. Other special functions

The gamma function is defined via a convergent improper integral

$$\Gamma(z) = \int_0^{\infty} x^{z-1} \exp\{-x\}\, dx,$$

where $\operatorname{Re} z > 0$. For any positive integer n, $\Gamma(n) = (n-1)!$. To calculate its value one can run the command $\mathbf{Gamma}(z)$.

The beta function, also called the Euler integral of the first kind, is also defined via another integral

$$\mathrm{B}(x, y) = \int_0^1 t^{x-1}(1-t)^{y-1}\, dt,$$

where both inequalities hold $\operatorname{Re} x > 0$ and $\operatorname{Re} y > 0$. It is closely related to the gamma function because $\mathrm{B}(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$.

To calculate its value one can run the command $\mathbf{Beta}(x, y)$. For example, let us verify the equality $B(2, 3) = 1/12$:

```
SPACE = R64[];
FLOATPOS = 4;
\Beta(2, 3);
```

The output is equal to 0.0833.

The binomial coefficients are $\mathbf{binom}(n, k) = \begin{pmatrix} n \\ k \end{pmatrix} = \dfrac{n!}{k!(n-k)!}$. For suitable function f, the Laplace transform is the integral $\displaystyle\int_0^{\infty} f(t) e^{-st}\, dt$.

To calculate the Laplace transform one can run **laplaceTransform**(). The inverse Laplace transform can be calculated by **inverseLaplaceTransform**(). Let us consider an example:

```
SPACE = R64[t];
L = \laplaceTransform(\exp(3t));
```

The output is $L = \dfrac{1.0}{t-3.0}$.

Next, let us calculate the inverse transform:

```
SPACE = R64[t];
F = \inverseLaplaceTransform(1/(t - 3));
```

The output is $F = e^{3t}$.

3. The Lagutinski determinant

The Lagutinski method allows us to search for rational integrals of a given differential ring [21], [24], [25]. Therefore, it can be used to integrate ordinary differential equations in symbolic form [7], [23].

Let us consider the differential ring $\mathbb{Q}[x, y]$ of bivariate polynomials over the field $\mathbb{Q}$, where the differentiation is given by $D = p(x, y)\dfrac{\partial}{\partial x} + q(x, y)\dfrac{\partial}{\partial y}$.

Let us consider an infinite matrix whose entries are monomials. The first row consists of all bivariate monomials with graduated lexicographical ordering m_1, m_2, ... The second row consists of the first derivatives Dm_1, Dm_2, ... The third row consists of the second derivatives D^2m_1, D^2m_2, ..., and so on. In particular, both monomials m_2 and m_3 are linear. For $N = \dfrac{1}{2}(d+1)(d+2)$, the monomial m_N is the last monomial of degree d.

The Lagutinski determinant of order n with respect to the differentiation D is a leading principal minor of order n in this matrix. Of course, the first order Lagutinski determinant is equal to 1. To calculate the Lagutinski determinant of order n with respect to the differentiation D one can run the command $\det \mathbf{L}(n, [p, x, q, y])$.

The significance of this determinant is explained by the following result that was previously obtained by Lagutinski [24], [25], but presented here in a modern formulation, cf. [7], [23]. A non-constant rational function $f \in \mathbb{Q}(x, y)$ is called an integral when Df vanishes identically.

Theorem 1 (Lagutinski). *Given a differentiation D and a positive integer $d > 0$. The Lagutinski determinant of order $N = \dfrac{1}{2}(d+1)(d+2)$ vanishes if and only if there exists a rational integral whose numerator and denominator are of degree at most d.*

For example, if the differentiation is given by $D = \dfrac{\partial}{\partial x} + \dfrac{\partial}{\partial y}$, then $D(x - y) = 0$. In accordance with Theorem 1, the third order Lagutinski determinant vanishes:

```
SPACE = Q[x, y];
p = 1; q = 1;
\detL(3, [p, x, q, y]);
```

The output is equal to zero.

Next, if the differentiation is given by $D = x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y}$, then $D(xy) = 0$. In accordance with Theorem 1, the sixth order Lagutinski determinant vanishes. Moreover, the fifth order Lagutinski determinant vanishes too because the fifth monomial coincides with the integral:

```
SPACE = Q[x, y];
p = x; q = -y;
\detL(5, [p, x, q, y]);
```

The output is equal to zero. But the third order Lagutinski determinant is equal to $-2xy$. Thus, there does not exist any integral whose numerator and denominator are linear. Contrariwise, if the differentiation is given by $D = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}$, then $D\left(\frac{x-y}{x+y}\right) = 0$. In accordance with Theorem 1, the third order Lagutinski determinant vanishes:

```
SPACE = Q[x, y];
p = x; q = y;
\detL(3, [p, x, q, y]);
```

The output is equal to zero.

4. Conclusion

The MathPartner service has become better and allows us to solve new problems in geometry and physics. MathPartner supports both symbolic and numerical integration of elementary functions. Moreover, some special functions can be calculated using fast algorithms.

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Вычисление интегралов в MathPartner

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В статье рассмотрены возможности сервиса MathPartner по вычислению определённых и неопределённых интегралов. MathPartner содержит программную реализацию алгоритма Риша и предоставляет пользователям возможность вычислять первообразные для элементарных функций. Некоторые интегралы, в том числе несобственные, можно вычислить с помощью численных алгоритмов. В этом случае каждый пользователь может указать необходимую точность, с которой ему необходимо знать числовое значение интеграла. Отметим специальные функции, которые позволяют вычислять полные эллиптические интегралы. К ним относятся функции для вычисления арифметико-геометрического среднего и геометрическо-гармонического среднего, которые позволяют вычислять полные эллиптические интегралы первого рода. Набор также включает модифицированное арифметико-геометрическое среднее, которое предложил Семён Адлай, что позволяет вычислять полные эллиптические интегралы второго рода и длину (периметр) эллипса. Особый интерес представляет алгоритм Лагутинского. Для данного дифференцирования в поле рациональных функций от двух переменных можно решить, существует ли рациональный интеграл. Алгоритм основан на вычислении определителя Лагутинского. В этом году мы отмечаем 150-летие со дня рождения Михаила Лагутинского.

Ключевые слова: система компьютерной алгебры, MathPartner, интеграл, арифметико-геометрическое среднее, модифицированное арифметико-геометрическое среднее, определитель Лагутинского

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Quantum mereology in finite quantum mechanics

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Any Hilbert space with composite dimension can be factored into a tensor product of smaller Hilbert spaces. This allows us to decompose a quantum system into subsystems. We propose a model based on finite quantum mechanics for a constructive study of such decompositions.

Key words and phrases: quantum mereology, closed quantum system, quantum subsystems, finite quantum mechanics, quantum entanglement, energy

1. Introduction

Mereology is the study of the part-to-whole and part-to-part relations within a whole. In *quantum mereology*, the whole is a closed quantum system ("the Universe")[1] in a given pure state, undergoing a given unitary (Schrödinger) evolution. Quantum mereology studies the interrelations between singled out subsystems of the Universe ("observable system", "observer", "environment", etc.), the emergence of geometry and even time (Page–Wootters mechanism [1]) from quantum entanglement, and other fundamental issues of quantum mechanics [2]–[4].

The division of the whole into parts is somewhat arbitrary and depends on the used separation criteria. There are two different facets of the separability between quantum systems.

1. Quantum systems are separated if the interaction energy between them is small. This is a more visible, material criterion that agrees well with the usual concept of locality. Quantitatively, the interaction energy between subsystems A and B can be represented as

$$\Delta E(A, B) = E(A \cup B) - E(A) - E(B)\,. \tag{1}$$

[1]Obviously, in the exact sense, closed systems do not exist (or they are fundamentally unobservable), with the possible exception of the Universe as a whole.

2. Quantum systems are separated if the quantum correlations between them are small. This criterion is more subtle and has non-local manifestations. Quantitatively, the entanglement between subsystems can be described, for example, by *mutual information*

$$\mathcal{I}(A, B) = S(A) + S(B) - S(A \cup B)\,, \tag{2}$$

where S denotes entropy.

There is a certain structural similarity between expressions (1) and (2). However, they describe completely different types of connections between subsystems.

For example, in the Page–Wootters model of emergent time, it is assumed that the whole timeless Universe is divided into two subsystems: the "clock", C, and the rest of the Universe, R. It is assumed that the Hamiltonian of the Universe has the form $H = H_C \otimes \mathbb{1}_R + \mathbb{1}_C \otimes H_R$, which means that the interaction energy between C and R is zero. On the other hand, the existence of nontrivial quantum correlations between C and R is assumed.

It would be interesting to take a closer look at the interplay between these two different, energy and information, aspects of quantum separability.

We develop and implement algorithms based on computer algebra techniques to perform the following. An isolated quantum system, constructed in the framework of finite quantum mechanics, is decomposed into a tensor product of subsystems. By reducing the "universe" quantum state, we obtain mixed states for subsystems. This allows us to study energy interactions and quantum correlations between subsystems and their time evolution.

2. Decomposition of a quantum system

Tensor product of Hilbert spaces. The (*global*) Hilbert space $\mathcal{H}$ of a K-component quantum system is the tensor product of the (*local*) Hilbert spaces $\mathcal{H}_k$ of the components:

$$\mathcal{H} = \bigotimes_{k=1}^{K} \mathcal{H}_k\,. \tag{3}$$

If $\dim \mathcal{H} = \mathcal{N}$ and $\dim \mathcal{H}_k = d_k$, then $\mathcal{N} = \prod_{k=1}^{K} d_k$.

For any d-dimensional Hilbert space, the ith orthonormal basis element is denoted by $|i\rangle$, that is,

$$|0\rangle = (1, 0, \dots)^\top,\ |1\rangle = (0, 1, 0, \dots)^\top, \dots,\ |d-1\rangle = (0, 0, \dots, 1)^\top.$$

Tensor monomials of local basis elements form an orthonormal basis in the global Hilbert space:

$$|i\rangle = |i_1\rangle \otimes \cdots \otimes |i_k\rangle \otimes \cdots \otimes |i_K\rangle\,, \tag{4}$$

where $|i\rangle \in \mathcal{H}$, $|i_k\rangle \in \mathcal{H}_k$ and

$$i = i_1 \prod_{m=2}^{K} d_m + \ldots + i_k \prod_{m=k+1}^{K} d_m + \ldots + i_K. \tag{5}$$

Tensor factorization of a Hilbert space. We can reverse the procedure, since (4) is a one-to-one correspondence: the sequence $i_1, \ldots, i_K$ is uniquely recovered from i by a simple procedure based on formula (5):

$$\begin{array}{l} k \leftarrow K,\ \tilde{\imath} \leftarrow i \\ \textbf{while } k \geqslant 1 \textbf{ do} \\ \quad i_k \leftarrow \tilde{\imath} \mod d_k,\ \tilde{\imath} \leftarrow \lfloor \tilde{\imath}/d_k \rfloor,\ k \leftarrow k-1 \\ \textbf{end while} \end{array} \tag{6}$$

Given an orthonormal basis in an $\mathcal{N}$-dimensional Hilbert space $\mathcal{H}$ and a decomposition $\mathcal{N} = d_1 \cdots d_K$, we can construct a particular bijection of the form (3).

When constructing a bijection, we must take into account the freedom in the choice of bases in Hilbert spaces. Any two orthonormal bases are related by a unitary transformation.

It is easy to show that general unitary changes of bases in all involved spaces are equivalent to a single change in the global space.

Namely, any vector of the global space can be represented as a sum of tensor products of elements of local spaces

$$|\psi\rangle = \sum_{\ell} \bigotimes_{k=1}^{K} |\psi_k^\ell\rangle,\ |\psi_k^\ell\rangle \in \mathcal{H}_k,\ |\psi\rangle \in \mathcal{H}. \tag{7}$$

Applying unitary transformations to all vectors in (7) and using the properties of the tensor product, we have

$$U|\psi\rangle = \sum_{\ell} \bigotimes_{k=1}^{K} U_k |\psi_k^\ell\rangle = \bigotimes_{k=1}^{K} U_k \sum_{\ell} \bigotimes_{k=1}^{K} |\psi_k^\ell\rangle$$

$$\Downarrow$$

$$U'|\psi\rangle = \sum_{\ell} \bigotimes_{k=1}^{K} |\psi_k^\ell\rangle,\ \text{where } U' = \left(\bigotimes_{k=1}^{K} U_k \right)^{-1} U.$$

Thus, to specify the factorization of the Hilbert space $\mathcal{H}$ we need two things[2]

1. an *integer decomposition* $\dim \mathcal{H} = d_1 \cdots d_K$, and
2. a *unitary transformation* U, which fixes a basis in $\mathcal{H}$.

[2]Another approach, in which the tensor factorization of a Hilbert space is specified by a set of observables, was proposed in [5], [6].

Decomposition of a pure quantum state. Any mixed state of a quantum system can be obtained from a pure state in a larger Hilbert space by taking a partial trace. It is natural to assume that at the fundamental level the state of an isolated system must be pure.[3] For a given factorization $\mathcal{H} = \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_K$, we introduce the set of indices (which can be thought of as *"geometric points"*)

$$X = \{1, \dots, K\}\,.$$

Subsystems are identified with subsets $A \subseteq X$. The density matrix of the pure state $|\psi\rangle \in \mathcal{H}$ of the entire system is $\rho_X = \dfrac{|\psi\rangle\langle\psi|}{\langle\psi \mid \psi\rangle}$. According to the laws of quantum mechanics, the statistical behavior of the subsystem A is correctly described by the reduced density matrix $\rho_A = \operatorname{tr}_{X\setminus A} \rho_X$ calculated by taking the partial trace over the complement to A.

In more detail, the calculation of the reduced density matrix is as follows. According to (4), the basis of the global Hilbert space can be represented as the Cartesian product of the local bases

$$B_X = \prod_{k\in X} B_k\,.$$

In a similar way we introduce the sets

$$B_A = \prod_{k\in A} B_k \quad \text{and} \quad B_{X\setminus A} = \prod_{k\in X\setminus A} B_k\,.$$

In components, the global density matrix can be written as

$$\rho_X = (\rho_X)_{i_X j_X} |i_X\rangle\langle j_X|\,,$$

where $i_X \simeq \{i_1, \dots, i_K\} \in B_X$ and $j_X \simeq \{j_1, \dots, j_K\} \in B_X$, and the equivalence $\simeq$ is provided by formula (5) and procedure (6). The procedure for calculating the reduced density matrix is obvious from the formula

$$(\rho_A)_{i_A j_A} = \sum_{\substack{m_{X\setminus A} \in B_{X\setminus A}\\ i_X = i_A \sqcup m_{X\setminus A}\\ j_X = j_A \sqcup m_{X\setminus A}}} (\rho_X)_{i_X j_X}\,, \text{ where } i_A, j_A \in B_A\,.$$

3. Finite quantum mechanics

We use a version of quantum theory [8]–[10] in which the groups of unitary evolutions are replaced by linear representations of finite groups, and the field

[3] This belief (an instance of Occam's razor), expressed by the metaphor "Church of the Larger Hilbert Space" (J.A. Smolin), allows one to obtain all probabilities in quantum theory from the only fundamental probability that is described by Gleason's theorem [7] (Born's rule).

of complex numbers is replaced by its dense constructive subfields, which naturally arise from the non-negative integers and roots of unity.

Permutation Hilbert space. *Any* linear (hence *unitary*) representation of a finite group is a subrepresentation of some permutation representation. This implies that the formalism of quantum mechanics can be completely[4] reproduced based on permutations of some set

$$\Omega = \{e_1, \dots, e_{\mathcal{N}}\} \cong \{1, \dots, \mathcal{N}\} \tag{8}$$

of primary (*"ontic"*) objects on which a permutation group $G \leqslant \mathsf{S}_{\mathcal{N}}$ acts.

The Hilbert space on Ω, needed for calculations in quantum theory, can be most economically constructed on the basis of two primitive concepts:

1. *natural numbers* $\mathbb{N} = \{0, 1, \dots\}$, abstraction of *counting*, and
2. *roots of unity*, abstraction of *periodicity*.

To construct a field $\mathcal{F}$ sufficient for all the needs of the quantum formalism, in particular, for splitting any representation of any subgroup of G into irreducible components, we can proceed as follows. We extend the semiring $\mathbb{N}$ to the ring $\mathbb{N}\left[\zeta_\ell\right]$, where ζ_ℓ is the ℓth primitive root of unity, and ℓ is the LCM of the periods of the elements of G. The *algebraic integer* ζ_ℓ can be written in complex form as $\zeta_\ell = \mathrm{e}^{2\pi\mathrm{i}/\ell}$. Finally, constructing the *quotient field* of the ring $\mathbb{N}\left[\zeta_\ell\right]$, we arrive at the *cyclotomic extension* of the rationals $\mathcal{F} = \mathbb{Q}\left(\mathrm{e}^{2\pi\mathrm{i}/\ell}\right)$. For $\ell > 2$, the field $\mathcal{F}$, being a dense subfield of $\mathbb{C}$, is empirically indistinguishable from $\mathbb{C}$.

Treating the set Ω as a basis, we obtain an $\mathcal{N}$-dimensional Hilbert space $\mathcal{H}_{\mathcal{N}}$ over $\mathcal{F}$. The action of G on Ω determines the *permutation representation* $\mathcal{P}$ in $\mathcal{H}_{\mathcal{N}}$ by the matrices $\mathcal{P}(g)_{i,j} = \delta_{ig,j}$, where ig denotes the (right) action of $g \in G$ on $i \in \Omega$.

Decomposition of permutation representation. The permutation representation of any group G has the *trivial* one-dimensional subrepresentation in the space spanned by the *all-ones* vector

$$|\omega\rangle = (\underbrace{1, 1, \dots, 1}_{\mathcal{N}})^\top.$$

The complement to the trivial subrepresentation is called the *standard representation.* The operator of projection onto the $(\mathcal{N}-1)$-dimensional *standard space* $\mathcal{H}_\star$ has the form

$$\mathrm{P}_\star = \mathbb{1}_{\mathcal{N}} - \frac{|\omega\rangle\langle\omega|}{\mathcal{N}}.$$

Quantum mechanical behavior (interference, etc.) manifests itself precisely in $\mathcal{H}_\star$. Tom Banks made a profound observation [11] that the projection of classical permutation evolutions in the whole $\mathcal{H}_{\mathcal{N}}$ leads to truly quantum evolutions in the subspace $\mathcal{H}_\star$. Banks also showed that the choice $G = \mathsf{S}_{\mathcal{N}}$,

[4] *Modulo* empirically insignificant elements of traditional formalism such as infinities of various kinds.

where $\mathcal{N}$ is the number of fundamental (Planck) elements,[5] "can accurately reproduce all of the results of conventional quantum mechanics". In order to clarify a correspondence between finite quantum mechanics and traditional theory based on continuous unitary groups, Banks pointed out the connection between the symmetric group on $\mathcal{N}$ elements and the unitary group in $\mathcal{N}-1$ dimensions. Namely, for sufficiently large $\mathcal{N}$ (according to [12] $\mathcal{N} \geqslant 72$), the most general finite subgroup, G, of $\mathsf{SU}(\mathcal{N}-1)$ has the structure of a semidirect product of a finite Abelian group, A, and the group $\mathsf{S}_{\mathcal{N}}$

$$G = A \rtimes \mathsf{S}_{\mathcal{N}} < \mathsf{SU}(\mathcal{N}-1)\,.$$

Ontic vectors. $\mathsf{S}_{\mathcal{N}}$ is a *rational-representation group*, i.e., its every irreducible representation (the standard representation is one of them) is realizable over $\mathbb{Q}$. This means that to describe evolutions in $\mathcal{H}_\star$, it is sufficient to consider only vectors with rational components.[6]

It is easy to show that any quantum state in $\mathcal{H}_\star$ can be obtained as the projection of an integer vector from the non-negative orthant $\mathcal{H}_{\mathcal{N}}^{+} \subset \mathcal{H}_{\mathcal{N}}$. Let $|x\rangle = \left(x_1, \dots, x_{\mathcal{N}}\right)^\top \in \mathcal{H}_{\mathcal{N}}^{+}$ be a vector with non-negative rational components. Then its projection to $\mathcal{H}_\star$ is an $(\mathcal{N}-1)$-dimensional vector of the form

$$|y\rangle = \left(y_1, \dots, y_{\mathcal{N}-1}\right)^\top = \mathrm{P}_\star \, |x\rangle\,. \tag{9}$$

The set $\{|0\rangle - |\mathcal{N}-1\rangle, \dots, |\mathcal{N}-2\rangle - |\mathcal{N}-1\rangle\}$ is one of the bases in $\mathcal{H}_\star$, where $\{|0\rangle, \dots, |\mathcal{N}-1\rangle\}$ is a basis in $\mathcal{H}_{\mathcal{N}}$. In this basis, equation (9) is equivalent to the set of relations

$$y_1 = x_1 - x_{\mathcal{N}}\,, \dots,\, y_i = x_i - x_{\mathcal{N}}\,, \dots,\, y_{\mathcal{N}-1} = x_{\mathcal{N}-1} - x_{\mathcal{N}}\,.$$

Obviously, *any* set of values $y_1, \dots, y_{\mathcal{N}-1}$ can be obtained using *only non-negative* values $x_1, \dots, x_{\mathcal{N}}$.

Since quantum states are rays in Hilbert space, we can replace non-negative rational vectors $|x\rangle$ with natural vectors $|n\rangle = (n_1, \dots, n_{\mathcal{N}})^\top \in \mathbb{N}^{\mathcal{N}} \subset \mathcal{H}_{\mathcal{N}}^{+}$. To build constructive models (to remain in the finite realm), one needs to select a finite subset in $\mathbb{N}^{\mathcal{N}}$. The simplest choice is vectors with coordinates from the set $\{0, 1\}$, i.e., bit strings of length $\mathcal{N}$. We call them *ontic vectors* or *ontic states*. These states are attractive for both ontological and computational reasons.

Interpreting ontic state $|q\rangle$ as a *characteristic function*, we can identify it with the subset $q \subset \Omega$ or, equivalently, with the *partition* of the ontic set (8) into two nontrivial subsets $\Omega = q \sqcup {\sim}q$, ${\sim}q = \Omega \setminus q$, where $\sim$ denotes

[5] By the current cosmological data, the number $\mathcal{N}$ is estimated as $\sim \mathrm{Exp}(\mathrm{Exp}(20))$ and $\sim \mathrm{Exp}(\mathrm{Exp}(123))$ for 1 cm^3 of matter and for the entire Universe, respectively.

[6] Complex numbers — i.e., nontrivial elements of cyclotomic extensions — may be needed only in problems that require splitting representations of some proper subgroups of $\mathsf{S}_{\mathcal{N}}$ into irreducible components.

set complement operation (or *bitwise inversion*). The complete set of ontic states is $Q = 2^{\Omega} \setminus \{\emptyset, \Omega\}$. The number of ontic states, $|Q| = 2^{\mathcal{N}} - 2$, depends exponentially on $\mathcal{N}$, so they present a fairly large set of quantum states in the standard space for large $\mathcal{N}$.

The complement operation applied to an ontic state induces a change in the sign of the corresponding quantum state in the standard space:

$$|\psi\rangle = \mathrm{P}_\star |q\rangle \implies -|\psi\rangle = \mathrm{P}_\star |{\sim} q\rangle .$$

The inner product of normalized projections of the ontic vectors $|q\rangle$ and $|r\rangle$ onto $\mathcal{H}_\star$ is

$$S(q,r) \equiv \frac{\langle q |\mathrm{P}_\star| r|q |\mathrm{P}_\star| r\rangle}{\sqrt{\langle q |\mathrm{P}_\star| q|q |\mathrm{P}_\star| q\rangle \langle r |\mathrm{P}_\star| r|r |\mathrm{P}_\star| r\rangle}} = \frac{\mathcal{N}\langle q \,\&\, r\rangle - \langle q\rangle \langle r\rangle}{\sqrt{\langle q\rangle \langle {\sim} q\rangle \langle r\rangle \langle {\sim} r\rangle}} ,$$

where & is the bitwise AND for bit strings, and $\langle \cdot \rangle$ denotes *population number* (or *Hamming weight*). The obvious identities $\langle {\sim} a\rangle = \mathcal{N} - \langle a\rangle$ and $\langle a \,\&\, b\rangle + \langle a \,\&\, {\sim} b\rangle = \langle a\rangle$ imply the folowing symmetries with respect to the complement operations on the ontic states

$$S(q,r) = -S({\sim} q, r) = -S(q, {\sim} r) = S({\sim} q, {\sim} r) .$$

4. Ontic and energy bases

Ontic basis. The original permutation basis in the space $\mathcal{H}_{\mathcal{N}}$, i.e., the set Ω, will be called the *ontic basis.* In this basis, the density matrix in $\mathcal{H}_\star$ associated with the ontic state $|q\rangle \in \mathcal{H}_{\mathcal{N}}$ has the form

$$\rho^o_q = \frac{\mathrm{P}_\star |q\rangle\langle q| \mathrm{P}_\star}{\langle q |\mathrm{P}_\star| q|q |\mathrm{P}_\star| q\rangle} = \frac{1}{\mathcal{N}} \frac{(|q\rangle - \alpha |\omega\rangle) (\langle q| - \alpha \langle \omega|)}{\alpha (1-\alpha)} , \tag{10}$$

where $\alpha = \langle q\rangle /\mathcal{N}$ is the *population density.* There is an obvious duality: the expression for the density matrix $\rho^o_{\sim q}$ is obtained from (10) by replacements $q \to {\sim} q$ and $\alpha \to 1-\alpha$

$$\rho^o_q \xrightarrow[]{\substack{q \to {\sim} q \\ \alpha \to 1-\alpha}} \rho^o_{\sim q} .$$

Energy basis. In continuous quantum mechanics, the evolution of an isolated system is described by the one-parameter unitary group $U_t = \mathrm{e}^{-\mathrm{i}Ht}$ generated by the Hamiltonian H whose eigenvalues are called *energy eigenvalues.*

In finite quantum mechanics, the evolution is described by a cyclic group $U(g)^t$ generated by an element $U(g) \in \mathcal{P}(G)$, where t is an integer parameter. We call the *energy basis* an orthonormal basis in which the matrix $U(g)$ is diagonal.

Planck's formula $E = h\nu$ relates the energy E to the frequency ν, which is defined as the inverse of the period of the corresponding cyclic process.

Any permutation can be represented as a product of disjoint cycles. It is instructive to see how often cycles of different lengths occur in the group of all permutations $\mathsf{S}_{\mathcal{N}}$. A simple combinatorial calculation shows that the total number of cycles of length ℓ in the whole group $\mathsf{S}_{\mathcal{N}}$ is $\mathcal{N}!/\ell$, and, therefore, the expected number of ℓ-cycles in a single permutation is $1/\ell$. That is, high-energy evolutions prevail in our permutation-based model of the Universe.[7]

The ℓ-cycle matrix has the form

$$C_\ell = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

i.e., $\left(C_\ell\right)_{ij} = \delta_{i-j+1 \pmod{\ell}}$. The diagonal form of this matrix is

$$F_\ell C_\ell F_\ell^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \zeta_\ell & 0 & \cdots & 0 \\ 0 & 0 & \zeta_\ell^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \zeta_\ell^{\ell-1} \end{pmatrix},$$

where $\zeta_\ell = \mathrm{e}^{2\pi\mathrm{i}/\ell}$ is the ℓth ("*ground*") primitive root of unity, and

$$F_\ell = \frac{1}{\sqrt{\ell}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \zeta_\ell^{-1} & \zeta_\ell^{-2} & \cdots & \zeta_\ell^{-(\ell-1)} \\ 1 & \zeta_\ell^{-2} & \zeta_\ell^{-4} & \cdots & \zeta_\ell^{-2(\ell-1)} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & \zeta_\ell^{-(\ell-1)} & \zeta_\ell^{-2(\ell-1)} & \cdots & \zeta_\ell^{-(\ell-1)(\ell-1)} \end{pmatrix}$$

is the *Fourier transform* matrix. F_ℓ is both unitary and symmetric, therefore

$$F_\ell^{-1} = F_\ell^\dagger = F_\ell^* \implies \left(F_\ell^{-1}\right)_{ij} = \frac{1}{\sqrt{\ell}} \zeta_\ell^{(i-1)(j-1)}.$$

In general, the matrix of the permutation representation of an element $g \in \mathsf{S}_{\mathcal{N}}$ is the direct sum of cyclic matrices $U(g) = \bigoplus_{m=1}^{M} C_{\ell_m}$, and the corresponding

[7] Of course, it would be more adequate to calculate the energy distribution for a given individual permutation evolution, but this is a more difficult combinatorial problem.

diagonalizing matrix is $F = \bigoplus_{m=1}^{M} F_{\ell_m}$, which is the transition matrix from the *ontic basis* to the *energy basis*.

The density matrix of the whole system in the energy basis can be calculated from (10) by the formula $\rho_q^{\varepsilon} = F \rho_q^{o} F^{*}$.

5. Entanglement measures

Quantitatively, quantum correlations are described by *measures of entanglement*, which are based on the concept of entropy. The most commonly used in physics is the *von Neumann entropy*

$$S_1(\rho) = -\operatorname{tr}(\rho \log \rho)\,. \tag{11}$$

Also often used are entropies from the *Rényi family* [13]

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \log \operatorname{tr}(\rho^\alpha)\,, \quad \alpha \geqslant 0,\ \alpha \neq 1. \tag{12}$$

The common feature of the von Neumann and Rényi entropies is their additivity on combinations of independent probability distributions determined by the eigenvalues of the density matrices. The von Neumann entropy is preferred because it additionally satisfies a stronger requirement, the chain rule for conditional entropies. In fact, the von Neumann entropy (11) can also be included in family (12) by going to the limit $\alpha \to 1$.

In our calculations, we use the 2nd Rényi entropy (also called the *collision entropy*) $S_2(\rho) = -\log \operatorname{tr}(\rho^2)$ for the following reasons:

— It is easy to calculate. For $n \times n$ density matrix ρ we have

$$S_2(\rho) = -\log\left(\sum_{i=1}^{n} \rho_{ii}^2 + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \left|\rho_{ij}\right|^2\right).$$

— $\operatorname{tr}(\rho^2)$ is the so-called *purity* of the state ρ.

— $\operatorname{tr}(\rho^2)$ coincides with the Born probability: "the system observes itself."

— $\operatorname{tr}(\rho^2) \equiv \langle\rho\rangle_\rho$ is the *expectation value* of the *observable* ρ in the state ρ.

— $\operatorname{tr}(\rho^2) \equiv \|\rho\|_{\mathrm{F}}^2$ is the square of the *Frobenius* (*Hilbert-Schmidt*) *norm* of the density matrix.

The *Frobenius inner product* for two matrices (or *Hilbert-Schmidt inner product* for two operators) a and b is defined as $\langle a \mid b\rangle_{\mathrm{F}} = \operatorname{tr}(a^\dagger b)$. The corresponding *Frobenius norm* is $\|a\|_{\mathrm{F}} = \sqrt{\langle a \mid a\rangle_{\mathrm{F}}}$. It can be shown that any constructions used in the study of quantum correlations and based on the von Neumann entropy can be reformulated in terms of matrix metrics.

For example, in emergent geometry models [3], [14], [15], the distances between subsystems A and B are described by functions of *mutual information*

$$\mathcal{I}(A,B) = S_1(\rho_A) + S_1(\rho_B) - S_1(\rho_{A\cup B}) \ . \tag{13}$$

Replacing in (13) the von Neumann entropy with the 2nd Rényi entropy, we obtain the expression

$$\mathcal{I}_2(A,B) = S_2(\rho_A) + S_2(\rho_B) - S_2(\rho_{A\cup B}) \tag{14}$$

whose exponential has the form

$$\frac{\operatorname{tr}(\rho_{A\cup B}^2)}{\operatorname{tr}(\rho_A^2)\operatorname{tr}(\rho_B^2)} \equiv \frac{\|\rho_{A\cup B}\|_{\mathrm{F}}^2}{\|\rho_A \otimes \rho_B\|_{\mathrm{F}}^2} \, . \tag{15}$$

Obviously, both (14) and (15), although (14) does not have a probabilistic interpretation of (13), also describe quite well the deviation from separability caused by entanglement.

6. Some computational observations

We are developing a C program for constructing tensor decompositions and calculating quantum correlations in the ontic and energy bases.

To illustrate the calculations, consider a homogeneous quantum system, i.e., a system whose Hilbert space is decomposed into a product of local spaces of the same dimension

$$\mathcal{H} = \bigotimes_{x\in X} \mathcal{H}_x \, ,$$

where $X = \{1,\dots,|X|\}$ (a set of "geometric points"), $\dim \mathcal{H}_x = d$ for all $x \in X$.

Preliminary calculations indicate that decompositions with smaller local dimension d exhibit more interesting behavior. Consider, e.g., the case $d = 2$ and $|X| = 23$, in which $\dim \mathcal{H} = 8\,388\,608$. We will treat here the analogue of mutual information (14) as a measure of the distance between points. Calculations of (14) on all edges $(x,y) \in X \times X$ of the complete graph on X show a spread of values by two orders of magnitude: a typical example is

$$\mathcal{I}_2(x,y) \in \left[5.3 \times 10^{-8}, 7 \times 10^{-6}\right] \, .$$

A large scatter in the distances between points can be considered a sign of the non-triviality of the geometry.

For the case with a slightly larger local dimension, $d = 7$ and $|X| = 7$ (hence $\dim \mathcal{H} = 823\,543$), similar calculations give $\mathcal{I}_2(x,y) \in [0.0037, 0.0041]$. That is, the geometry is close to trivial — all points are almost equidistant. More detailed calculations show that the main contribution to the non-triviality of geometry is made by the local dimension d, and not by the number of points $|X|$.

Figure 1 shows examples of calculating the entropies of subsystems of all possible sizes for quantum systems with $d = 2$, and $|X| = 6$ ("small" case) and

$|X| = 12$ ("large" case). In both cases, 10 randomly generated ontic states were used — the legends show their Hamming weights. The data presented in the figure demonstrates the following features:

— The trend towards universality (weak dependence on the quantum state) with the growth of $|X|$: visually, all graphs are almost identical in the "large" case.

— Symmetry $S_2(\rho_A) = S_2\left(\rho_{X\setminus A}\right)$ is a manifestation of the *Schmidt decomposition* [16] of a pure state: both matrices ρ_A and $\rho_{X\setminus A}$ have identical sets of nonzero eigenvalues.

— For the subsystem size $|A|$ noticeably smaller than $|X|/2$, the reduced state is close to the *maximally mixed* state: $S_2\left(\rho_{_A}\right) \approx |A| \log d$. Recall that a maximally mixed state is a state whose density matrix describes a uniform probability distribution, i.e., all its eigenvalues are equal.

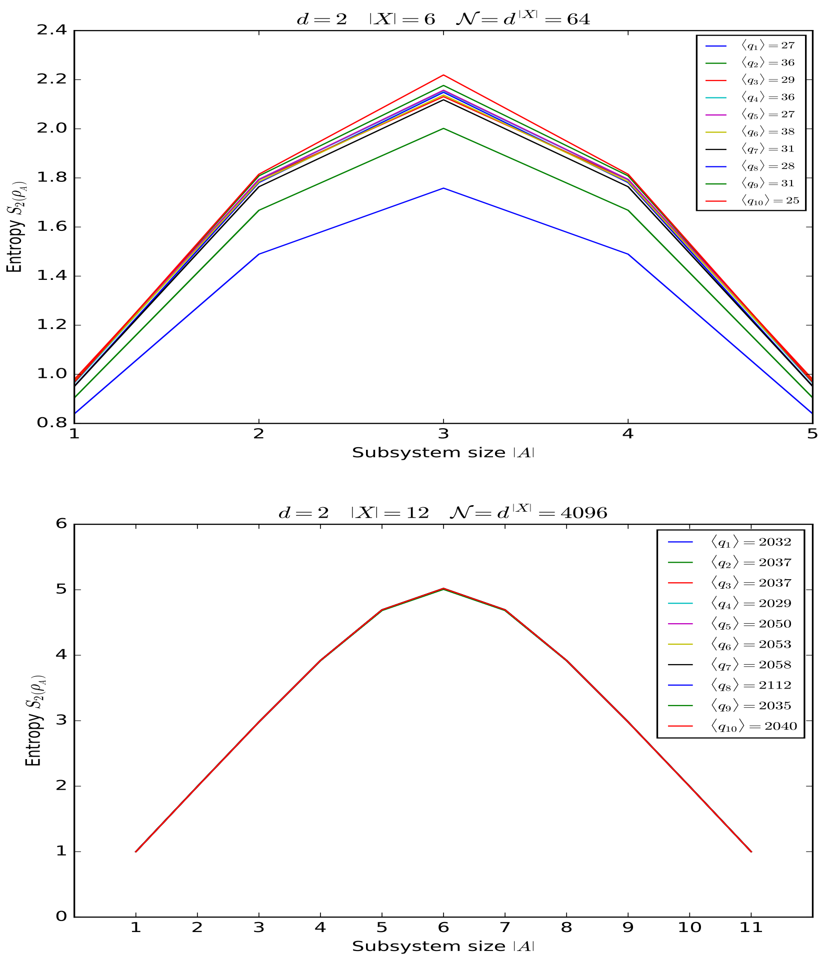

Figure 1. Entropies of subsystems

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Квантовая мереология в конечной квантовой механике

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Любое гильбертово пространство составной размерности можно разложить в тензорное произведение меньших гильбертовых пространств. Такая факторизация дает возможность разложить квантовую систему на подсистемы. Мы предлагаем модель, основанную на конечной квантовой механике, для конструктивного изучения таких разложений.

Ключевые слова: квантовая мереология, замкнутая квантовая система, квантовые подсистемы, конечная квантовая механика, квантовая запутанность, энергия

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Parameterizing qudit states

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Quantum systems with a finite number of states at all times have been a primary element of many physical models in nuclear and elementary particle physics, as well as in condensed matter physics. Today, however, due to a practical demand in the area of developing quantum technologies, a whole set of novel tasks for improving our understanding of the structure of finite-dimensional quantum systems has appeared.

In the present article we will concentrate on one aspect of such studies related to the problem of explicit parameterization of state space of an N-level quantum system. More precisely, we will discuss the problem of a practical description of the unitary $SU(N)$-invariant counterpart of the N-level state space $\mathfrak{P}_N$, i.e., the unitary orbit space $\mathfrak{P}_N/SU(N)$. It will be demonstrated that the combination of well-known methods of the polynomial invariant theory and convex geometry provides useful parameterization for the elements of $\mathfrak{P}_N/SU(N)$. To illustrate the general situation, a detailed description of $\mathfrak{P}_N/SU(N)$ for low-level systems: qubit ($N = 2$), qutrit ($N = 3$), quatrit ($N = 4$) — will be given.

Key words and phrases: density matrix parameterization, quantum system, qubit, qutrit, quatrit, qudit, polynomial invariant theory, convex geometry

1. Introduction

Quantum mechanics is a unitary invariant probabilistic theory of finite-dimensional systems. Both basic features, the invariance and the randomness, strongly impose on the mathematical structure associated with the state space $\mathfrak{P}$ of a quantum system. In particular, the geometrical concept of the convexity of the state space originates from the physical assumption of an ignorance about the quantum states. Furthermore, the convex structure of the state space, according to the Wigner [1] and Kadison [2] theorems about quantum symmetry realization, leads to unitary or anti-unitary invariance of the probability measures (short exposition of the interplay between these two theorems see e.g. in [3]). In turn of the action of unitary/anti-unitary transformations $\varrho \longrightarrow \varrho' = U\varrho U^\dagger$ sets the equivalence relation $\varrho \simeq \varrho'$ between the states $\varrho, \varrho' \in \mathfrak{P}$ and defines the factor space $\mathfrak{P}/U$. This space is a fundamental object containing all physically relevant information about a quantum system. An efficacious way to describe $\mathcal{O}[\mathfrak{P}_N] := \mathfrak{P}_N/SU(N)$ for an N-level quantum system is a primary motivation of the present article. The properties of $\mathcal{O}[\mathfrak{P}_N]$, as a semi-algebraic variety, are reflected in the structure of the center of the enveloping algebra $\mathfrak{U}(\mathfrak{su}(N))$. Hence, it is pertinently to describe $\mathcal{O}[\mathfrak{P}_N]$ using the algebra of real $SU(N)$-invariant polynomials defined over the state space $\mathfrak{P}_N$. Following this observation in a series of our previous publications [4]–[8], we develop description of $\mathcal{O}[\mathfrak{P}_N]$ using the classical invariant theory [9].

It is worth noting that within this description of the state space the entanglement properties of binary composite systems can be analyzed as well. In [5], [6] qubit-qubit and qubit-qutrit pairs were studied from this standpoint. In particular, the optimal integrity basis for the polynomial $SU(2) \times SU(2)$ invariant ring of a two-qubit system was proposed and the separability criterion was formulated via polynomial inequalities in three $SU(4)$ Casimir invariants and two determinants of the so-called correlation and the Schlienz–Mahler entanglement matrices, which are the $SU(2) \times SU(2)$ polynomial scalars.

On the other hand, $\mathfrak{P}_N/SU(N)$ is related to the co-adjoint orbits space $\mathfrak{su}^*(N)/SU(N)$ and hence it is natural to describe $\mathfrak{P}_N/SU(N)$ directly in terms of non-polynomial variables — the spectrum of density matrices. Below we will describe a scheme which combines these points of view and provides description of the orbit space $\mathfrak{P}_N/SU(N)$ in terms of one second order polynomial invariant, the Bloch radius of a state and additional non-polynomial invariants, the angles corresponding to the projections of a unit $(N-2)$-dimensional vector on the weight vectors of the fundamental representation of $SU(N)$.

The article is organised as follows. The next section is devoted to brief statements of general results about the state space $\mathfrak{P}_N$ of N-dimensional quantum systems, including discussion of its convexity (Section 2.1) and semi-algebraic structure (Section 2.2). Particularly, the set of polynomial inequalities in an (N^2-1)-dimensional Bloch vector and the equivalent set of inequalities in $N-1$ polynomial $SU(N)$-invariants will be presented for arbitrary N-level quantum systems. Section 3 contains information on the orbit space $\mathcal{O}[\mathfrak{P}_N]$ — the factor space of the state space under equivalence relation against the unitary group adjoint action. In Section 3.3.1 we introduce a new type of parameterization of a qubit, a qutrit and a quatrit based on the representation of the orbit space of a qudit as a spherical polyhedron on $\mathbb{S}_{N-2}$. This parameterization allows us to give a simple formulation of the conception of the hierarchy of subsystems inside one another. In Section 3.3.2 we present formal elements of the suggested scheme for an arbitrary final-dimensional system. Section 4 contains a few remarks on possible applications of the introduced version of the qudit parameterization.

2. The state space

The state space of a quantum system $\mathfrak{P}_N$ comes in many faces. One can discuss its mathematical structure from several points of view: as a topological set, as a measurable space, as a convex body, as a Riemannian manifold.[1] Below we concentrate mainly on a brief description of $\mathfrak{P}_N$ as a convex body realized as a semi-algebraic variety in $\mathbb{R}^{N^2-1}$ following in general the publications [4]–[8].

2.1. The state space as a convex body

According to the Hilbert space formulation of the quantum theory, a possible state of a quantum system is associated to a self-adjoint, positive semi-definite *"density operator"* acting on a Hilbert space. Considering a non-relativistic N-dimensional system whose Hilbert space $\mathcal{H}$ is $\mathbb{C}^N$, the density operator can be identified with the Hermitian, unit trace, positive semi-definite $N \times N$ *density matrix* [14], [15].

The set of all possible density matrices forms the *state space* $\mathfrak{P}_N$ of an N-dimensional quantum system. It is a subset of the space of complex $N \times N$ matrices:

$$\mathfrak{P}_N = \{\varrho \in M_N(\mathbb{C}) \,|\, \varrho = \varrho^\dagger,\ \varrho \geqslant 0,\ \operatorname{Tr} \varrho = 1\}.$$

A generic non-minimal rank matrix ϱ describes the *mixed state*, while the singular matrices with $\operatorname{rank}(\varrho) = 1$ are associated to *pure states.* Since the set of N-th order Hermitian matrices has a real dimension N^2, and due to the finite trace condition $\operatorname{Tr}(\varrho) = 1$, the dimension of the state space is $\dim(\mathfrak{P}_N) = N^2 - 1$. The semi-positivity condition $\varrho \geqslant 0$ restricts it further to a certain (N^2-1)-dimensional *convex body.* The convexity of $\mathfrak{P}_N$ is the fundamental property of the state space. The next propositions summarize results on a general pattern of the state space $\mathfrak{P}_N$ as a convex set with an interior $\operatorname{Int}(\mathfrak{P}_N)$ and a boundary $\partial\mathfrak{P}_N$ [10].

Proposition 1. Given two states $\varrho_1, \varrho_2 \in \operatorname{Int}(\mathfrak{P}_N)$ and a "probability" $p \in [0,1]$, consider the convex combination

$$\varrho_p := (1-p)\varrho_1 + p\varrho_2,$$

then $\varrho_p \in \operatorname{Int}(\mathfrak{P}_N)$.

Proposition 2. The boundary $\partial\mathfrak{P}_N$ consists of non-invertible matrices of all possible non-maximal ranks:

$$\partial\mathfrak{P}_N = \{\varrho \in \mathfrak{P}_N \,|\, \det(\varrho) = 0\}\,.$$

[1]Here is a short and extremely subjective list of publications on these issues [10]–[13].

The subset of pure states $\mathfrak{F}_N \subset \partial\mathfrak{P}_N$, $\mathfrak{F}_N = \{\varrho \in \partial\mathfrak{P}_N \,|\, \mathrm{rank}(\varrho) = 1\}$, contains N extreme boundary points $\mathscr{P}_i(\varrho)$ which generate the whole $\mathfrak{P}_N$ by taking the convex combination:

$$\varrho = \sum_{i=0}^{N} r_i \mathscr{P}_i(\varrho), \quad \sum_{i=0}^{N} r_i = 1, \quad r_i \geqslant 0. \tag{1}$$

In (1) every extreme component $\mathscr{P}_i(\varrho)$ can be related to the standard rank-one projector by a common unitary transformation $U \in SU(N)$ and transposition $P_{i(1)}$ interchanging the first and i-th position:

$$\mathscr{P}_i(\varrho) = U P_{i(1)}\, \mathbf{diag}(1, 0, \dots, 0)\, P_{i(1)}\, U^{\dagger}.$$

For any dimension of the quantum system the subset of extreme states provides important information about the properties of all possible states, even the pure states comprise a manifold of a real dimension $\dim(\mathfrak{F}_N) = 2N - 2$, smaller than that dimension of the whole state space boundary $\dim(\partial\mathfrak{P}_N) = N^2 - 2$.

2.2. The state space as a semi-algebraic variety

According to the decomposition (1), the neighbourhood of a generic point of $\mathfrak{P}_N(\mathbb{R}^{N^2-1})$ is locally homeomorphic to $\big(U(N)/U(1)^N\big) \times D^{N-1}$, where the component D^{N-1} is an $(N-1)$-dimensional disc (cf. [10], [13]). Following this result, below we will describe how the state space $\mathfrak{P}_N$ can be realized as a convex body in $\mathbb{R}^{N^2-1}$ defined via a finite set of polynomial inequalities involving the Bloch vector of a state. In order to formalize the description of the state space, we consider the universal enveloping algebra $\mathfrak{U}(\mathfrak{su}(\mathrm{N}))$ of the Lie algebra $\mathfrak{su}(\mathrm{N})$. Choosing the orthonormal basis $\lambda_1, \lambda_2, \dots, \lambda_{N^2-1}$ for $\mathfrak{su}(\mathrm{N})$,

$$\mathfrak{su}(\mathrm{N}) = \sum_{i=1}^{\mathrm{N}^2-1} \xi_i \lambda_i, \tag{2}$$

the density matrix will be identified with the element from $\mathfrak{U}(\mathfrak{su}(\mathrm{N}))$ of the form:

$$\varrho(N) = \frac{1}{N}\mathbb{I}_N + \sqrt{\frac{N-1}{2N}} \sum_{i=1}^{\mathrm{N}^2-1} \xi_i \lambda_i. \tag{3}$$

The analysis (see e.g. consideration in [4], [6]) shows the possibility of description of the state space via polynomial constraints on the Bloch vector of an N-level quantum system.

Proposition 3. If a real (N^2-1)-dimensional vector $\vec{\xi} = (\xi_1, \xi_2, \dots, \xi_{N^2-1})$ in (3) satisfies the following set of polynomial inequalities:

$$S_k(\vec{\xi}) \geqslant 0, \quad k = 1, 2, \dots N, \tag{4}$$

where $S_k(\vec{\xi})$ are coefficients of the characteristic equation of the density matrix ϱ:

$$\det\|x-\varrho\| = x^N - S_1 x^{N-1} + S_2 x^{N-2} - \dots + (-1)^N S_N = 0, \qquad (5)$$

then the equation (3) defines the states $\varrho \in \mathfrak{P}_N$.

The inequalities (4), which guarantee the semi-positivity of the density matrix, remain unaffected by unitary changes of the basis of the Lie algebra and thus the semi-algebraic set (4) can be equivalently rewritten in terms of the elements of the $SU(N)$-invariant polynomial ring $\mathbb{R}[\mathfrak{P}_N]^{\mathrm{SU(N)}}$. This ring can be equivalently represented by the integrity basis in the form of homogeneous polynomials $\mathcal{P} = (t_1, t_2, \dots, t_N)$,

$$\mathbb{R}\left[\xi_1, \xi_2, \dots, \xi_{N^2-1}\right]^{\mathrm{SU(N)}} = \mathbb{R}\left[t_1, t_2, \dots, t_N\right].$$

The useful, from a computational point of view, polynomial basis $\mathcal{P}$ is given by the *trace invariants* of the density matrix:

$$t_k := \mathrm{Tr}(\varrho^k). \qquad (6)$$

The coefficients S_k, being $SU(N)$-invariant polynomial functions of the density matrix elements, are expressible in terms of the trace invariants via the well-known determinant formulae:

$$S_k = \frac{1}{k!}\det\begin{pmatrix} t_1 & 1 & 0 & \cdots & 0 \\ t_2 & t_1 & 2 & \cdots & 1 \\ t_3 & t_2 & t_1 & \cdots & \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & k-1 \\ t_k & t_{k-1} & t_{k-2} & \cdots & t_1 \end{pmatrix}.$$

Aiming at more economic description of $\mathfrak{P}_N$, we pass from N^2-1 Bloch variables to $N-1$ independent trace variables t_k. Pay for such a simplification is necessity to take into account additional constraints on t_k which reflect the Hermicity of the density matrix. Below we give the explicit form of these constraints in terms of $\mathcal{P} = (t_1, t_2, \dots, t_N)$.

In accordance with the classical results, the *Bézoutian*, the matrix $\mathrm{B} = \Delta^T\Delta$, constructed from the Vandermonde matrix Δ, accommodates information on the number of distinct roots (via its rank), numbers of real roots (via its signature), as well as the Hermicity condition. A real characteristic polynomial has all its roots *real and distinct* if and only if the Bézoutian is positive definite. For generic invertible density matrices — matrices with all eigenvalues different, the positivity of the Bézoutian reduces to the requirement

$$\det\|\mathrm{B}\| > 0. \qquad (7)$$

Noting that the entries of the Bézoutian are simply the trace invariants:

$$\mathrm{B}_{ij} = t_{i+j-2}, \qquad (8)$$

one can get convinced that the determinant of the Bézoutian is nothing else than the *discriminant* of the characteristic equation of the density matrix, $\mathrm{Disc} = \prod_{i>j} \left(r_i - r_j\right)^2$, rewritten in terms of the trace polynomials[2]

$$\mathrm{Disc}(t_1, t_2, \dots, t_N) := \det \|\mathrm{B}\|. \tag{9}$$

Hence, we arrive at the following result.

Proposition 4. The following set of inequalities in terms of the trace $SU(N)$-invariants,

$$\mathrm{Disc}\left(t_1, t_2, \dots, t_N\right) \geqslant 0, \quad S_k\left(t_1, t_2, \dots, t_N\right) \geqslant 0, \quad t_1 = 1, \tag{10}$$

define the same semi-algebraic variety as the inequalities (4) in $N^2 - 1$ Bloch coordinates do.

3. Orbit space $\mathfrak{P}_N/SU(N)$

3.1. Parameterizing $\mathfrak{P}_N/SU(N)$ via polynomial invariants

Proposition 4 is a useful starting point for establishing a stratification of the $\mathfrak{P}_N$ under the adjoint action of the $SU(N)$ group. It turns out that, due to the unitary invariant character of the inequalities (10), they accommodate all nontrivial information on possible strata of unitary orbits on the state space $\mathfrak{P}_N$. Indeed, it is easy to find the link between the description of $\mathfrak{P}_N$ given in the previous section and the well-known method developed by Abud–Sartori–Procesi–Schwarz (ASPS) for construction of the orbit space of compact Lie group [16]–[18]. The basic ingredients of this approach can be very shortly formulated as follows.

Consider a compact Lie group G acting linearly on a real d-dimensional vector space V. Let $\mathbb{R}[V]^{\mathrm{G}}$ be the corresponding ring of the G-invariant polynomials on V. Assume $\mathcal{P} = \left(t_1, t_2, \dots, t_q\right)$ is a set of homogeneous polynomials that form the integrity basis, $\mathbb{R}[\xi_1, \xi_2, \dots, \xi_d]^{\mathrm{G}} = \mathbb{R}[t_1, t_2, \dots, t_q]$. Elements of the integrity basis define the polynomial mapping:

$$t: \; V \to \mathbb{R}^q; \quad (\xi_1, \xi_2, \dots, \xi_d) \to \left(t_1, t_2, \dots, t_q\right). \tag{11}$$

Since the map t is constant on the orbits of G, it induces a homeomorphism of the orbit space V/G and the image X of t-mapping; $V/G \simeq X$ [19]. In order to describe X in terms of $\mathcal{P}$ uniquely, it is necessary to take into account the *syzygy ideal* of $\mathcal{P}$, i.e.,

$$I_{\mathcal{P}} = \left\{h \in \mathbb{R}\left[y_1, y_2, \dots, y_q\right] : h\left(p_1, p_2, \dots, p_q\right) = 0, \text{ in } \mathbb{R}[V]\right\}.$$

Let $Z \subseteq \mathbb{R}^q$ denote the locus of common zeros of all elements of $I_{\mathcal{P}}$, then Z is an algebraic subset of $\mathbb{R}^q$ such that $X \subseteq Z$. Denoting by $\mathbb{R}[Z]$ the restriction

[2] The dependence of the discriminant on trace invariants only up to order N pointed in the left side of (9) assumes that all higher trace invariants t_k with $k > N$ in (9) are expressed via polynomials in $t_1, t_2, \dots, t_N$ (the Cayley–Hamilton Theorem).

of $\mathbb{R}[y_1, y_2, \dots, y_q]$ to Z, one can easily verify that $\mathbb{R}[Z]$ is isomorphic to the quotient $\mathbb{R}[y_1, y_2, \dots, y_q]/I_{\mathcal{P}}$ and thus $\mathbb{R}[Z] \simeq \mathbb{R}[V]^{\mathrm{G}}$. Therefore, the subset Z essentially is determined by $\mathbb{R}[V]^{\mathrm{G}}$, but to describe X the further steps are required. According to [17], [18], the necessary information on X is encoded in the structure of the $q \times q$ matrix with elements given by the inner products of gradients, $\mathrm{grad}(t_i)$:

$$\|\mathrm{Grad}\|_{ij} = \left(\mathrm{grad}\,(t_i)\,, \mathrm{grad}\,\left(t_j\right)\right). \tag{12}$$

Hence, applying the ASPS method to the construction of the orbit space $\mathfrak{P}_N/SU(N)$, one can prove the following proposition.

Proposition 5. The orbit space $\mathfrak{P}_N/SU(N)$ can be identified with the semi-algebraic variety, defined as points satisfying two conditions:

a) The integrity basis for $SU(N)$-invariant ring contains only N independent polynomials, i.e., the syzygy ideal is trivial and the integrity basis elements of $\mathbb{R}[\mathfrak{P}_N]^{\mathrm{SU}(N)}$ are subject to only semi-positivity inequalities

$$S_k\,(t_1, t_2, \dots, t_N) \geqslant 0;$$

b) ASPS inequality $\mathrm{Grad}(z) \geqslant 0$ is equivalent to the semi-positivity of the Bézoutian, provided by existence of the d-tuple where $\chi = (1, 2, \dots, d)$:

$$\mathrm{Grad}\,(t_1, t_2, \dots, t_d) = \chi \mathrm{B}\,(t_1, t_2, \dots, t_d)\,\chi^T. \tag{13}$$

3.2. $\mathfrak{P}_N/SU(N)$ — as a Δ_{N-1}-simplex of eigenvalues

The decomposition of the density matrix (1) over the extreme states explicitly displays the equivalence relation between states,

$$\varrho \overset{SU(N)}{\simeq} \varrho' \text{ if } \varrho' = U\varrho U^\dagger, \quad U \in SU(N).$$

Matrices with the same spectrum are unitary equivalent. Furthermore, since the eigenvalues of the density matrix $\mathbf{r} = (r_1, r_2, \dots, r_N)$ in (1) can be always disposed in a decreasing order, the orbit space $\mathfrak{P}_N/SU(N)$ can be identified with the following ordered $(N-1)$-simplex:

$$\Delta_{N-1} = \left\{ \mathbf{r} \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^{N} r_i = 1,\, 1 \geqslant r_1 \geqslant r_2 \geqslant \cdots \geqslant r_N \geqslant 0 \right\}. \tag{14}$$

3.3. $\mathfrak{P}_N/SU(N)$ — as a spherical polyhedron on $\mathbb{S}_{N-2}$

We are now ready to combine the above stated methods of the description of the state space $\mathfrak{P}_N$, the polynomial invariant theory and convex geometry for writing down certain parameterization of density matrices. Based on the extreme decomposition of states (1), the parameterization of the elements of $\mathfrak{P}_N$ reduces to fixing the coordinates on the flag manifolds of $SU(N)$ and the simplex Δ_N of eigenvalues of density matrices. In the remaining part of the article, we will describe $\mathfrak{P}_N/SU(N)$ in terms of the second order polynomial invariant, which is determined uniquely by the Euclidean length r of the Bloch vector, and $N-2$ angles on the sphere $\mathbb{S}_{N-2}$, whose radius in its turn is given as $\sqrt{\frac{N-1}{N}}\,r$.

3.3.1. Qubit, qutrit and quatrit

In order to demonstrate the main idea of the parameterization, we start with its exemplification by considering three the lowest-level systems, qubit, qutrit and quatrit and afterwards the general case of an N-level system will be briefly outlined.

Qubit. A two-level system, the qubit, is described by a three-dimensional Bloch vector $\vec{\xi} = \{\xi_1, \xi_2, \xi_3\}$:

$$\varrho(2) = \frac{1}{2}\left(\mathbb{I}_2 + \xi_i \sigma_i\right). \tag{15}$$

The qubit state with the spectrum $\mathbf{r} = \{r_1, r_2\} \in \Delta_1$ is characterized by the only one independent second order $SU(2)$-invariant polynomial $t_2 = r_1^2 + r_2^2$. Introducing the length of the qubit Bloch vector, $r = \sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}$, we see that[3]

$$t_2 = \frac{1}{2} + \frac{1}{2}\,r^2.$$

Hence, the eigenvalues of the qubit density matrix (15) can be parameterized as

$$r_i = \frac{1}{2} + r\mu_i. \tag{16}$$

It will be explained later that the coincidence of the constants $\mu_1 = 1/2$ and $\mu_2 = -1/2$ in (16) with the standard weights of the fundamental $SU(2)$ representation, when the diagonal Pauli matrix σ_3 is used for the Cartan element of $\mathfrak{su}(2)$ algebra, is not accidental. Below we will give a generalization of (16) for the qudit, an arbitrary N-level system. With this aim it is sapiential to start with considering the $N = 3$ and $N = 4$ cases.

Qutrit. We assume that a generic qutrit state ($N = 3$) has the spectrum $\mathbf{r} = \{r_1, r_2, r_3\}$ from the simplex Δ_2 and thus is an eight-dimensional object. According to the normalization chosen in (3), it is characterized by the 8-dimensional Bloch vector $\vec{\xi} = (\xi_1, \xi_2, \dots, \xi_8)$,

$$\varrho(3) = \frac{1}{3}\,\mathbb{I}_3 + \frac{1}{\sqrt{3}}\sum_{i=1}^{8} \xi_i \lambda_i. \tag{17}$$

[3]The semi-positivity of state (15) dictates the constraint, $S_2 = 1/2(1 - t_2) \geqslant 0$, which restricts the value of the Bloch vector length: $0 \leqslant r \leqslant 1$.

A qutrit has two independent $SU(3)$ trace invariant polynomials, the first one, $t_2 = r_1^2 + r_2^2 + r_3^2$, is expressible via the Euclidean length of the Bloch vector, $r^2 = \sum_{i=1}^{8} \xi_i^2$,

$$t_2 = \frac{1}{3} + \frac{2}{3}\, r^2, \tag{18}$$

and the third order polynomial invariant, $t_3 = r_1^3 + r_2^3 + r_3^3$, which rewritten in terms of eight components of the Bloch vectors reads:

$$\begin{aligned} t_3 = \frac{1}{9} + \frac{2}{3} r^2 + \frac{2}{\sqrt{3}} \xi_1\ (\xi_4\xi_6 + \xi_5\xi_7) + \\ + \frac{2}{\sqrt{3}}\, \xi_2\, (\xi_5\xi_6 - \xi_4\xi_7) + \frac{1}{\sqrt{3}}\, \xi_3\, (\xi_4^2 + \xi_5^2 - \xi_6^2 - \xi_7^2) + \\ + \frac{1}{9} \xi_8\, (6\,(\xi_1^2 + \xi_2^2 + \xi_3^2) - 3\,(\xi_4^2 + \xi_5^2 + \xi_6^2 + \xi_7^2) - 2\xi_8^2)\,. \end{aligned} \tag{19}$$

Now we want to rewrite (19) in terms of the Bloch vector of a length r and an additional $SU(3)$ invariant. Having this in mind, it is convenient to pass to new coordinates linked to the structure of the Cartan subalgebra of $\mathfrak{su}(3)$. Choosing the latter as the span of the diagonal SU(3) Gell-Mann matrices and noting that the state (17) is $SU(3)$-equivalent to the diagonal state:

$$\varrho(3) \overset{SU(3)}{\simeq} \frac{1}{3}\, \mathbb{I}_3 + \frac{1}{\sqrt{3}}\, (\mathcal{J}_3\lambda_3 + \mathcal{J}_8\lambda_8), \tag{20}$$

one can consider two coordinates $(\mathcal{J}_3, \mathcal{J}_8)$ in the Cartan subalgebra of $\mathfrak{su}(3)$ as independent coordinates in $\mathfrak{P}_3/SU(3)$. Taking into account that for the given values of the second trace invariant (18) the coefficients obey relation $\mathcal{J}_3^2 + \mathcal{J}_8^2 = r^2$, we pass to the polar coordinates on the $(\mathcal{J}_3, \mathcal{J}_8)$-plane,

$$\mathcal{J}_3 = r\, \cos\left(\frac{\varphi}{3}\right), \quad \mathcal{J}_8 = r\, \sin\left(\frac{\varphi}{3}\right). \tag{21}$$

In terms of new variables (r, φ) the expression (19) for the $SU(3)$-polynomial invariant t_3 simplifies,

$$t_3 = \frac{1}{9} + \frac{2}{3}\, r^2 + \frac{2}{9} r^3 \sin\varphi, \tag{22}$$

and the image of the ordered simplex Δ_2 in $(\mathcal{J}_3, \mathcal{J}_8)$-plane under the mapping (21) is given by the triangle $\triangle ABC$:

$$\Delta_2 \mapsto \left\{ 0 \leqslant \mathcal{J}_3 \leqslant \frac{\sqrt{3}}{2}, \quad \frac{1}{\sqrt{3}}\, \mathcal{J}_3 \leqslant \mathcal{J}_8 \leqslant \frac{1}{2} \right\},$$

depicted in the figure 1.

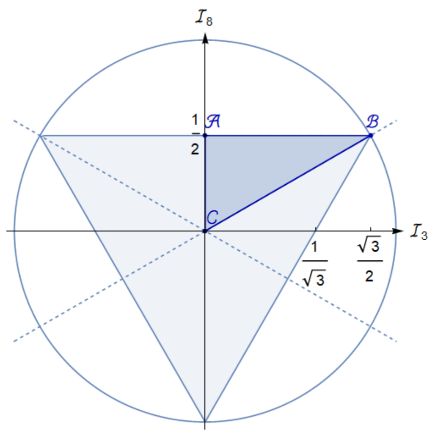

Figure 1. The image of the ordered simplex Δ_2 in $(\mathcal{I}_3, \mathcal{I}_8)$-plane under the mapping (21)

In the figure 1 the Δ_2-simplex of the qutrit eigenvalues is mapped to the triangle $\triangle ABC$ inscribed in a unit-radius circle $\mathcal{I}_3^2 + \mathcal{I}_8^2 = 1$. Its inner part $\triangle ABC$ comprises the points of the maximal rank-3 states $\mathfrak{P}_{3,3}$ with $1 > r_1 > r_2 > r_3 > 0$. All these points generate the *regular* $SU(3)$ orbits $\mathcal{O}_{123}$ of dimension $\dim(\mathcal{O}_{123}) = 6$. The points on the line AB also generate regular orbits $\mathcal{O}_{123}$, however the corresponding states have $\operatorname{rank}(\varrho) = 2$. In contrast to the above case, the line $AC/\{A\}$ and line $BC/\{B\}$ correspond to the subspace of $\mathfrak{P}_{3,3}$, but now the eigenvalues of the states are degenerate, either $r_1 = r_2 > r_3$, or $r_1 > r_2 = r_3$, hence representing the *degenerate orbits* $\mathcal{O}_{1|23}$ and $\mathcal{O}_{12|3}$, respectively. The dimensions of both types of orbits are the same, $\dim(\mathcal{O}_{1|23}) = \dim(\mathcal{O}_{12|3}) = 4$. Finally, the single point $C(0,0)$ represents a maximally mixed state which belongs also to the set of rank-3 states.

The polar form of the invariants (21) prompts us to introduce a unit 2-vector $\vec{n} = (\cos(\varphi/3), \sin(\varphi/3))$ and represent the qutrit eigenvalues as

$$r_i = \frac{1}{3} + \frac{2}{\sqrt{3}}\, r\, \vec{\mu}_i \cdot \vec{n}, \tag{23}$$

with the aid of the weights of the fundamental $SU(3)$ representation:

$$\vec{\mu}_1 = \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \quad \vec{\mu}_2 = \left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \quad \vec{\mu}_3 = \left(0, -\frac{1}{\sqrt{3}}\right). \tag{24}$$

Gathering all together, we convinced that the representation (23) is nothing else than the well-known trigonometric form of the roots of the 3-rd order characteristic equation of the qutrit density matrix:

$$\begin{gathered} r_1 = \frac{1}{3} - \frac{2}{3}\, r\, \sin\left(\frac{\varphi + 4\pi}{3}\right), \quad r_2 = \frac{1}{3} - \frac{2}{3}\, r\, \sin\left(\frac{\varphi + 2\pi}{3}\right), \\ r_3 = \frac{1}{3} - \frac{2}{3}\, r\, \sin\left(\frac{\varphi}{3}\right). \end{gathered} \tag{25}$$

It is in order to present a 3-dimensional geometric picture associated to the parameterization (23). The three drawings in the figure 2 with different values of r show that (23) are parametric form of the arc of the red circle which is the intersection $\Delta_2 \cap \mathbb{S}_1(\sqrt{2/3}\,r)$.

The picture in the figure 2 illustrates a geometrical meaning of the parameterization of qutrit eigenvalues (25) in terms of the Bloch radius r and the angle $\varphi \in [0, \pi]$. Consider an intersection of a qutrit simplex Δ_2 with 2-sphere $r_1^2 + r_2^2 + r_3^2 = 1/3 + (2/3)r^2$. The intersection depends on a value of a qutrit Bloch vector. For $r = 0$ the sphere and the simplex Δ_2 intersect at point $C = (1/3, 1/3, 1/3)$, while for $0 < r < 1$ the intersection is an arc $\mathcal{C}_r$ of a circle on the plane $r_1 + r_2 + r_3 = 1$ of the radius $\sqrt{2/3}\,r$ centered at the point $C(1/3, 1/3, 1/3)$. The intersection for $r = 1$ takes place at $B(1, 0, 0)$. The ordering of eigenvalues $1 \geqslant r_1 \geqslant r_2 \geqslant r_3 \geqslant 0$ determines the length of the arc $\mathcal{C}_r$. For any r, the arc $\mathcal{C}_r$ is described by (25), the depicted curve in the figure corresponds to the fixed value $r = 1/4$. Furthermore, varying r within the interval $r \in [0, 1]$, provides the slices covering the whole simplex $\Delta_2 = [0, \pi] \times \mathcal{C}_r$.

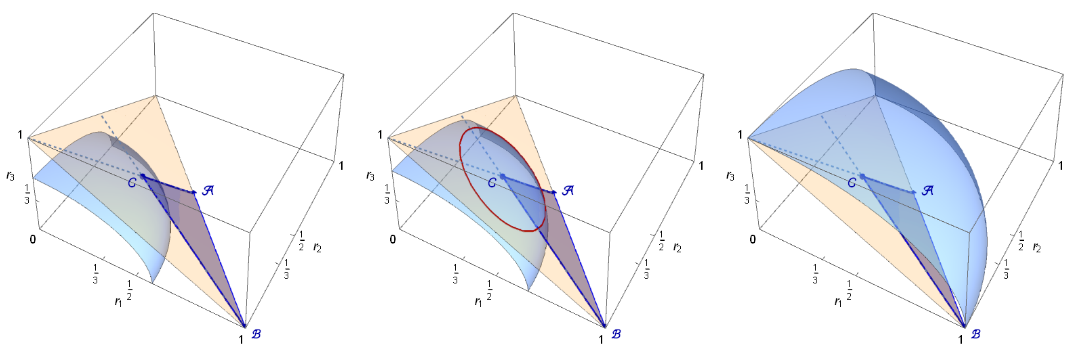

Figure 2. The geometrical meaning of the parameterization of qutrit eigenvalues (25) in terms of the Bloch radius r and the angle $\varphi \in [0, \pi]$

Qutrit Boundary. The introduced parameterization is very useful for analyzing the structure of a qutrit boundary states. The qutrit space $\mathfrak{P}_3$ admits decomposition

$$\mathfrak{P}_3 = \mathfrak{P}_{3,3} \cup \mathfrak{P}_{3,2} \cup \mathfrak{P}_{3,1} \tag{26}$$

into 8d-component of maximal rank-3, 7d-component of rank-2 and extreme pure states. Every component of (26) can be associated with the corresponding domains in the orbit space $\partial\mathcal{O}[\mathfrak{P}_3]$. Particularly, the boundary $\partial\mathcal{O}[\mathfrak{P}_3]$ consists of two components and is described as follows:

— **Qubit inside Qutrit.** For a chosen decreasing order of the qutrit eigenvalues, $r_1 \geqslant r_2 \geqslant r_3$, the rank-2 states belong to the edge Δ_3, given by equation $r_3 = 0$, which in the parameterization (25) reads:

$$\text{rank-2 states}: \quad \left\{ r = \frac{1}{2\,\sin(\varphi/3)} \text{ for } \varphi \in [0,\pi) \right\}. \tag{27}$$

Considering (27) as a polar equation for a plane curve, we find that the rank-2 states $\mathfrak{P}_{3,2}$ can be associated to the part of a 3-order plane curve. Indeed, rewriting (27) in Cartesian coordinates $x = r\cos\varphi$, $y = r\sin\varphi$,

$$(x^2+y^2)(y-3a)+4a^3 = 0,$$

we identify this curve with the famous Maclaurin trisectrix with a special choice of $a = 1/2$.

For the boundary states (27), the equations (25) reduce to

$$r_1 = \frac{1}{2}(1 + r^*_{2\subset 3}), \quad r_2 = \frac{1}{2}(1 - r^*_{2\subset 3}), \tag{28}$$

where

$$r^*_{2\subset 3} = \frac{2}{\sqrt{3}}\sqrt{r^2 - \frac{1}{4}}. \tag{29}$$

These expressions for non-vanishing eigenvalues of a qutrit indicate the existence of a "qubit inside qutrit" whose effective radius is $r^*_{2\subset 3}$. Since the radius of the Bloch vector of rank-2 states associated to a qubit in qutrit lies in the interval $1/2 \leqslant r < 1$, the length of its Bloch vector, $r^*_{2\subset 3}$, takes the same values as a single isolated qubit, $0 \leqslant r^*_{2\subset 3} < 1$.

— **Orbit space of pure states of qutrit.** The boundary $\partial\mathcal{O}[\mathfrak{P}_{3,1}]$ corresponding to all pure states $\mathfrak{P}_{3,1}$ is attainable by $SU(3)$ transformation from the point, $r = 1$ for $\varphi = \pi$.

Quatrit. Now, following the qutrit case, consider a 4-level system, the quatrit, whose mixed state is described by the Bloch vector $\vec{\xi} = \{\xi_1, \xi_2, \dots, \xi_{15}\}$,

$$\varrho(4) = \frac{1}{4}\,\mathbb{I}_4 + \frac{3}{2\sqrt{6}}\sum_{i=1}^{15}\xi_i\lambda_i.$$

The integrity basis for a quatrit ring of $SU(4)$-invariant polynomials $\mathbb{R}[\xi_1, \dots, \xi_{15}]^{\mathrm{SU}(4)}$ consists of three polynomials $\mathbb{R}[t_2, t_3, t_4]$. Using the compact notations (see details in Appendix 5.1), they can be represented in terms of the Casimir invariants of $\mathfrak{su}(4)$ algebra in the following form:

$$\begin{gathered} t_2 = \frac{1}{4} + \frac{3}{4}r^2, \quad t_3 = \frac{1}{16} + \frac{9}{16}r^2 + \frac{3}{16}\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi}, \\ t_4 = \frac{1}{64} + \frac{9}{32}r^2 + \frac{3}{16}\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi} + \frac{9}{64}r^4 + \frac{1}{64}\vec{\xi}\vee\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi}. \end{gathered} \tag{30}$$

From the expressions (30) one can see that apart from the length r of the Bloch vector, there are two independent parameters required to unambiguously characterize the quatrit eigenvalues. To find them, let us proceed as in the qutrit case. Consider the diagonal form corresponding to a quatrit state:

$$\varrho(4) \overset{SU(4)}{\simeq} \frac{1}{4}\mathbb{I}_4 + \frac{3}{2\sqrt{6}}\left(\mathcal{J}_3\lambda_3 + \mathcal{J}_8\lambda_8 + \mathcal{J}_{15}\lambda_{15}\right). \tag{31}$$

The coefficients $\mathcal{J}_3, \mathcal{J}_8$ and $\mathcal{J}_{15}$ in (31) are invariants under the adjoint $SU(4)$ transformations of ϱ. By equivalence relation (31), the quatrit state space is projected to the following convex body:

$$0 \leqslant \mathcal{J}_3 \leqslant \sqrt{\frac{2}{3}}, \quad \frac{\mathcal{J}_3}{\sqrt{3}} \leqslant \mathcal{J}_8 \leqslant \frac{\sqrt{2}}{3}, \quad \frac{\mathcal{J}_8}{\sqrt{2}} \leqslant \mathcal{J}_{15} \leqslant \frac{1}{3}. \tag{32}$$

The 2-dimensional slice $\mathcal{J}_{15} = 1/3$ of this body corresponds to rank-3 states, see the figure 3. In terms of new invariants, all states with a given length of Bloch vector r belong to a 2-sphere: $\mathcal{J}_3^2 + \mathcal{J}_8^2 + \mathcal{J}_{15}^2 = r^2$. Hence, the corresponding spherical angles φ and θ of these invariants,

$$\mathcal{J}_3 = r\sin\theta\cos\frac{\varphi}{3}, \quad \mathcal{J}_8 = r\sin\theta\sin\frac{\varphi}{3}, \quad \mathcal{J}_{15} = r\cos\theta, \tag{33}$$

can be used as two additional parameters needed for the parameterization of a quatrit eigenvalues.

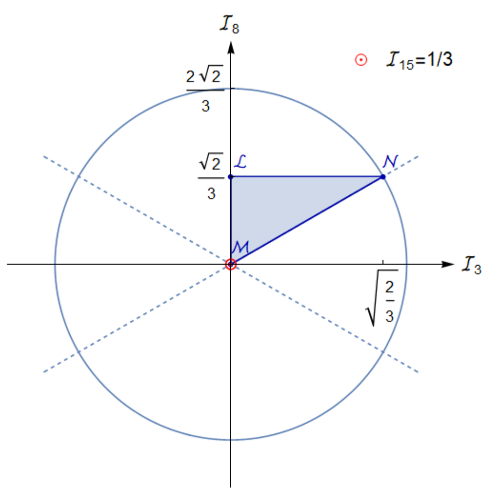

Figure 3. Slice of the convex body (32) as a result of cutting by the plane $\mathcal{J}_{15} = 1/3$

Let us now, in accordance with (33), introduce the unit 3-vector $\vec{n} = (\sin\theta\cos(\varphi/3), \sin\theta\sin(\varphi/3), \cos\theta)$ and parameterize 4-tuple of the eigenvalues of the density matrix $\mathbf{r} = (r_1, r_2, r_3, r_4)$ via the following projections:

$$r_i = \frac{1}{4} + \sqrt{\frac{3}{2}}\, r\,\vec{n}\cdot\vec{\mu}_i, \tag{34}$$

where 3-vectors $\vec{\mu}_1, \vec{\mu}_2, \vec{\mu}_3$ and $\vec{\mu}_4$ denote the weights of the fundamental $SU(4)$. Explicitly the weights read:

$$\begin{aligned} \vec{\mu}_1 &= \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}, \frac{1}{2\sqrt{6}}\right), \quad \vec{\mu}_2 = \left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}, \frac{1}{2\sqrt{6}}\right), \\ \vec{\mu}_3 &= \left(0, -\frac{1}{\sqrt{3}}, \frac{1}{2\sqrt{6}}\right), \quad \vec{\mu}_4 = \left(0, 0, -\frac{3}{2\sqrt{6}}\right). \end{aligned} \tag{35}$$

Note that the weights $\vec{\mu}_i$ are normalised in a way leading to a unit norm of the simple roots of algebra $\mathfrak{su}(4)$ and obey relations:

$$\sum_{i=1}^{4} \vec{\mu}_i = 0, \quad \text{and} \quad \sum_{i=1}^{4} \mu_i^\alpha \, \mu_i^\beta = \frac{1}{2}\,\delta^{\alpha\beta}. \tag{36}$$

Using these expressions, we arrive at the following parameterization of a quatrit eigenvalues:

$$\begin{aligned} r_1 &= \frac{1}{4} - \frac{1}{\sqrt{2}}\, r \left(\sin\theta \sin\frac{\varphi + 4\pi}{3} - \frac{1}{2\sqrt{2}}\cos\theta\right), \\ r_2 &= \frac{1}{4} - \frac{1}{\sqrt{2}}\, r \left(\sin\theta \sin\frac{\varphi + 2\pi}{3} - \frac{1}{2\sqrt{2}}\cos\theta\right), \\ r_3 &= \frac{1}{4} - \frac{1}{\sqrt{2}}\, r \left(\sin\theta \sin\frac{\varphi}{3} - \frac{1}{2\sqrt{2}}\cos\theta\right), \\ r_4 &= \frac{1}{4} - \frac{3}{4}\, r\cos\theta. \end{aligned} \tag{37}$$

To ensure the chosen ordering of the eigenvalues $r_i \in \Delta_3$, the Bloch radius should vary in the interval $r \in [0, 1]$ and angles φ, θ be defined over the domains:

$$\frac{\pi}{6} < \frac{\varphi}{3} < \frac{\pi}{2}, \quad \cot\theta \geqslant \frac{1}{\sqrt{2}}\sin\left(\frac{\varphi}{3}\right). \tag{38}$$

A geometric interpretation of (37), in full analogy with the qutrit case, is described in figure 4.

In the figure 4 the 3-sphere $\sum_i^4 r_i^2 = 1/4 + (3/4)r^2$ intersects the hyperplane $\sum_i^4 r_i = 1$ in the positive quadrant. The intersection occurs iff $1/4 \leqslant 1/4 + (3/4)r^2 \leqslant 1$, and represents the 2-sphere $\mathbb{S}_2(\frac{\sqrt{3}}{2}\, r)$ centered at the point $D = (1/4, 1/4, 1/4, 1/4)$. The intersection with the ordered simplex Δ_3 is given by a spherical polyhedron with 3 or 4 vertices, depending on the Bloch radius r.

The boundary of a quatrit orbit space $\partial\mathcal{O}[\mathfrak{P}_4]$ can be decomposed into 2d-component of rank-3, 1d-component of rank-2 and extreme zero-dimensional component of rank-1, corresponding to pure states:

$$\partial\mathcal{O}[\mathfrak{P}_4] = \partial\mathcal{O}[\mathfrak{P}_{4,3}] \cup \partial\mathcal{O}[\mathfrak{P}_{4,2}] \cup \partial\mathcal{O}[\mathfrak{P}_{4,1}].$$

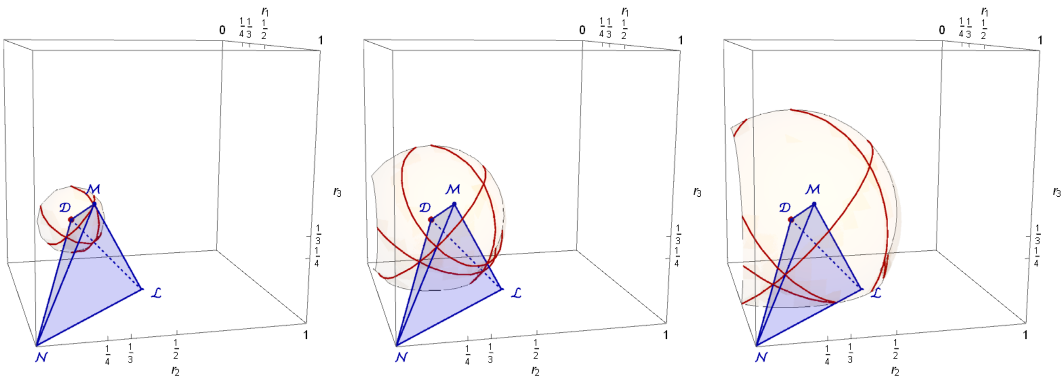

Figure 4. A geometric illustration of (37)

Qutrit inside Quatrit. The boundary component $\mathcal{O}[\mathfrak{P}_{4,3}]$ of rank-3 states is determined by the intersection of 3D simplex Δ_3 with the hyperplane:

$$r_4 = 0. \tag{39}$$

Parameterizing quatrit eigenvalues in terms of angles, the solution to the equation (39) is

$$\cos\theta = \frac{1}{3\,r}, \quad \text{if} \;\; r \in \left[\frac{1}{3}, 1\right]. \tag{40}$$

Hence, the parametric form of the 2-dimensional surface $\mathcal{O}[\mathfrak{P}_{4,3}]$ is given in terms of the remaining three non-vanishing eigenvalues:

$$\begin{gathered} r_1 = \frac{1}{3} - \frac{1}{\sqrt{2}}\, f(r)\, \sin\left(\frac{\varphi + 4\pi}{3}\right), \quad r_2 = \frac{1}{3} - \frac{1}{\sqrt{2}}\, f(r)\, \sin\left(\frac{\varphi + 2\pi}{3}\right), \\ r_3 = \frac{1}{3} - \frac{1}{\sqrt{2}}\, f(r) \sin\left(\frac{\varphi}{3}\right), \end{gathered} \tag{41}$$

where $f(r) = \sqrt{r^2 - \frac{1}{9}}$.

Consequences of the above derived formulae deserve few comments.

1. According to the formula (41) for the eigenvalues of boundary rank-3 states, their expressions are similar to the qutrit eigenvalues given in (25). This observation prompts us to introduce the conception of the *"effective qutrit inside quatrit"*, whose Bloch radius value is determined by the Bloch radius of a quatrit:

$$r^{*}_{3\subset 4} = \frac{3}{2\sqrt{2}}\sqrt{r^2 - \frac{1}{9}}.$$

Note that since the admissible range of the Bloch radius of rank-3 quatrit states is $r \in [1/3, 1]$, then the effective radius $r^{*}_{3\subset 4}$ takes values in the interval $0 \leqslant r^{*}_{3\subset 4} < 1$.

2. The idea to identify qutrit inside quatrit is based on the establishing correspondence on the level of orbit spaces $\mathfrak{P}_{4,3}$ and $\mathfrak{P}_{3,3}$. The generic qutrit state in (26) is 8-dimensional, while $\dim(\mathfrak{P}_{4,3}) = 14$. Thus, one can speak about the correspondence between quatrit rank-3 states and qutrit states only modulo unitary transformations.
3. In favour of the idea considering "effective qutrit inside quatrit" is a relation between the polynomial invariants for states on bulk and boundary. Particularly, using expressions for trace polynomials given in Appendix 5.2, we get:
$$t_2^{(4,3)}(r) = t_2^{(3,3)}\left(r^*_{3\subset 4}\right).$$

Qubit inside Qutrit inside Quatrit. In Δ_3 the rank-2 boundary component $\mathcal{O}[\mathfrak{P}_{4,2}]$ is comprised from points on a line given by its intersection with two hypersurfaces:
$$r_4 = 0, \quad r_3 = 0.$$

Following in complete analogy with the rank-3 states, we arrive at "matryoshka" structure with "effective qubit inside qutrit which in turn is inside quatrit". The Bloch radius of this effective qubit is given by the Bloch radius of a quatrit:
$$r^*_{2\subset 3\subset 4} = \frac{3}{\sqrt{6}}\sqrt{r^2 - \frac{1}{3}}.$$

Note that for rank-2 states $r \in [1/\sqrt{3}, 1]$ and hence $0 < r^*_{2\subset 3\subset 4} < 1$.

Finally, the rank-1 boundary component $\mathcal{O}[\mathfrak{P}_{4,1}]$ is generated by one point $\mathbf{r} = (1, 0, 0, 0)$ which represents all pure states in Δ_3.

3.3.2. Generalization to N-level system

Now after examining main features of the introduced parameterization for a qutrit and quatrit, we are ready to give a straightforward generalization to the case of an arbitrary N-level system. With this aim, we will use the Cartan subalgebra of $SU(N)$ as span of the following diagonal $N \times N$ Gell-Mann matrices:
$$H_1 = \operatorname{diag}(1, -1, 0, \dots, 0),$$
$$H_2 = \frac{1}{\sqrt{3}}\operatorname{diag}(1, 1, -2, \dots, 0),$$
$$H_k = \frac{2}{\sqrt{2k(k-1)}}\operatorname{diag}\left(\overbrace{1, 1, \dots, 1}^{k\ times}, -k, 0, \dots, 0\right),$$
$$H_{N-1} = \frac{2}{\sqrt{2N(N-1)}}\operatorname{diag}\left(\overbrace{1, 1, \dots, 1}^{(N-1)\ times}, -(N-1)\right).$$

The corresponding weights of the fundamental $SU(N)$ representation are

$$\vec{\mu}_1 = \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_2 = \left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_3 = \left(0, -\frac{2}{2\sqrt{3}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_k = \left(\overbrace{0, 0, \dots, 0}^{(k-2)\ times}, -\sqrt{\frac{k-1}{2k}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_N = \left(\overbrace{0, 0, \dots, 0}^{(N-2)\ times}, \dots, -\sqrt{\frac{N-1}{2N}}\right).$$

It is easy to verify that the following relations are true:

$$\sum_{i=1}^{N} \vec{\mu}_i = 0, \quad \text{and} \quad \sum_{i=1}^{N} \mu_i^{\alpha}\, \mu_i^{\beta} = \frac{1}{2}\, \delta^{\alpha\beta}.$$

Taking into account these observations, one can write down the following parameterization for the roots $\mathbf{r}$ of the Hermitian $N \times N$ matrix:

$$r_i = \frac{1}{N} + \sqrt{\frac{2(N-1)}{N}}\, r\, \vec{\mu}_i \cdot \vec{n}, \tag{42}$$

where $\vec{n} \in \mathbb{S}_{N-2}(1)$ and parameter r provides the fulfillment of the correspondence with a value of the second order invariant,

$$t_2 = \frac{1}{N} + \frac{N-1}{N}\, r^2.$$

Writing the traceless part of the density matrix as the expansion over the Cartan subalgebra H of $\mathfrak{su}(N)$,

$$\varrho(N) - \frac{1}{N}\mathbb{I}_N \overset{SU(N)}{\simeq} \sqrt{\frac{(N-1)}{2N}} \sum_{\lambda \in H} \mathcal{J}_s \lambda_s,$$

we see that $N-2$ angles of the unit norm vector $\vec{n}$ (42) are related to the invariants $\mathcal{J}_3^2, \mathcal{J}_8^2, \dots, \mathcal{J}_{N^2-1}^2$, whose values are constrained by the Bloch radius r:

$$\sum_{s=2}^{N} \mathcal{J}_{s^2-1}^2 = r^2. \tag{43}$$

Finally, it is worth to give the geometric arguments which are emphasizing the introduced parameterization (42) of qudit eigenvalues. With this goal consider the intersection $\mathbb{S}_{N-1}(R) \cap \Sigma_{N-1}$ of $(N-1)$-sphere of radius R and hyperplane $\Sigma_{N-1} : \sum_i^N r_i = 1$ in $\mathbb{R}^N$. Let us describe the hyperplane in parametric form, with parameters $s_1, s_2, \dots, s_{N-1}$:

$$\mathbf{r} = \mathbf{d} + \mathbf{e}^{(1)} s_1 + \mathbf{e}^{(2)} s_2 + \cdots + \mathbf{e}^{(N-1)} s_{N-1}, \tag{44}$$

where N-vector $\mathbf{d}$ fixes the point $P \in \Sigma_{N-1}$ and the basis vectors (Darboux frame) obey conditions:

$$\mathbf{d} \cdot \mathbf{e}^{(\alpha)} = 0, \quad \mathbf{e}^{(\alpha)} \cdot \mathbf{e}^{(\beta)} = \delta^{\alpha\beta}, \quad \alpha, \beta = 1, 2, \dots, N-1.$$

Using this parameterization, the equation for $(N-1)$-sphere reduces to the constraint

$$\mathbf{d}^2 + s_1^2 + s_2^2 + \cdots + s_{N-1}^2 = R^2$$

for all points of intersection $\mathbb{S}_{N-1}(R) \cap \Sigma_{N-1}$. Hence, the intersection is nothing else as the $(N-2)$-sphere of radius $R_{N-2} = \sqrt{R^2 - \mathbf{d}^2}$ centered at a point associated to the vector $\mathbf{d} \in \Sigma_{N-1}$. Now if we fix the point P such that $\mathbf{d} = (1/N, \dots, 1/N)$, express the parameters in (44) in terms of the Bloch radius and the components of the unit vector by relation $s_\alpha = \sqrt{2(N-1)/N}\, r\, n_\alpha$ and define the frame vectors $\mathbf{e}^{(\alpha)}$, so that[4]

$$e_i^{(\alpha)} = \sqrt{2}\, \mu_\alpha^{(i)}, \quad i = 1, 2, \dots, N, \quad \text{while} \quad \alpha = 1, 2, \dots, N-1,$$

we arrive at the representation (42) with the radius of intersection sphere $R_{N-2} = \sqrt{(N-1)/N}\, r$.

Passing from hyperplane Σ_{N-1} to its subset, the simplex Δ_{N-1}, we note that $\mathbb{S}_{N-1}(R) \cap \Delta_{N-1}$ will be determined uniquely for every chosen order of the eigenvalues and the value of r. For an arbitrary N, a special analysis is required to write down explicitly $\mathbb{S}_{N-1}(R) \cap \Delta_{N-1}$. Here we only note that the intersection is given by one out of all possible tillings of $\mathbb{S}_{N-2}$ by the spherical polyhedra. For $N = 3$ such polyhedron degenerates to an arc of a circle, whereas for $N = 4$ the intersection will be given by two types of polyhedra, either a spherical triangle, or a spherical quadrilateral, depending on the value of the Bloch radius r.

4. Concluding remarks

Since the introduction of the concept of mixed quantum states, the problem of an efficient parameterization of density matrices in terms of independent variables became one of the important tasks of numerous studies. Starting with the famous Bloch vector parameterization [20], several alternative types of "coordinates" for points of quantum states have been suggested [21]–[30]. According to the generalization of Bloch vector parameterization, initially introduced for a 2-level system, the Bloch vector for an N-level system is a real

[4] Here α component of i-th weights $\vec{\mu}^{(i)}$ determines i-th component of basis vector $\mathbf{e}^{(\alpha)}$.

(N^2-1)-dimensional vector. However, owing to the unitary symmetry of an isolated quantum system, those N^2-1 parameters can be divided into two special subsets. The first subset is given by $N-1$ unitary invariant parameters, and the second one is compiled from the coordinates on a certain flag manifold constructed from the $SU(N)$ group. Introduction of the coordinates on both subsets has a long history. A description of the former set of $SU(N)$-invariant parameters is related to the classical problem of determination of roots of a polynomial equation, while the latter corresponds to a description of the homogeneous spaces of $SU(N)$ group [5].

In the present article we have discussed the first part of the problem of parameterization of $N \times N$ density matrices and proposed a general form of parameterization of N-tuple of its eigenvalues in terms of a length r of the Bloch vector and $N-2$ angles on sphere $\mathbb{S}_{N-2}(\sqrt{(N-1)/N}r)$. We expect that this parameterization will be useful from a computational point of view in many physical applications including the models of elementary particles. Particularly, in forthcoming publications it will be used for the evaluation of very recently introduced indicators of quantumness/classicality of quantum states which are based on the potential of the Wigner quasidistributions to attain negative values [35]–[37].

5. Appendix

5.1. Constructing Casimir invariants for $\mathfrak{su}(N)$ algebra

In this Appendix we collect few notions and formulae explaining the construction of the polynomial Casimir invariants on the Lie algebra $\mathfrak{g} = \mathfrak{su}(N)$ of the group $G = SU(N)$.

Consider algebra $\mathfrak{g} = \sum_i^{N^2-1} \xi_i \lambda_i$, spanned by the orthonormal basis $\{\lambda_i\}$ with the multiplication rule

$$\lambda_i \lambda_j = \frac{2}{N}\delta_{ij} + (d_{ijk} + \imath f_{ijk})\,\lambda_k, \tag{45}$$

defined via the symmetric d_{ijk} and anti-symmetric f_{ijk} structure constants. Let $\{\omega^i\}$ be the dual basis in $\mathfrak{g}^*$, i.e., $\omega^i(\lambda_j) = \delta^i_j$, and introduce the G-invariant symmetric tensor S of order r:

$$S = S_{i_1 i_2 \dots i_r}\,\omega^{i_1} \otimes \omega^{i_2} \cdots \otimes \omega^{i_r}. \tag{46}$$

The G-invariance of tensor S means that

$$\sum_{s=1}^{r} f^{m}_{\ i i_s} S_{i_1 i_2 \dots i_{s-1} m i_{s+1} \dots i_r} = 0. \tag{47}$$

[5] Among the important contributions to the problem of parameterizing $SU(N)$, we would like to mention the following publications that influenced the present work: [31]–[34].

Using the tensor S, one can construct the elements of the enveloping algebra $\mathcal{U}(\mathfrak{g})$:

$$C_r = S_{i_1 i_2 \dots i_r} \lambda_{i_1} \lambda_{i_2} \dots \lambda_{i_r}, \tag{48}$$

which turns to belong to the center of $\mathcal{U}(\mathfrak{g})$, i.e., $[C_r, \lambda_i] = 0$, for all generators λ_i. Having in mind the solution to the invariance equations (47), one can build the polynomials in N^2-1 real variables $\vec{\xi} = (\xi_1, \xi_2, \dots \xi_{N^2-1})$:

$$\mathfrak{C}_r(\vec{\xi}\,) = \sum_i S_{i_1 i_2 \dots i_r} \xi_{i_1} \xi_{i_2} \dots \xi_{i_r},$$

which are invariant under the adjoint $SU(N)$-transformations:

$$p(\overrightarrow{\mathrm{Ad}_g(\xi)}) = p(\vec{\xi}\,).$$

It can be proved that the symmetric tensors $k^{(r)}$ defined in the given basis of algebra as $k^{(r)}_{i_1 i_2 \dots i_r} = \mathrm{Tr}\left(\lambda_{\{i_1} \lambda_{i_2} \dots \lambda_{i_r\}}\right)$, satisfy invariance equation (47) and form the basis for the polynomial ring of G-invariants. The tensors $k^{(r)}$ admit decomposition with the aid of the lowest symmetric invariants tensors, δ_{ij} and d_{ijk}. Particularly, the following combinations are valid candidates for the basis:

$$k^{(4)}_{i_1 i_2 i_3 i_4} = d_{\{i_1 i_2\}s} d_{\{i_3 i_4\}s},$$
$$k^{(5)}_{i_1 i_2 i_3 i_4 i_5} = d_{\{i_1 i_2\}s} d_{s i_3 t} d_{\{i_4 i_5\}t},$$
$$k^{(6)}_{i_1 i_2 i_3 i_4 i_5 i_6} = d_{\{i_1 i_2\}s} d_{s i_3 t} d_{t, i_4, u} d_{\{i_5 i_6\}u}.$$

As an example, for N-level system the G-invariant polynomials up to order six read:

$$\begin{aligned}
\mathfrak{C}_2 &= (N-1)\,\vec{\xi}^{\,2},\\
\mathfrak{C}_3 &= (N-1)\,\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi},\\
\mathfrak{C}_4 &= (N-1)\,\vec{\xi}\vee\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi},\\
\mathfrak{C}_5 &= (N-1)\,\vec{\xi}\vee\vec{\xi}\vee\vec{\xi}\vee\vec{\xi}\cdot\vec{\xi},\\
\mathfrak{C}_6 &= (N-1)\,(\vec{\xi}\vee\vec{\xi}\vee\vec{\xi}\,)^2.
\end{aligned} \tag{49}$$

In the equation (49) the Casimir invariants are represented in a dense vectorial notation using the auxiliary (N^2-1)-dimensional vector defined via the symmetrical structure constants d_{ijk} of the algebra $\mathfrak{su}(N)$:

$$(\vec{\xi}\vee\vec{\xi}\,)_k := \sqrt{\frac{N(N-1)}{2}}\, d_{ijk}\, \xi_i \xi_j.$$

5.2. Polynomial $SU(N)$-invariants on $\mathfrak{P}_N$

In this section the explicit formulae for polynomial invariants for quatrit will be given in terms of the suggested parameterization of density matrices. Since the traceless part of the density matrices, $\varrho - \frac{1}{N} I_N = \sqrt{\frac{(N-1)}{2N}}\ \mathfrak{g}$, belongs to the algebra $\mathfrak{su}(N)$, all trace polynomials t_k can be expanded over the $\mathfrak{su}(N)$ Casimir invariants. The corresponding decomposition of independent polynomials for the quatrit ($N = 4$) read:

$$t_2 = \frac{1}{4}(1 + 3\mathfrak{C}_2),$$

$$t_3 = \frac{1}{4^2}(1 + 3\mathfrak{C}_2 + \mathfrak{C}_3),$$

$$t_4 = \frac{1}{4^3}\left(1 + 6\mathfrak{C}_2 + 4\mathfrak{C}_3 + \mathfrak{C}_2^2 + \mathfrak{C}_4\right).$$

In order to derive the explicit form of polynomials $\mathfrak{C}_2$ and $\mathfrak{C}_3$, the knowledge of components of the symmetric structure tensor d is needed. It is convenient at first to express the invariants for diagonal states, characterized by $\mathcal{J}_3$, $\mathcal{J}_8$ and $\mathcal{J}_{15}$, and afterwards rewrite them for generic states using parameterization (33). With this aim, we collect (up to permutations) in the table 1 all non-zero coefficients d_{ijk} for the Cartan subalgebra of $\mathfrak{su}(3)$ and $\mathfrak{su}(4)$.

Table 1

Symmetric structure constants for the Cartan subalgebra of $\mathfrak{su}(3)$ and $\mathfrak{su}(4)$

i.j.k	3.3.8	3.3.15	8.8.8	8.8.15	15.15.15
$d_{ijk}^{\mathrm{SU}(4)}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$-\sqrt{\frac{2}{3}}$
$d_{ijk}^{\mathrm{SU}(3)}$	$\frac{1}{\sqrt{3}}$		$-\frac{1}{\sqrt{3}}$		

Taking into account the values for structure constant d from the table 1, the Casimir invariants of the third and fourth order of a quatrit read:

$$\mathfrak{C}_3 = 9\,\mathcal{J}_{15}\left(\mathcal{J}_3^2 + \mathcal{J}_8^2\right) + 9\sqrt{2}\,\mathcal{J}_8\left(\mathcal{J}_3^2 - \frac{1}{3}\,\mathcal{J}_8^2\right) - 6\,\mathcal{J}_{15}^3, \tag{50}$$

$$\mathfrak{C}_4 = 9\,\left(\mathcal{J}_3^2 + \mathcal{J}_8^2\right)^2 + 36\sqrt{2}\,\mathcal{J}_8\,\mathcal{J}_{15}\left(\mathcal{J}_3^2 - \frac{1}{3}\,\mathcal{J}_8^2\right) + 12\,\mathcal{J}_{15}^4. \tag{51}$$

Finally, plugging expressions (33) into (50) and (51), we arrive at the representation of the $\mathfrak{su}(4)$ Casimir invariants in terms of quatrit Bloch radius r and two angles (θ, φ):

$$\mathfrak{C}_3 = \frac{3}{4}\,r^3\left[4\sqrt{2}\sin^3(\theta)\sin(\varphi) - 3\cos(\theta) - 5\cos(3\theta)\right],$$

$$\mathfrak{C}_4 = \frac{3}{8}r^4\left[32\sqrt{2}\sin^3(\theta)\cos(\theta)\sin(\varphi) + 4\cos(2\theta) + 7\cos(4\theta) + 21\right],$$

as well as directly for the trace polynomial invariants,

$$t_2 = \frac{1}{4} + \frac{3}{4}r^2,$$

$$t_3 = \frac{1}{16} + \frac{9}{16}r^2 + \frac{3}{64}r^3\left(4\sqrt{2}\sin^3\theta\sin\varphi - 3\cos\theta - 5\cos(3\theta)\right),$$

$$t_4 = \frac{1}{64} + \frac{9}{32}r^2 + \frac{3}{64}r^3\left(4\sqrt{2}\,\sin^3\theta\sin\varphi - 3\cos\theta - 5\cos(3\theta)\right) + \\ + \frac{3}{512}r^4\left(32\sqrt{2}\sin^3\theta\cos\theta\sin\varphi + 4\cos(2\theta) + 7\cos(4\theta) + 45\right).$$

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Квантовые системы с конечным числом состояний всегда были основным элементом многих физических моделей в ядерной физике, физике элементарных частиц, а также в физике конденсированного состояния. Однако сегодня, в связи с практической потребностью в области развития квантовых технологий, возник целый ряд новых задач, решение которых будет способствовать улучшению нашего понимания структуры конечномерных квантовых систем.

В статье мы сфокусируемся на одном из аспектов исследований, связанных с проблемой явной параметризации пространства состояний N-уровневой квантовой системы. Говоря точнее, мы обсудим вопрос практического описания унитарного пространства орбит — $SU(N)$-инвариантного аналога N-уровневого пространства состояний $\mathfrak{P}_N$. В работе будет показано, что сочетание хорошо известных методов теории полиномиальных инвариантов и выпуклой геометрии позволяет получить удобную параметризацию для элементов $\mathfrak{P}_N/SU(N)$. Общая схема параметризации $\mathfrak{P}_N/SU(N)$ будет детально проиллюстрирована на примере низкоуровневых систем: кубита ($N = 2$), кутрита ($N = 3$), куатрита ($N = 4$).

Ключевые слова: параметризация матрицы плотности, квантовая система, кубит, кутрит, куатрит, кудит, теория полиномиальных инвариантов, выпуклая геометрия

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On involutive division on monoids

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We consider an arbitrary monoid M, on which an involutive division is introduced, and the set of all its finite subsets $\operatorname{Set} M$. Division is considered as a mapping $d : \operatorname{Set} M \times M$, whose image $d(U, m)$ is the set of divisors of m in U. The properties of division and involutive division are defined axiomatically. Involutive division was introduced in accordance with the definition of involutive monomial division, introduced by V. P. Gerdt and Yu. A. Blinkov. New notation is proposed that provides brief but explicit allowance for the dependence of division on the $\operatorname{Set} M$ element. The theory of involutive completion (closures) of sets is presented for arbitrary monoids, necessary and sufficient conditions for completeness (closedness) — for monoids generated by a finite set X. The analogy between this theory and the theory of completely continuous operators is emphasized. In the last section, we discuss the possibility of solving the problem of replenishing a given set by successively expanding the original domain and its connection with the axioms used in the definition of division. All results are illustrated with examples of Thomas monomial division.

Key words and phrases: involutive monomial division, Gröbner basis

1. Introduction

The creation of the technique of involutive bases as an alternative to the classical Gröbner bases and its application to the study of ideals in polynomial and differential rings is undoubtedly one of the most important contributions made by V. P. Gerdt and his disciples in computer algebra.

The concept of involutive division came to algebras from the compatibility studies of systems of partial differential equations, dating back to the works of Riquier [1], Janet [2], Thomas [3]. Since the mid-1990s, V. P. Gerdt and his students A. Yu. Zharkov and Yu. A. Blinkov have published a series of papers in which this concept was developed in an abstract algebraic form and indicated the wide possibilities of using involutive bases as an alternative to the usual Gröbner bases. The first example of involutive division — Pomare division — was introduced by Zharkov in 1993 [4]–[7].

In general terms, the concept of involutive division was introduced by Gerdt and Blinkov in [8]–[11]. V. P. Gerdt strove for an axiomatic presentation of the concept of involutive division, especially emphasizing this in his report made at RUDN University in November 2020 [12]. In our opinion, the theory of divisions on monoids, cleared of applied issues, looks like a self-sufficient and very elegant theory, which is complete only to the extent that was of interest for applied researchers. We have tried to present it in general terms.

We based on §1.2 from the Dr. Sci. thesis by Blinkov [13], but have significantly revised the terminology. The fact is that the creators of this theory obviously intended to give it a topological interpretation, but, unfortunately, they never did it. Therefore, a number of terms (continuity of division, closure of sets) refer to this so far unknown topology. In our opinion, this topology is the Zariski topology, and therefore incidental analogies taken from the $\mathbb{R}$ topology greatly hinder its development.

2. Divisions on monoids

Definition 1. A set is called a monoid if a binary associative operation called multiplication is specified on it, and there is an element 1 such that $1m = m$ for any $m \in M$.

The set of all finite subsets of the set M will be denoted as $\operatorname{Set} M$. For definiteness, we will assume that $\emptyset \in \operatorname{Set} M$.

Definition 2. By division on the monoid M we mean the mapping

$$d: \operatorname{Set} M \times M \to \operatorname{Set} M,$$

having the following properties:

1. $d(U, m) \subset U$,
2. $u \in d(U, u)$,
3. if $u \in d(U, m)$, then there is an element $m^* \in M$ such that $m = um^*$,
4. if $u \in d(U, mu)$ and $u \in d(U, m'u)$, then $u \in d(U, mm'u)$,
5. if $U' \subset U$, then $d(U, m) \cap U' \subset d(U', m)$,

valid for any $U, U' \in \operatorname{Set} M$, $u \in U$, $m, m' \in M$. Elements of the image $d(U, m)$ will be called divisors of m in U and m is said divisible by elements of $d(U, m)$.

Remark 1. We have split the definition of involutive division from [13, def. 5] into the definition of division in general and involutive division (def. 4 below). The notation has been changed. The notation $u|_{\mathcal{L}(U)}m$ used in [13] is now changed for $u \in d(U, m)$.

Example 1. Assuming $d(U, m) = \{u \in U : \exists m^* \in M : m^*u = m\}$, we will define the standard division on the monoid.

If there is a set $X \in \operatorname{Set} M$ such that any element of the set M other than 1 can be represented as a product of elements from X, then the monoid is said to be generated by the set X. If such a representation is unique for an element of the set M, then M is said to be a set of monomials, and the elements of the set X are treated as variables.

Definition 3. An element $x \in X$ will be called multiplicative for u with respect to U if $u \in d(U, xu)$.

The set of all multiplicative elements for u relative to U will be denoted as $X_d(U, u)$.

Theorem 1. *If $x_1, \dots, x_s$ are multiplicative elements of X for u with respect to U, then $u \in d(U, x_1^{j_1} \dots x_s^{j_s} u)$.*

Proof. Corollary of the 4th property of definition 2. □

To difine division on a monoid generated by the set X, it is enough to specify X_d.

Theorem 2. *Suppose that a finite set X generates a monoid M and some mapping is given $X_d : \operatorname{Set} M \times M \to \operatorname{Set} X$.*

Let us define the function $d : \operatorname{Set} M \times M \to \operatorname{Set} M$ as follows: $u \in d(U, m)$ if and only if $u \in U$ and there exists a product of m^* elements from $X_d(U, u)$ such that $m = m^* u$. The function d defines division by M if and only if the embedding $U' \subset U$ implies

$$X_d(U, u) \subset X_d(U', u) \quad \forall u \in U'. \tag{1}$$

Remark 2. In [13] it was noted that “involutive division for a monomial can be specified by defining sets of multiplicative and non-multiplicative variables”. We have formulated this idea in the form of theorems 1 and 2. They seem to be mutually inverse. However, according to theorem 1

$$v = \prod_{x \in X} x^{j_x} \Longrightarrow u \in d(U, vu),$$

and theorem 2 does not reverse the arrow, but asserts that if the condition (1) is satisfied, we can define a division by M such that

$$v = \prod_{x \in X} x^{j_x} \Longleftrightarrow u \in d(U, vu).$$

Proof. Property 1 of definition 2 is fulfilled, since by construction of d, the element $u \in d(U, m)$ only if $u \in U$. Property 2 is satisfied, since for $m = u$ one can take $m^* = 1$. Property 3 is fulfilled because m^* is explicitly specified when constructing d.

Property 4 is fulfilled, since by the construction of d the embeddings $u \in d(U, mu)$ and $u \in d(U, m'u)$ mean that there exist products v, v' of elements from $X_d(U, u)$ such that $mu = vu$ and $m'u = v'u$. But then $mm'u = vv'u$ and, since vv' is the product of elements from $X_d(U, u)$, $u \in d(U, mm'u)$.

Now we turn to property 5. Let $U' \subset U$ and $u \in d(U,m) \cap U'$, then $u \in U'$ and there exists a product of m^* of elements from $X_d(U,u)$ such that $m = m^* u$. From this it follows that $u \in d(V,m)$ if and only if $X_d(U,u) \subset X_d(U',u)$, i.e., the ratio (1) is true. □

Example 2. Consider the set M of all monomials generated by the n variables $X = (x_1, \dots, x_n)$. Let us agree to write $\partial_i x_1^{j_1} \dots x_n^{j_n} = j_i$.

Thomas division is determined by the formula

$$x_i \in X_d(U,u) \Leftrightarrow \partial_i u = \max_{v \in U} \partial_i v.$$

Let us check the condition (1). Let $u \in U' \subset U$. If $x_i \in X_d(U,u)$, then the maximum of $\partial_i v$ on U is achieved when $v = u \in U'$. Since $U' \subset U$,

$$\max_{v \in U'} \partial_i v \leqslant \max_{v \in U} \partial_i v$$

and, therefore, the maximum is attained at $v = u$. This is what condition (1) asserts.

3. Involutive divisions on monoids

Definition 4. A division d will be called involutive if for any $U \in \operatorname{Set} M$ and $m \in M$ the set $d(U,m)$

1. is empty,
2. consists of one element,
3. consists of several elements, and then for any $u, u' \in d(U,m)$, it is strictly true that either $u \in d(U,u')$, or $u' \in d(U,u)$.

The maximum number of distinct elements that make up $d(U,m)$ for any $U \in \operatorname{Set} M$ and $m \in M$ will be called the rank of the involutive division of d.

Remark 3. Simultaneous execution of equalities $u \in d(U,u')$, $u' \in d(U,u)$ by virtue of property 3 of definition 2, implies the existence of two elements $v, v' \in M$ such that $u' = vu$ and $u = v'u'$. In a monomial set, the simultaneous fulfillment of these equalities means that $v = v' = 1$ and therefore $u = u'$. Thus, only one of them can be fulfilled in definition 4. Definition 4 implies that only one of these equalities holds in the case of an arbitrary monoid.

Definition 4 allows ordering the linearly finite set $d(U,m)$:

$$u \in d(U,u') \ \text{ and } \ u \neq u' \Leftrightarrow u < u'.$$

Therefore, there exists a single maximal element, i.e., an element u such that $d(U,m) \subset d(U,u)$. This can be taken as a definition of involutivity, equivalent to the previous one.

Definition 5. A division d will be called involutive if, for any $U \in \operatorname{Set} M$ and $m \in M$, there exists and, moreover, a unique element $u \in U$ such that

$$d(U,m) \subset d(U,u).$$

Example 3. Let us describe the Thomas division in more detail. Let U be a finite subset of the set M_n of all monomials in n variables. For brevity we put

$$r_i = \max_{w \in U} \partial_i w.$$

These numbers only depend on U. Let $u \in d(U, m)$, then there is a product of v variables from $X_d(U, u)$ such that $m = uv$. Then $\partial_i m = \partial_i u + \partial_i v$.

If $x_i \in X_d(U, u)$, then $\partial_i v \geqslant 0$ and $\partial_i u = r_i$, whence $\partial_i v = \partial_i m - r_i \geqslant 0$.

If $x_i \notin X_d(U, u)$, then $\partial_i v = 0$ and $\partial_i u < r_i$, where $r_i > \partial_i u = \partial_i m - 0$.

Thus, combining both cases,

$$\partial_i v = \begin{cases} \partial_i m - r_i & \partial_i m \geqslant r_i \\ 0 & \partial_i m < r_i \end{cases}$$

and

$$\partial_i u = \partial_i \frac{m}{v} = \begin{cases} r_i & \partial_i m \geqslant r_i \\ \partial_i m & \partial_i m < r_i \end{cases} = \min(\partial_i m, r_i).$$

Thus, u is uniquely determined by specifying U and m. It is already clear from this that the Thomas division is an involutive division of the 1st rank. However, we also obtained an explicit formula for $d(U, m)$. If $\partial_i u = \min(\partial_i m, r_i)$ specifies an element u from U, then $d(U, m)$ consists of this one element. If this element does not belong to U, then $d(U, m)$ is empty.

4. Complete sets and completely involutive divisions

Let again $U \in \operatorname{Set} M$.

Definition 6. A set of elements of the form mu, where $u \in U$ and $m \in M$, will be called a cone generated by the set U and denoted as $C(U)$.

Definition 7. The set of elements $m \in M$ such that $d(U, m) \neq \emptyset$, will be called an involutive cone generated by the set U and denoted as $I_d(U)$.

By virtue of property 3 of definition 2, $I_d(U) \subseteq C(U)$.

Definition 8. A set $U \in \operatorname{Set} M$ is called complete with respect to the involutive division of d if the involutive cone generated by it coincides with the usual one, i.e., $I_d(U) = C(U)$.

Remark 4. In [13], instead of 'complete sets', the term 'closed sets' is used. We prefer the term 'complete' because it does not give rise to connotations with some topology on $\operatorname{Set} M$.

Example 4. In M_n the embedding $m \in C(U)$ means that there is an element $u \in U$ such that $\partial_i m \geqslant \partial_i u \quad \forall i = 1, 2, \dots, n$. With respect to Thomas division, $m \in C(U)$ is divisible by U if and only if v with $\partial_i v = \min(\partial_i m, r_i)$ belongs to U. Let U contain all monomials u satisfying the inequalities

$$c_i \leqslant \partial_i u \leqslant r_i \quad \forall i = 1, 2, \dots, n,$$

where $c_1, \dots, c_n$ are non-negative integers. Then

$$\partial_i m \geqslant \partial_i u \geqslant c_i \quad \forall i = 1, 2, \dots, n,$$

and therefore $c_i \leqslant \partial_i v = \min(\partial_i m, r_i) \leqslant r_i$ and $v \in U$. Therefore, such a set U is complete with respect to the Thomas division.

Definition 9. A set $U^* \in \operatorname{Set} M$ is called a completion of the set $U \in \operatorname{Set} M$ with respect to division d if

1. U is a subset of the set U^*,
2. U^* is a complete set with respect to division of d, that is, $I_d(U^*) = C(U^*)$,
3. $C(U) = C(U^*)$.

Definition 10. An involutive division d is called completely involutive if each set from $\operatorname{Set} M$ has completion with respect to this division.

Remark 5. In [13], such divisions are called Noetherian, which requires a rather lengthy explanation of the connection between the issue and the finiteness of the ideal bases.

Example 5. For the Thomas division, the completion can be described explicitly: the completion of U is the set $U^* \in \operatorname{Set} M_n$ formed by the monomials v with the following property: there exists a monomial $u \in U$ such that

$$\partial_i u \leqslant \partial_i v \leqslant r_i.$$

Indeed, by the construction of U^*, $U \subseteq U^*$ holds, that is, property 1 of definition 9. The fulfillment of the 3rd property is also obvious, since $U^* \subset C(U)$ by construction.

Let us check the second property. Let $m \in C(U^*)$, that is, there is a monomial $u^* \in U^*$ and a monomial $v \in M_n$ such that $m = u^* v$, where $\partial_i m \geqslant \partial_i u^*$.

By the construction of U^*, this implies that for m one can specify a monomial $u \in U$ such that $\partial_i m \geqslant \partial_i u$. On the other hand, the monomial m is divisible by U^* if and only if the monomial u^* with $\partial_i u^* = \min(\partial_i m, r_i)$ belongs to U^*. But this is indeed the case, since $\partial_i u \leqslant \min(\partial_i m, r_i) \leqslant r_i$.

This means that $C(U^*) = I_T(U^*)$, that is, U^* is a complete set. This is the second property.

Remark 6. Historically, the concept of Pomare division was first introduced, it is involutive, and not completely involutive, which is a source of various kinds of pathological examples, see [13, example 55] and also [4], [14], [15].

5. Necessary and sufficient conditions for the completeness of a set

Theorem 3 (necessary completeness condition). *Let the monoid M be generated by elements of a finite set X. For the set M to be complete with respect to the division of d, it is necessary that*

$$d(U, xu) \neq \emptyset \quad \forall u \in U, \forall x \in X. \tag{2}$$

This condition is sufficient only for a certain class of divisions.

Definition 11. A sequence $\{u_0, u_1 \dots,\}$ of elements of the set U will be called fundamental if for any i there is an element $x_i \in X$ such that:

1. $u_i \notin d(U, x_i u_i)$,
2. $u_{i+1} \in d(U, x_i u_i)$.

Definition 12. A division of d by the monoid M will be called finite if every fundamental sequence is finite.

Remark 7. In [13], division is called continuous if every finite fundamental sequence does not contain two identical terms. In this case, any piece of an infinite fundamental sequence is shorter than the total number of elements in U and the division is finite in the sense of our definition. However, to prove theorem 4, the 'continuity' requirement can be weakened to that described in our definition.

Remark 8. In our opinion, this construction is much more similar to the concept of a completely continuous mapping, and not just a continuous one. For this reason, we call the sequences from definition 11 fundamental, and the property described in the definition 10, complete involutivity.

Theorem 4. *If d is a finite involutive division on the monoid M generated by elements of the finite set X, then for the set U to be complete it is necessary and sufficient that condition* (2) *be satisfied.*

Proof. Let condition (2) be satisfied for the set U. Take $u \in U$ and $m \in M$ in an arbitrary way and construct a divisor of mu in U as follows.

Let us take u as the first element u_0 of the sequence of elements U. If $u_0 \in d(U, um)$, then we will not do anything. If $u_0 \notin d(U, um)$, then among the factors m from X there is x_0 such that $u_0 \notin d(U, u_0 x_0)$ by theorem 1. But by virtue of (2) then there exists $u_1 \in U$ such that $u_1 \in d(U, u_0 x_0)$.

If $u_1 \in d(U, um)$, then we will not do anything. Otherwise, there is an element $x_1 \in X$ such that $u_1 \notin d(U, u_1 x_1)$.

Then, by virtue of (2), there is an element $u_2 \in U$ such that $u_2 \in d(U, u_1 x_1)$.

Proceeding on like this, we get a sequence $\{u_0, u_1, \dots\}$ of U elements.

The described sequence is fundamental (definition 11). Under the conditions of the theorem being proved, it is indicated that d is a finite division, therefore every fundamental sequence is finite. By construction, its last element is a divisor of um in U.

Thus, every element um has a divisor in U, that is, U is a complete set. □

Example 6. In the case of Thomas division, the set $d(U, u_i x_{k_i})$ consists of one element u_{i+1}, and $\partial_j u_{i+1} = \min(\partial_j u_i x_{k_i}, r_j)$.

For $j \neq k_i$

$$\partial_j u_{i+1} = \min(\partial_j u_i, r_j) = \partial_j u_i.$$

since $u_i \in U$. For $j = k_i$

$$\partial_{k_i} u_{i+1} = \min(\partial_{k_i} u_i + 1, r_{k_i}) = \partial_{k_i} u_i + 1,$$

because otherwise it would be $\partial_{k_i} u_i + 1 > r_{k_i}$, which contradicts $u_i \in U$. Thus, $u_{i+1} = u_i x_{k_i}$.

From this, in particular, it is clear that there are no coinciding elements among the elements. Since there is a finite number of products of U and X, the fundamental sequence is finite.

6. Set completion

Problem. Given $U \in \mathrm{Set}\, M$ and a finite completely involutive division of d by M, it is required to find its completion with respect to d.

In the specified class of divisions, this problem always has a solution (definition 10). For Thomas division, we know its explicit solution (example 5). For other divisions, it would be desirable to solve the problem, gradually supplementing U with new elements.

So, let U be given. By searching over two finite sets, we seek all pairs $u \in U$ and $x \in X$ such that $d(U, xu) = \emptyset$.

If there is no such pair, then the completion $U^* = U$ (theorem 4) and the problem is solved. If there are such pairs, then we add one of the products xu obtained in this way to the set U and obtain the set U_1. Proceeding on like this, we will expand U more and more, while remaining inside the cone $C(U)$. If this process is interrupted at the n-th step, then the resulting set is complete by virtue of theorem 4. This will be the completion U^* of the set U by definition 9. However, the finiteness of U^* does not imply finiteness of the described process, since we can get sets that contain elements that are absent in U^*. To avoid this, it is necessary to indicate a rule for choosing a pair from the set of pairs $u \in U_n$ and $x \in X$ such that $d(U_n, xu) = \emptyset$, which guarantees the embedding $U_n \subset U^*$ at each step.

The simplest option is to take an element that is in some sense minimal, but for this purpose we have to restrict ourselves to the special case when the monoid is the set of monomials in n variables that make up the set X. Let this set be given a monomial order, say, deglex.

Given U, among the pairs $u \in U$ and $x \in X$ such that $d(U, xu) = \emptyset$, we take the one for which the product ux is minimal. By virtue of property 5 of definition 2

$$d(U^*, xu) \cap U \subset d(U, xu) = \emptyset.$$

That is why $v \in d(U^*, xu) \notin U$.

By virtue of property 3 of definition 2 there is an element $m \in M$ such that $xu = vm$. If $m = 1$, then $xu = v \in U^*$ and $U_1 = U \cup \{xu\} \subset U^*$ and you can go to the next step.

Regarding the second option, when $m > 1$, one can notice the following.

Theorem 5. *If $m > 1$, then $d(U, v)$ is not empty.*

Proof. Since $v \in U^* \subset C(U)$, there exists a pair $u_1 \in U$ and $m_1 \in M$ such that $v = m_1 u_1$.

If $m_1 = 1$, then $v = u_1 \in U$, which is impossible. Therefore, $m_1 > 1$. Therefore, $xu = u_1 m m_1$, $m, m_1 > 1$.

This means that $u_1 y < ux$ for any $y \in X$. Since we initially chose the minimum pair, $d(U, u_1 y) \neq \emptyset \quad \forall y \in X$.

Let us denote the set of variables that are included in m_1 as Y.

If $u_1 \in d(U, u_1 y) \quad \forall y \in Y$, then by virtue of theorem 1, $u_1 \in d(U, u_1 m_1) = d(U, v)$, i.e., $d(U, v)$ is not empty.

Otherwise, there is $y_1 \in Y$ such that $u_1 \notin d(U, u_1 y_1)$.

The set $d(U, u_1 y_1)$ itself is not empty, let $u_2 \in U$ belong to it, then $u_1 \neq u_2$ and there exists $m_2 \in M$ such that $u_1 y_1 = u_2 m'$. But then

$$v = u_1 m_1 = u_2 m_2, \quad m_2 = \frac{m_1 m'}{y_1},$$

and m_1 is divisible by y_1, since $y_1 \in Y$. Thus, we get the first elements u_1, u_2 of the fundamental sequence, and $v = u_1 m_1 = u_2 m_2$.

Repeating the above considerations in relation to the representation $v = u_2 m_2$, we get either $u_2 \in d(U, v)$, or the next element of the sequence. Since every fundamental sequence is finite, at some step we get $u_n \in d(U, v)$, that is, $d(U, v) \neq \emptyset$. □

The process of solving the problem described above will stop if the following condition is met:

$$d(U, v) = \emptyset \quad \forall v \in (U^* - U). \tag{3}$$

It does not follow from property 5 of definition 2 and should be somehow imposed on the division in question.

Example 7. For the Thomas division, the completion U^* of the set U was described in example 5: it is formed by monomials v for which there exists a monomial $u \in U$ such that $\partial_i u \leqslant \partial_i v \leqslant r_i$.

The criterion of emptiness for $d(U, v)$ is indicated at the end of example 3: $d(U, v)$ is empty if and only if $\partial_i w = \min(\partial_i v, r_i)$ specifies an element w that is not in U. For $v \in U^*$ this equality reduces to the trivial $\partial_i w = \partial_i v$, that is, $w = v$. By hypothesis, $v \notin U$, so $d(U, v)$ is empty.

7. Discussion

As easily seen, all the basic concepts are introduced for arbitrary monoids. The sufficient criterion for completeness (theorem 4) is proved for monoids generated by a finite set, and the algorithm for successive completion of a set only for a set of monomials. Moreover, axiom 5 of definition 2 of division appears only in the last section and, by and large, it is lacking in the proof of the correctness of the completion algorithm. Possibly, this part of the definition of division could be slightly corrected.

This axiom is the only one that suggests changing the domain. In fact, all the results presented, except for theorem 5, are satisfied for a fixed U, that is, the function d is considered as a function of one argument. Division is not a good functor from Set M to Set M. Many questions here seem to be unclear. The focus was on the completion of a set, but not the uniqueness of such a completion. Moreover, there can be obviously sets enclosed between a complete set and its cone, 'overfull' sets. They hamper proving theorem 5, but what is their true role in division theory?

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Об инволютивном делении на моноидах

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Рассматривается произвольный моноид M, на котором введено инволютивное деление, и множество всех его конечных подмножеств $\operatorname{Set} M$. Деление рассматривается как отображение $d : \operatorname{Set} M \times M$, образ которого $d(U, m)$ — множество делителей m в U. Свойства деления и инволютивного деления задаются аксиоматически. Понятия инволютивного деления введено в соответствии с определением инволютивного мономиального деления, введённым В. П. Гердтом и Ю. А. Блинковым. Предложен ряд новых обозначений, позволяющих коротко, но явно учитывать зависимость деления от элемента $\operatorname{Set} M$. Теория инволютивного пополнения (замыкания) множеств изложена для произвольных моноидов, необходимые и достаточные условия полноты (замкнутости) — для моноидов, порождённых конечным множеством X. Подчёркнута аналогия между этой теорией и теорией вполне непрерывных операторов. В последнем разделе обсуждена возможность решения задачи о пополнении заданного множества путём последовательного расширения исходной области и её связь с аксиомами, используемыми в определении деления. Все результаты проиллюстрированы примерами о мономиальном делении Томаса.

Ключевые слова: инволютивное мономиальное деление, базис Грёбнера