Research Article

Discrete Vector Models for Catalysis and Autocatalysis

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Based on Ruch's concept of diagram lattices formed by Young diagrams we investigated the possibility to transform incomparable diagrams into comparable ones by means of vector catalysis. Ruch's diagram lattices allow a very general description of comparing frequency distributions by their mixing-character as an order relation which is equivalent to majorisation in the mathematical theory of inequalities. Dealing with Young diagrams or vectors containing only integer components, respectively, vector catalysis is strongly related to entanglement catalysis in quantum informatics. In a very systematic way the diagram lattices of the partitions up to the number $n = 20$ have been searched for incomparable pairs which can be catalysed. This concept opens the opportunity for regarding vector catalysis as a universal phenomenon which is not restricted to the quantum mechanical idea of entanglement catalysis. Such a general approach offers the possibility to compare vector catalysis with chemical ideas of catalysis and autocatalysis in a very fundamental sense. We emphasize that vector catalysis is a universally valid procedure for classification purposes, where incomparable sequences of symbols are transformed into comparable ones in a much higher dimensional space ignoring any physical interpretation of these symbols.

1. Introduction

Catalysis is very old but still an unsolved problem in chemistry and biochemistry, although there exist a lot of experimental and theoretical publications on this topic. The term *catalysis* was introduced 1835/36 into chemistry by Berzelius [1] to describe the ability of substances *to awake affinities, which are asleep at a particular temperature, by their mere presence and not by their own affinity (the catalytic power seems actually to consist in the fact that substances are able to*

awake affinities, which are asleep at a particular temperature, by their mere presence and not by their own affinity). In other words, reactions which do not occur on their own or spontaneously take place only at the presence of an additional substance—the so-called *catalyst*. It took about hundred years to develop the almost generally accepted idea of catalysis. Now, this classical definition of catalysis is given by Ostwald in 1894 on the basis of the theory of chemical reaction rate [2–4]; *catalysis is the acceleration of a slowly preceding chemical reaction through the presence of a foreign substance, which may participate intermediately but is not consumed by the reaction*.

Abel (85th Meeting of German Natural and Medical Scientists, Vienna 1913) claimed in a much more abstract and modern way that only reactions, but no substances are catalysing and that there do not exist catalysts in general, "the speaker comes to the conclusion that according to the general view of current research on homogeneous catalysis one can clearly deduce *not substances, but only reactions are catalysing* . . . . Since only reactions, but not substances are catalysing it is strange that in the presence of several catalysts they do not act additively, even though the catalysing reaction paths can be well interleaved . . . . *Catalysis emerges in case of chemical activity of the catalyst by extension of the reaction path and in case of physical interference of the catalyst by shifting of the reaction level*" [5].

Most of the theoretical works on chemical catalysis deal with numerical quantum-chemical treatment on the molecular level. Nonlinear dynamics based on the ideas of Prigogine [6, 7] and Haken [8, 9] favoured the old idea of autocatalysis in order to describe macroscopic pattern formation in chemical systems. In heterogeneous catalysis, enormous scientific effort has been made in order to close the gap between high vacuum investigations on molecular processes on surfaces [10–12] on the one hand and the technical level of catalysis at normal and high pressure [13–15] on the other hand. Although the atomic structure of elementary steps in the catalytic formation of NH_3 [16–20] or the oxidation of CO on single crystal surfaces in vacuum meanwhile has been figured out in great detail [21–27], there still remains an unavoidable gap. Furthermore, there exists another question which rises from the assumption of the existence of a catalytic centre (catalytic sites) which is created by separation from its surrounding. There are a lot of fancy descriptions like "spill over effects" in heterogeneous catalysis or "steric effects" in enzyme catalysis, which are connected with this artificial separation [28].

It is somehow a miracle that one needs large molecular systems like enzymes or haemoglobin in order to catalyse very small molecules. In heterogeneous catalysis, one needs surfaces or large clusters to catalyse small molecular systems. However, if the system to be catalysed is of medium size, one only needs catalysts of medium sizes to arrange the reaction.

In recent years, the term catalysis was introduced in quite another field than chemistry, that is, in the mathematics of quantum information theory [29]. Starting point was the observation that entangled quantum states can be transformed with certainty into each other by local transformations, if the distribution of ordered Schmidt coefficients of one state is majorising the corresponding distribution of the other state [30]. This connects entanglement with the linear algebraic theory of majorisation [31–33]. As a consequence, entangled quantum states cannot be transformed with certainty, if their distributions of Schmidt coefficients are incomparable in terms of majorisation. But in some special cases, there exists an additional entangled quantum state that enhances the local transformation of two incomparable quantum states without changing itself at the end [29]. This additional state is called *catalyst* in analogy

to chemistry and the corresponding transformation of quantum states as *entanglement catalysis*. Although some progress was made in the last few years for special types of incomparable states and catalysts, the problem of entanglement catalysis is far away from being well understood [34–41].

On the first view, catalysis in chemistry and entanglement catalysis have nothing in common. But besides the name there are even more aspects related to catalysis which suggest a connection between both fields, that is, the application of quantum logic [42, 43] and majorisation theory [31]. For this reason, we are strongly convinced that entanglement catalysis and catalysis are much more general phenomena than considered until now.

The idea of majorisation was adopted to chemistry for the first time when Ruch together with Schönhofer introduced a *greater* relation for *Young diagrams* [44–47] in order to answer questions in connection with the theory of chirality functions. Later on, Ruch generalised this concept in his articles *on diagram lattices as structural principle* [48], on *the principles of increasing mixing* [49] and on *information extent, and information distance* [50]. These powerful ideas have been applied recently to rank biodiversity indices for the comparison of water quality of lakes [51].

Taking into account the concepts of Ruch, we investigated in our previous articles the decay of beer foam and its bubble size distributions as well as—more generally—diffusion processes by diagram lattices and variants of majorisation using discrete partition vectors [52–55]. More precisely, the foam decay is described by a bubble size distribution function and its variation in time. As a consequence, we consider distribution functions which are transformed into each other. Assuming that any distribution function describes a snapshot of a certain situation or "state" during foam decay, these states are compared by majorisation. Depending on the kind of beer and the conditions of decay, we observe transitions between incomparable distributions, which are not yet fully understood. It seems that we have similar phenomena than those observed in quantum informatics.

In this paper, we will extend our previous approaches to *discrete vector catalysis*, that is, we investigate the question under which circumstances two discrete (distribution or state) vectors containing only integer components, which are incomparable in terms of majorisation, can be made comparable by a third discrete state vector of integer components, which we call *catalyst vector*. This corresponds in a discrete formulation to the problem in quantum informatics of enabling a certain transformation of two quantum states by a third quantum state which cannot be done without this latter state.

We are convinced that the results can be transferred uniquely to entanglement catalysis in quantum informatics. Recall that the Schmidt coefficients of the orthonormal bases of the entangled quantum states are distributions of nonnegative real numbers that can be arranged as ordered vectors summing up to one. On the other hand, in all numeric examples of normalised distributions or—equivalently—proportions with sum "1" the space of real numbers $\mathbb{R}$ is projected onto the space of rational numbers $\mathbb{Q}$. Furthermore, since the sets of rational numbers $\mathbb{Q}$ and of nonnegative integers $\mathbb{N}^0$ are of the same cardinality, all results obtained for discrete vector catalysis by comparing vectors with nonnegative integer numbers should analogously be valid for entanglement catalysis. It is therefore our aim to treat the problem of catalytic majorisation on this simplest possible system and to show some fundamental aspects of discrete vector catalysis.

2. Mathematical background

2.1. Partition lattices and incomparable pairs of partitions

Using discrete mathematical model state vectors can be described in terms of partition diagrams. Let $u_1 + u_2 + \cdots + u_d = n$ with $d \leq n$ and $u_i \geq u_{i+1}$ for $i = 1, 2, \ldots, d - 1$ a partition of natural number n with d positive integers. It can be represented graphically by a partition diagram or *Young diagram* [45–47] consisting of n boxes, arranged in rows and columns in such a way that the ith row has u_i boxes and the first box in each row lies in the first column. For example, the partition "$3 + 2 + 1$" of $n = 6$ is represented by the *Young diagram*.

$$(2.1)$$

If one introduces a greater relation in the sense of majorisation [31], the set of partitions of a natural number n forms a lattice, the so-called diagram lattice ([48, 52], see Figure 1 for $n = 6$).

Ruch formulated this greater relation with respect to *Young diagrams* as follows. *A diagram γ is called greater than a diagram γ', if γ' can be constructed from γ by moving boxes upward, that is, from shorter rows into longer or equal ones* [48]. Starting from this definition, he summarised in his fundamental article about the diagram lattice as a structural principle all lattices up to $n = 10$. With regard to the following investigation we like to emphasise that diagram lattices of $n \geq 6$ are partially ordered, that is, they exhibit pairs of diagrams which are not comparable in sense of majorisation by the partial order of the lattice (see Figure 1(a)).

Each of the partition diagrams can also be expressed by a (column) vector $\mathbf{u}$ with trace n,

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_d \end{pmatrix}, \qquad \mathrm{tr}(\mathbf{u}) = \sum_{j=1}^{d} u_j = n \tag{2.2}$$

containing d nonzero components which are ordered in decreasing (nonincreasing) sequences (see Figure 1(b)). For comparison of different partitions, partition vectors are filled with additional zeros up to totally n components such that the numbers of components in a vector pair are equal.

In the terminology of (classical) majorisation [31], a partition vector $\mathbf{u}$ is said to be majorised by a partition vector $\mathbf{v}$, denoted $\mathbf{u} \prec \mathbf{v}$, if (i) the partial sums $\mathbf{o}_{\mathbf{u},i}$ of $\mathbf{u}$ are less or equal to the partial sums $\mathbf{o}_{\mathbf{v},i}$ of $\mathbf{v}$ for all $i = 1, \ldots, n - 1$ and (ii) both the sums of components of $\mathbf{u}$ and $\mathbf{v}$ are equal to n (see (2.3)), which is the natural number of the diagram or partition lattice,

$$\mathbf{u} \prec \mathbf{v} \quad \text{if} \begin{cases} (\text{i}) \left(\mathbf{o}_{\mathbf{u},i} = \sum_{j=1}^{i} u_j \right) \leq \left(\mathbf{o}_{\mathbf{v},i} = \sum_{j=1}^{i} v_j \right), \quad i = 1, \ldots, n - 1, \\[3mm] (\text{ii}) \left(\mathbf{o}_{\mathbf{u},n} = \sum_{j=1}^{n} u_j \right) = \left(\mathbf{o}_{\mathbf{v},n} = \sum_{j=1}^{n} v_j \right) = n. \end{cases} \tag{2.3}$$
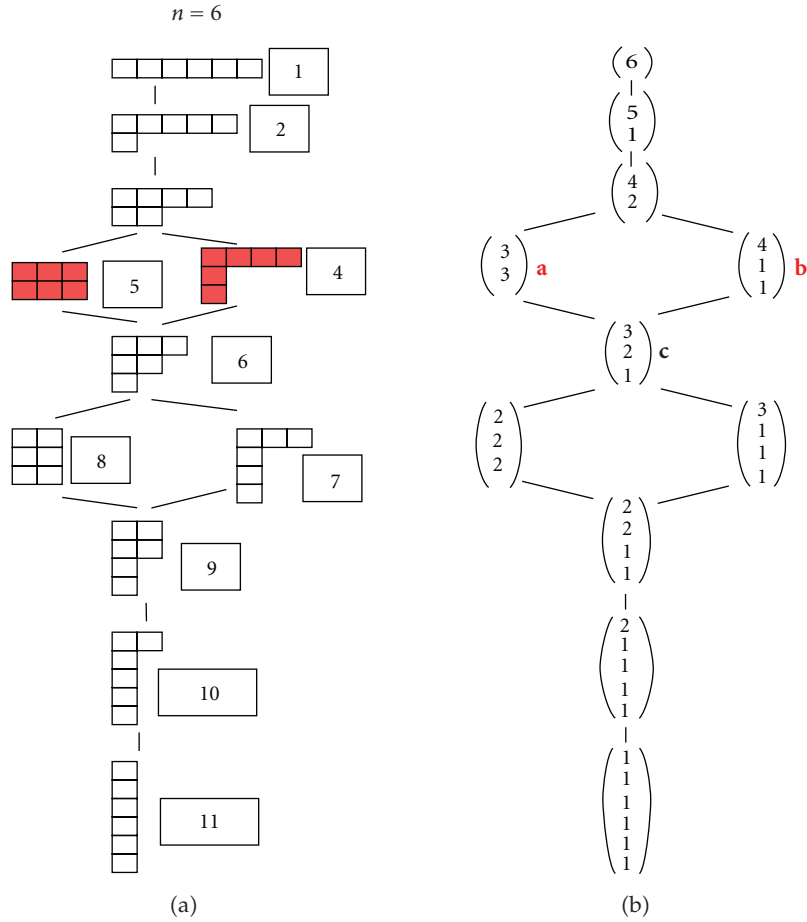
Figure 1: (a) Ruch's lattice of the partition diagrams of the natural number $n = 6$ with 11 diagrams; (b) corresponding lattice of partition vectors. The diagrams no. 4 and 5 and partition vectors **a** and **b** which are marked in magenta show examples for incomparable structures.

If condition (i) of (2.3) does not hold, the vectors **u** and **v** are said to be incomparable, denoted by $(\mathbf{u} \nsucc \mathbf{v}) \wedge (\mathbf{u} \nprec \mathbf{v})$, abbreviated $\mathbf{u} \ntrianglelefteq \mathbf{v}$ (see also Table 7). As an example of an incomparable vector pair in the sense of majorisation we consider diagrams no. 5 and no. 4, or partition vectors **a** and **b** of Figure 1. The discrete distribution function of the components of **a** and **b** is shown in Figure 2. Forming the vectors of the partial sums $\mathbf{o_a}$ and $\mathbf{o_b}$, respectively, one can easily show that $\mathbf{a} \ntrianglelefteq \mathbf{b}$, that is, there exists a component j, where $\mathbf{o}_{\mathbf{a},j} < \mathbf{o}_{\mathbf{b},j}$, and another component j' with $\mathbf{o}_{\mathbf{a},j'} > \mathbf{o}_{\mathbf{b},j'}$,

$$\mathbf{o_a} = \begin{pmatrix} 3 \\ 6 \\ 6 \end{pmatrix}, \quad \mathbf{o_b} = \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix}, \quad \begin{array}{l} 3 < 4, \quad j = 1, \\ 6 > 5, \quad j' = 2, \quad \mathbf{a} \ntrianglelefteq \mathbf{b}. \\ 6 = 6, \end{array} \tag{2.4}$$

If one of the partition vectors **u** and **v** is majorising the other, there exists always a doubly stochastic matrix [53] which transforms the vector **u** into **v** or vice versa. In a physical interpretation, the vectors **u** and **v** may be any probability vectors or states and the doubly stochastic matrix describes the transition between these states. On the other hand, if **u** and **v** are incomparable, such as **a** and **b** in the example above ($\mathbf{a} \ntrianglelefteq \mathbf{b}$, see Figure 2), it follows that

$a = (3\ 3\ 0)$
$b = (4\ 1\ 1)$
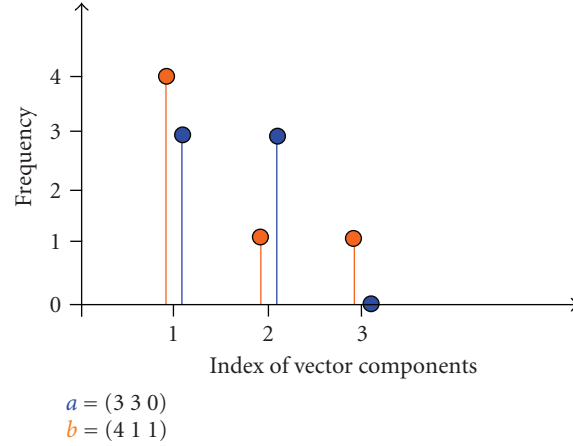
Figure 2: The components of the two vectors **a** (blue) and **b** (red) of Figure 1 as a discrete function of the corresponding row numbers. Both distribution (probability) functions are incomparable.

there does not exist a doubly stochastic matrix [53] which transforms the vectors into each other, that is, there is no transition between both states.

2.2. Introduction of catalyst partition vector

However, one may ask if there exists another vector **c** (see, e.g., Figure 1(b)) which enables the vectors **a** and **b** to be transformed into each other, that is, to become comparable. This question is usually answered by comparing the nonincreasingly ordered set of elements of the tensor products of the vectors **a** and **b** with the transpose $\mathbf{c}^T$ a third vector **c**, respectively. The tensor product of two vectors is a rectangular matrix, where each component of the first vector is multiplied with each component of the second one. Arranging the elements of these matrices in a list with decreasing (nonincreasing) order one gets ordered vectors $\boldsymbol{\theta}_{\mathbf{b}\otimes\mathbf{c}}$ and $\boldsymbol{\theta}_{\mathbf{a}\otimes\mathbf{c}}$ of the same dimension as of the rectangular matrix which can now be investigated with respect to their comparability. For this purpose, one has to form the vectors $\mathbf{o}_{\mathbf{b}\otimes\mathbf{c}}$ and $\mathbf{o}_{\mathbf{a}\otimes\mathbf{c}}$ of the partial sums of the components of the new vectors $\boldsymbol{\theta}_{\mathbf{b}\otimes\mathbf{c}}$ and $\boldsymbol{\theta}_{\mathbf{a}\otimes\mathbf{c}}$,

$$\mathbf{b}\otimes\mathbf{c}^T = \begin{pmatrix} 4 \\ 1 \\ 1 \end{pmatrix}\otimes\begin{pmatrix} 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 12 & 8 & 4 \\ 3 & 2 & 1 \\ 3 & 2 & 1 \end{pmatrix} \Longrightarrow \boldsymbol{\theta}_{\mathbf{b}\otimes\mathbf{c}}^T = (\ 12\ 8\ 4\ 3\ 3\ 2\ 2\ 1\ 1\ ),$$

$$\mathbf{a}\otimes\mathbf{c}^T = \begin{pmatrix} 3 \\ 3 \\ 0 \end{pmatrix}\otimes\begin{pmatrix} 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 9 & 6 & 3 \\ 9 & 6 & 3 \\ 0 & 0 & 0 \end{pmatrix} \Longrightarrow \boldsymbol{\theta}_{\mathbf{a}\otimes\mathbf{c}}^T = (\ 9\ 9\ 6\ 6\ 3\ 3\ 0\ 0\ 0\ ),$$

$$\mathbf{o}_{\mathbf{b}\otimes\mathbf{c}}^T = (\ 12\ 20\ 24\ 27\ 30\ 32\ 34\ 35\ 36\ ),$$

$$\mathbf{o}_{\mathbf{a}\otimes\mathbf{c}}^T = (\ 9\ 18\ 24\ 30\ 33\ 36\ 36\ 36\ 36\ ),$$

$$\mathbf{o}_{\mathbf{b}\otimes\mathbf{c}}^T - \mathbf{o}_{\mathbf{a}\otimes\mathbf{c}}^T = (\ +3\ +2\ 0\ -3\ -3\ -4\ -2\ -1\ 0\ ).$$

(2.5)

If there is a change of the signs of the components in the difference vector $\mathbf{o}_{\mathbf{b}\otimes\mathbf{c}} - \mathbf{o}_{\mathbf{a}\otimes\mathbf{c}}$ (as shown for the actual choice of **a**, **b**, and **c**), the new tensor vectors $\boldsymbol{\theta}_{\mathbf{a}\otimes\mathbf{c}}$ and $\boldsymbol{\theta}_{\mathbf{b}\otimes\mathbf{c}}$ still remain incomparable. In other words, the elements of the difference vector have to be semidefinite.

Difference of partial sums of ordered tensor product vectors
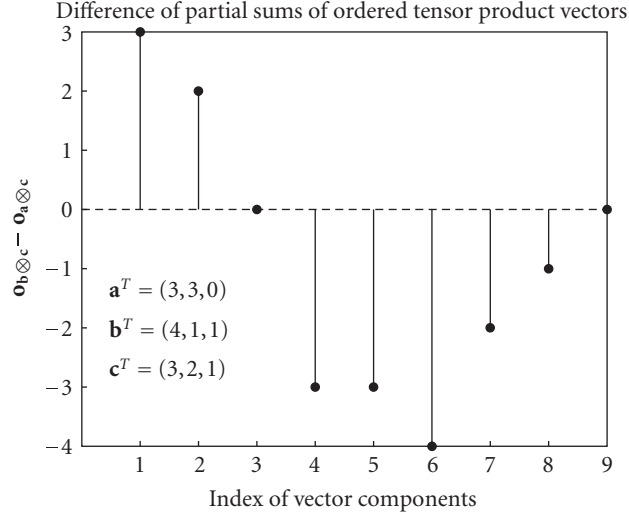
Figure 3: The components of the difference vector $\mathbf{o}_{\mathbf{b}\otimes\mathbf{c}} - \mathbf{o}_{\mathbf{a}\otimes\mathbf{c}}$ as a discrete function of the position count of the vector components.

To illustrate the property of incomparableness graphically, in Figure 3 the difference $\mathbf{o}_{\mathbf{b}\otimes\mathbf{c}} - \mathbf{o}_{\mathbf{a}\otimes\mathbf{c}}$ is shown as a discrete function of the position count of vector components. The existence of negative deviations from the zero line indicates that the compared partition vectors are incomparable.

But there exist pairs of incomparable vectors which can be catalysed by a third vector, such that the resulting tensor vectors are comparable. One of the simplest examples is given in the following.

Consider the pair of vectors

$$\mathbf{d} = \begin{pmatrix} 5 \\ 4 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \qquad \mathbf{e} = \begin{pmatrix} 6 \\ 2 \\ 2 \\ 2 \\ 0 \end{pmatrix} \tag{2.6}$$

of the partition lattice with $n = 12$. These partition vectors are obviously incomparable, $\mathbf{d} \not\gtrless \mathbf{e}$, but can be catalysed by a third vector
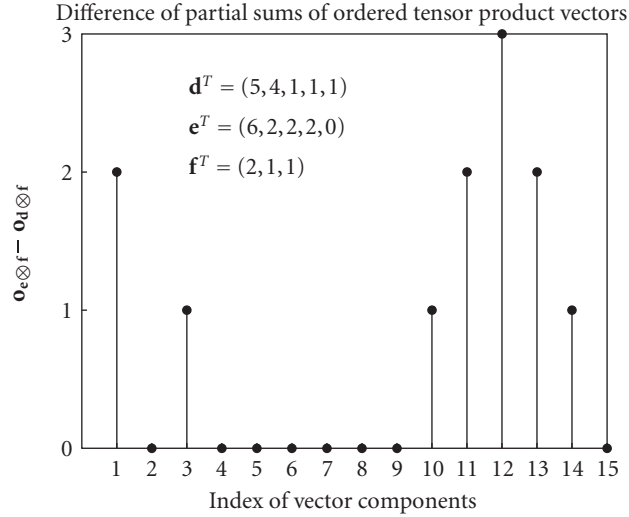
$$\mathbf{f}^T = (\, 2 \ \ 1 \ \ 1 \,). \tag{2.7}$$

Calculating the tensor products $\mathbf{d} \otimes \mathbf{f}^T$ and $\mathbf{e} \otimes \mathbf{f}^T$, and ordering their components in decreasing sequence, respectively, one obtains the following tensor vectors $\boldsymbol{\theta}_{\mathbf{e}\otimes\mathbf{f}}$ and $\boldsymbol{\theta}_{\mathbf{d}\otimes\mathbf{f}}$,

$$\begin{aligned} \boldsymbol{\theta}_{\mathbf{e}\otimes\mathbf{f}}^T &= (\, 12 \ \ 6 \ \ 6 \ \ 4 \ \ 4 \ \ 4 \ \ 2 \ \ 2 \ \ 2 \ \ 2 \ \ 2 \ \ 2 \ \ 0 \ \ 0 \ \ 0 \,), \\ \boldsymbol{\theta}_{\mathbf{d}\otimes\mathbf{f}}^T &= (\, 10 \ \ 8 \ \ 5 \ \ 5 \ \ 4 \ \ 4 \ \ 2 \ \ 2 \ \ 2 \ \ 1 \ \ 1 \ \ 1 \ \ 1 \ \ 1 \,). \end{aligned} \tag{2.8}$$

Constructing their partial sums $\mathbf{o}_{\mathbf{e}\otimes\mathbf{f}}$ and $\mathbf{o}_{\mathbf{d}\otimes\mathbf{f}}$, and building the difference $\mathbf{o}_{\mathbf{e}\otimes\mathbf{f}} - \mathbf{o}_{\mathbf{d}\otimes\mathbf{f}}$ yields,

$$\begin{aligned} \mathbf{o}_{\mathbf{e}\otimes\mathbf{f}}^T &= (\, 12 \ \ 18 \ \ 24 \ \ 28 \ \ 32 \ \ 36 \ \ 38 \ \ 40 \ \ 42 \ \ 44 \ \ 46 \ \ 48 \ \ 48 \ \ 48 \ \ 48 \,), \\ \mathbf{o}_{\mathbf{d}\otimes\mathbf{f}}^T &= (\, 10 \ \ 18 \ \ 23 \ \ 28 \ \ 32 \ \ 36 \ \ 38 \ \ 40 \ \ 42 \ \ 43 \ \ 44 \ \ 45 \ \ 46 \ \ 47 \ \ 48 \,), \\ \mathbf{o}_{\mathbf{e}\otimes\mathbf{f}}^T - \mathbf{o}_{\mathbf{d}\otimes\mathbf{f}}^T &= (\, +2 \ \ 0 \ \ +1 \ \ 0 \ \ 0 \ \ 0 \ \ 0 \ \ 0 \ \ +1 \ \ +2 \ \ +3 \ \ +2 \ \ +1 \ \ 0 \,). \end{aligned} \tag{2.9}$$

Difference of partial sums of ordered tensor product vectors

Figure 4: The components of the difference vector $\mathbf{o}_{\mathbf{e} \otimes \mathbf{f}} - \mathbf{o}_{\mathbf{d} \otimes \mathbf{f}}$ as a discrete function of the position count of the vector components.

If one draws the difference $\mathbf{o}_{\mathbf{e} \otimes \mathbf{f}} - \mathbf{o}_{\mathbf{d} \otimes \mathbf{f}}$ as a discrete function over the position numbers of the vector components, one obtains the graph represented in Figure 4, which is touching but not crossing the abscissa. This indicates that the corresponding pair of ordered tensor product vectors is comparable in the sense of majorisation.

The catalyst vector $\mathbf{f}$ is the minimum partition vector catalysing the incomparable pair of vectors $\mathbf{d}$ and $\mathbf{e}$, that means it is the partition with the smallest natural number n which is the trace of the vector catalyst. In addition to this catalyst vector one can find an infinite number of catalysing partitions for this couple of vectors (and also for any other pair of vectors which can be catalysed), for example, (4 2 2), (6 3 3), and so on.

3. Results and discussion

In the following, we present a systematic approach to discrete vector catalysis by considering vectors of integer components with sum (trace) n which can be correlated to partition diagrams of n boxes forming the diagram lattice according to Ruch [48]. For this purpose, we have written a computer program in C++, which calculates all incomparable pairs of partition vectors which occur in partition lattices up to $n = 20$. Also, we computed for any catalysable couple of partition vectors the list of all catalyst vectors which can be found in partition lattices up to $n = 20$. In addition, we determined some more catalysts of partition lattices with $n > 20$ using the functional language *Haskell* and an empirical method. The notation being used is summarised in Tables 7 and 8.

3.1. Minimal global properties of discrete vector catalysis

Concerning minimal global properties of discrete vector catalysis, one may ask the following questions, the answers of which are listed in Table 1.

(a) What is the minimal component sum (trace) n, for which one can find an incomparable pair $\mathbf{u}$ and $\mathbf{v}$ of partition vectors which can be catalysed?

Table 1: Incomparable, catalysable pairs of partition vectors and their corresponding catalyst partition vectors with distinguished minimal global properties of discrete vector catalysis. The significant minimal global properties are marked in bold italic letters.

	n	m	$n \cdot m$	$d_{\mathbf{u},\mathbf{v}}$	$d_{\mathbf{c}}$	$d_{\mathbf{u},\mathbf{v}} \cdot d_{\mathbf{c}}$	Incomparable, catalysable pair of partition vectors		Catalyst partition vector
							$\mathbf{u}^T$	$\mathbf{v}^T$	$\mathbf{c}^T$
(a)	**11**	42	482	5	9	45	$(4, 4, 1, 1, 1)$	$(5, 2, 2, 2, 0)$	$(10, 6, 5, 5, 4, 3, 3, 3, 3)$
(b)	12	410	4 920	**4**	38	152	$(5, 5, 1, 1)$	$(6, 3, 3, 0)$	$(36, 24, 20, 20, 16, 16, 15, 15, 12, 12, 12, 12, 10, 10, 10, 10, 9, 9, 9, 9, 8, 8, 8, 8, 8, 8, 8, 6, 6, 6, 6, 6, 6, 6, 6, 6)^*$
(c)	14	**3**	42	4	**2**	8	$(6, 6, 1, 1)$	$(8, 3, 3, 0)$	$(2, 1)$
(d)	14	3	**42**	4	2	8	$(6, 6, 1, 1)$	$(8, 3, 3, 0)$	$(2, 1)$

* Catalyst partition vector may not be minimal.

> (b) What is the minimal dimension $d_{\mathbf{u},\mathbf{v}}$ of an incomparable pair of partition vectors $\mathbf{u}$ and $\mathbf{v}$ which can be catalysed and the natural number n of its first occurrence?
>
> (c) What is the smallest catalyst partition vector $\mathbf{c}$ and its corresponding pair of incomparable partition vectors $\mathbf{u}$ and $\mathbf{v}$?
>
> (d) What are the smallest balanced combinations consisting of a catalysable pair of incomparable partition vectors $\mathbf{u}$ and $\mathbf{v}$ and its smallest catalyst $\mathbf{c}$, that is, where either $(n \cdot m)$ or $(d_{\mathbf{u},\mathbf{v}} \cdot d_{\mathbf{c}})$ is minimal?

Answering question, (a) follows that the smallest number n for which one can find an incomparable but catalysable vector pair is $n = 11$, and the corresponding partition vectors are $\mathbf{u}^T = (4, 4, 1, 1, 1)$ and $\mathbf{v}^T = (5, 2, 2, 2, 0)$, respectively. Thus, the first diagram or partition lattice with the possibility of vector catalysis is that of 11 boxes. The minimal catalyst vector of the smallest catalysable pair is $\mathbf{c}^T = (10, 6, 5, 5, 4, 3, 3, 3, 3)$, which belongs to a lattice of the integer $m = 42$. As a consequence, both the dimension $d_{\mathbf{u},\mathbf{v}} \cdot d_{\mathbf{c}}$ and the trace (no. of boxes) $n \cdot m$ of the resulting tensor product space in which vector catalysis occurs are rather high. This corresponds to the observation in chemistry that small molecules are often catalysed by large catalysts.

This analogy turns out even stronger, if one considers—as in question (b)—the tensor product space of the *first* occurrence of an incomparable but catalysable pair $\mathbf{u}$ and $\mathbf{v}$ of smallest dimension $d_{\mathbf{u},\mathbf{v}}$. Jonathan and Plenio have already proven in their fundamental article on entanglement catalysis [29] that incomparable states with less than four components cannot be catalysed, hence the minimal dimension of catalysable pairs of partition vectors is $d_{\mathbf{u},\mathbf{v}} = 4$. The first such a pair is $\mathbf{u}^T = (5, 5, 1, 1)$ and $\mathbf{v}^T = (6, 3, 3, 0)$ with $n = 12$. It can be catalysed, but the smallest catalyst which we found by extended calculations contains $d_{\mathbf{c}} = 38$ components and has a trace of $m = 410$ (see Table 1) yielding a tensor product space with $d_{\mathbf{u},\mathbf{v}} \cdot d_{\mathbf{c}} = 152$ and $n \cdot m = 4\,920$. Such a highly dimensional space of vector catalysis may possibly be related to enzyme catalysis in chemistry or biochemistry.

On the other hand, the answers to questions (c) and (d), that is, to the smallest catalyst partition vector $\mathbf{c}$ and to the smallest balanced combinations of $\mathbf{u}/\mathbf{v}$ and $\mathbf{c}$ lead to a tensor product space of comparatively low dimensionality ($d_{\mathbf{u},\mathbf{v}} \cdot d_{\mathbf{c}} = 8$, $n \cdot m = 42$). This result

Table 2: Incomparable pairs of partition vectors which may be catalysable from partition lattices up to $n = 13$ and corresponding catalyst partition vectors.

n	$d_{\mathbf{u,v}}$	$\mathbf{u}^T$	$\mathbf{v}^T$	m	$d_{\mathbf{c}}$	$\mathbf{c}^T$	$N_{\mathbf{c},20}$
11	5	(4, 4, 1, 1, 1)	(5, 2, 2, 2, 0)	42	9	(10, 6, 5, 5, 4, 3, 3, 3, 3)	0
12	4	(5, 5, 1, 1)	(6, 3, 3, 0)	410	38	(36, 24, 20, 20, 16, 16, 15, 15, 12, 12, 12, 12, 10, 10, 10, 10, 9, 9, 9, 9, 8, 8, 8, 8, 8, 8, 8, 6, 6, 6, 6, 6, 6, 6, 6, 6, 6)*	0
12	5	(5, 4, 1, 1, 1)	(6, 2, 2, 2, 0)	4	3	(2, 1, 1)	87
12	6	(4, 4, 1, 1, 1, 1)	(5, 2, 2, 2, 1, 0)	42	9	(10, 6, 5, 5, 4, 3, 3, 3, 3)	0
12	6	(3, 3, 3, 1, 1, 1)	(4, 2, 2, 2, 2, 0)	37	5	(12, 8, 7, 5, 5)*	0
13	4	(6, 5, 1, 1)	(7, 3, 3, 0)	31	6	(10, 6, 5, 4, 3, 3)*	0
13	5	(6, 4, 1, 1, 1)	(7, 2, 2, 2, 0)	4	3	(2, 1, 1)	120
13	5	(5, 5, 1, 1, 1)	(7, 2, 2, 2, 0)	4	3	(2, 1, 1)	229
13	5	(5, 5, 1, 1, 1)	(6, 3, 3, 1, 0)	410	38	(36, 24, 20, 20, 16, 16, 15, 15, 12, 12, 12, 12, 10, 10, 10, 10, 9, 9, 9, 9, 8, 8, 8, 8, 8, 8, 8, 6, 6, 6, 6, 6, 6, 6, 6, 6, 6)*	0
13	5	(5, 5, 1, 1, 1)	(6, 3, 2, 2, 0)	?**	?**	?**	?**
13	6	(5, 4, 1, 1, 1, 1)	(6, 2, 2, 2, 1, 0)	4	3	(2, 1, 1)	87
13	6	(4, 4, 2, 1, 1, 1)	(5, 2, 2, 2, 2, 0)	42	9	(10, 6, 5, 5, 4, 3, 3, 3, 3)	0
13	7	(4, 4, 1, 1, 1, 1, 1)	(5, 2, 2, 2, 2, 0, 0)	16	4	(6, 4, 3, 3)	9
13	6	(4, 3, 3, 1, 1, 1)	(5, 2, 2, 2, 2, 0)	4	3	(2, 1, 1)	134
13	7	(4, 4, 1, 1, 1, 1, 1)	(5, 2, 2, 2, 1, 1, 0)	42	9	(10, 6, 5, 5, 4, 3, 3, 3, 3)	0
13	7	(3, 3, 3, 1, 1, 1, 1)	(4, 2, 2, 2, 2, 1, 0)	37	5	(12, 8, 7, 5, 5)*	0

*Catalyst partition vector may not be minimal for the respective pair.
**A catalyst could not yet be found by our investigations. We assume that a catalyst vector for this pair does not exist.

corresponds in chemistry particularly to homogeneous catalysis of medium-sized molecules by medium-sized catalysts.

3.2. Incomparable vector pairs and necessary conditions for vector catalysis

Table 2 summarises all incomparable pairs $\mathbf{u}$ and $\mathbf{v}$ of partition lattices up to $n = 13$ which may be catalysable together with a (minimal) catalyst partition vector $\mathbf{c}$, if such was found by systematic calculation or empirical investigation. Also, the number of incomparable pairs—denoted by $N_{\mathbf{c},20}$—which are catalysed by a catalyst partition vector of a partition lattice with $n \leq 20$ is given in Table 2.

In the case of partition lattices with $n \leq 10$ no incomparable pair exists which can be catalysed, as will be shown in the following.

An important question is now under which circumstances two incomparable pairs of a partition lattice with natural number n can be catalysed by a third partition vector. A necessary condition was given by Jonathan and Plenio [29] which can be expressed using the terminology of discrete partition vectors as follows.

Let $\mathbf{u}^T = (\ u_1\ u_2\ \cdots\ u_i\ \cdots\ u_{d_{\mathbf{u},\mathbf{v}}}\ )$ and $\mathbf{v}^T = (\ v_1\ v_2\ \cdots\ v_i\ \cdots\ v_{d_{\mathbf{u},\mathbf{v}}}\ )$ a pair of incomparable partition vectors of length $d_{\mathbf{u},\mathbf{v}}$, then this pair can be catalysed be a third (catalytic) partition vector only if both

$$u_1 \leq v_1, \qquad u_{d_{\mathbf{u},\mathbf{v}}} \geq v_{d_{\mathbf{u},\mathbf{v}}} \tag{3.1}$$

hold. If one can find such a catalyst vector, denoted by $\mathbf{c}^T = (\ c_1\ c_2\ \cdots\ c_{d_c}\ )$, the resulting ordered tensor product $\mathbf{v} \otimes \mathbf{c}^T$ majorises the ordered tensor product $\mathbf{u} \otimes \mathbf{c}^T$. Accordingly, in the interpretation of quantum information theory the corresponding entangled quantum states can be transformed with *entanglement-assisted local transformation and classical communication* (ELQCC) [29]. As mentioned above, Jonathan and Plenio have also shown that incomparable partitions of dimension $d_{\mathbf{u},\mathbf{v}} < 4$ cannot be catalysed [29].

In the following, we suggest a stronger necessary condition for vector catalysis which is based on the concept of majorisation.

Proposition 3.1. *A pair of incomparable partition vectors of dimension $d_{\mathbf{u},\mathbf{v}}$ ($d_{\mathbf{u},\mathbf{v}} \geq 4$) can be catalysed only if there exist two indices i_1 and i_2 with $1 < i_1 < i_2 < d_{\mathbf{u},\mathbf{v}}$ such that for the partial sums $\mathbf{o}_{\mathbf{u},i}$ and $\mathbf{o}_{\mathbf{v},i}$ holds*

$$
\begin{aligned}
\text{(I)} \quad & \mathbf{o}_{\mathbf{v},i} \geq \mathbf{o}_{\mathbf{u},i} \quad \textit{for } 1 \leq i < i_1, \\
\text{(II)} \quad & \mathbf{o}_{\mathbf{v},i} < \mathbf{o}_{\mathbf{u},i} \quad \textit{for } i = i_1, \\
& \mathbf{o}_{\mathbf{v},i} \leq \mathbf{o}_{\mathbf{u},i} \quad \textit{for } i_1 + 1 \leq i < i_2, \\
\text{(III)} \quad & \mathbf{o}_{\mathbf{v},i} > \mathbf{o}_{\mathbf{u},i} \quad \textit{for } i = i_2, \\
& \mathbf{o}_{\mathbf{v},i} \geq \mathbf{o}_{\mathbf{u},i} \quad \textit{for } i_2 + 1 \leq i \leq d_{\mathbf{u},\mathbf{v}}.
\end{aligned}
\tag{3.2}
$$

In addition, for the $d_{\mathbf{u},\mathbf{v}}$th vector component the majorisation condition

$$\mathbf{o}_{\mathbf{v},i} = \mathbf{o}_{\mathbf{u},i} = n \tag{3.3}$$

is fulfilled.

Although we cannot give yet a strict mathematical proof, our proposition can be confirmed by the following consideration. In the case of the largest partition values, that is, interval (I) in (3.2), one partition vector (**v**) obviously "majorises" the other (**u**). Since the pair is incomparable, there must follow an interval (II) with partition values such that the second partition vector (**u**) "majorises" the first (**v**). Finally, in order to enable majorisation after building the ordered tensor products with a catalyst vector, it seems to be necessary to have a last interval (III) with the smallest partition values, where the first partition vector (**v**) takes over "majorisation" again.

For a pair of incomparable partition vectors **u** and **v** with these properties, we suggest to introduce the notation "$\mathbf{v} \succ\!<\!\succ \mathbf{u}$" or—equivalently—"$\mathbf{u} \prec\!>\!\prec \mathbf{v}$" (see also Table 7).
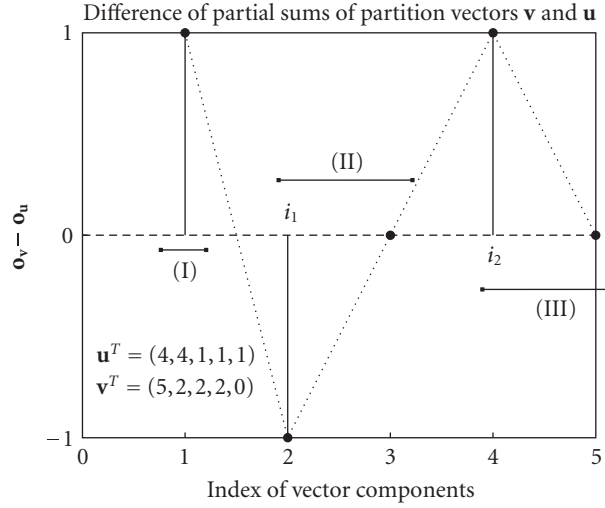
Figure 5: The components of the difference vector $\mathbf{o}_\mathbf{v}^T - \mathbf{o}_\mathbf{u}^T$ of the partial sums of partitions $\mathbf{u}^T = (4, 4, 1, 1, 1)$ and $\mathbf{v}^T = (5, 2, 2, 2, 0)$ as a discrete function of the position count of the vector components.

The condition (3.2) will be illustrated at the example of the incomparable pair $\mathbf{u}^T = (4, 4, 1, 1, 1)$ and $\mathbf{v}^T = (5, 2, 2, 2, 0)$ with $d_{\mathbf{u},\mathbf{v}} = 5$ and $n = 11$. The corresponding partial sums are $\mathbf{o}_\mathbf{u}^T = (4, 8, 9, 10, 11)$ and $\mathbf{o}_\mathbf{v}^T = (5, 7, 9, 11, 11)$. Thus,

$$
\begin{aligned}
(\mathbf{o}_{\mathbf{v},1} = 5) &> (4 = \mathbf{o}_{\mathbf{u},1}), & \text{interval (I)}, \\
(\mathbf{o}_{\mathbf{v},2} = 7) &< (8 = \mathbf{o}_{\mathbf{u},2}), & \text{interval (II)}, \\
(\mathbf{o}_{\mathbf{v},3} = 9) &= (9 = \mathbf{o}_{\mathbf{u},3}), & \text{interval (II)}, \\
(\mathbf{o}_{\mathbf{v},4} = 11) &> (10 = \mathbf{o}_{\mathbf{u},4}), & \text{interval (III)}, \\
(\mathbf{o}_{\mathbf{v},5} = 11) &= (11 = \mathbf{o}_{\mathbf{u},5}), & \text{interval (III)},
\end{aligned}
\tag{3.4}
$$

and hence $i_1 = 2$ and $i_2 = 4$.

A graphical representation of the resulting difference vector $\mathbf{o}_\mathbf{v}^T - \mathbf{o}_\mathbf{u}^T = (1, -1, 0, 1, 0)$ is drawn in Figure 5, where also the interval boundaries i_1 and i_1 as well as the intervals (I), (II), and (III) are indicated, respectively. The dotted line shows the limiting curve (envelope) between the values of the difference of partial sums. Note that this curve is crossing twice the (dashed) zero line of the diagram indicating a twofold change of sign of the difference vector $\mathbf{o}_\mathbf{v}^T - \mathbf{o}_\mathbf{u}^T$; in other word, the envelope exhibits three extremal points (nodes).

Keeping in mind that the necessary condition (3.2) for vector catalysis of the given pair $\mathbf{u}$ and $\mathbf{v}$ is fulfilled one would like to find a suitable—possibly minimal—catalyst partition vector $\mathbf{c}$. This can be done by calculating the ordered tensor product vectors $\mathbf{u} \otimes \mathbf{c}^T$ and $\mathbf{v} \otimes \mathbf{c}^T$ with all possible partition vectors of partition diagrams with $n \geq 3$ and test them with respect to majorisation. Although one can exclude systematically many partitions, this method of testing grows exponentially with increasing n and is only feasible up to $n \approx 150$–200 due to this problem of NP complexity.

Another way of finding catalysts is to minimise the negative deviation of the difference vector $\mathbf{o}_\mathbf{v}^T - \mathbf{o}_\mathbf{u}^T$ (see Figure 5) which occurs in interval (II), where $\mathbf{o}_{\mathbf{u},i} \geq \mathbf{o}_{\mathbf{v},i}$. If a catalyst exists, this difference must "converge" towards zero by comparing the ordered tensor products of $\mathbf{u}$ and $\mathbf{v}$ with varying catalyst vectors $\mathbf{c}$. In the case of the above example, a catalyst vector $\mathbf{c}^T =$
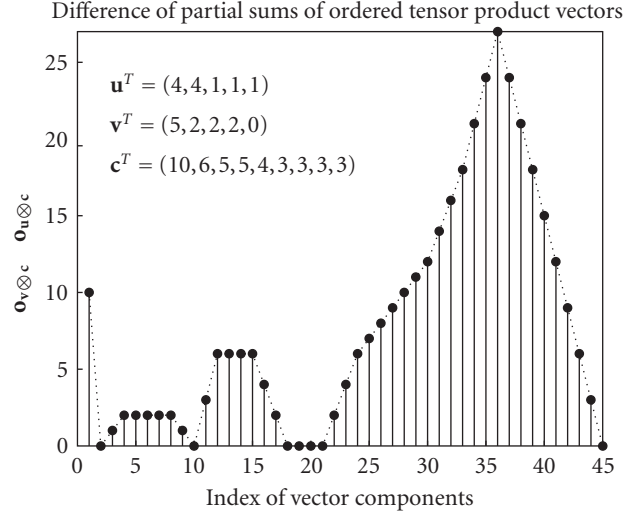
Figure 6: The components of the difference vector $\mathbf{o}_{\mathbf{v}\otimes\mathbf{c}} - \mathbf{o}_{\mathbf{u}\otimes\mathbf{c}}$ *for* $\mathbf{u}^T = (4,4,1,1,1)$, $\mathbf{v}^T = (5,2,2,2,0)$, and $\mathbf{c}^T = (10,6,5,5,4,3,3,3,3)$ as a discrete function of the position count of the vector components.

$(10,6,5,5,4,3,3,3,3)$ was found for the limiting case, where the negative deviation vanishes (see Figure 6).

As mentioned above, the proposition (3.2) is more restrictive than condition (3.1) of Jonathan and Plenio. This can be verified by the example of the incomparable pair $\mathbf{u}^T = (4,4,1,1)$ and $\mathbf{v}^T = (5,2,2,1)$ with $d_{\mathbf{u},\mathbf{v}} = 4$ and $n = 10$ [29]. Clearly, $\mathbf{u}_1 < \mathbf{v}_1$ and $\mathbf{u}_{d_{\mathbf{u},\mathbf{v}}} = \mathbf{v}_{d_{\mathbf{u},\mathbf{v}}}$, and therefore the necessary condition (3.1) for catalysis is fulfilled. On the other hand, starting from the partial sums $\mathbf{o}_{\mathbf{v}} = (5,7,9,10)$ and $\mathbf{o}_{\mathbf{u}} = (4,8,9,10)$ one obtains

$$
\begin{aligned}
\left(\mathbf{o}_{\mathbf{v},1} = 5\right) &> \left(4 = \mathbf{o}_{\mathbf{u},1}\right), &\text{interval (I)},\\
\left(\mathbf{o}_{\mathbf{v},2} = 7\right) &< \left(8 = \mathbf{o}_{\mathbf{u},2}\right), &\text{interval (II)},\\
\left(\mathbf{o}_{\mathbf{v},3} = 9\right) &= \left(9 = \mathbf{o}_{\mathbf{u},3}\right), &\text{interval (II)},\\
\left(\mathbf{o}_{\mathbf{v},4} = 10\right) &= \left(10 = \mathbf{o}_{\mathbf{u},4}\right), &\text{interval (II)}.
\end{aligned}
\tag{3.5}
$$

This means, there is no interval (III) where at least one partial sum of $\mathbf{v}$ is greater than that of $\mathbf{u}$ and thus condition (3.2) does not hold. As a consequence, the pair $(5, 2, 2, 1)$ and $(4, 4, 1, 1)$ should not be catalysable according to proposition (3.2) which agrees with the results listed in Table 2.

Concluding the discussion of necessary conditions for vector catalysis of an incomparable pair we would like to give an idea, how proposition (3.2) can be extended. Starting from the concept of intervals (I), (II),..., where $\mathbf{v}$ and $\mathbf{u}$ are alternately "majorising" each other we conjecture that an incomparable pair may be (nontrivially) catalysable only if the number of these intervals is odd, that is, it equals $2k + 1$ ($k = 1, 2, \ldots$). Conversely, if the number of such intervals is even ($2k, k = 1, 2, \ldots$), the corresponding incomparable pair cannot be catalysed.

To get a symbolic formulation for alternately "majorising" pairs of partition vectors, we suggest the following notation (see also Table 7).

Notation 1. If the number of intervals is even, the "sequentially changing majorisation property" should be denoted by $\mathbf{v}(\succ\prec)_k\mathbf{u}$ or $\mathbf{u}(\prec\succ)_k\mathbf{v}$ and in the case of odd intervals by $\mathbf{v} \succ (\prec\succ)_k\mathbf{u}$ or $\mathbf{u} \prec (\succ\prec)_k\mathbf{v}$ with $k \in \mathbb{N}$. Then, the above conjecture is stated by the following.

An incomparable pair of partition vectors is potentially catalysable only if $\mathbf{v} > (<>)_k \mathbf{u}$ or, equivalently, $\mathbf{u} \prec (><)_k \mathbf{v}$.

A tantamount statement of this supposition is as follows.

Proposition 3.2. *An incomparable pair is catalysable only if the number of crossings of the limiting curve for the difference vector $\mathbf{o_v} - \mathbf{o_u}$ of partial sums of the incomparable partitions $\mathbf{u}$ and $\mathbf{v}$ is even or—equivalently—the number of nodes of this curve (envelope) is odd.*

This proposition is a nice analogy to odd/even rules in chemistry which possibly may also lead to a deeper understanding of vector catalysis.

3.3. Autocatalysis

3.3.1. Reaction kinetics

Beside the classical ideas of catalysis as mentioned above, one can observe self-accelerating chemical processes in solid-solid reactions, such as the historical tin-refuse reaction or the decomposition of silver oxide (Lewis, 1897). In solutions the Landolt-reaction (1896) obeys a velocity dependence of the formation of iodide on its own concentration.

For such types of reactions, the idea of autocatalysis is fully accepted. Autocatalysis became a very powerful heuristic idea with the concept of self-organisation introduced by Prigogine [56, 57] in order to describe chemical oscillations in homogenous fluid systems and enzymatic reactions assuming autocatalytic reaction steps like

$$A + X \xrightarrow{k_2} 2X \tag{3.6}$$

or

$$A + 2X \xrightarrow{k_3} 3X, \tag{3.7}$$

where k_2 and k_3 are reaction rate constants.

This symbolic formulation of chemical reactions is expressed in the nonlinear kinetics by

$$\frac{dX}{dt} = k_2 A X,$$
$$\frac{dX}{dt} = k_3 A X^2, \tag{3.8}$$

respectively, by introducing a dissipative term into the dynamics. The formal equations (3.6) and (3.7) are not really chemical equations in the classical sense. Only in their reduced form (3.9) they fulfill the rules for writing down chemical equations,

$$A \xrightarrow{k_1} X. \tag{3.9}$$
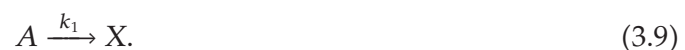
This reduced equation will give a conservative dynamics (3.10),

$$\frac{dX}{dt} = k_1 A, \tag{3.10}$$

which is not in agreement with the typical structure formation as can be observed in dissipative chemical systems. It seems that the so-called autocatalytic equations (3.6) and (3.7) are auxiliary constructions in order to introduce dissipative terms in the dynamics by typical methods to derive chemical kinetics.

Both autocatalytic reactions equations (3.6) and (3.7) seem to accentuate the classical idea of catalysis, but the differential equations (3.8) of the correlated chemical kinetics indicate that it is the dynamics of the reaction which is catalysing because of the nonlinear dissipation terms. This is in total agreement with the ideas of Abel [58] that reactions are catalysing and generating autocatalysis as well.

3.3.2. Mathematical classification

Similarly, one can define autocatalysis in vector catalysis, if one of the partitions $\mathbf{u}$ or $\mathbf{v}$ of the incomparable pair $\mathbf{u} \not\approx \mathbf{v}$ is identical with the catalysing partition vector,

$$\mathbf{u} \otimes \mathbf{u} \approx \mathbf{u} \otimes \mathbf{v}, \quad \mathbf{v} \otimes \mathbf{v} \approx \mathbf{u} \otimes \mathbf{v}, \quad \text{with } \mathbf{u} \not\approx \mathbf{v}. \tag{3.11}$$

As in the discussion up to now we choose without loss of generality the partition vector $\mathbf{v}$ as the one which is able to majorise $\mathbf{u}$ by forming the respective tensor products.

Several kinds of autocatalysis can be distinguished.

(i) The catalyst partition is identical to the partition vector $\mathbf{v}$, the resulting ordered tensor product vector $\mathbf{v} \otimes \mathbf{v}$ of which is majorising the other tensor product vector $\mathbf{u} \otimes \mathbf{v}$ (3.12). We suggest to call this type *Master-Autocatalysis*:

$$\text{Master-Autocatalysis} := (\mathbf{u} \not\approx \mathbf{v}) \wedge (\mathbf{u} \otimes \mathbf{v} \prec \mathbf{v} \otimes \mathbf{v}). \tag{3.12}$$

Our calculations show that the first diagram or partition lattice, where Master-autocatalysis occurs is that of natural number 16 (see Table 3).

(ii) The catalyst partition is identical to the partition vector $\mathbf{u}$, the resulting ordered tensor product vector $\mathbf{u} \otimes \mathbf{u}$ of which is majorised by the other tensor product vector $\mathbf{u} \otimes \mathbf{v}$ (3.13). For this type we propose the term *Slave-Autocatalysis*:

$$\text{Slave-Autocatalysis} := (\mathbf{u} \not\approx \mathbf{v}) \wedge (\mathbf{u} \otimes \mathbf{u} \prec \mathbf{u} \otimes \mathbf{v}). \tag{3.13}$$

Slave-Autocatalysis occurs for the first time in the partition lattice with $n = 16$, as can be shown by our calculations (see Table 3).

(iii) Both partition vectors $\mathbf{u}$ and $\mathbf{v}$ act as catalyst partition, that is, the resulting ordered tensor product vector $\mathbf{v} \otimes \mathbf{v}$ is majorising the other tensor product vector $\mathbf{u} \otimes \mathbf{v}$ and—simultaneously—the ordered tensor product vector $\mathbf{u} \otimes \mathbf{u}$ is majorised by $\mathbf{u} \otimes \mathbf{v}$ (3.14). In other word, Master-Autocatalysis and Slave-Autocatalysis occur concurrently. For this type we propose the term *Mutual Autocatalysis*:

$$\text{Mutal Autocatalysis} := (\mathbf{u} \not\approx \mathbf{v}) \wedge (\mathbf{u} \otimes \mathbf{v} \prec \mathbf{v} \otimes \mathbf{v}) \wedge (\mathbf{u} \otimes \mathbf{u} \prec \mathbf{u} \otimes \mathbf{v}). \tag{3.14}$$

According to our calculations, Mutual Autocatalysis can be found for the first time in partition lattices with $n = 22$.

Table 3: Incomparable pairs of partition vectors **u** and **v** which exhibit Master- or Slave-Autocatalysis and are contained in partition lattices up to $n = 17$, and incomparable pairs showing Mutual Autocatalysis of partition lattice with $n = 22$. In addition, the type of autocatalysis and the minimal catalyst vector $\mathbf{c}_{min}$ for **u** and **v** are listed.

n	$\mathbf{u}^T$	$\mathbf{v}^T$	Autocatalytic partition	Type of autocatalysis	$\mathbf{c}_{min}^T$
15	$(6, 3, 3, 1, 1, 1)$	$(7, 2, 2, 2, 2, 0)$	**u**	Slave	$(2, 1, 1)$
16	$(6, 3, 3, 1, 1, 1, 1)$	$(7, 2, 2, 2, 2, 1, 0)$	**u**	Slave	$(2, 1, 1)$
16	$(4, 4, 4, 1, 1, 1, 1)$	$(6, 3, 2, 2, 2, 1, 0)$	**v**	Master	$(2, 1)$
16	$(5, 3, 3, 1, 1, 1, 1, 1)$	$(6, 2, 2, 2, 2, 2, 0, 0)$	**u**	Slave	$(2, 1, 1)$
17	$(7, 4, 3, 1, 1, 1)$	$(9, 2, 2, 2, 2, 0)$	**u**	Slave	$(2, 1)$
17	$(6, 3, 3, 2, 1, 1, 1)$	$(7, 2, 2, 2, 2, 2, 0)$	**u**	Slave	$(2, 1, 1)$
17	$(6, 3, 3, 1, 1, 1, 1, 1)$	$(7, 2, 2, 2, 2, 2, 0, 0)$	**u**	Slave	$(2, 1, 1)$
17	$(5, 4, 3, 2, 1, 1, 1)$	$(7, 2, 2, 2, 2, 2, 0)$	**u**	Slave	$(2, 1)$
17	$(6, 3, 3, 1, 1, 1, 1, 1)$	$(7, 2, 2, 2, 2, 1, 1, 0)$	**u**	Slave	$(2, 1, 1)$
17	$(4, 4, 4, 1, 1, 1, 1, 1)$	$(6, 3, 2, 2, 2, 2, 0, 0)$	**v**	Master	$(2, 1)$
17	$(4, 4, 4, 1, 1, 1, 1, 1)$	$(6, 3, 2, 2, 2, 1, 1, 0)$	**v**	Master	$(2, 1)$
17	$(5, 3, 3, 1, 1, 1, 1, 1, 1)$	$(6, 2, 2, 2, 2, 2, 1, 0, 0)$	**u**	Slave	$(2, 1, 1)$
22	$(7, 5, 4, 3, 1, 1, 1)$	$(10, 4, 2, 2, 2, 2, 0)$	**u, v**	Mutual	$(2, 1)$
22	$(8, 5, 3, 3, 1, 1, 1)$	$(10, 3, 3, 2, 2, 2, 0)$	**u, v**	Mutual	$(2, 1, 1)$
22	$(8, 4, 4, 3, 1, 1, 1)$	$(10, 3, 3, 2, 2, 2, 0)$	**u, v**	Mutual	$(2, 1)$
22	$(6, 5, 3, 3, 1, 1, 1, 1, 1)$	$(9, 3, 2, 2, 2, 2, 2, 0, 0)$	**u, v**	Mutual	$(2, 1)$
22	$(6, 4, 4, 3, 1, 1, 1, 1, 1)$	$(9, 3, 2, 2, 2, 2, 2, 0, 0)$	**u, v**	Mutual	$(2, 1)$
22	$(6, 5, 3, 3, 1, 1, 1, 1, 1)$	$(9, 3, 2, 2, 2, 2, 1, 1, 0)$	**u, v**	Mutual	$(2, 1)$

Table 3 lists all autocatalytic pairs which can be found in partition lattices from $n = 15$ to $n = 17$ as well as all mutually autocatalytic pairs for $n = 22$.

As can be seen from Table 3, surprisingly the minimal nonautocatalytic catalyst partition vector $\mathbf{c}_{min}^T$ is always $(2, 1)$ or $(2, 1, 1)$, that is, its dimension $d_{c,min}$ and its trace m_{min} is much smaller than that of the autocatalysts. This means that simple vector catalysis with a catalyst vector $\mathbf{c} \neq \mathbf{u}, \mathbf{v}$ can take place in a space of much lower dimensionality as compared to autocatalysis.

Recently, Uhlman [59] suggested to use the term "autocatalysis" for entanglement transformations of multiple copies of bipartite quantum states (MLOCC or multiple-copy local operation and classical communication), a phenomenon in quantum informatics which was discovered by Bandyopadhyay et al. [60]. We suggest to call this type *Multiple-Copy Autocatalysis* (3.15),

$$\text{Multiple-Copy Autocatalysis} := (\mathbf{u} \neq \mathbf{v}) \wedge \left\{ \exists (p \in \mathbb{N}) > 1, \text{ such that: } \mathbf{u}^{\otimes p} \approx \mathbf{v}^{\otimes p} \right\}, \tag{3.15}$$

where $\mathbf{u}^{\otimes p}$ and $\mathbf{v}^{\otimes p}$ denote tensor exponentiation by the exponent p, that is, **u** and **v**, respectively, are p-times multiplied by tensor products with itself (3.16),

$$\mathbf{u}^{\otimes p} = \underbrace{\mathbf{u} \otimes \mathbf{u} \otimes \cdots \otimes \mathbf{u}}_{p\text{-times}}, \qquad \mathbf{v}^{\otimes q} = \underbrace{\mathbf{v} \otimes \mathbf{v} \otimes \cdots \otimes \mathbf{v}}_{p\text{-times}}. \tag{3.16}$$

Note that the exponentiation with $p = 0$ yields the unity vector (2.3) with one component equal to "1."

Table 4: Conditions for special cases of autocatalysis derived from unified autocatalysis.

Type of autocatalysis	Conditions for exponents p, q, r, and s
Master-autocatalysis	$(p = 1) \wedge (q \geq 1) \wedge (r = 0) \wedge (s = q + 1)$
Slave-autocatalysis	$(p \geq 2) \wedge (q = 0) \wedge (r = p - 1) \wedge (s = 1)$
Multiple-copy autocatalysis	$(p = s \geq 2) \wedge (q = r = 0)$

Using tensor exponentiation our idea of Master- and Slave-Autocatalysis in vector catalysis can be generalised by (3.17),

$$(\mathbf{u} \not\approx \mathbf{v}) \wedge \left\{ \exists (p \in \mathbb{N}) > 1, \text{ such that: } \mathbf{u}^{\otimes p} \approx \mathbf{u}^{\otimes(p-1)} \otimes \mathbf{v} \right\}. \tag{3.17}$$

A combination of both concepts of autocatalysis leads to (3.18) and will be denoted by *Unified Autocatalysis*.

$$\text{Unified Autocatalysis} := (\mathbf{u} \not\approx \mathbf{v}) \wedge \left\{ \exists p, q, r, s \in \mathbb{N}^0 \text{ such that:} \right.$$
$$\left. (p + q = r + s \geq 2) \wedge \left(\mathbf{u}^{\otimes p} \otimes \mathbf{v}^{\otimes q} \approx \mathbf{u}^{\otimes r} \otimes \mathbf{v}^{\otimes s} \right) \right\}. \tag{3.18}$$
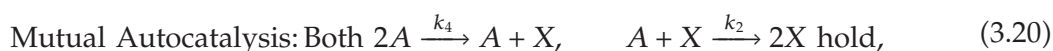
The individual cases of autocatalysis can be derived from (3.18) by setting the exponents p, q, r, and s as shown in Table 4.

Allowing $p + q = r + s = 1$ for an arbitrary vector pair $\mathbf{u}$ and $\mathbf{v}$, one gets (classical) majorisation.
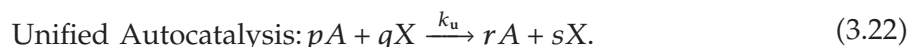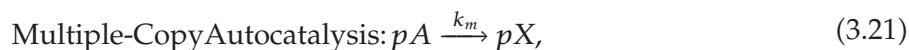
3.3.3. Relation to chemistry

Let us identify the reaction arrow "$\rightarrow$" in formal chemical kinetics with the majorisation relation symbol "$\prec$." This approach corresponds to the observation that common spontaneous reactions occur towards higher disorder and thus in downward direction within the diagram lattices of Ruch [48].

Then the classical autocatalytic reaction equation (3.6) is related to (3.13) of Slave-Autocatalysis in the mathematical framework. Analogously, one can formulate formal kinetic equations for the other types of autocatalysis:

$$\text{Master-Autocatalysis: } 2A \xrightarrow{k_4} A + X, \tag{3.19}$$

$$\text{Mutual Autocatalysis: Both } 2A \xrightarrow{k_4} A + X, \qquad A + X \xrightarrow{k_2} 2X \text{ hold,} \tag{3.20}$$

where k_2 and k_4 correspond to different reaction conditions,

$$\text{Multiple-Copy Autocatalysis: } pA \xrightarrow{k_m} pX, \tag{3.21}$$

$$\text{Unified Autocatalysis: } pA + qX \xrightarrow{k_u} rA + sX. \tag{3.22}$$

A typical example for autocatalysis is the so-called tin pest, that is, the conversion of white β-tin into grey α-tin [61, 62]. The velocity of this autocatalytic reaction is—apart from temperature—depending on size and shape of the growing seeds. Such reactions are also called *collectively autocatalytic* [63], that is, the reactions produce themselves as reaction products such that the

entire set of reactions is self sustaining and accelerating. Without going into details, we suggest that the kinetic equations (3.6) and (3.19) to (3.22) may serve as an adequate description of such processes.

A similar phenomenon can be observed in case of heterogeneous catalysis which takes place by processes of adsorption from the gas phase, reaction at solids or solid surfaces and desorption into the gas phase. During these processes adsorption clusters are formed which are the reactive units of catalysis. These units can be local adsorption complexes at "active centres," clusters at larger surface domains, the adsorption layer or even the adsorbate together with the bulk [64]. The catalytic properties are strongly depending upon the size of the reactive units which may be considered as an accelerating autocatalytic set combined with structure formation. In other words, the reaction is determined by the distribution function of the adsorption clusters which catalyse theirs own formation and decay.

As a particular example, one may consider the oxidation of CO on Palladium supported catalysts [13–15, 21–27]. By model studies one can show that the phase transition between Pd and PdO occurs faster with decreasing size of the catalytic Pd clusters [13–15]. As a result, it comes to resonance phenomena between catalysts of different sizes whereupon self-affine patterns are formed the overall shape of which depends on the particle size distribution. The synchronised CO oxidation as well as the fast loss of catalytic activity in the oxidised state of the catalyst particles is indicative for autocatalytic processes. A detailed description of this model is given in [13–15].

3.4. Counting properties of partition lattices for $n = 1$ to $n = 20$

To give an impression of the complexity of the discrete approach to vector catalysis, in Table 5 some counting properties of partition lattices up to $n = 20$ are given. All characteristics listed in this table are increasing exponentially due to NP complexity of the problem.

The following notations are used in Table 5.

(i) N: No. of partition vectors $\mathbf{u}$ and $\mathbf{v}$ with $\mathrm{tr}(\mathbf{u}) = \mathrm{tr}(\mathbf{v}) = n$ which is identical to the no. of diagrams of Ruch's diagram lattices with natural number n;

(ii) $N_{\mathbf{u},\mathbf{v}}$: No. of all possible pairs of partition vectors $\mathbf{u}$ and $\mathbf{v}$ in a partition lattice with natural no. n;

(iii) $N_{\mathbf{u}-\mathbf{v}}$: No. of all adjacent pairs in a partition lattice with natural no. n, that is, couples of partition vectors $\mathbf{u}$ and $\mathbf{v}$, where one of them is directly majorising the other;

(iv) $N_{\mathbf{u}\not\gtrless\mathbf{v}}$: No. of all incomparable pairs of partition vectors $\mathbf{u}$ and $\mathbf{v}$ in a partition lattice with natural no. n;

(v) $N_{\mathbf{u(pot)v}}$: No. of all incomparable pairs of partition vectors $\mathbf{u}$ and $\mathbf{v}$ in a partition lattice with natural no. n which are potentially catalysable, that is, which fulfill the condition $\mathbf{v} \succ (\mathord{<}\mathord{>})_k \mathbf{u}$ with $k \in \mathbb{N}$ (see Section 3.2 and Table 7);

(vi) $N_{\mathbf{u(c\leq 20)v}}$: No. of all incomparable pairs of partition vectors $\mathbf{u}$ and $\mathbf{v}$ in a partition lattice with natural number n which are catalysed by a catalyst partition vector $\mathbf{c}$ of a partition lattices with $n \leq 20$;

(vii) $N_{\mathbf{u(auto)v}}$: No. of all incomparable pairs of partition vectors $\mathbf{u}$ and $\mathbf{v}$ in a partition lattice with natural no. n which are autocatalysed according to (3.12) or (3.13) by one of the partition vectors of the incomparable pair;

Table 5: Counting values of partition vectors **u** and **v** and their properties concerning vector catalysis depending on the natural number n of the partition lattice.

| n	N	$N_{\mathbf{u},\mathbf{v}} = \binom{N}{2}$	$N_{\mathbf{u}-\mathbf{v}}$	$N_{\mathbf{u}\not\sim\mathbf{v}}$	$N_{\mathbf{u}(\text{pot})\mathbf{v}}$	$N_{\mathbf{u}(c\leq20)\mathbf{v}}$	$N_{\mathbf{u}(\text{auto})\mathbf{v}}$	$N_{\mathbf{u}(\text{Master})\mathbf{v}}$	$N_{\mathbf{u}(\text{Slave})\mathbf{v}}$
1	1	—	—	—	—	—	—	—	—
2	2	1	1	—	—	—	—	—	—
3	3	3	2	—	—	—	—	—	—
4	5	10	4	—	—	—	—	—	—
5	7	21	6	—	—	—	—	—	—
6	11	55	12	2	—	—	—	—	—
7	15	105	17	4	—	—	—	—	—
8	22	231	28	15	—	—	—	—	—
9	30	435	41	35	—	—	—	—	—
10	42	861	62	85	—	—	—	—	—
11	56	1 540	87	170	1	—	—	—	—
12	77	2 926	128	385	4	1	—	—	—
13	101	5 050	175	712	11	5	—	—	—
14	135	9 045	247	1 405	28	14	—	—	—
15	176	15 400	335	2 583	69	34	1	—	1
16	231	26 565	459	4 771	149	74	3	1	2
17	297	43 956	611	8 307	313	161	8	2	6
18	385	73 920	824	14 798	630	324	27	7	20
19	490	119 805	1 081	24 976	1 215	631	78	25	53
20	627	196 251	1 430	42 805	2 286	1 192	171	57	114

Table 6: Counting values of partition vectors **u** and **v** and their properties concerning vector catalysis depending on the natural number n of the partition lattice.

Counting value	a	$\ln(a)$	b	R^2
N	5.2 e−02	−3.0	2.1	0.99992
$N_{\mathbf{u},\mathbf{v}} = \binom{N}{2}$	1.0 e−03	−6.9	4.3	0.99996
$N_{\mathbf{u}-\mathbf{v}}$	2.9 e−02	−3.5	2.4	0.99997
$N_{\mathbf{u}\not\sim\mathbf{v}}$	3.5 e−05	−10.2	4.7	0.99996
$N_{\mathbf{u}(\text{pot})\mathbf{v}}$	2.3 e−08	−17.6	5.7	0.99992
$N_{\mathbf{u}(c\leq20)\mathbf{v}}$	9.5 e−09	−18.5	5.7	0.99989
$N_{\mathbf{u}(\text{auto})\mathbf{v}}$[*]	2.4 e−11	−24.5	6.6	0.99984
$N_{\mathbf{u}(\text{Master})\mathbf{v}}$[*]	3.3 e−13	−28.7	7.3	0.99997
$N_{\mathbf{u}(\text{Slave})\mathbf{v}}$[*]	1.2 e−10	−22.8	6.2	0.99941

[*]Counting values were calculated up to $n = 24$.

(viii) $N_{\mathbf{u}(\text{Master})\mathbf{v}}$: No. of all incomparable pairs of partition vectors **u** and **v** in a partition lattice with natural no. n which show Master-Autocatalysis according to (3.12);

(ix) $N_{\mathbf{u}(\text{Slave})\mathbf{v}}$: No. of all incomparable pairs of partition vectors **u** and **v** in a partition lattice with natural no. n which show Slave-Autocatalysis according to (3.13).

Table 7: Notations for pairs of partition vectors and majorisation.

$n \in \mathbb{N}$	Positive integer (natural number) to be partitioned.
$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{d_\mathbf{u}} \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{d_\mathbf{v}} \end{pmatrix}$	Discrete partition vectors (column vectors) with non-negative integers u_i and v_i as components ($i, u_i, v_i \in \mathbb{N}$). They are used as *pair of partition vectors* to be compared with respect to majorisation and discrete vector catalysis. The following conventions are assumed. If a pair of different vectors $\mathbf{u}$ and $\mathbf{v}$ ($\mathbf{u} \neq \mathbf{v}$) is compared with respect to majorisation, $\mathbf{u}$ is chosen as the vector with the first occurrence of a component $\mathbf{u}_i < \mathbf{v}_i$.
$d_\mathbf{u}, d_\mathbf{v} \in \mathbb{N}$	Dimensions, that is, number of nonzero components, of $\mathbf{u}$ and $\mathbf{v}$, respectively. In general, $d_\mathbf{u}$ and $d_\mathbf{v}$ are different.
$d_{\mathbf{u},\mathbf{v}} = \sup\left(d_\mathbf{u}, d_\mathbf{v}\right)$	Supremum of dimensions $d_\mathbf{u}$ and $d_\mathbf{v}$. The vector with the lower dimension is filled up with zeros to $d_{\mathbf{u},\mathbf{v}}$ components.
$n_\mathbf{u} = \text{tr}(\mathbf{u}) = \sum_{j=1}^{d_{\mathbf{u},\mathbf{v}}} u_j,$ $n_\mathbf{v} = \text{tr}(\mathbf{v}) = \sum_{j=1}^{d_{\mathbf{u},\mathbf{v}}} v_j, \quad n_\mathbf{u}, n_\mathbf{v} \in \mathbb{N}$	Trace (sum of components) of $\mathbf{u}$ and $\mathbf{v}$, respectively; (classical) majorisation, $n_\mathbf{u} = n_\mathbf{v} = n$.
$\mathbf{o_u} = \begin{pmatrix} \mathbf{o}_{\mathbf{u},1} \\ \mathbf{o}_{\mathbf{u},2} \\ \vdots \\ \mathbf{o}_{\mathbf{u},d_{\mathbf{u},\mathbf{v}}} \end{pmatrix}, \quad \mathbf{o_v} = \begin{pmatrix} \mathbf{o}_{\mathbf{v},1} \\ \mathbf{o}_{\mathbf{v},2} \\ \vdots \\ \mathbf{o}_{\mathbf{v},d_{\mathbf{u},\mathbf{v}}} \end{pmatrix}$ $\mathbf{o}_{\mathbf{u},i} = \sum_{j=1}^{i} u_j, \quad \mathbf{o}_{\mathbf{v},i} = \sum_{j=1}^{i} v_j, \quad i = 1, 2, \ldots, d_{\mathbf{u},\mathbf{v}}$	Vectors of partial sums of partition vectors $\mathbf{u}$ and $\mathbf{v}$, respectively.
$\prec, \succ:$ $\mathbf{u} \prec \mathbf{v} \equiv \mathbf{v} \succ \mathbf{u} := \mathbf{o}_{\mathbf{u},i} \le \mathbf{o}_{\mathbf{v},i}, \quad i = 1, 2, \ldots, d_{\mathbf{u},\mathbf{v}}$	(Classical) majorisation relation. Comparable pair, where $\mathbf{u}$ is being majorised by $\mathbf{v}$ and $\mathbf{v}$ is majorising. $\mathbf{u}$ In quantum informatics the corresponding transition of entangled states is possible with certainty by LOCC (local operation and classical communication).
$\mathbf{u} \approx \mathbf{v}: = (\mathbf{u} \prec \mathbf{v}) \vee (\mathbf{u} \succ \mathbf{v})$	Pair of partition vectors which is comparable with respect to majorisation.
$\mathbf{u} \not\approx \mathbf{v} = \neg(\mathbf{u} \approx \mathbf{v})$	Pair of partition vectors which is incomparable with respect to majorisation.
$\mathbf{u} \diamond \mathbf{v} \equiv \mathbf{v} \diamond\!\!\!\diamond \mathbf{u}$	Incomparable pair, where both $\mathbf{u}$ and $\mathbf{v}$, respectively, are divided in two subsections of contiguous components, such that in the first section all partial sums $\mathbf{o_v}$ of $\mathbf{v}$ are greater or equal to $\mathbf{o_u}$ of $\mathbf{o_u}$ and in the second section vice versa. (For this and the following definitions see also Section 3.2).
$\mathbf{u} (\diamond)_k \mathbf{v} \equiv \mathbf{v} (\diamond\!\!\!\diamond)_k \mathbf{u}, \ k \in \mathbb{N}$	Same as $\mathbf{u} \diamond \mathbf{v}$ but changing subsections of components are repeated k times; in case of $k = 1$ one obtains the notation above.
$\mathbf{u} \diamond\!\!\!\diamond \mathbf{v} \equiv \mathbf{v} \diamond\!\!\!\diamond \mathbf{u}$	Incomparable pair, where both $\mathbf{u}$ and $\mathbf{v}$, respectively, are divided in three subsections of contiguous components, such that in the first and last (third) section all partial sums $\mathbf{o_v}$ of $\mathbf{v}$ are greater or equal to $\mathbf{o_u}$ of $\mathbf{u}$ and in the second section vice versa.
$\mathbf{u} \prec (\succ\!\prec)_k \mathbf{v} \equiv \mathbf{v} \succ (\prec\!\succ)_k \mathbf{u}, \ k \in \mathbb{N}^0$	Same as $\mathbf{u} \diamond\!\!\!\diamond \mathbf{v}$ but changing subsections of components are repeated k times; in case of $k = 1$ one obtains the notation above, in case of $k = 0$ one gets the majorisation relation $\succ$ ($\prec$).
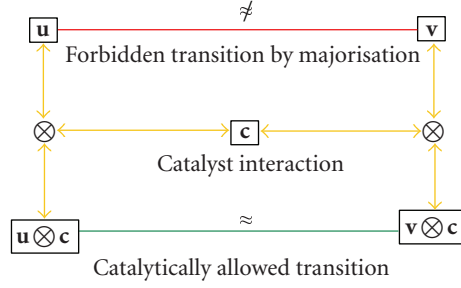
Figure 7: Incomparable pair **u** and **v** corresponding to a forbidden transition, which will be allowed by a third vector **c** as catalyst.

The number series of Table 5 can roughly be approximated by the power law

$$y = ae^{bn^{0.5}} \qquad \text{or} \qquad \ln y = \ln a + bn^{0.5}, \tag{3.23}$$

where y are the least square fits of each of the counting values as a function of n with R^2 values of about 0.9999. The coefficients of these fits are listed in Table 6.

As can be seen from coefficients b, the counting numbers of properties correlated to all and to the incomparable partition pairs are growing about twice as fast as the number N of partition vectors and the number $N_{\mathbf{u-v}}$ of directly majorising partitions. The calculated coefficients b for properties which are attributed to vector catalysis are even larger, but may be less significant, because a fewer number of values are included in the fits; if one takes a sufficiently large number of counting values the coefficients b for catalysable or catalytic pairs cannot exceed that for incomparable pairs.

4. Conclusion and summary

Our mathematical model of discrete vector catalysis is based on partition vectors, the components of which are only natural numbers including zero. The set of all these vectors forms a special, discrete vector space V_{disc} which—in analogy to real vector spaces—is based on d-dimensional vectors $\mathbf{u} = (u_1, \ldots, u_d)$ with u_i, $d \in \mathbb{N}^0$ and $\text{tr}(\mathbf{u}) = n \in \mathbb{N}^0$, a direct sum "$\oplus$" of vector components, a multiplier $\mu \in \mathbb{N}^0$ and a scalar multiplication "$\cdot$" such that

$$
\begin{aligned}
\mathbf{u}, \mathbf{v}, \mathbf{w}, \mathbf{0} \equiv (0), \quad \mathbf{0}_d \equiv \Big(\underbrace{0 \ \ 0 \ \cdots \ 0}_{d\text{-times}} \Big) &\in V_{\text{disc}}, \quad \mu \in \mathbb{N}^0 \Longrightarrow \mathbf{0} \oplus \mathbf{u} = \mathbf{u}, \quad 0 \cdot \mathbf{u} = \mathbf{0}_d, \\
\mathbf{u} \oplus (\mathbf{v} \oplus \mathbf{w}) = (\mathbf{u} \oplus \mathbf{v}) \oplus \mathbf{w}, &\quad 1 \cdot \mathbf{u} = \mathbf{u}, \\
\mathbf{u} \oplus \mathbf{v} = \mathbf{v} \oplus \mathbf{u}, &\quad \mu \cdot \mathbf{u} = \mathbf{u} \cdot \mu, \\
\mu \cdot (\mathbf{u} \oplus \mathbf{v}) = \mu \cdot \mathbf{u} &\oplus \mu \cdot \mathbf{v}.
\end{aligned}
\tag{4.1}
$$

On this discrete vector space the majorisation relation "$\prec, \succ, \approx$" and the tensor product "$\otimes$" are defined as described in the previous sections and in Tables 7 and 8. The restriction to such a discrete space enabled us to develop some powerful rules for describing vector catalysis for an effective search of correlated catalysts. On the other hand, this method is of great advantage for discussing our results in the number-theoretical framework of Young diagrams and Ruch's diagram lattices. Particularly, with regard to further investigations on discrete vector catalysis

we would like to represent the procedure, that a transition which is forbidden by majorisation due to incomparable vector pairs becomes allowed by participation of a third catalyst vector, schematically as shown in Figure 7.

    The results can be summarised as follows.

(i) We could verify numerically that not all pairs of incomparable diagrams or partition vectors, respectively, can be catalysed. The smallest possible lattice, which contains a catalytic vector pair, is the diagram lattice for $n = 11$ with the catalysable vector pair $(4, 4, 1, 1, 1)$ and $(5, 2, 2, 2, 0)$, and the catalytic partition vector $(10, 6, 5, 5, 4, 3, 3, 3, 3)$ the trace of which is $m = 42$.

(ii) The smallest nontrivial catalyst vector is $(2, 1)$ belonging to the diagram lattice for $n = 3$; and the smallest incomparable vector pair $(6, 6, 1, 1) \not\succ (8, 3, 3, 0)$ which is catalysable by this catalyst is contained in the diagram lattice with $n = 14$.

(iii) We have introduced the ideas of nonprimitively catalysable incomparable vector pairs and of potentially catalysable vectors pairs. Moreover, we have presented a selection rule which distinguishes between potentially catalysable and noncatalysable incomparable vector pairs by considering alternately majorising subsections in an incomparable pair. This can be seen as a nice analogy to odd/even rules in chemistry.

(iv) In connection with potentially catalysable vector pairs we have sketched a semiempirical/graphical method for finding catalyst vectors by minimising the negative deviation of the difference vector of the partial sums of the ordered tensor products. Using this procedure a catalyst with 38 components and trace of value 410 could be found for the smallest 4-dimensional pair $(5, 5, 1, 1) \not\succ (6, 3, 3, 0)$ belonging to the diagram lattice with $n = 12$.

(v) For any catalysable pair of incomparable vectors, a countable infinite number of catalysts exist. The set of the catalyst vectors assigned to the same pair can be grouped into different classes based upon the component structure and the tensor powers of the catalysts. This will be discussed in detail in a further paper.

(vi) In analogy to chemistry we have adopted the term "autocatalysis" as a special type of vector catalysis, at which at least one partition vector of the incomparable pair acts as catalyst. Depending upon the partition vectors which are catalysing we distinguish between Master-, Slave-, and Mutual Autocatalysis. The smallest diagram lattice in which autocatalysis occurs is that with $n = 15$ and the respective incomparable pair is $(6, 3, 3, 1, 1, 1) \not\succ (7, 2, 2, 2, 2, 0)$ with $(6, 3, 3, 1, 1, 1)$ serving as Slave-Autocatalyst. Mutual Autocatalysis takes place at the first time in a diagram lattice with $n = 22$, and there exist already 6 incomparable pairs with this property. We would like to mention that there are remarkable connections between vector catalysis and the structure of diagram lattices which we consider in a forthcoming publication.

Comparing the chemical ideas of catalysis and autocatalysis with the idea of vector catalysis, it seems on a first view that vector catalysis reflects the old chemical idea of a substance as a catalyst. But the formation of tensor products implies that with help of a catalyst much larger vector spaces of the entangled systems are created. These systems can be interpreted as new pure states which are now comparable by majorisation, and therefore the transition between these entangled states occurs in a high-dimensional space—as opposed to the forbidden noncatalysed transition in the lower-dimensional space (see also Figure 7).

Table 8: Notations for tensor operations and discrete vector catalysis.

$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{d_\mathbf{c}} \end{pmatrix}$ $\mathbf{c}^T = \begin{pmatrix} c_1 & c_2 & \cdots & c_{d_\mathbf{c}} \end{pmatrix}$	Catalyst partition vector, represented as column vector $\mathbf{c}$ or as row vector $\mathbf{c}^T$; it will be used for tensor multiplication with $\mathbf{u}$ or $\mathbf{v}$, respectively, in vector catalysis.
$d_\mathbf{c} \in \mathbb{N}$	Dimension (number of nonzero components) of catalyst partition vector $\mathbf{c}$.
$m = \text{tr}(\mathbf{c}) = \sum_{j=1}^{d_\mathbf{c}} c_j, \quad m \in \mathbb{N}$	Trace (sum of components) of catalyst partition vector $\mathbf{c}$.
$\otimes$	Symbol for tensor product relation.
$\mathbf{u} \otimes \mathbf{c}^T$, $\mathbf{v} \otimes \mathbf{c}^T$ (vector product notation) $\mathbf{u} \otimes \mathbf{c}$, $\mathbf{v} \otimes \mathbf{c}$ (tensor product notation)	Tensor products of $\mathbf{u}$ with $\mathbf{c}(\mathbf{c}^T)$ and $\mathbf{v}$ with $\mathbf{c}(\mathbf{c}^T)$, respectively, in both cases represented as a $(d_{\mathbf{u},\mathbf{v}} \times d_\mathbf{c})$-matrix.
$\boldsymbol{\theta}_{\mathbf{u} \otimes \mathbf{c}}$, $\boldsymbol{\theta}_{\mathbf{v} \otimes \mathbf{c}}$	Vectors of tensor products $\mathbf{u} \otimes \mathbf{c}$ and $\mathbf{v} \otimes \mathbf{c}$, respectively, where all components (tensor product elements) are arranged in decreasing (nonincreasing) order.
$d_{\mathbf{u} \otimes \mathbf{c}} = d_{\mathbf{v} \otimes \mathbf{c}} = d_{\mathbf{u},\mathbf{v}} \cdot d_\mathbf{c}$	Dimension (number of components) of tensor product vectors, that is, dimension $d_{\mathbf{u},\mathbf{v}}$ of partition pair vectors multiplied with dimension $d_\mathbf{c}$ of catalyst vector.
$n_{\mathbf{u} \otimes \mathbf{c}} = n_{\mathbf{v} \otimes \mathbf{c}} = n \cdot m$	Trace (sum of components) of tensor product vectors, that is, trace of partition vectors multiplied with trace of catalyst vector.
$\mathbf{o}_{\mathbf{u} \otimes \mathbf{c}}$, $\mathbf{o}_{\mathbf{v} \otimes \mathbf{c}}$	Vectors of partial sums of tensor product vectors $\boldsymbol{\theta}_{\mathbf{u} \otimes \mathbf{c}}$ and $\boldsymbol{\theta}_{\mathbf{v} \otimes \mathbf{c}}$, respectively.
$\mathbf{u}^{\otimes p} = \underbrace{\mathbf{u} \otimes \mathbf{u} \otimes \cdots \otimes \mathbf{u}}_{p\text{-times}},$ $\mathbf{v}^{\otimes q} = \underbrace{\mathbf{v} \otimes \mathbf{v} \otimes \cdots \otimes \mathbf{v}}_{q\text{-times}},$ $p, q \in \mathbb{N}^0$	Tensor exponentiation of partition vectors $\mathbf{u}$ and $\mathbf{v}$ with exponents p and q, respectively. Special cases, $\mathbf{u}^{\otimes 1} = \mathbf{u}, \mathbf{v}^{\otimes 1} = \mathbf{v}$, $\mathbf{u}^{\otimes 0} = \mathbf{v}^{\otimes 0} = (1)$.

But catalysis means also that there is a possibility that the catalyst can be extracted again after a catalytic transition. The decomposition of the new entangled vectors into the catalyst and the original vectors is possible if one knows the one of them. In general, there are several alternatives to disaggregate, that is, the decomposition; it is by no means unique.

On the other side, recall that the process of vector catalysis is enabled by formation of the tensor product matrices of the partition pair vectors and the catalyst vector, respectively, followed by downwards reorganisation of the matrix elements into vectors with monotonously decreasing order of their components, such that the resulting vector states are comparable. As a consequence of this rearrangement, the components of the initial partition pair vectors and the catalyst vector are mixed within the ordered tensor product vectors, and thus the distribution relations are changed. In other words, the new ordered vectors of the entangled states are not at all simple linear combinations of the source vectors but result of a complex transformation combined with the loss of identity of the catalyst vector. Indeed, not only the formation of tensor products in a high-dimensional space but primarily the process of reorganisation causes

catalysis. This is a nice analogy to the statement in chemistry that not substances but only reactions are catalysing [5].

We are convinced that in future the comparison of chemical catalysis and entanglement catalysis will be fruitful for both sides.

Acknowledgments

References

 [1] J. J. Berzelius, "Einige Ideen über eine bei der Bildung organischer Verbindungen in der lebenden Natur wirksame, aber bisher nicht bemerkte Kraft," *Jahres-Berkcht über die Fortschritte der Chemie*, vol. 15, pp. 237–245, 1836.
 [2] W. Ostwald, "Definition der Katalyse," *Zeitschrift für Physikalische Chemie*, vol. 15, pp. 705–706, 1894.
 [3] W. Ostwald, "Über Katalyse," *Physikalische Zeitschrift*, vol. 3, pp. 313–322, 1901.
 [4] W. Ostwald, "Über Katalyse," *Annalen der Naturphilosophie*, vol. 9, pp. 1–25, 1910.
 [5] E. Abel, "Arbeiten allgemeinen inhalts," *Colloid & Polymer Sciences*, vol. 14, no. 2, pp. 109–110, 1914.
 [6] I. Prigogine, *Vom Sein zum Werden—Zeit und Komplexität in den Naturwissenschaften*, Piper, Munchen, Germany, 1979.
 [7] I. Prigogine, *From Being to Becoming—Time and Complexity in Physical Sciences*, Freeman, San Francisco, Calif, USA, 1980.
 [8] H. Haken, *Synergetik—Eine Einführung*, Springer, Berlin, Germany, 1990.
 [9] H. Haken, *Synergetics: An Introduction*, vol. 1 of *Springer Series in Synergetics*, Springer, Berlin, Germany, 3rd edition, 1983.
[10] G. Ertl, "Dynamik der Wechselwirkung von Molekülen mit Oberflächen," *Berichte der Bunsengesellschaft für Physikalische Chemie*, vol. 99, no. 11, pp. 1282–1294, 1995.
[11] G. Ertl, "Surface science and catalysis," *Pure and Applied Chemistry*, vol. 52, pp. 2051–2060, 1980.
[12] G. Ertl, "Elementarschritte bei der Katalyse an Metallen," in *Leopoldina-Diskussionskreis Chemische Elementarreaktionen und Reaktionsmechanismen*, Halle (Saale), Germany, 1979.
[13] P. J. Plath, K. Möller, and N. I. Jaeger, "Cooperative effects in heterogeneous catalysis—part II: analysis and modelling of the temperature dependence of the catalytic oxidation of CO on a palladium Al_2O_3-supported catalyst," *Journal of the Chemical Society, Faraday Transactions I*, vol. 84, no. 6, pp. 1751–1771, 1988.
[14] P. Svensson, N. I. Jaeger, and P. J. Plath, "Phase and frequency relations with forced oscillations of the heterogeneous catalytic oxidation of carbon monoxide on supported palladium," *Journal of Physical Chemistry*, vol. 92, no. 7, pp. 1882–1888, 1988.
[15] C. Ballandis and P. J. Plath, "A new discrete model for the non-isothermic dynamics of the exothermic CO-oxidation on Palladium supported catalyst," *Journal of Non-Equilibrium Thermodynamics*, vol. 25, no. 3-4, pp. 301–324, 2000.
[16] M. Grunze, F. Bozso, G. Ertl, and M. Weiss, "Interaction of ammonia with Fe(111) and Fe(100) surfaces," *Applications of Surface Science*, vol. 1, no. 2, pp. 241–265, 1978.
[17] M. Weiss, G. Ertl, and F. Nitschké, "Adsorption and decomposition of ammonia on Fe(110)," *Applications of Surface Science*, vol. 2, no. 4, pp. 614–535, 1979.
[18] G. Ertl and N. Thiele, "XPS studies with ammonia synthesis catalysts," *Applications of Surface Science*, vol. 3, no. 1, pp. 99–112, 1979.

[19] G. Ertl, M. Weiss, and S.-B. Lee, "The role of potassium in the catalytic synthesis of ammonia," *Chemical Physics Letters*, vol. 60, no. 3, pp. 391–394, 1979.

[20] A. Hornung, D. Zemlyanov, M. Muhler, and G. Ertl, "The catalytic reduction of NO by H_2 on Ru(0001): observation of NH_{ads} species," *Surface Science*, vol. 600, no. 2, pp. 370–379, 2006.

[21] R. Imbihl, M. P. Cox, and G. Ertl, "Kinetic oscillations in the catalytic CO oxidation on Pt(100): experiments," *Journal of Chemical Physics*, vol. 84, no. 6, pp. 3519–3534, 1986.

[22] P. Möller, K. Wetzl, M. Eiswirth, and G. Ertl, "Kinetic oscillations in the catalytic CO oxidation on Pt(100): computer simulations," *Journal of Chemical Physics*, vol. 85, no. 9, pp. 5328–5336, 1986.

[23] K. Krischer, R. Rico-Martinez, I. G. Kevrekidis, H. H. Rotermund, G. Ertl, and J. L. Hudson, "Model identification of a spatiotemporally varying catalytic reaction," *AIChE Journal*, vol. 39, no. 1, pp. 89–98, 1993.

[24] N. Hartmann, K. Krischer, and R. Imbihl, "The role of adsorbate-adsorbate interaction in the rate oscillations on catalytic CO oxidation on Pd (110)," *Journal of Chemical Physics*, vol. 101, no. 8, pp. 6717–6727, 1994.

[25] J. Starke, C. Reichert, M. Eiswirth, H. H. Rotermund, and G. Ertl, "Fluctuation-induced pattern formation in a surface reaction," *Europhysics Letters*, vol. 73, pp. 820–825, 2006.

[26] C. Beta, A. S. Mikhailov, H. H. Rotermund, and G. Ertl, "Defect-mediated turbulence in a catalytic surface reaction," *Europhysics Letters*, vol. 75, pp. 868–874, 2006.

[27] P. S. Bodega, P. Kaira, C. Beta, et al., "High frequency periodic forcing of the oscillatory catalytic CO oxidation on Pt(110)," *New Journal of Physics*, vol. 9, no. 3, p. 61, 2007.

[28] A. Amann, "Molecules coupled to their environment," in *Large-Scale Molecular Systems: Quantum and Stochastic Aspects—Beyond the Simple Molecular Picture*, W. Gans, A. Blumen, and A. Amann, Eds., vol. 258 of *NATO ASI Series B. Physics*, pp. 3–22, Plenum Press, New York, NY, USA, 1991.

[29] D. Jonathan and M. B. Plenio, "Entanglement-assisted local manipulation of pure quantum states," *Physical Review Letters*, vol. 83, no. 17, pp. 3566–3569, 1999.

[30] M. A. Nielsen, "Conditions for a class of entanglement transformations," *Physical Review Letters*, vol. 83, no. 2, pp. 436–439, 1999.

[31] A. W. Marshall and I. Olkin, *Inequalities: Theory of Majorization and Its Applications*, vol. 143 of *Mathematics in Science and Engineering*, Academic Press, New York, NY, USA, 1979.

[32] P. M. Alberti and A. Uhlmann, *Dissipative Motion in State Spaces*, vol. 33 of *Teubner-Texte zur Mathematik*, BSB B. G. Teubner, Leipzig, Germany, 1981.

[33] P. M. Alberti and A. Uhlmann, *Stochasticity and Partial Order: Doubly Stochastic Maps and Unitary Mixing*, vol. 9 of *Mathematics and Its Applications*, D. Reidel, Dordrecht, The Netherlands, 1982.

[34] J. Eisert and M. Wilkens, "Catalysis of entaglement manipulation for mixed states," *Physical Review Letters*, vol. 85, no. 2, pp. 437–440, 2000.

[35] Z.-W. Zhou and G.-C. Guo, "Basic limitations for entanglement catalysis," *Physics Letters A*, vol. 277, no. 2, pp. 70–74, 2000.

[36] P. H. Anspach, "Two-qubit catalysis in a four-state pure bipartite system," arXiv:quant-ph/0102067v1, preprint, 2001.

[37] S. Daftuar and M. Klimesh, "Mathematical structure of entanglement catalysis," *Physical Review A*, vol. 64, no. 4, Article ID 042314, 6 pages, 2001.

[38] X. Sun, R. Duan, and M. Ying, "The existence of quantum entanglement catalysts," *IEEE Transactions on Information Theory*, vol. 51, no. 1, pp. 75–80, 2005.

[39] Y. Feng, R. Duan, and M. Ying, "Catalyst-assisted probabilistic entanglement transformation," *IEEE Transactions on Information Theory*, vol. 51, no. 3, pp. 1090–1101, 2005.

[40] G. Aubrun and J. Nechita, "Catalytic majorization and l_p norms," arXiv:quant-ph/0702153v2, preprint, 2007.

[41] S. Turgut, "Necessary and sufficient conditions for the trumping relation," *Journal of Physics A*, vol. 40, pp. 12185–12212, 2007.

[42] H. Primas, *Chemistry, Quantum Mechanics and Reductionismml: Perspectives in Theoretical Chemistry*, vol. 24 of *Lecture Notes in Chemistry*, Springer, Berlin, Germany, 1981.

[43] P. J. Plath, *Diskrete Physik Molekularer Umlagerungen*, vol. 19 of *Teubner Texte zur Physik*, BSB B.G. Teubner, Leipzig, Germany, 1988.

[44] E. Ruch and A. Schönhofer, "Theorie der Chiralitätsfunktionen," *Theoretica Chimica Acta*, vol. 19, no. 3, pp. 225–287, 1970.

[45] A. Young, "On quantitative substitutional analysis," *Proceedings of the London Mathematical Society*, vol. 33, no. 1, pp. 97–145, 1900.

[46] A. Young, "On quantitative substitutional analysis," in *The Collected Papers of Alfred Young (1873–1940)*, Mathematical Expositions no. 21, pp. 42–91, University of Toronto Press, Toronto, Ont, Canada, 1977.

[47] A. Young, "On quantitative substitutional analysis (Third Paper) (1927)," in *The Collected Papers of Alfred Young (1873–1940)*, Mathematical Expositions no. 21, pp. 352–389, University of Toronto Press, Toronto, Ont, Canada, 1977.

[48] E. Ruch, "The diagram lattice as structural principle," *Theoretica Chimica Acta A*, vol. 38, no. 3, pp. 167–183, 1975.

[49] E. Ruch and A. Mead, "The principle of increasing mixing character and some of its consequences," *Theoretica Chimica Acta A*, vol. 41, no. 2, pp. 95–117, 1976.

[50] E. Ruch and B. Lesche, "Information extent and information distance," *The Journal of Chemical Physics*, vol. 69, no. 1, pp. 393–401, 1978.

[51] R. Brüggemann, N. Walz, M. Brauns, and W. Ostendorp, "Beitragsserie: Seeufer, ein vergessenes Ökoton, Beitrag 3," *UWST-Z. Umweltchemie Ökotox*, vol. 16, no. 1, pp. 48–56, 2004.

[52] S. Sauerbrei, E. C. Haß, and P. J. Plath, "The Apollonian decay of beer foam bubble size distribution and the lattices of Young diagrams and their correlated mixing functions," *Discrete Dynamics in Nature and Society*, vol. 2006, Article ID 79717, 35 pages, 2006.

[53] S. Sauerbrei, U. Sydow, and P. J. Plath, "On the characterization of foam decay with diagram lattices and majorization," *Zeitschrift für Naturforschung*, vol. 61, no. 3-4, pp. 153–165, 2006.

[54] S. Sauerbrei and P. J. Plath, "Diffusion without constraints," *Journal of Mathematical Chemistry*, vol. 42, no. 2, pp. 153–175, 2007.

[55] S. Sauerbrei, K. Knicker, E. C. Hass, and P. J. Plath, "Weak majorization as an approach to non-equilibrium foam decay," *Applied Mathematical Sciences*, vol. 1, no. 11, pp. 527–550, 2007.

[56] I. Prigogine, "Zeit, struktur und fluktuationen (Nobel-Vortrag)," *Angewandte Chemie*, vol. 90, no. 9, pp. 704–715, 1978.

[57] I. Prigogine and R. Lefever, "Symmetry breaking instabilities in dissipative systems II," *Journal of Chemical Physics*, vol. 48, no. 4, pp. 1695–1700, 1968.

[58] E. Abel, "Katalytische Studien IV. H^+-Ionen-Katalyse und—Autokatalyse der katalytisch abgelenkten Wasserstoffsuperoxyd-thiosulfat-Reaktion," vorgelegt in der Sitzung vom 20, February 1913.

[59] A. Uhlmann, Private communication (lecture at Fritz-Haber Institute of Max-Planck-Gesellschaft), August 2007.

[60] S. Bandyopadhyay, V. Roychowdhury, and U. Sen, "Classification of nonasymptotic bipartite pure-state entanglement transformations," *Physical Review A*, vol. 85, no. 5, Article ID 052315, 4 pages, 2002.

[61] J. Eggert, *Lehrbuch der Physikalischen Chemie in Elementarer Darstellung*, S. Hirzel, Stuttgart, Germany, 1960.

[62] A. F. Hollemann and E. Wiberg, *Lehrbuch der Anorganischen Chemie*, Walter de Gruyter, Berlin, Germany, 1964.

[63] B. McMullin, "Some remarks on autocatalysis and autopoiesis," in *Proceedings of the Work-Shop on Closure: Emergent Organizations and Their Dynamics*, University of Ghent, Ghent, Belgium, May 1999.

[64] P. J. Plath and H. Prüfer, "Ein stochastischer zellulärer automat als modell einer heterogen katalysierten reaktion," *Zeitschrift für Physikalische Chemie*, vol. 268, no. 2, pp. 235–249, 1987.

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