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Fock space approach to Schnakenberg model

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FOCK SPACE APPROACH TO SCHNAKENBERG MODEL

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Everything you want's a dream away
(Coldplay)

Resumo

Este trabalho tem como objetivo estudar a relação entre espaços de Fock, operadores de mecânica quântica e sistemas de reações químicas usados para modelar diversos processos estocásticos com motivação biológica, como crescimento populacional, batimentos cardíacos e metabolismo celular. Em particular, vamos trabalhar com uma generalização do modelo de Schnakenberg, em suas versões determinística e estocástica, e que pode ser utilizado para descrever o processo de glicólise celular. Como é uma área recente e ao mesmo tempo interdisciplinar, envolvendo conhecimento em processos estocásticos, física teórica, química e biomatemática, este texto procura ser autocontido, incluindo todos os fundamentos necessários para o estudo do tema, visando contribuir para o melhor entendimento entre estas diversas áreas.

Palavras-chave: Espaços de Fock. Reações químicas. Osciladores biológicos. Modelo de Schnakenberg.

Abstract

This work has as objective to study the relationship between Fock spaces, quantum operators and chemical reaction systems used to model many stochastic processes with biological motivation, such as population growth, heartbeats and cell metabolism. In particular, we work with a generalization of Schnakenberg model, in its deterministic and stochastic versions, and which is used to describe the process of cellular glycolysis. As it is a new and at the same time a interdisciplinary area, involving knowledge in stochastic processes, theoretical physics, chemistry and biomathematics, this text seeks to be self-contained, including all the elements needed for the study of theme, for the purpose of contribute to the better understanding between these diverse areas.

Key-words: Fock spaces. Chemical reactions. Biological oscillators. Schnakenberg model.

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Introduction

At first sight, it not seems to exist a logical relation between food chain, chemical reaction systems and statistics. In fact, for many people it is hard to have some connection between mathematics and natural sciences, and further an area where they are all related. However, the study of a difficult problem may be more comfortable if we use concepts developed in other areas of knowledge.

For example, in Physics we have Statistical Mechanics, that uses Probability Theory - a mathematical construction - to study the behaviour of systems whose trajectories are uncertain or, saying, "not behaved". In biology or in medicine, there are systems of this type, called biological oscillators. Then, an interesting way to study biological systems can be done using the tools of Statistical Physics.

However, how to make this connection? An oscillator can be written as a system of chemical reactions; in turn, each reaction can be described as an Ordinary Differential Equation (ODE), and hence we can find physical and mathematical applications.

Meantime, an imperfection in this process is the fact that, usually, the system of ODE's is treated with numerical methods. Not that this is a severe problem that affects the entire study of the biological system, but the treatment in this way brings restricted results, which can, in some cases, compromise the study of the general system, because not always the particular results can be generalized. Thus, the natural way is to seek analytical solutions to the biological system, which are more accurate and more general than the numeric solutions. The problem is that this is not as easy as it sounds; in some cases, the calculations can be long, difficult and discouraging. Then, we will try to implement an important link between biology, maths and physics.

An interesting alternative to confront this challenge is to use the Quantum Field Theory operators, based on two naive concepts: creation and annihilation operators. The idea of their use is simplistic: for example, to move one particle from a point i to a point j, simply annihilate the particle in point i and create the particle in point j. As a chemical reaction is a mixture of various particles of various species in search of equilibrium, then it can be written in terms of these operators.

The objective of this work is to use this idea, along with other concepts already mentioned and some definitions of Fock Space and Linear Algebra, to study the behaviour of the Schnakenberg model, a system that can be used to describe the glycolysis, a set of biological process for the absorption of glucose by cells. The entire method is written in this text.

For a better explanation of all the necessary content for the study, this dissertation is divided into three parts. In the first part, there is a summary of all the mathematical and physical concepts necessary for the study of the subject. In the second part, we make the connection between biological oscillators, statistical physics, Fock spaces and linear algebra. The result of these areas together and the application to the Schnakenberg model are described in third part.

Whenever necessary, there are references to other books and articles on the theme in question. Good reading.

Part I

Prologue

1 Chemical reactions and biological systems

One way used to model biological systems, such as population's growth, constitutes in assembly chemical reactions, which can be rewritten and used in the study of larger systems, such as protein folding (see (1) and (2)), heart beats ((3)) and analysis of endemics diseases ((4)). To study in detail such systems, we will use tools from various areas, such as probability and quantum mechanics((5)), for example.

Both deterministic and stochastic models can be described macroscopically. The deterministic model can be seen as a Partial Differential Equation (PDE) and be analysed by the qualitative behaviour of the structure of the reaction network. However, some more complex models feature "exotic" situations such as oscillatory, multistationary and chaotic behaviour, and have been more intensive and detailed subject investigated in the last 50 years.

In some cases, stochastic models can be seen as a Markovian process, i.e., a process in which the future state depends only on the current state and the previous state of the system don't exert influence on the reaction. A system with this characteristic has useful properties which simplify the study, although not always makes it easier.

The overall goal of the theory of chemical kinetics is to describe the interactions between the components (in this case the species) of a chemical system. As we will see later in this text, we use n-dimensional vectors for this, and the dimension of the vector space which contains the vector is the number of interacting species, and vector module describes the quantities of species. Hence, reactions occur between the components, causing changes in their quantities.

Traditionally, a chemical reaction is conceived as a process where some chemical components are transformed into other chemical components. Within this process, there are two issues to be investigated. The first is to analyze the algebraic structure of transformations, by calculating the change in the composition that occur due to the reaction; this is the goal of stoichiometry. The other issue is to see how long occur the reaction, i.e., the time from which the reactions between the components will stop and the system will become stable.

There are several approaches to solving these problems, and one of them is to use the rate equations and the master equation associated to the reaction. They provide valuable information of the processes involved in the system, the last of which gives more detail, so it is most required in the studies, as will be seen later in this text.

2 Notions of probability

If we want throw a ping-pong ball down, we can precisely calculate the total distance and the time she spends until it stops in the soil. Likewise, we can determine the boiling temperature of the milk put in stove.

Known certain conditions, it is perfectly possible to answer these and other questions before performing these experiments and even if they are repeated countless times. They are called deterministic experiments because in them the results can be predicted.

Already if we roll one dice, we cannot conclude precisely what number is obtained as result. Even if the experiment is repeated many times, the results are different, and we say that this is a random experiment.

At first, a random phenomenon seems to have regularity, and therefore would not be subject to study. However, after a closer look, we see that it is indeed possible to have some sort of regularity. Returning to the example of the dices, if we roll infinite dices and observe the results, we see that after a sequence of rolls, the results obtained follow a model. If we observe another sequence of dices, we see that the model will repeat. This is the regularity that we can observe in random phenomena.

The study of random phenomena is made by the union of three theories - probability, stochastic processes and stochastic dynamic - and two key concepts: the concept of probability and the concept of random variable. The definition of probability is built upon various results of an experiment, joined in sets, which are assigned non-negative real numbers whose sum is 1. However, this definition is too general for what we will study later. This is because the interpretation of probability does not follow directly from its definition; for us, the probability of an outcome is the frequency of occurrence of this result.

Below, we list some definitions of statistical physics, the branch of physics that uses methods of probability and statistics to describe a variety of systems with inherently stochastic nature. There are several books on this topic, but in this text we use as reference (6) and (7).

Before, first it is important to make a logical clarification. In this dissertation, stochastic and random are the same thing. Indeed, a variable is called random if it depends on a parameter x; if x means the time, then the variable is labeled stochastic (7). As we often work with time in statistical physics, it is natural that stochastic and random, in the end, being related to the same object. However, in the probability in general, stochastic and random are treated as equals.

2.1 Random variables

When we roll one dice, we know that the value x of the face up will be a number between 1 and 6, although it is not possible to predict the correct value. Similarly, when we install a lamp, do not know the total life time t until it burn.

In both cases, "roll the dice" and "lamp on" are two experiments; x and t are random variables or stochastic variables. The sets $\{1, 2, 3, 4, 5, 6\}$ and $[0, +\infty)$ are the respective sample spaces. An event is a subset of a sample space, for example, odd number on the face up of dice: $\{1, 3, 5\}$.

Mathematically, a random variable is a function $x : S \to \mathbb{R}$ that associates elements of a sample space S to real numbers. It is a quantitative variable, whose result (value) depends of experiment. Furthermore, for all event $E \subset S$, the probability of x admit a value $e \in E$ is $p(e \in E) = p(E)$, which is well defined, although it is not always possible to calculate it. Thus, it is always possible to obtain a probability distribution function defined around the sample space.

Consider a random variable x that takes only integer values and suppose that each value of x is associated with a real number

$$p_x \geq 0 \tag{2.1}$$

such that

$$\sum_x p_x = 1. \tag{2.2}$$

If this happens, x is a discrete random variable and p_x is the probability distribution of random variable x. For example, the Poisson distribution

$$p_x = e^{-\alpha} \frac{\alpha^x}{x!}, \tag{2.3}$$

for $\alpha > 0$ and $x \in \mathbb{Z}^+$, is a discrete probability distribution, because

$$\sum_{x=0}^{\infty} p_x = e^{-\alpha} \sum_{x=0}^{\infty} \frac{\alpha^x}{x!} = 1.$$

Consider, now, a continuous random variable x, that takes any real value. In this case, the probability is associated with an interval of $\mathbb{R}$. Thus, the probability of x be in the interval $[a, b]$ is

$$\int_a^b \rho(x) dx, \tag{2.4}$$

where $\rho(x)$ is the probability density function, with the properties

$$\rho(x) \geq 0 \tag{2.5}$$

and

$$\int_{-\infty}^{\infty} \rho(x) dx = 1. \tag{2.6}$$

The cumulative distribution function $F(x)$ is defined by

$$F(x) = \int_{-\infty}^{x} p(y)dy \tag{2.7}$$

and is a monotonically increasing function.

As famous example of probability density function, we have the Gaussian distribution

$$\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{x^2}{2\sigma^2}). \tag{2.8}$$

2.2 Averages, variance and characteristic function

Henceforth, we will focus our study on continuous variables, which will be most useful in our work. Consider a function $f(x)$ and let be $\rho(x)$ the probability density associated with x. The average $\langle f(x)\rangle$ is defined by

$$\langle f(x)\rangle = \int f(x)\rho(x)dx. \tag{2.9}$$

The moments are defined by

$$\mu_n = \langle x^n\rangle = \int x^n \rho(x)dx. \tag{2.10}$$

The first moment μ_1 is the average of x. The dispersion or variance is defined by

$$\sigma^2 = \langle (x - \langle x\rangle)^2\rangle \tag{2.11}$$

and is always non-negative. Using the property

$$\langle af(x) + bg(x)\rangle = a\langle f(x)\rangle + b\langle g(x)\rangle, a, b \in \mathbb{R}, \tag{2.12}$$

we have

$$\begin{aligned} \langle (x - \langle x\rangle)^2\rangle &= \langle (x^2 - 2x\langle x\rangle + \langle x\rangle^2)\rangle \\ &= \langle x^2\rangle - 2\langle x\rangle^2 + \langle x\rangle^2 \\ &= \langle x^2\rangle - \langle x\rangle^2 \end{aligned}$$

Therefore, we have

$$\sigma^2 = \mu_2 - \mu_1^2. \tag{2.13}$$

The characteristic function $g(k)$ of a random variable x is defined by the Fourier transform of probability density function associated with x, that is,

$$g(k) = \int \rho(x)e^{ikx}dx = \langle e^{ikx}\rangle, \tag{2.14}$$

with the properties

$$g(0) = 1 \text{ and } |g(k)| \leq 1. \tag{2.15}$$

The characteristic function always exists. However, it is not always possible to extend it in Taylor series; this means that the probability distribution does not have moments.

The characteristic function also serves to generate the cumulants κ_n, which are defined by

$$g(k) = exp(\sum_{n=1}^{\infty} \frac{(ik)^n}{n!} \kappa_n). \tag{2.16}$$

Taking the example of Gaussian distribution, the characteristic function is given by:

$$g(k) = exp(-\frac{\sigma^2 k^2}{2}) \tag{2.17}$$

and the expansion in Taylor series is

$$g(k) = 1 + \sum_{i=1}^{\infty} \frac{(ik)^n}{n!} \mu_n. \tag{2.18}$$

Taking the logarithm of 2.16 and comparing with 2.18, we have the relation between cumulants and moments:

$$\begin{gathered} \kappa_1 = \mu_1, \\ \kappa_2 = \mu_2 - \mu_1^2, \\ \kappa_3 = \mu_3 - 3\mu_2\mu_1 + 2\mu_1^3, \\ \kappa_4 = \mu_4 - 4\mu_3\mu_1 - 3\mu_2^2 + 12\mu_2\mu_1^2 - 6\mu_1^4, \\ \text{etc.} \end{gathered} \tag{2.19}$$

Note that every the cumulants of Gaussian distribution, after third, are null.

2.3 Joint probability distribution

Let be x and y two random variables. The probability of find x in interval $[a, b]$ and y in interval $[c, d]$ is

$$\int_a^b \int_c^d \rho(x, y) dx dy, \tag{2.20}$$

where $\rho(x, y)$ is the joint probability density of x and y. It has the properties

$$\rho(x, y) \geq 0 \text{ and } \int \int \rho(x, y) dx dy = 1. \tag{2.21}$$

Thenceforward, we can obtain the marginal probability density $\rho_1(x)$ of x and $\rho_2(y)$ of y, given, respectively, by

$$\rho_1(x) = \int \rho(x, y) dy \tag{2.22}$$

and

$$\rho_2(y) = \int \rho(x, y) dx. \tag{2.23}$$

The random variables x and y are independent if $\rho(x,y) = \rho_1(x)\rho_2(y)$. In this case, the average of product of functions $X(x)$ and $Y(y)$ is equal to product of the averages:

$$\langle X(x)Y(y)\rangle = \langle X(x)\rangle\langle Y(y)\rangle. \tag{2.24}$$

If we have a third random variable z which depends of x and y by $z = f(x,y)$, we can calculate the probability distribution $\rho_3(z)$ by

$$\rho_3(z) = \int\int \delta(z - f(x,y))\rho(x,y)dxdy. \tag{2.25}$$

If we have two random variables u and v, which depends of x and y by $u = f_1(x,y)$ and $v = f_2(x,y)$, the joint probability distribution $\rho_3(u,v)$ is

$$\rho_3(u,v) = \int\int \delta(u - f_1(x,y))\delta(v - f_2(x,y))\rho(x,y)dxdy. \tag{2.26}$$

If the transformation $(x,y) \to (u,v)$ is a bijection, then

$$\rho_3(u,v)dudv = \rho(x,y)dxdy. \tag{2.27}$$

2.4 Markov process

Consider, now, a random/stochastic process where the time and the random variable are discretized by a parameter t. Suppose that the stochastic variable x_t takes integer values and t the values $0, 1, 2, 3...$ A stochastic process is well defined until the instant ℓ by joint probability distribution

$$P_\ell(n_0, n_1, n_2, ..., n_\ell) \tag{2.28}$$

of x_t take the value n_0 at instant $t = 0$, the value n_1 at $t = 1$,..., and the value n_ℓ at $t = \ell$.

Next, consider the conditional probability

$$P_{\ell+1}(n_{\ell+1}|n_0, n_1, ..., n_\ell) \tag{2.29}$$

of the stochastic variable x_t take the value $n_{\ell+1}$ at instant $t = \ell + 1$, given that it has taken the value n_0 at instant $t = 0$, n_1 at $t = 1$,..., and n_ℓ at $t = \ell$. If this probability is equal to conditional probability

$$P_{\ell+1}(n_{\ell+1}|n_\ell) \tag{2.30}$$

of the stochastic variable x_t take the value $n_{\ell+1}$ at instant $t = \ell+1$, given that it has taken only the value n_ℓ at instant $t = \ell$, then the stochastic process is a Markovian process.

In other words, in a Markov process the conditional probability of x_t take a given value in a given time t depends only of value that it has taken in immediately previous instant, not on the sequence of events that preceded it. In addition, because of the definition of conditional probability, we have

$$P_\ell(n_0, n_1, n_2, ..., n_\ell) = P_\ell(n_l|n_{l-1})...P_2(n_2|n_1)P_1(n_1|n_0)P_0(n_0), \tag{2.31}$$

and thus we conclude that the Markov process is completely defined by the initial probability $P_0(n_0)$ and the conditional probability $P_{\ell+1}(n_{\ell+1}|n_\ell)$.

In a Markov process, the probability $P_\ell(n_\ell)$ of the variable x_t take the value n_ℓ at $t = \ell$ is given by

$$P_\ell(n_\ell) = \sum P_\ell(n_0, n_1, n_2, ..., n_\ell), \tag{2.32}$$

where the sum is over $(n_0, n_1, n_2, ...)$ but no over n_ℓ. If we use the above formula, we obtain

$$P_\ell(n_\ell) = \sum_{n_{\ell-1}} P_\ell(n_\ell|n_{\ell-1})P_{\ell-1}(n_{\ell-1}). \tag{2.33}$$

That is, we can obtain $P_\ell(n_\ell)$ at any time using only $P_0(n_0)$.

The conditional probability $P_\ell(n_\ell|n_{\ell-1})$ can be interpreted as the transition probability between the states $n_{\ell-1}$ and n_ℓ. At first, this transition may depend of considered time, but in this work, we consider only Markov process whose transition probabilities not vary with the time. Then, we write $P_\ell(n_\ell|n_{\ell-1}) = T(n_\ell, n_{\ell-1})$ and we have

$$P_\ell(n_\ell) = \sum_{n_{\ell-1}} T(n_\ell, n_{\ell-1})P_{\ell-1}(n_{\ell-1}), \tag{2.34}$$

or, in simplified form,

$$P_\ell(n) = \sum_m T(n, m)P_{\ell-1}(m). \tag{2.35}$$

$T(n, m)$ can be interpreted as element of a matrix T, that has the properties:

1. $T(n, m) \geq 0$, because $T(n, m)$ is a probability; and
2. $\sum_n T(n, m) = 1$, because T must be normalized. That is, the sum of the elements of a column is equal to 1.

Any square matrix that has these two properties is called stochastic matrix.

If we define a matrix P_ℓ as the column vector whose elements are $P_\ell(n)$, then the equation 2.35 can be written in form of matrix product,

$$P_\ell = TP_{\ell-1}. \tag{2.36}$$

In this way, given the initial column vector P_0, we obtain P_ℓ by

$$P_\ell = T^\ell P_0 \tag{2.37}$$

and the problem of determine $P_\ell(n)$ reduces to calculate the ℓth power of the stochastic matrix T. This equation may be written in form

$$P_\ell(n) = \sum_m T^\ell(n,m) P_0(m), \tag{2.38}$$

where the matrix element $T^\ell(n,m)$ is the transition probability of state m to state n in ℓ steps, that is, the probability of variable x_t take the value n at instant t given that it has taken the value m at previous instant $t-\ell$.

3 Chemical Kinetics, Probability and Quantum Field Theory

3.1 Law of mass action and rate equation

Chemical systems do not always react with the same speed. Some reactions are very fast, such as neutralization reactions; others take hours, days, or even years to reach equilibrium, such as radioactive decay (8). The speed of a chemical reaction consists in measuring the change in concentration of the reactants and products in a given unit of time.

There are several factors that influence the rate of a chemical reaction, such as the concentration and physical state of the reactants, the temperature and ambient light, besides the presence of a catalyst or inhibitor in the reaction.

The progress (extension) of a chemical reaction is measured as the amount of substance that reacted. The speed (rate) of a chemical reaction is a derivative of the extent of reaction with respect to time. For homogeneous reactions, the progress is measured in terms of the concentration (c) or partial pressure (p), while the speed is measured as the derivative or instantaneous speed, dc/dt and dp/dt.

Since there is no equipment for measuring instantaneous speeds s, what has been done is to measure the extent of reaction in terms of p and c at different times. The difference between two successive measurements of extent of successive reaction times results in a differential increment dc/dt or dP/dt, which is the average reaction rate during that time interval. As the time between successive measurements becomes smaller, the difference approaches the derivative.

Then, the average velocity during the time interval (difference) becomes a good approximation for the instantaneous speed (derivative) and may be used in its place. Nevertheless, it can be experimentally found that the reaction rate may not be constant over time.

Chemical experiments over the years have shown that there is a correspondence between the reaction rate and the concentration of the reactants. This correspondence is represented by a proportionality constant k, called reaction rate coefficient (for more information, see (9) and (8)).

There is a mathematical method to study and predict the behaviour of chemical reactions in equilibrium using the masses of reactants, called law of mass action. This law involves two aspects: the composition of the mixture in equilibrium; and the rate equations of reactions that lead the system to this state.

According to the law of mass action, the production rate of a chemical species is proportional to the product of the reactants. For example, consider the reversible reaction given by

$$mA + nB \underset{k_-}{\overset{k_+}{\rightleftharpoons}} pC,$$

where m, n and p are stoichiometric constants of substances A, B and C respectively, in the reaction. Using the law of mass action, the differential equations of the outward reaction are:

$$\begin{aligned} \tfrac{d[A]}{dt} &= -mk_+[A]^m[B]^n \\ \tfrac{d[B]}{dt} &= -nk_+[A]^m[B]^n \\ \tfrac{d[C]}{dt} &= pk_+[A]^m[B]^n \end{aligned} \tag{3.1}$$

The reaction back, $pC \underset{k_-}{\rightarrow} mA + nB$, have differential equations given by:

$$\begin{aligned} \tfrac{d[A]}{dt} &= mk_-[C]^p \\ \tfrac{d[B]}{dt} &= nk_-[C]^p \\ \tfrac{d[C]}{dt} &= -pk_-[C]^p \end{aligned} \tag{3.2}$$

Thus, for the general reaction, we "add" their equations (in reality, we sum the terms of second member of equations whose first member are equal) and get:

$$\begin{aligned} \tfrac{d[A]}{dt} &= -mk_+[A]^m[B]^n + mk_-[C]^p \\ \tfrac{d[B]}{dt} &= -nk_+[A]^m[B]^n + nk_-[C]^p \\ \tfrac{d[C]}{dt} &= pk_+[A]^m[B]^n - pk_-[C]^p \end{aligned} \tag{3.3}$$

Taking as an example the reaction of oxidation of ammonia,

$$4NH_3 + 3O_2 \overset{k}{\rightarrow} 2N_2 + 6H_2O,$$

we will have the following rate equations:

$$\begin{cases} \tfrac{d[NH_3]}{dt} = -4k[NH_3]^4[O_2]^3 \\ \tfrac{d[O_2]}{dt} = -3k[NH_3]^4[O_2]^3 \\ \tfrac{d[N_2]}{dt} = 2k[NH_3]^4[O_2]^3 \\ \tfrac{d[H_2O]}{dt} = 6k[NH_3]^4[O_2]^3 \end{cases}$$

3.2 Master equation

The master equation is a more accurate version than the rate equation, because it is based on transition probabilities and not just on the rate of the change of species between two states. Therefore, there are more useful properties, and it is more interesting to our study. There are many books and handouts about this topic, but in this text we relied in Raul (10), Van Kampen (6) and Hizanidis(11).

Consider a situation where there is an alternation between two states, 1 and 2. For example, in the reaction $Na + Cl \leftrightarrow NaCl$, the sodium atom cannot be switched on (state 1) or is bonded to the chlorine atom (state 2). Let be $W(1 \to 2)$ the rate at which something passes, uniformly and randomly, from state 1 to state 2 at time $(t, t + dt)$

The reverse process of passing from state 2 to 1 may or may not occur. A radioactive substance, for example, cannot return to the original state from the deteriorated state. However, in reversible chemical reactions, product molecules can be divided to form the reacting species. If the reverse reaction can occur we represent with a probability $W(2 \to 1)$.

Given an initial time t_0, we want to know what are the probabilities $P_1(t)$ and $P_2(t)$ at time t. To answer this question, the ideal is to deduce an equation for $P_1(t)$, knowing that $P_1(t) + P_2(t) = 1$. For this, the relationship between the probability in t and $t + dt$ will be analysed using implicitly the Markov property, assuming the transition rate between states in the range $(t, t + dt)$ is independent of what happened before t.

Thus, the probability $P_1(t + dt)$ of the particle is in state 1 at time $(t + dt)$ has two contributions: one $P_j(t)$ to be in state 1 at time t and not jumped to 2, that is, $[1 - (W(1 \to 2)dt)]$; and other, $P_{j-1}(t)$, to be in second state and jump to first state $W(2 \to 1)dt$. Summarizing these cases and using the rules of conditional probability, we have

$$P_1(t + dt) = P_1(t)[1 - W(1 \to 2)dt] + P_2(t)W(2 \to 1)dt + O(dt^2) \tag{3.4}$$

The terms in $O(t^2)$ could appear if the particle was in the state 1 during $t + dt$ time, because it could have made two jumps from 1 to 2 and 2 to 1 during the interval $(t, t + dt)$, which could contribute to $P_j(t)$, as $W(1 \to 2)dt \times W(2 \to 1)dt$. Similarly, there could be particles jumping from 2 to 1 and then from 1 to 2. Fortunately, these events do not interfere in the results in the limit $dt \to 0$; thereby obtaining the following differential equation:

$$\frac{dP_1(t)}{dt} = -W(1 \to 2)P_1(t) + W(2 \to 1)P_2(t) \tag{3.5}$$

Similar reasoning leads to an equivalent equation for $P_2(t)$:

$$\frac{dP_2(t)}{dt} = -W(2 \to 1)P_2(t) + W(1 \to 2)P_1(t) \tag{3.6}$$

These equations are a very simple example of master equations, equations to find the probability that a stochastic particle jump from one state to another at time t.

A generalization of the master equation can be made from the Chapman-Kolmogorov equation[1]. Actually, the master equation is a more simplified version of this, since it is obtained from the time difference dt in limit $dt \to 0$.

Let be T_t the transition probability $P(y_t, t; y_{t-1}, t-1)$. Since the coefficient $1 - W(1 \to 2)dt$ is the probability of no transition during dt, and using the Chapman-Kolmogorov equation, we get

$$T_{t+dt}(1 \to 3) = [1 - W(3 \to 2)dt]T_{dt}(1 \to 3) + dt \int W(2 \to 3)T_t(1 \to 2)d2,$$

where $d2$ means the integration over the state 2. Dividing by dt, and taking the limit $dt \to 0$, have

$$\frac{\partial}{\partial t}T_{dt}(1 \to 3) = \int [W(2 \to 3)T_{dt}(1 \to 2) - W(3 \to 2)T_{dt}(1 \to 3)]d2 \qquad (3.7)$$

The master equation can be written in a simplified and intuitive way, relating two states y and y':

$$\frac{\partial P(y,t)}{\partial t} = \int [W(y' \to y)P(y',t) - W(y \to y')P(y,t)]dy' \qquad (3.8)$$

If we are working with a discrete state space with n times, the equation reduces to

$$\frac{dp_n(t)}{dt} = \sum_n [W_{nn'}p_{n'}(t) - W_{n'n}p_n(t)]$$

Note, from this case, that the master equation is an equation of loss-gain of the probabilities of the states n. The first term is the gain of the n-th state due to transitions to other states n', and the second term is the loss due to transitions in from other states.

A property of the master equation is that when $t \to \infty$, all solutions tend to the stationary solution, although this is strictly true for a finite number of discrete states. For an infinite number of states, and for continuous state space, there are some exceptions, for example the random walk. In physics, this is useful because it is known that many systems tend towards equilibrium.

3.3 Operators in Fock Space and second quantization

In classical mechanics, we can determine the position and velocity of a particle in the system at a given time t; however, with microscopic particles this process is somewhat more complex.

In quantum mechanics, the study of these properties is based in Heisenberg's uncertainty principle - as the name suggests, the statement tell us that there is a fuzziness

[1] $P_{1|1}(y_3, t_3|y_1, t_1) = \int P_{1|1}(y_3, t_3|y_2, t_2)P_{1|1}(y_2, t_2|y_1, t_1)dy_2$(6)

in nature, a fundamental limit to what we can know about the behaviour of quantum particles and, therefore, the smallest scales of nature. Of these scales, the most we can hope for is to calculate probabilities for where things are and how they will behave (12). Then, to describe the state of a quantum system - a system consisting of microscopic particles -, it resorts to a wave function $\psi(x, t)$, depending on the position x and time t.

The wave function contains some information about the system, and most important, they obey a general wave equation, known as Schrödinger equation. This idea of describing the behaviour of particles as if they were waves is known in quantum mechanics as the first quantization.

The reverse situation, called second quantization, is to describe wave functions using operators used to describe the behaviour of particles as a quantum field, and which meet the Schrödinger equation. The term "second quantization" was coined in beginning of quantum mechanics, to extend it to quantum field theory.

The process of formalism of second quantization in this dissertation is based in texts of Lancaster e Blundell(13) and Lima(14). We start by defining a state of many particles: $|n_1, n_2, ..., n_i, ...\rangle$, where n_i is the number of particles with eigenvalue k_i is an operator. The space formed by these kets is a Hilbert space (a complete normed vector space) and is called the Fock space.

For the construction of Fock space, it is important to consider that the state of particles that interact with each other can be written on a basis of independent particles, as eigenkets of operators of one particle with eigenvalue k_i. We consider, also, that there are two special states:

1. The vacuum or absence of particles: $|0\rangle \equiv |0, 0, ..., 0, ...\rangle$
2. The state with one particle $|k_i\rangle \equiv |0, 0, ..., n_i = 1, ...\rangle$

Next, we define a "field operator" $a_i^\dagger$, whose function will be increases in 1 the number of particles with eigenvalue k_i. This operator is called creation operator and is described as

$$a_i^\dagger |n_1, n_2, ..., n_i, ...\rangle \propto |n_1, n_2, ..., n_i + 1, ...\rangle, \tag{3.9}$$

where the proportionality constant is defined using normalization criteria.

Let be $a_i^\dagger|0\rangle = |0, 0, ..., n_i = 1, ...\rangle = |k_i\rangle$, with $\langle k_i|k_i\rangle = 1$. With this, we have $1 = \langle k_i|k_i\rangle = [\langle 0|a_i][a_i^\dagger|0\rangle] = \langle 0|a_i a_i^\dagger|0\rangle$, what implies that $a_i a_i^\dagger|0\rangle = |0\rangle$.

Therefore, we can define the annihilation operator – that destroys a particle with eigenvalue k_i – as $a_i|k_i\rangle = a_i|0, 0, ..., n_i = 1, ...\rangle = |0\rangle$. Thus,

$$a_i|n_1, n_2, ..., n_i, ...\rangle \propto n_i|n_1, n_2, ..., n_i - 1, ...\rangle \tag{3.10}$$

With this definition, we see that $a_i|0\rangle = 0$ and $a_i|k_j\rangle = 0, i \neq j$. Note that the action of permutate two particles can be seen as a comparison between put first a particle in k_i and then another in k_j with put first a particle in k_j and then another in k_i. Thus, for a two-particle system is expected that

$$a_i^\dagger a_j^\dagger|0\rangle = \pm a_j^\dagger a_i^\dagger|0\rangle, \tag{3.11}$$

Where the positive sign applies to bosons and the negative sign applies to fermions. Bosons are particles that represent totally symmetric states, while the fermions represent antisymmetric states. Thus, we have an anticommutator in the case of fermions.

$$\begin{cases} a_i^\dagger a_j^\dagger - a_j^\dagger a_i^\dagger = [a_i^\dagger, a_j^\dagger] = 0 \Rightarrow \text{bosons} \\ a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = \{a_i^\dagger, a_j^\dagger\} = 0 \Rightarrow \text{fermions} \end{cases} \tag{3.12}$$

For a system with N particles the logic is the same. Note that the Pauli Exclusion Principle is automatically incorporated into the formalism because $a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0 \rightarrow a_i^\dagger a_i^\dagger = 0$, if $i = j$, that is, it must not take two particles in the same state.

Finally, we define an operator that counts particles. If we have $[a_i, a_j^\dagger] = 1$, an analogy with the counter of quantum of energy of the harmonic oscillator show us that the definition $N = a_i^\dagger a_i$ is useful. In the case of bosons, this condition is sufficient to define the operator that counts particles.

In the case of fermions, the number of particles in a state k_i can only be 0 or 1: $\{a_i, a_j^\dagger\} = \delta_{ij}$. Thus,

$$N_i|n_1, n_2, ...n_i, ...\rangle = \begin{cases} (a_i^\dagger a_i|n_1, n_2, ..., n_i = 0, ...\rangle = 0|n_1, n_2, ..., n_i = 0, ...\rangle \\ a_i \text{ in } 0 \text{ is } 0 \\ \\ a_i^\dagger a_i|n_1, n_2, ..., n_i = 1, ...\rangle = 1|n_1, n_2, ..., n_i = 1, ...\rangle \\ \text{Using the fact that } a_i^\dagger a_i = 1 - a_i a_i^\dagger. \end{cases} \tag{3.13}$$

Thus, for both types of particles, bosons and fermions, we can define the operator that counts the particles by $N = \sum\limits_i a_i^\dagger a_i$.

But how to build an operator in the second quantization language that do more than count particles? If we look for an additive operator, such as the kinetic energy of the system (the sum of the kinetic energies of the individual particles), the account is simple. In such a case, if the system is, for example, in a Fock space $|n_1, n_2, ..., n_i, ...\rangle$, where each particle n_i have energy k_i, the kinetic energy of system is $\sum_i n_i k_i$, which is eigenvalue of operator $H = \sum_i k_i N_i = \sum_i a_i^\dagger a_i$

There is another case to be examined, which is when the Fock space is written on a basis $\{l_i\rangle\}$ which isn't diagonal (i.e., $H|l_i\rangle \neq k_i|l_i\rangle$), that is, a basis different of the basis

$\{k_i\}$. In this case, it's know that $k_i\rangle = \sum_j |l_j\rangle\langle l_j|k_i\rangle$, then $a_i^\dagger = \sum_j b_j^\dagger \langle l_j|k_i\rangle$, which implies $a_i = \sum_j \langle l_j|k_i\rangle * b_j = \sum_j \langle k_i|l_j\rangle * b_j$.

Replacing in H, have

$$\begin{aligned} H &= \textstyle\sum_i k_i \sum_{mn} b_m^\dagger \langle l_m|k_i\rangle\langle k_i|l_n\rangle b_n \\ &= \textstyle\sum_{mn} b_m^\dagger b_n \sum_i \langle l_m|k_i\rangle k_i \langle k_i|l_n\rangle \\ &= \textstyle\sum_{mn} b_m^\dagger b_n \sum_i \langle l_m|[H|l_i\rangle\langle k_i]|l_n\rangle \\ &= \textstyle\sum_m n b_m^\dagger b_n \langle l_m|H|l_n\rangle \end{aligned} \tag{3.14}$$

Note that this formula H is for writing any operator that operates in the individual particles in the second quantization language. It can be said that this expression applies to operators who do not express interactions between the particles.

One application of this formalism is in condensed matter physics. Consider a net formed by infinite squares with side L, each one with an electron positioned at one end any i. The kinetic energy of the particle is $E_n = \frac{1}{2m}(\frac{n\pi}{L})^2$. Note that the lower the G, larger the energy. On the other hand, the kinetic energy may cause the electron to move in a larger volume. Thus, in a tight-binding model[2] (as this process is called), electrons can expend energy jumping from one lattice to another.

To handle the discrete structure of this model, it is necessary to work on a basis where the creation operator $a_i^\dagger$ creates a particle at position i. The kinetic energy of the particle used to make her jump from j to i is called t_{ij}. The Hamiltonian H is a summation of all the jumps of electrons between the sites, so

$$H = \sum_i j(-t_{ij}) a_i^\dagger a_j. \tag{3.15}$$

Note that each term of this sum is equivalent to the annihilation of a particle in j and creation at position i, through the energy t_{ij}. Note that if $t_{ij} = t$ to neighbouring positions and $t = 0$ in other cases, we can write H as:

$$H = -t \sum_{i\tau} a_i^\dagger a_{i+\tau}, \tag{3.16}$$

where the sum of τ is on nearby neighbours.

3.4 Master equation and quantum operators

In this section we rewrite the master equation of similar way to the Schrödinger equation for imaginary time, which is described as

$$H(t)|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle, \tag{3.17}$$

2 The name "tight-binding" of this electronic band structure model suggests that this quantum mechanical model describes the properties of tightly bound electrons in solids

where i is the imaginary number, $\hbar$ is the Planck constant divided by 2π and $H(t)$ is a self-adjoint operator.

Thus, a single Hamiltonian sums up the whole dynamics of the system, even if there are changes in the process; and the hierarchy of moment is summarized in a single equation for the dynamics of the moment-generating functional, similarly to initially made by Doi(15).

Suppose a model with k different species, where $p(n_1, ..., n_k)$ is the probability of have n_i objects in i-th specie. Thus, the master equation is a way to study the behaviour of these probabilities at a time t. For the sake of notation, we will write $n = (n_1, ..., n_k) \in \mathbb{N}^k$.

Then, taking all probability distributions $p(n) = p_n$ and using the notation of Dirac ("brackets"), we can write the probabilistic state of the system as a vector

$$|v\rangle = \sum_n p_n |n\rangle. \tag{3.18}$$

Now consider the creation $a^\dagger$ and annihilation a operators and the commutation relation $aa^\dagger - a^\dagger a = 1$. By the fact of $a^\dagger$ "to create" particles, we have the vector $(a^\dagger)^n|0\rangle$, which is the probability distribution where there is exactly n particles, that is, $|n\rangle = (a^\dagger)^n|0\rangle$. Then, we can write the state as

$$|v\rangle = \sum_n p_n (a^\dagger)^n |0\rangle. \tag{3.19}$$

Consider, too, the reference state $0\rangle = e^{a^\dagger}|0\rangle$. It will be useful because it is the state that corresponds to the probability distribution that satisfies the normalization condition $|v\rangle = 1$, which is equivalent to $\sum_n p_n = 1$. Thus, the expected number of particles in state $|v\rangle$ is $n = n|v\rangle$. As the master equation is linear, can be written similar to the Schrödinger equation:

$$\frac{d}{dt}|v\rangle = -H|v\rangle \tag{3.20}$$

The linear operator H is the same Hamiltonian seen in section 3.3. It varies according to the model we are studying, but if we use the equation 3.18, we can write it in terms of bosonics operators.

Suppose we have a model with a set of transitions T. Let be $r(\tau)$ the constant rate of the transition $\tau \in T$, and let be $n(\tau)$ and $m(\tau)$ the input vectors and output τ. Then, we can write

$$H = \sum_{\tau \in T} r(\tau)({a^\dagger}^{n(\tau)} - {a^\dagger}^{m(\tau)})a^{m(\tau)} \tag{3.21}$$

Note that each portion of the sum is formed by the difference of two terms, which correspond to two situations that occur within a same transition τ. The first term, ${a^\dagger}^{n(\tau)} a^{m(\tau)}$, describes how $m_i(\tau)$ particles of i-th specie are annihilated, and $n_i(\tau)$ particles of i-th specie are created. The second term, ${a^{\dagger}}^{m(\tau)} a^{m(\tau)}$, describes the probability that nothing happens as time passes - i.e., the i-th state remains the same way to the end of the transition.

Furthermore, the second term has the function of ensuring the conservation of probability. That is, if we have $\sum_n p_n = 1$ at $t = 0$, the term quoted ensures that this sum of probability distributions remain equal to 1 in later times.

4 Occupation number representation

One of the applications of the theory seen so far is the study of chemical reactions. Basically, a reaction can be understood as the destruction of a molecule and its subsequent creation in another "site". This procedure can be used for the simplest reactions, as well as to complex systems involving many different species, for example the reaction-diffusion processes, which are well studied by science (see (16), (17), (18), (19), (20), (21) and (22)).

One of the objects of study of chemical reactions are the conditions that they meet to reach equilibrium, that is, the situation in which the proportion between the quantities of reactants and products remain constant over time. One way of looking at this is to write the master equation of the chemical reaction, and thus we can resolve two issues: The first point aims to verify the existence of an alleged steady state; already the second question, much more difficult, is to find out how this state is reached. This is done by looking at the long-time behaviour of such systems.

There is a well-defined path to write the master equation of a chemical system. However, instead of we list the method using generic species, we will stick to the most common and useful examples to our work, in particular the Lotka-Volterra model, which is very didactic in this case.

4.1 Chemical reaction $A \rightleftharpoons B$

Consider the situation where a particle can switch between two states, generically called 1 and 2; for example, consider a radioactive atom which has not disintegrated in state 1, whereas the state 2 is the atom after the disintegration.

We can represent the transitions between the states 1 and 2 as random events that happen at some rates (10). Let be one particle which jump from site 1 to site 2 with rate $\omega_{1\to 2}$; the inverse process, jump from site 2 to site 1, occurs at a constant rate $\omega_{2\to 1}$. If the particle is in the form A in state 1 and is in the form B in state 2, we can indicate the process by

$$A \underset{\omega_{2\to 1}}{\overset{\omega_{1\to 2}}{\rightleftharpoons}} B \tag{4.1}$$

We can study each step of reaction separately, then let us consider the reaction $A \to B$. Let be n_1 the quantity of particles of specie A (or in state 1), n_2 the quantity of particles of specie B (or in state 2), and $N = n_1 + n_2$ the total quantity of particles in system. We want to know the probability $p(n_1, n_2, t)$ that at a given time t there are exactly n_1 elements of A in state 1 and n_2 elements of B in state 2, and for this we deduce a differential equation for $p(n_1, n_2, t)$.

As before, we will describe the probabilities at times t and $t+dt$. What can happen in the interval $(t, t+dt)$? We have two situations:

1. No particle jumps from state 1 to state 2 in this period. The probability that one particle doesn't jump from 1 to 2 is $1 - \omega_{1\to 2}dt$, thence for n_1 particles we have $(1 - \omega_{1\to 2}dt)^{n_1}$. Expanding to first order in dt, we have $1 - n_1\omega_{1\to 2}dt + O(dt^2)$.

2. There is $n_1 + 1$ particles in state 1 and one particle jumps from 1 to 2 during the interval. The probability that one particle jumps is $\omega_{1\to 2}dt$, then the probability that any of the $n_1 + 1$ particles jumps from 1 to 2 is the sum of all these probabilities, i.e., $(n_1 + 1)\omega_{1\to 2}dt$.

Then, we write:

$$\begin{aligned} p(n_1, n_2, t+dt) = &\; p(n_1, n_2, t) \times \text{ Prob(no particle jumped)} \\ + &\; p(n_1+1, n_2-1, t) \times \text{ Prob(any of the } n_1 \text{ particles jump from 1 to 2)} \\ = &\; p(n_1, n_2, t) \cdot (1 - n_1\omega_{1\to 2}dt) \\ + &\; p(n_1+1, n_2-1, t) \cdot (n_1+1)\omega_{1\to 2}dt + O(dt^2) \end{aligned} \tag{4.2}$$

Rearranging and taking the limit $dt \to 0$ we obtain the master equation

$$\frac{\partial p(n_1, n_2, t)}{\partial t} = -n_1\omega_{1\to 2}p(n_1, n_2, t) + (n_1+1)\omega_{1\to 2}p(n_1+1, n_2-1, t) \tag{4.3}$$

We can describe this chemical reaction using quantum operations. Initially, we define the state vector as (9)

$$|\psi(t)\rangle = \sum_{n_1, n_2} P(n_1, n_2, t)|n_1, n_2\rangle = \sum_{n_1, n_2} P(n_1, n_2, t)(a^\dagger)^{n_1}(b^\dagger)^{n_2}|0\rangle \tag{4.4}$$

Then, we have

$$\begin{aligned} \tfrac{\partial}{\partial t}|\psi(t)\rangle = &\; \textstyle\sum_{n_1, n_2} \tfrac{\partial}{\partial t}P(n_1, n_2, t)(a^\dagger)^{n_1}(b^\dagger)^{n_2}|0\rangle \\ = &\; \textstyle\sum_{n_1, n_2} (-n_1\omega_{1\to 2}p(n_1, n_2, t) + (n_1+1)\omega_{1\to 2}p(n_1+1, n_2-1, t))(a^\dagger)^{n_1}(b^\dagger)^{n_2}|0\rangle \end{aligned} \tag{4.5}$$

Using the conversion

$$(n+1)(a^\dagger)^n = (1 + a^\dagger a)(a^\dagger)^n = aa^\dagger(a^\dagger)^n = a(a^\dagger)^{n+1} \tag{4.6}$$

we continue writing

$$\begin{aligned} \tfrac{\partial}{\partial t}|\psi(t)\rangle = &\; \textstyle\sum_{n_1, n_2} \omega_{1\to 2}p(n_1+1, n_2-1, t)(a^\dagger)^{n_1+1}(b^\dagger)^{n_2-1}b^\dagger a|0\rangle \\ - &\; \textstyle\sum_{n_1, n_2} \omega_{1\to 2}p(n_1, n_2, t)(a^\dagger)^{n_1}(b^\dagger)^{n_2}a^\dagger a|0\rangle \\ = &\; \omega_{1\to 2}(b^\dagger a - a^\dagger a)|\psi(t)\rangle \end{aligned} \tag{4.7}$$

Therefore, we conclude that the Hamiltonian for the reaction is

$$H_{1\to2} = \omega_{1\to2}(b^\dagger a - a^\dagger a) \tag{4.8}$$

The back hopping from state 2 to state 1 leads in the same way, and we obtain

$$H_{2\to1} = \omega_{2\to1}(a^\dagger b - b^\dagger b), \tag{4.9}$$

and the total Hamiltonian for the reaction $A \rightleftharpoons B$ is the sum $H = H_{1\to2} + H_{2\to1}$; if we have $\omega_{2\to1} = -\omega_{1\to2}$, then

$$H = \omega_{1\to2}(b^\dagger a - a^\dagger a + a^\dagger b - b^\dagger b) = \omega_{1\to2}(b^\dagger - a^\dagger)(b - a). \tag{4.10}$$

4.2 Chemical reaction $A + B \to C$

The quantization process can be useful for studying the properties of chemical reactions, especially the larger and more complex (see (23), (24) and (25)); in this section, we rely on (10).

Consider the chemical reaction $A + B \to C$, where molecules of A react with elements of molecule B, resulting in a molecule C; for simplicity, the reaction is not reversible. An atom A can react (state 1) or no (state 2) with the atom B, to form C.

Consider the situation in which initially there are the same number N of particles A and B, and haven't C-molecules. We have that $n(t)$ is the number of the A-particles in state 1 at time t, thus the number of B particles will also be $n(t)$ (since one atom A combines with one atom B), and the number of particles of C is $N - n(t)$.

The rate of the combination of A with B to form C is denoted by $\omega(1 \to 2)$, and since there isn't reverse reaction, $\omega(2 \to 1) = 0$. Unlike the previous case, not always $\omega(1 \to 2)$ is constant; to A react with B, first the molecules of each species have find each other, in a relationship which will depend on various factors, such as the number n of elements and the volume of the container in which they are contained. To highlight these variations, it is more convenient to write $\omega[n]$ instead of $\omega(1 \to 2)$.

To deal with this difficulty, we consider each individual element that interferes in amount of elements of A, during the time interval $(t, t + dt)$. In this case, there are two situations to consider:

1. There are n elements of A at time t, but neither reacts with B, then no particle C is formed. The probability of this happen is

$$(1 - \omega(1 \to 2)[n]dt)^n(1 - \omega(2 \to 1)[n]dt)^{N-n} = 1 - n\omega[n]dt + O(dt^2).$$

2. There are $n+1$ particles of A at time t, and one them react with only one of $n+1$ particles of B. The probability of that one of particles of A react is $\omega[n+1]dt$; already the probability that any of the $n+1$ particles react is $(n+1)\omega[n+1]dt$.

Combining these two cases, we have

$$\begin{aligned} P(n;t+dt) &= P(n;t)[1-n\omega[n]dt] \\ &\quad +P(n+1;t)[(n+1)\omega[n+1]dt] \end{aligned}.$$

Making the operations and taking the limit $dt \to 0$, we come to

$$\frac{\partial P(n;t)}{\partial t} = -n\omega[n]P(n;t) + (n+1)\omega[n]P(n+1;t) \tag{4.11}$$

As in the previous case, we can describe this chemical reaction using quantum operations, and this is similar to the previous case, because we have two states, although we have three species. Defining $n_1 = n$ and $n_2 = (N-n)$, we can write the state vector as

$$|\psi(t)\rangle = \sum_{n_1,n_2} P(n_1,n_2,t)|n_1,n_1,n_2\rangle = \sum_{n_1,n_2} P(n_1,n_2,t)(a^\dagger)^{n_1}(b^\dagger)^{n_1}(c^\dagger)^{n_2}|0\rangle \tag{4.12}$$

Then, we have

$$\begin{aligned} \tfrac{\partial}{\partial t}|\psi(t)\rangle &= \sum_{n_1,n_2} \tfrac{\partial}{\partial t}P(n_1,n_2,t)(a^\dagger)^{n_1}(b^\dagger)^{n_1}(c^\dagger)^{n_2}|0\rangle \\ &= \sum_{n_1,n_2} (-n_1\omega[n]p(n_1,n_2,t) + (n_1+1)\omega[n]p(n_1+1,n_2-1,t))(a^\dagger)^{n_1}(b^\dagger)^{n_1}(c^\dagger)^{n_2}|0\rangle \\ &= \sum_{n_1,n_2} \omega[n]p(n_1+1,n_2-1,t)(a^\dagger)^{n_1+1}(b^\dagger)^{n_1+1}(c^\dagger)^{n_2-1}c^\dagger ba|0\rangle \\ &- \sum_{n_1,n_2} \omega[n]p(n_1,n_2,t)(a^\dagger)^{n_1}(b^\dagger)^{n_1}(c^\dagger)^{n_2}a^\dagger ab^\dagger b|0\rangle \\ &= \omega[n](c^\dagger ab - b^\dagger ba^\dagger a)|\psi(t)\rangle \end{aligned} \tag{4.13}$$

Therefore, we define the Hamiltonian as

$$H = -\omega[n](c^\dagger ab - b^\dagger ba^\dagger a) = -\omega[n](c^\dagger b - b^\dagger a^\dagger)ba \tag{4.14}$$

4.3 Self-annihilation

Let us now study a type reaction where one element A self-destructs, that is, $A + A \to \emptyset$. This case, which a pair of particles annihilate, can be treated as a similar case of a diffusion process (see (9)).

Note that if $n+2$ react with each other in a time t, $P(n;t)$ is increased; already a reaction of two particles in a state with occupation number n leads to a decrease of $P(n;t)$. If this occurs at a rate ω, we can write the master equation to $P(n;t)$ as

$$\frac{\partial P(n;t)}{\partial t} = \omega(n+2)(n+1)\cdot P(n+2;t) - \omega n(n-1)\cdot P(n;t). \tag{4.15}$$

Substituting the above equation in the equation for the state vector $v = |\psi(t)\rangle$, seen earlier in this dissertation, we have:

$$\begin{aligned} \tfrac{\partial P(n;t)}{\partial t}|\psi(t)\rangle &= \sum_n \tfrac{\partial P(n;t)}{\partial t}(a^\dagger)^n|0\rangle \\ &= \sum_n(\omega(n+2)(n+1)\cdot P(n+2;t) - \omega n(n-1)\cdot P(n;t))(a^\dagger)^n|0\rangle \end{aligned} \tag{4.16}$$

Knowing that

$$(n+2)(n+1)(a^\dagger)^n = (n+2)[a(a^\dagger)^{n+1}] = a^2(a^\dagger)^{n+2}, \tag{4.17}$$

and that

$$\begin{aligned} n(n-1)(a^\dagger)^n &= (n^2-n)(a^\dagger)^n \\ &= ((a^\dagger a)^2 - (a^\dagger a))(a^\dagger)^n \\ &= a^\dagger a)(a^\dagger a) - (a^\dagger a))(a^\dagger)^n \\ &= (a^\dagger(\mathbb{I} + a^\dagger a)a - (a^\dagger a))(a^\dagger)^n \\ &= (a^\dagger)^2 a^2 (a^\dagger)^n \end{aligned} \tag{4.18}$$

we can continue writing

$$\begin{aligned} \tfrac{\partial P(n;t)}{\partial t}|\psi(t)\rangle &= \omega\textstyle\sum_n P(n+2;t)a^2(a^\dagger)^{n+2}|0\rangle - \omega\sum_n P(n;t)(a^\dagger)^2a^2(a^\dagger)^n|0\rangle \\ &= \omega(a^2-(a^\dagger)^2a^2)|\psi(t)\rangle \end{aligned} \tag{4.19}$$

Therefore, of the last equality and according by (9), we conclude that the Hamiltonian for the reaction in question is

$$H = \omega(a^2 - (a^\dagger)^2 a^2) \tag{4.20}$$

.

4.4 Diffusion on the lattice

Consider another simple case of diffusion, the particles jump from a site i to a site j at a constant rate D. The probability $P(n_i, n_j, t)$ increases when the particle is in configuration $\eta = (n_i + 1, n_j - 1)$ and jump to site j; likewise, $P(n_i, n_j, t)$ decreases if the particle jumps from i to j in a configuration $\eta = (n_i, n_j)$. Thus, we can write the master equation as:

$$\frac{\partial}{\partial t}P(n_i,n_j,t) = D(n_i+1)\cdot P(n_i+1,n_j-1,t) - Dn_i\cdot P(n_i,n_j,t), \tag{4.21}$$

The vector state $v = |\psi(t)\rangle$ is given by

$$|\psi(t)\rangle = \sum_{n_i,n_j} P(n_i,n_j,t)|n_i,n_j\rangle = \sum_{n_i,n_j} P(n_i,n_j,t)(a_i^\dagger)^{n_i}(a_j^\dagger)^{n_j}|0\rangle \tag{4.22}$$

Therefore, we have

$$\begin{aligned}
\frac{\partial}{\partial t}|\psi(t)\rangle &= \textstyle\sum_{n_i,n_j} \frac{\partial}{\partial t} P(n_i,n_j,t)(a_i^\dagger)^{n_i}(a_j^\dagger)^{n_j}|0\rangle \\
&= \textstyle\sum_{n_i,n_j}(D(n_i+1)\cdot P(n_i+1,n_j-1,t) - Dn_i \cdot P(n_i,n_j,t))(a_i^\dagger)^{n_i}(a_j^\dagger)^{n_j}|0\rangle \\
&= \textstyle\sum_{n_i,n_j} D\cdot P(n_i+1,n_j-1,t)a_j^\dagger a_i (a_i^\dagger)^{n_i+1}(a_j^\dagger)^{n_j-1}|0\rangle \\
&\quad -\textstyle\sum_{n_i,n_j} D\cdot P(n_i,n_j,t)a_i^\dagger a_i (a_i^\dagger)^{n_i}(a_j^\dagger)^{n_j}|0\rangle \\
&= D(a_j^\dagger a_i - a_i^\dagger a_i)|\psi(t)\rangle
\end{aligned} \tag{4.23}$$

Thus, we define

$$H_{i\to j} = -D(a_j^\dagger a_i - a_i^\dagger a_i). \tag{4.24}$$

For the back process, of site j to site i, the process is similar, getting

$$H_{j\to i} = D(a_i^\dagger a_j - a_j^\dagger a_j). \tag{4.25}$$

Thus, the total hopping Hamiltonian between sites i and j is the sum of $H_{i\to j}$ with $H_{j\to i}$, that is,

$$H = D(a_j^\dagger - a_i^\dagger)(a_j - a_i). \tag{4.26}$$

We can generalize the result for the lattice, since the particles are allowed to jump only to the neighbouring site. So we have

$$H_{diff}(i) = D\cdot \sum_{\langle i,j\rangle}(a_i^\dagger - a_j^\dagger)(a_i - a_j), \tag{4.27}$$

where the sum is taken over nearby neighborhoods $\langle i,j\rangle$.

4.5 A useful generalization

Based in the previous examples, one can deduce a method for write the Hamiltonian of a chemical reaction without resort to the master equation.

Consider the reaction $aA + bB \to cC$, where A, B, C are species and a, b, c are the quantities. Suppose, also, that the reaction occurs at a rate ω. Then, using the fact that the particles of A and B are annihilated and particles of C are created, as particles in a box, we write the Hamiltonian H as

$$H = -\omega((C^\dagger)^c A^a B^b - (A^\dagger)^a A^a (B^\dagger)^b B^b) \tag{4.28}$$

Note that H has two parts. The first parcel refers to fact that the C is created and A and B are annihilated, while the second parcel refers to fact that it does not, that is, A and B are annihilated and created next.

4.6 Lotka-Volterra model

Let us study a well-known population dynamics model, the Lotka-Volterra model. In this model, a predator A can reproduce through the ingestion of prey B, which survives and reproduces by eating a natural resource. The system remains in balance thanks to the positive or negative variation of the amount of predators and prey.

There are many simplifications assumed in this model, which is considered as a simple outline for what happens in reality. However, it is widely used because it contains the essential details (but not all) of the process. In addition, it is a foundation for building more complex models, including in other areas such as epidemiology, such as the SIR and SIRS models, which are models of transmission of communicable disease through individuals, where S - susceptible, I - infected and R - removed; for more information, see (26), (24) and (27).

The Lotka-Volterra model is composed of three distinct situations:

1. The preys reproduce at a rate σ spontaneously: $B \to B + B$. The Hamiltonian for this reaction can be described as $H_1 = -\sigma((b^\dagger)^2 - b^\dagger)b$.

2. The prey are eaten by predators, which at same time reproduce each other at a constant rate λ: $A + B \to A + A$. The Hamiltonian for this reaction can be described as $H_2 = -\lambda((a^\dagger)^2 - (a^\dagger b^\dagger)ab$.

3. The predators die (naturally or not), at a rate μ: $A \to \emptyset$. In this case, the Hamiltonian is $H_3 = -\mu(\mathbb{I} - a^\dagger)a$.

The total Hamiltonian of Lotka-Volterra model is simply the sum of these three Hamiltonians: $H = H_1 + H_2 + H_3$.

As Lotka-Volterra model can also be interpreted as reaction-diffusion system (see (9)), its Hamiltonian should be written as the sum of two Hamiltonians, one to describe the dispersion of the elements on the environment, and one for the set of reactions governing the system. Therefore, in terms of bosonic operators, we have:

$$
\begin{aligned}
H_{LV} = \quad & H_{diff} + H_{react} \\
& [D_A \textstyle\sum_{\langle i,j \rangle}(a_i^\dagger - a_j^\dagger)(a_i - a_j) + D_B \sum_{\langle i,j \rangle}(b_i^\dagger - b_j^\dagger)(b_i - b_j)] \\
& [-\lambda \textstyle\sum_i((a_i^\dagger)^2 - (a_i^\dagger b_i^\dagger)a_i b_i - \mu \sum_i(\mathbb{I} - a_i^\dagger)a_i - \sigma \sum_i((b_i^\dagger)^2 - b_i^\dagger)b_i]
\end{aligned}
\tag{4.29}
$$

Part II

Theoretical frameworks

5 Approach to mass action systems

Previously, we saw that can write a chemical reaction with k species in terms of creation and annihilation operators. We also saw that the Master Equation of the system can be written in a way analogous to the Schrödinger equation:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -H|\psi(t)\rangle. \tag{5.1}$$

Note that, solving this ODE, obtain

$$|\psi(t)\rangle = \exp(-tH)|\psi(0)\rangle, \tag{5.2}$$

where $\psi(0)$ is the initial condition of the system.

So, our goal now is to find an explicit formula for $\psi(t)$, which can greatly help in the study of system properties. For a long time, it was made by means of numerical methods, which do not always provide the precision required for this type of study. If done manually, it is a long and time consuming multistep process (see, for example, the model studied in (28)). With the advent of computer graphics, the calculations became easier, but even then the focus continued on the numerical solutions of the system.

But, recently, Santos, Gadêlha e Gaffney(29) created a method to find analytical solutions for small stochastic systems, using only Linear Algebra resources. In order to use the method described in this article, we will also use some quantum field theory settings.

Note that the Fock space of the above system is formed by tensor product of each Hilbert space S_i corresponding to the k component species of the chemical reaction, that is, $F = S_1 \otimes ... \otimes S_k$. Thus, an interesting question is to find a matrix representing H associated with a base of F, which we can denote by $(v_1, v_2, ..., v_k)$ or $(|1\rangle, |2\rangle, ..., |k\rangle)$.

For this, we have established a maximum number $N_{max}(s_i)$ of each specie and generate every the Fock space $|i\rangle = |s_1...s_k\rangle$ possible, where $s_i \in 0, ..., N_{max}(s_i)$, such that each element of the matrix H will be a billinear form where each term is given by $H_{ij} = H(v_i, v_j) = \langle i|H|j\rangle$. The elements of basis in the Fock space are the solutions of diophantine equation

$$s_1 + s_2 + ... + s_k = \sum_{i=1}^{k} N_{max}(s_i),$$

while the quantity of these elements can be easily determined using the multiplication principle.

If it is possible to find the matrix H, the computing of $\exp(-tH)$ can be done in several ways (see (30), (31), (32) and (33), for example) and we have the solution of the problem, because we find the general state $\psi(t)$ of the system, given the initial condition $\psi(0)$.

How does it work? Suppose that the initial condition is given by $\psi(0)\rangle = |s_1^0 s_2^0 ... s_k^0\rangle$. Initially we search, in the basis of the Fock space, the vector equivalent to $|\psi(0)\rangle$, which is a vector $|i\rangle$ of the basis. Furthermore, from the Linear Algebra, this vector is equivalent to the vector e_i of the canonical basis of $\mathbb{R}^k$, and by a property, if A is a matrix of a linear transformation, the product $A \cdot [e_i]$ is the i-th column of the matrix (for more information, see (34)). That is, in our case, we have

$$|\psi(t)\rangle = \exp(-tH)|\psi(0)\rangle \Leftrightarrow \begin{bmatrix} \psi_1(t) \\ . \\ . \\ . \\ \psi_k(t) \end{bmatrix} = \begin{bmatrix} \\ \exp(-tH) \\ \\ \end{bmatrix} \begin{bmatrix} \\ e_i \\ \\ \end{bmatrix} \tag{5.3}$$

If we have the function $|\psi(t)\rangle$, is possible evaluate the averages $\langle s_j \rangle$ of elements of the system, in time t, under the initial condition $|\psi(0)\rangle$. Remember that each element of the basis of the Fock Space is of the form $|i\rangle = |i_1 i_2 i_3 ... i_n\rangle$; as we have $|\psi(t)\rangle = \sum_{i=1}^{k} \psi_i |i\rangle$, the average of the element s_j, in time t, is given by:

$$\langle s_j \rangle = \sum_{i=1}^{k} \psi_i \cdot i_j. \tag{5.4}$$

This result is useful to study the system properties that are not possible to be described analytically using other approaches, such as numerical simulations.

6 Biological oscillators

Oscillators are very common and extensively studied in physics. They may be forced - if there is an external force dependent of the time - and/or damped - if a frictional force proportional to the velocity is also present. If the system is not forced or damped, it is called simple. There are classic examples of these oscillators, such as mass-spring system and the simple pendulum.

This type of oscillator has a periodic behaviour. For example, a swinging pendulum returns the same point in space x at regular intervals; furthermore, its velocity v also rises and falls with regularity. The amplitude of the oscillations depends on the initial perturbation, i.e., the height from which it is released θ.

Therefore, while the oscillators, especially the simple harmonic, are only an idealization, their study is justified by the practical fact that in many cases of real analysis of oscillators of complex systems, it is possible and even desirable to reduce the treatment as if they were the ideal type . This represents huge gains in several respects. However, strictly speaking, each case requires specific physical and mathematical treatment.

There are complex biological systems that are at the same time efficently compact and highly ordered; which, however, cannot be modelled solely on the basis of a characteristic period, since there would be required to accurately to study the model; then, in such systems is also considered a characteristic amplitude. In phase space, their trajectories correspond to a limit cycle. So, if there is a disturbance in the system, it will automatically return to normal behaviour, i.e., to its limit cycle. Then, we say that such systems are modelled by biological oscillators.

In the biomedical sciences, the biological oscillators are common, appear in widely varying contexts, have high precision (in some cases greater than powerful computer) and can have periods from a few seconds to hours to days and even weeks. According to (3) and (4), some models that can be described in terms of biological oscillators are the periodic behaviour of the heart, the approximately 24-hour periodic emergence of fruit flies from their pupae, the propagation of impulses in neurons, lifecycles of cells, testosterone levels in men and even chemical castration processes[1].

The first oscillating system that we know has been described by Lotka in the 1910 (35), and it was perfected later by Volterra (36), becoming known as Lotka-Volterra model, which was previously described.

Note that, in all examples cited above, the systems are linked to biological clocks,

[1] This is done by decreasing the testosterone production, with the aid of drugs as Goserelin, Lupon or Depo-provera(3).

which in turn are associated with external periodic functions, but these external periodicities do not force the system. Therefore, we say that the limit cycle oscillators are open systems thermodynamic arguments.

Traditionally, a way of describing a biological oscillator is to use a set of differential equations with some feedback control mechanism, which can be positive or negative, depending on the situation; although systems with negative feedback (feedback inhibition) are much more common than systems with positive feedback, see (37) and (38) for example.

6.1 Autocatalysis

As seen above, many biological systems can be built using feedback controls, which are very important and must be carefully assembled. A list of feedback control systems and how they work can be found in (39) and (37). Basically, according by Murray(3), feedback is when the product of one step in a reaction of the sequence has an effect on other reaction steps in the sequence. The effect is generally nonlinear and may be to activate or inhibit these reactions. An important feedback control is the autocatalysis. In chemistry, it is characterized by a reaction in which one of the reactants acts as a catalyst for the reaction itself. The reaction speed will be increasing as the catalyst (product) will constitute. A didactic example of autocatalytic reaction is

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2B \tag{6.1}$$

The classical Lotka-Volterra model ((35), (36)) is an example of biological oscillator model with autocatalysis. As we saw in chapter 2, the systems is composed by three reactions:

$$\begin{cases} B \to 2B \\ A + B \to 2A \\ A \to \emptyset \end{cases} \tag{6.2}$$

Note that the two first reactions of the model are autocatalytics.

In almost all biological processes, we don't know the biochemical reactions involved. However, we can study the qualitative behaviour of the process if make a small variation in a known reactant or if change the system operating conditions. We can study the case if we make a small change in a known reagent or if we change the system operating conditions. Then, an illuminating method used in modelling biological processes is to study this behavioural variation in the test model, and then make predictions in a broad context. That is, if we can represent a set of reactions as a system of differential equations, we can build models that represent the behaviour of the model in view of the concentrations of the species given by the same differential equations. For more information about this, see (3) and (4).

The problem with this form of study of systems is that the differential equations don't always have exact solutions. In many cases, it is necessary to use numerical methods, which only give approximate results, and typically can distort the model construction. Moreover, the study of the system is restricted, and the use of algebraic computing systems it is necessary to analyse the various cases.

Our goal now is to use the method described in this thesis, described in (29) and constructed with results of Fock Space, Linear Algebra and Quantum Field Theory, to study a particular problem. Then, we compare the results obtained with the method described above, based on analysis of differential equations and widespread in the scientific community, to verify the validity and effectiveness of the new study model.

6.2 Schnackenberg model

There are general results for models involving oscillations between two or more species, which exhibit limit cycle under certain conditions. These models are often represented by a system of various chemical reactions, and some of which are difficult to study. However, Hanusse (40) showed that, in system involving only two species, to have limit cycle solutions, the quantity of chemical reaction of the system is exactly three.

At first, this quantity of reactions may be insufficient to describe the system accurately, but models like this, from high-order systems, can be describe by this way if there are catalytic reactions involved in the process, for example (see (3) for more informations). So, it's plausible to consider trimolecular reactions not only for mathematical convenience.

In 1979, Schnackenberg (41) described a class of trimolecular reactions which allow periodic solutions. The simplest system is given by

$$\begin{cases} A \xrightarrow{1} X \\ X + 2Y \xrightarrow{2} 3Y \\ Y \underset{4}{\overset{3}{\rightleftharpoons}} B \end{cases} \tag{6.3}$$

This system it is proposed by a rewrite the Selkov model (42), used to describe the process of glycolysis, a set of metabolic reactions that degrade glucose for energy production. The model does not show periodic behaviour in all cases; in his article, Schnakenberg described the criteria needed so that there is limit cycle solution.

We will study a generalization of the model described by Schnakenberg. In our case, all reactions are reversible and the A and B concentrations are also variable. Therefore, we have

$$\begin{cases} A \underset{k_{1_-}}{\overset{k_{1_+}}{\rightleftharpoons}} X \\ X + 2Y \underset{k_{2_-}}{\overset{k_{2_+}}{\rightleftharpoons}} 3Y \\ Y \underset{k_{3_-}}{\overset{k_{3_+}}{\rightleftharpoons}} B \end{cases} \tag{6.4}$$

Note that, in this case, it is possible to quantify the chemical driving force of the overall reaction $A \rightleftharpoons B$, which has chemical potential difference (43)

$$\Delta G_{AB} = k_B \log(\tfrac{k_{1+}k_{2+}k_{3+}}{k_{1-}k_{2-}k_{3-}}).$$

Under the biomedical point of view it is relevant to consider the variations A and B in the model, since the system is open, and in this case the quantities of A and B are so large that their variations is negligible, therefore such quantities are considered constant (44). However, in this text, we will consider the general case, i.e., the chemical reaction $A \rightleftharpoons B$ added of an intermediate cubic autocatalytic reaction, in a closed system.

Part III

Results

7 Deterministic method (via ODE)

As previously mentioned, the system we will study consists of the following chemical reactions:

$$\begin{cases} A \underset{k_{1_-}}{\overset{k_{1_+}}{\rightleftharpoons}} X \\ X + 2Y \underset{k_{2_-}}{\overset{k_{2_+}}{\rightleftharpoons}} 3Y \\ Y \underset{k_{3_-}}{\overset{k_{3_+}}{\rightleftharpoons}} B \end{cases} \tag{7.1}$$

7.1 The simplifed case

In the simplified case, we consider that the system is open, that is, the system has external interference and some species are infinitely availabe in the system. In this case, suppose that we can determine the initial concentrations of the reactant and of the product; therefore, a and b, which represent respectively the species A and B, are constants; and we work with two instead of four equations. Then, we write the system of ODE's as

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}x(t) = k_{1+}a - k_{1-}x(t) - k_{2+}x(t)(y(t))^2 + k_{2-}(y(t))^3 \\ \frac{\mathrm{d}}{\mathrm{d}t}y(t) = k_{2+}x(t)(y(t))^2 - k_{2-}(y(t))^3 - k_{3+}y(t) + k_{3-}b \end{cases} \tag{7.2}$$

It is worth noting that the existence of limit cycle in this system is subject to the appropriate choice of a and b. So, an interesting question is to determine what criteria these constants should comply to the system return a periodic solution. Didactically, we can divide our research in four cases, in ascending order of generalization:

1. The reactions are not reversible; in this condition, we have $k_{1_-} = k_{2_-} = k_{3_-} = 0$, thus the system becomes independent of value of b. This case was discussed in Ref. (44).

2. The situation where $k_{1_-} = k_{2_-} = 0$, that is, the first and second reactions aren't reversible. Note that this is the Schnakenberg model itself (41). In Murray(3), it is treated the case where the other constants are equal to 1.

3. The intermediate situation where $k_{1_-} = 0$, i.e., only the first reaction are not reversible.

4. The general case.

With the exception of the first case, to determine the parameters a and b we use a method described in Murray(3). The idea is simple: write a and b as functions of x or y (only one of two), and plot a graphic in axis Oab. If the graph delineates a compact region (bounded by the axes, if necessary), then any point (a, b) within the region returns a limit cycle. All the calculations are described in the Maple code in the Appendix of this text.

Thus, if we know this parameters a and b, we can study better the system using the Fock Space method. Below, we have a graphic of system with parameters which return limit cycle, discovered by method described above and detailed in Appendix.

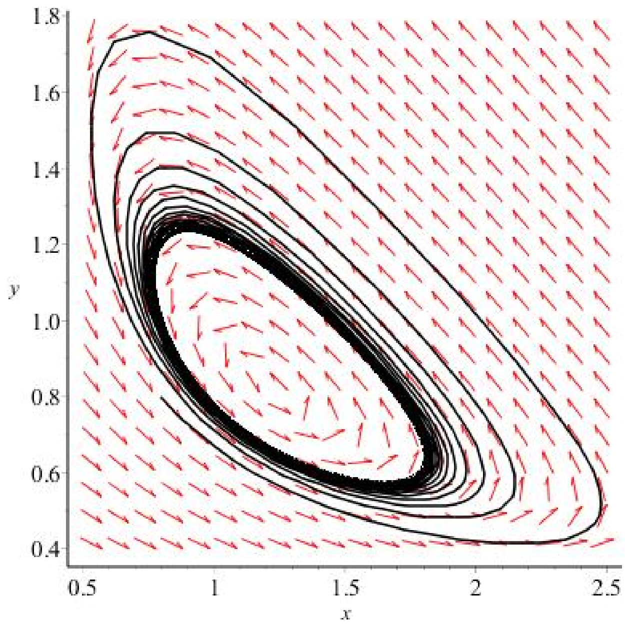

Figure 1 – Solution to the ODE system 7.2, with $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1, k_{1-} = k_{2-} = 0.1$ and $a = 0.9, b = 0.05$.

7.1.1 Irreversible reactions

In this case, we have $k_{1-} = k_{2-} = k_{3-} = 0$, as studied by Barragán (44). Note that, under this conditions, the system is independent of b.

The author used the traditional method to study of ODE's, which consists in linearize the system and analyze the fixed points. We found the fixed point and calculated the Jacobian of the system, obtaining respectively

$$(x_0, y_0) = \left(\frac{k_{3+}^2}{k_{2+}k_{1+}a}, \frac{k_{1+}a}{k_{3+}}\right) \text{ and } \tag{7.3}$$

$$J(x, y) = \begin{bmatrix} -k_{2+}\, y^2 & -2\, k_{2+}\, xy \\ k_{2+}\, y^2 & 2\, k_{2+}\, xy - k_{3+} \end{bmatrix}. \tag{7.4}$$

Now, we compute the Jacobian at the critical point:

$$J(x_0, y_0) = \begin{bmatrix} -\frac{k_{2+}\, a^2 k1c^2}{{k_{3+}}^2} & -2\,k_{3+} \\ \frac{k_{2+}\, a^2 k1c^2}{{k_{3+}}^2} & k_{3+} \end{bmatrix}. \tag{7.5}$$

The determinant and the trace of this matrix are

$$\frac{k_{2+}\, a^2 k1c^2}{k_{3+}} \text{ and } \frac{-k_{2+} a^2 k1c^2}{k_{3+}^2} + k_{3+}, \text{ respectively.} \tag{7.6}$$

Note that the determinant of the matrix is always greater than 0. So, we have a limit cycle if the trace of Jacobian is greater than 0 too, and we managed to get this relationship in terms of a^2, obtaining

$$a^2 = \frac{k_{3+}^3}{k_{2+} k_{1+}^2}. \tag{7.7}$$

Thus, if we take values such that

$$a^2 < \frac{k_{3+}^3}{k_{2+} k_{1+}^2},$$

the system returns a limit cycle. Indeed, it applies to the conditions below, for example, to $k_{1+} = k_{3+} = 0.2$ and $k_{2+} = 0.3$:

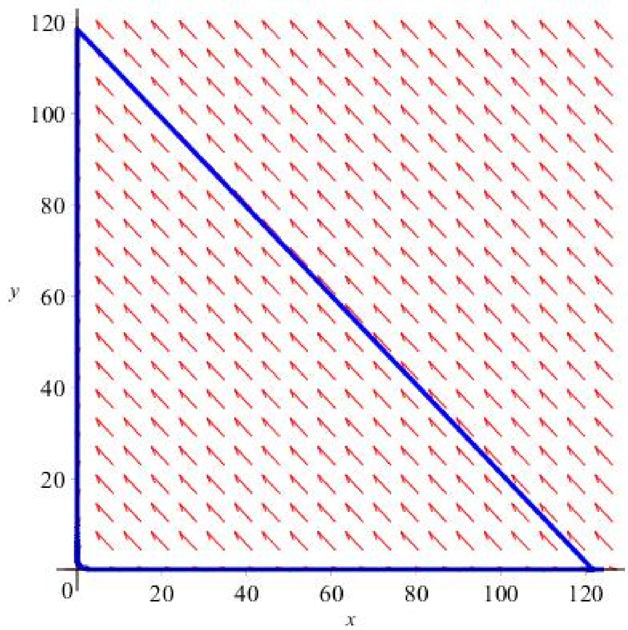

Figure 2 – Solution to the ODE system 7.2, with $k_{1+} = k_{3+} = 0.2, k_{2+} = 0.3, k_{1-} = 0, k_{2-} = 0, k_{3-} = 0$ and $a = \sqrt{0.66} - 0.1, b = 140$.

7.1.2 The Schnakenberg model

In this case, we have $k_{1-} = k_{2-} = 0$; it was described initially by Schnakenberg(41), and it is used as a teaching academic or pedagogical model for several authors in the study of biomathematics, among which Murray(3).

If we study the system using the previous method − i.e., finding the fixed points, computing the Jacobian, appling to the fixed point and calculating the determinant and the trace of the resulting matrix −, the study becomes more difficult if we follow this path. Therefore, we adopt the method described in Murray(3).

The fixed point of system is

$$(x_0, y_0) = \frac{ak_{1+}k_{3+}^2}{k_{2+}(ak_{1+} + bk_{3-})^2}, \frac{ak_{1+} + bk_{3-}}{k_{3+}}. \tag{7.8}$$

We will write x in terms of y; for this, from the fixed point, we isolate k_{3+}, obtaining

$$k_{3+} = \frac{ak_{1+} + bk_{3-}}{y} \tag{7.9}$$

and replace in x:

$$x = \frac{ak_{1+}}{k_{2+}y^2}, \tag{7.10}$$

obtaining the point

$$(x_0, y_0) = (\frac{ak_{1+}}{k_{2+}y^2}, y). \tag{7.11}$$

Thus, we replace this point at the Jacobian of the system:

$$\begin{bmatrix} -k_{2+}\, y^2 & -\frac{2k_{1+}\, a}{y} \\ k_{2+}\, y^2 & \frac{2k_{1+}\, a}{y} - k_{3+} \end{bmatrix}, \tag{7.12}$$

and calculate the determinant and the trace of the matrix, which are respectively:

$$k_{2+}k_{3+}y^2 \text{ and } -k_{2+}y^2 + \frac{2ak_{1+}}{y} - k_{3+}. \tag{7.13}$$

We have a Hopf bifurcation if the trace of the Jacobian is equal to 0. Therefore, solving the equation in terms of a, we get:

$$a = \frac{(k_{2+}y^2 + k_{3+})y}{2k_{1+}} \tag{7.14}$$

To find the value of b, we replace the value found in $y = \frac{ak_{1+}+bk_{3-}}{k_{3+}}$ and obtain

$$b = -\frac{y(k_{2+}y^2 - k_{3+})}{2k_{3-}} \tag{7.15}$$

Then, we plot the parametric graph $(\frac{(k_{2+}y^2+k_{3+})y}{2k_{1+}}, \frac{y(k_{2+}y^2-k_{3+}}{k_{3-}})$ in the axis Oab. For example, choosing every the non-zero constants equal to 1, we have the graph in figure 3.

For instance, take $(a, b) = (0.6, 0.1)$, we obtain a limit cycle plotted in figure 4.

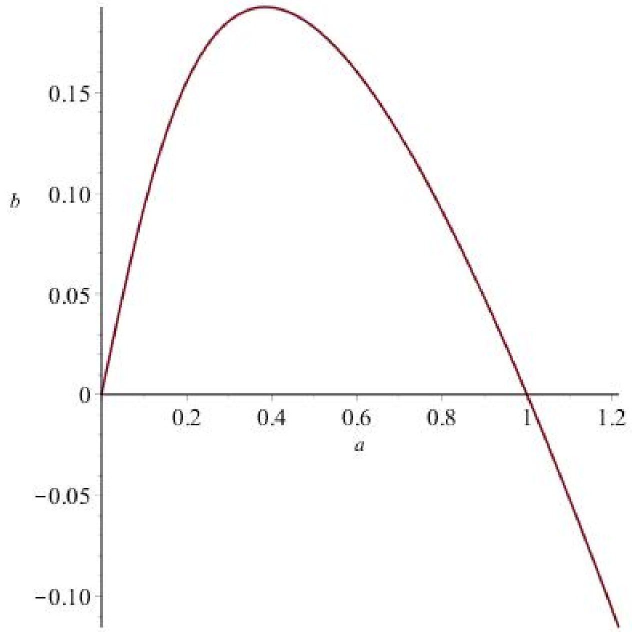

Figure 3 – Parametric graph in axis Oab for every non-zero constants equal to 1.

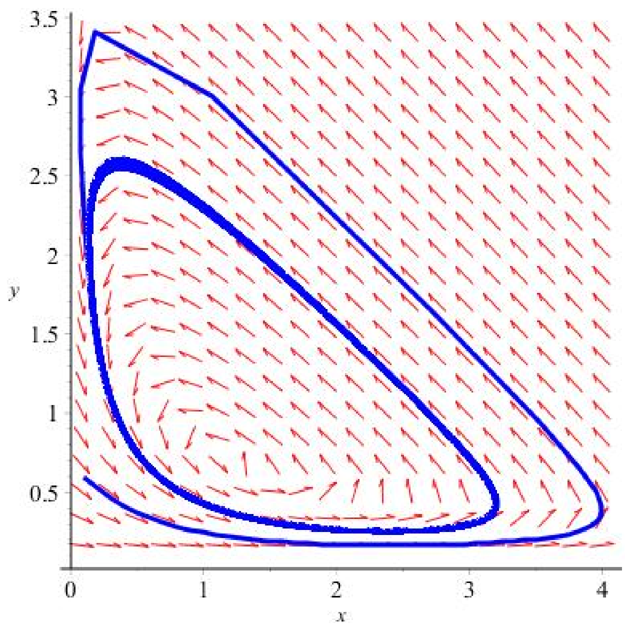

Figure 4 – Solution to the ODE system 7.2, with $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $a = 0.6, b = 0.1$.

7.1.3 The intermediate case

In this case, we have $k_{1-} = 0$. We will follow the same steps taken in previous case. First, we analyze the Jacobian at the fixed point found:

$$(x_0, y_0) = \frac{a^3 k_{1+}^3 k_{2-} + 3\,a^2 b k_{1+}^2 k_{2-} k_{3-} + 3\,ab^2 k_{1+} k_{2-} k_{3-}^2 + b^3 k_{2-} k_{3-}^3 + k_{1+} a k_{3+}^3}{k_{3+} k_{2+} \left(k_{1+} a + b k_{3-}\right)^2}, \frac{k_{1+} a + b k_{3-}}{k_{3+}} \tag{7.16}$$

Note that the fixed point found suggests that there is no easy job to find out the parameters a and b. Then, we apply the method described in Murray(3); at first, we write x in terms of y, from the fixed point found. Take $k_{3+} = \frac{k_{1+}a+bk_{3-}}{y}$ and substitute in x, obtaining:

$$x = \frac{k_{2-}y^3 + ak_{1+}}{k_{2+}y^2}. \tag{7.17}$$

We compute the Jacobian and its determinant and trace at the point $(\frac{k_{2-}y^3+ak_{1+}}{k_{2+}y^2}, y)$:

$$J(x_0, y_0) = \begin{bmatrix} -k_{2+}\,y^2 & -\frac{2\,k_{2-}\,y^3+2\,k_{1+}\,a}{y} + 3\,k_{2-}\,y^2 \\ k_{2+}\,y^2 & \frac{2\,k_{2-}\,y^3+2\,k_{1+}\,a}{y} - 3\,k_{2-}\,y^2 - k_{3+} \end{bmatrix}, \tag{7.18}$$

$$k_{2+}\,y^2 k_{3+} \text{ and } -k_{2+}\,y^2 + \frac{2\,k_{2-}\,y^3 + 2\,k_{1+}\,a}{y} - 3 \text{ and } k_{2-}\,y^2 - k_{3+}, \text{ respectively.} \tag{7.19}$$

We have a Hopf bifurcation when trace of matrix is equal to 0. Then, we obtain

$$a = \frac{(k_{2+}y^2 + k_{2-}y^2 + k_{3+})y}{2k_{1+}}. \tag{7.20}$$

and substitute the result in $y = \frac{ak_{1+}+bk_{3-}}{k_{3+}}$, we obtain

$$b = -\frac{y(k_{2+}y^2 + k_{2-}y^2 - k_{3+})}{2k_{3-}}. \tag{7.21}$$

Thus, we plot the parametric graph $(\frac{(k_{2+}y^2+k_{2-}y^2+k_{3+})y}{2k_{1+}}, -\frac{y(k_{2+}y^2+k_{2-}y^2-k_{3+})}{2k_{3-}})$ in axis Oab. For example, take every the non-zero constants equal to 1, we have:

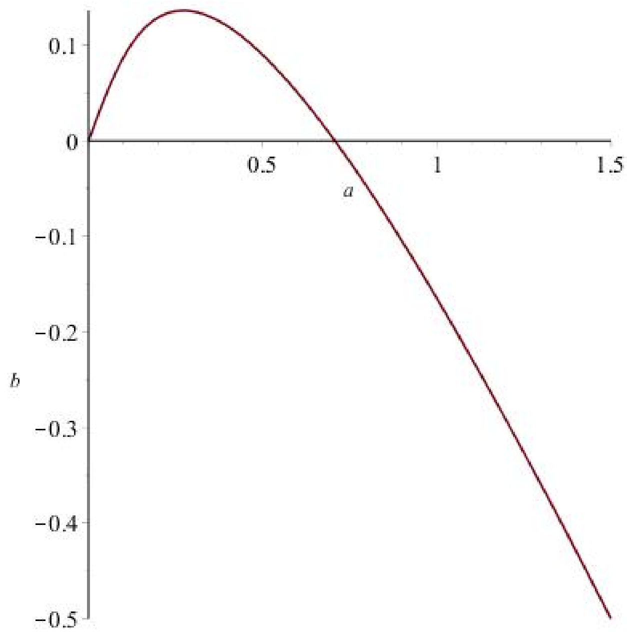

Figure 5 – Parametric graph in axis Oab for non-zero constants equal to 1.

For instance, if we take the parameters such that $(a, b) = (0.4, 0.1)$, we obtain a limit cycle. The initial condition of system, in this example, is $(0.1, 0.6)$:

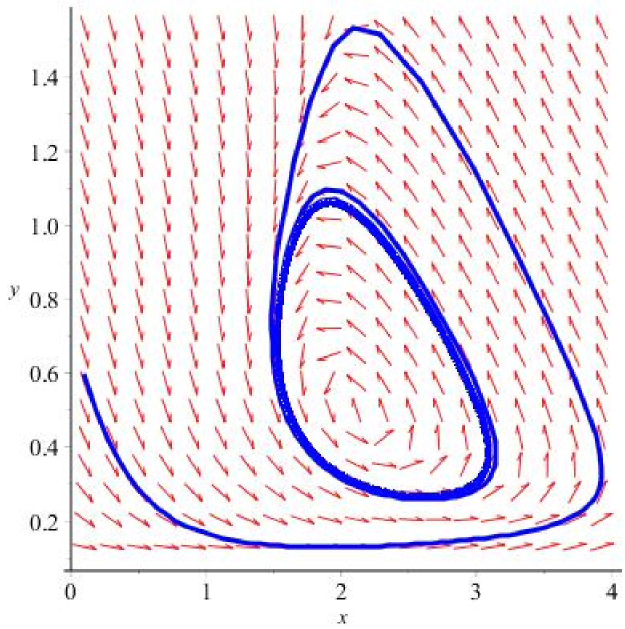

Figure 6 – Solution to the ODE system 7.2, with $k_{1+} = k_{2+} = k_{3+} = k_{2-} = k_{3-} = 1$ and $a = 0.6, b = 0.1$.

7.1.4 All reactions are reversible

This case is more complex than previous, regardless of the way forward. The difficulty starts from the calculation of the fixed point, which gives us one real fixed point and two complex fixed points, not suitable to be described here. In the Appendix, there is a Maple code to estimate numerically the Jacobian, its determinant and trace in specific cases.

Applying the method developed by Murray(3), we will try to write x in terms of y. For this, due to the cumbersome expressions involving the computation of the fixed points; we perform this computation using the command *RootOf* (see Appendix). We notice that, in this case, the x and y terms in the *RootOf* command are identical. Then, substituting y in x, we have

$$x = \frac{k_{2-}(ak_{1+} + bk_{3-})y^2 + k_{3+}^2 y - bk_{3+}k_{3-}}{(k_{1-}k_{2-} + k_{2+}k_{3+})y^2} \tag{7.22}$$

Next, we compute the Jacobian at the point $(x_0, y_0) = \frac{k_{2-}(ak_{1+}+bk_{3-})y^2+k_{3+}^2 y-bk_{3+}k_{3-})}{(k_{1-}k_{2-}+k_{2+}k_{3+})y^2}, y$, obtaining:

$$J(x_0, y_0) = \begin{bmatrix} -k_{2+}\, y^2 - k_{1-} & -\frac{2k_{2+}\left(k_{2-}\,(k_{1+}\,a+bk_{3-})y^2+k_{3+}^2 y-bk_{3+}\,k_{3-}\right)}{(k_{1-}\,k_{2-}+k_{2+}\,k_{3+})y} + 3\,k_{2-}\,y^2 \\ k_{2+}\,y^2 & \frac{2k_{2+}\left(k_{2-}\,(k_{1+}\,a+bk_{3-})y^2+k_{3+}^2 y-bk_{3+}\,k_{3-}\right)}{(k_{1-}\,k_{2-}+k_{2+}\,k_{3+})y} - 3\,k_{2-}\,y^2 - k_{3+} \end{bmatrix} \tag{7.23}$$

Its trace is

$$-k_{2+}\,y^2 - k_{1-} + 2\,\frac{k_{2+}\,\left(k_{2-}\,(k_{1+}\,a + bk_{3-})\,y^2 + k_{3+}^2 y - bk_{3+}\,k_{3-}\right)}{(k_{1-}\,k_{2-} + k_{2+}\,k_{3+})\,y} - 3\,k_{2-}\,y^2 - k_{3+} \tag{7.24}$$

The determinant is cumbersome, so it was left out of this text and it is described in the Appendix.

Note that the trace of Jacobian depends on a and b. Then, instead of simply solve $Trace(J(x_0, y_0)) = 0$, we will add other equation, which is the coordinate y_0. Thus, we have a system of equations which solution is:

$$a = \frac{k_{2+}^2 y^4 + k_{2+}\,k_{2-}\,y^4 + 2\,k_{1-}\,k_{2+}\,y^2 + 3\,k_{1-}\,k_{2-}\,y^2 + k_{2+}\,y^2 k_{3+} + k_{1-}^2 + k_{1-}\,k_{3+}}{2yk_{1+}\,k_{2+}} \tag{7.25}$$

$$b = -\frac{y\left(k_{2+}\,y^2 + k_{2-}\,y^2 + k_{1-} - k_{3+}\right)}{2k_{3-}} \tag{7.26}$$

Now, we can plot this graph in the axis Oab. Choosing $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $k_{1-} = k_{2-} = 0.1$, we have:

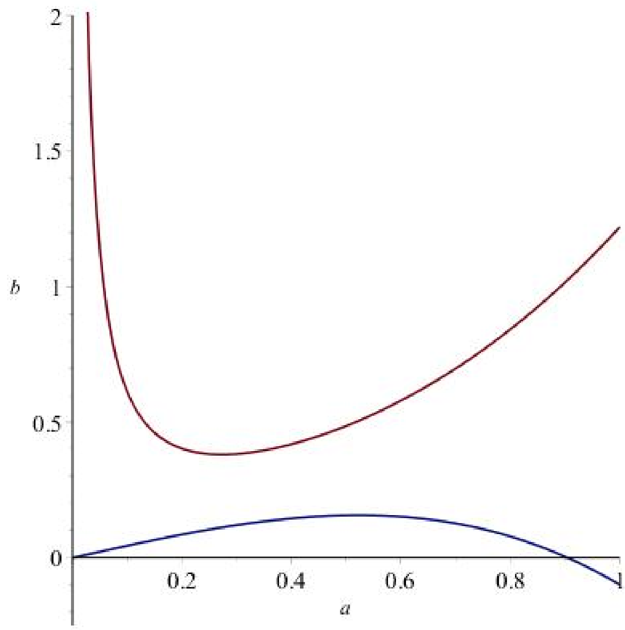

Figure 7 – Graph in axis Oab, for $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $k_{1-} = k_{2-} = 0.1$.

Note that the graph delineates various regions in plane AB, but there is only one closed region, which is delimited by the blue line. Then, the region is much smaller than in other cases. As example, choose at $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $k_{1-} = k_{2-} = 0.1, a = 0.75, b = 0.05$, with initial condition of system $x_0 = 0.8, y_0 = 0.6$:

7.2 The general case

If the system is closed, that is, there is no external interference, we have four ODE's to describe the system. Then, using the mass action law, we write the rate equations for

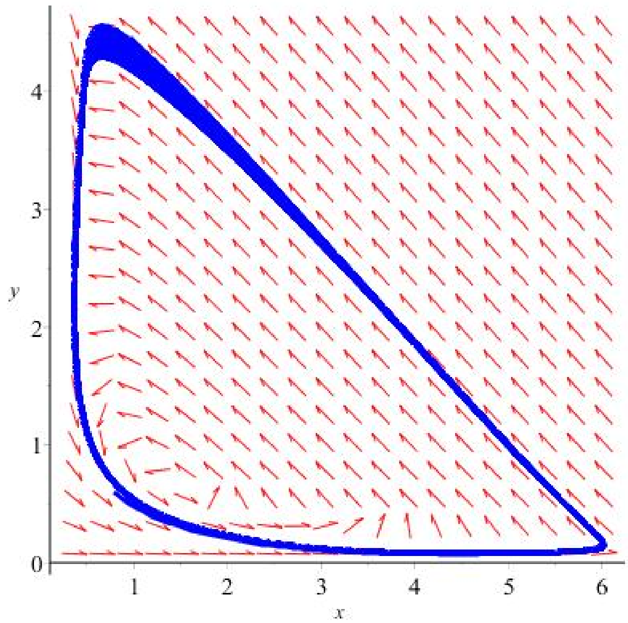

Figure 8 – Solution to the ODE system 7.2, with $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $k_{1-} = k_{2-} = 0.1, a = 0.75, b = 0.05$ and $x_0 = 0.8, y_0 = 0.6$.

the system 7.1 as:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}a\left(t\right) = -k_{1+}\,a\left(t\right) + k_{1-}\,x\left(t\right) \\ \frac{\mathrm{d}}{\mathrm{d}t}x\left(t\right) = k_{1+}\,a\left(t\right) - k_{1-}\,x\left(t\right) - k_{2+}\,x\left(t\right)\left(y\left(t\right)\right)^2 + k_{2-}\,\left(y\left(t\right)\right)^3 \\ \frac{\mathrm{d}}{\mathrm{d}t}y\left(t\right) = k_{2+}\,x\left(t\right)\left(y\left(t\right)\right)^2 - k_{2-}\,\left(y\left(t\right)\right)^3 - k_{3+}\,y\left(t\right) + k_{3-}\,b\left(t\right) \\ \frac{\mathrm{d}}{\mathrm{d}t}b\left(t\right) = k_{3+}\,y\left(t\right) - k_{3-}\,b\left(t\right) \end{cases} \tag{7.27}$$

This system has two fixed points $p_i = (a*, x*, y*, b*)$:

$$\begin{aligned} p_1 &= (\tfrac{k_{1-}}{k_{1+}}x(t), x(t), 0, 0) \\ p_2 &= (\tfrac{k_{1-}k_{2-}}{k_{2+}k_{1+}}y(t), \tfrac{k_{2-}}{k_{2+}}y(t), y(t), \tfrac{k_{3+}}{k_{3-}}y(t)) \end{aligned} \tag{7.28}$$

The Jacobian of this system is

$$J(x,y) = \begin{bmatrix} -k_{1+} & k_{1-} & 0 & 0 \\ k_{1+} & -k_{2+}\,y^2 - k_{1-} & -2\,k_{2+}\,xy + 3\,k_{2-}\,y^2 & 0 \\ 0 & k_{2+}\,y^2 & 2\,k_{2+}\,xy - 3\,k_{2-}\,y^2 - k_{3+} & k_{3-} \\ 0 & 0 & k_{3+} & -k_{3-} \end{bmatrix} \tag{7.29}$$

which applied in fixed points p_1 and p_2, results in

$$J_{p_1} = \begin{bmatrix} -k_{1+} & k_{1-} & 0 & 0 \\ k_{1+} & -k_{1-} & 0 & 0 \\ 0 & 0 & -k_{3+} & k_{3-} \\ 0 & 0 & k_{3+} & -k_{3-} \end{bmatrix} \tag{7.30}$$

and

$$J_{p_2} = \begin{bmatrix} -k_{1+} & k_{1-} & 0 & 0 \\ k_{1+} & -k_{2+}\,y^2 - k_{1-} & k_{2-}\,y^2 & 0 \\ 0 & k_{2+}\,y^2 & -k_{2-}\,y^2 - k_{3+} & k_{3-} \\ 0 & 0 & k_{3+} & -k_{3-} \end{bmatrix} \tag{7.31}$$

whose respective traces T_{p_i} are

$$T_{p_1} = -k_{1+} - k_{1-} - k_{3+} - k_{3-} \tag{7.32}$$

$$T_{p_2} = -k_{2+}\,y^2 - k_{2-}\,y^2 - k_{1+} - k_{1-} - k_{3+} - k_{3-} \tag{7.33}$$

Note that, in both cases, the trace is negative. In addition, the determinant of J_{p_1} and J_{p_2} are null.

The matrix J_{p_1} has three eigenvalues: 0 (with multiplicity 2), $-(k_{1+} + k_{1-})$ and $-(k_{3+} + k_{3-})$. By the other hand, the matrix J_{p_2} has four eigenvalues, some cumbersome and described in the program in Appendix B; but one of these eigenvalues is always 0 and the others three are negative, among which two can be complex and dependent on y. If we have $y = 0$, then the eigenvalues of J_{p_1} and J_{p_2} are equal.

With this, we can apply the Center Manifold Theorem[1] (for more information, see (45)) and we conclude that there are a one-dimensional center manifold in the system 7.3.

[1] Let $\mathbf{f} \in C^r(E)$, where E is an open subset of $\mathbb{R}^n$ containing the origin. If $\mathbf{f(0)=0}$ and the Jacobian matrix has n_S eigenvalues with negative real part, n_U eigenvalues with positive real part, and $n_C = n - n_S - n_U$ purely imaginary eigenvalues, then there exists an n_C-dimensional center manifold W_C of class C^r which is tangent to the center manifold E_C of the linearized system.

8 Quantum method (via Fock Space)

8.1 The simplified case

In the simplified case, where a and b are fixed and constant, we make a small adjustment in system: replace this species for empty ($\emptyset$), and then the first reaction will be creation of species X, while the last reaction becomes annihilation of species Y. This occurs because a and b can be found in infinite quantities in the system. Therefore, we have

$$\begin{cases} \emptyset \underset{k_{1_-}}{\overset{k_{1_+}}{\rightleftharpoons}} X \\ X + 2Y \underset{k_{2_-}}{\overset{k_{2_+}}{\rightleftharpoons}} 3Y \\ Y \underset{k_{3_-}}{\overset{k_{3_+}}{\rightleftharpoons}} \emptyset \end{cases} \tag{8.1}$$

As we have just two species, then the Fock space is $F = X \bigotimes Y$. Writing in terms of quantum operators, where x and y represent respectively the species X and Y, the Hamiltonians of the system are

$$\begin{aligned} H_{1_+} &= -k_{1_+}(x^\dagger \cdot 1 - 1 \cdot 1), \\ H_{1_-} &= -k_{1_-}(1 \cdot x - x^\dagger x), \\ H_{2_+} &= -k_{2_+}((y^\dagger)^3 y^2 x - (y^\dagger)^2 y^2 x^\dagger x), \\ H_{2_-} &= -k_{2_-}((y^\dagger)^2 x^\dagger y^3 - (y^\dagger)^3 y^3), \\ H_{3_+} &= -k_{3_+}(1 \cdot y - y^\dagger y), \\ H_{3_-} &= -k_{3_-}(y^\dagger \cdot 1 - 1 \cdot 1). \end{aligned} \tag{8.2}$$

and the total Hamiltonian, $H = H_{1_+} + H_{1_-} + H_{2_+} + H_{2_-} + H_{3_+} + H_{3_-}$, is

$$\begin{aligned} H = \; & -k_{1_+}(x^\dagger - 1) - k_{1_-}(1 - x^\dagger)x - k_{2_+}((y^\dagger)^3 - (y^\dagger)^2 x^\dagger) y^2 x \\ & -k_{2_-}((y^\dagger)^2 x^\dagger - (y^\dagger)^3) y^3 - k_{3_+}(1 - y^\dagger) y - k_{3_-}(y^\dagger - 1). \end{aligned} \tag{8.3}$$

The basis that spans the system is constituted by all kets $|x_i\, y_i\rangle$, with $x_i \in X$ and $y_i \in Y$. In this case, the basis for only one particle is given by

$$|1\rangle = |0\ 0\rangle, |2\rangle = |0\ 1\rangle, |3\rangle = |1\ 0\rangle, |4\rangle = |1\ 1\rangle. \tag{8.4}$$

The nonzero contribution for the Matrix representation, obtained according to the procedure explained in Chapter 5, are:

$$\begin{aligned} H_{ij} = & -\delta_{y_i,y_j-1} \left(k_{2-}\ (y_j - 1)\,(y_j - 2)\,\delta_{x_i,x_j+1} + k_{3+}\,\delta_{x_i,x_j} \right) y_j - \left(k_{2+}\ x_j\, y_j\ (y_j - 1)\,\delta_{x_i,x_j-1} + k_{3-}\,\delta_{x_i,x_j} \right) \delta_{y_i,y_j+1} + \\ & \delta_{y_i,y_j} \left(\left(k_{2-}\ {y_j}^3 + (k_{2+}\ x_j - 3\,k_{2-})\,{y_j}^2 + (-k_{2+}\ x_j + 2\,k_{2-} + k_{3+})\,y_j + k_{1-}\ x_j + k_{1+} + k_{3-} \right) \delta_{x_i,x_j} - k_{1-}\ x_j\,\delta_{x_i,x_j-1} - k_{1+}\,\delta_{x_i,x_j+1} \right), \end{aligned}$$

and the matrix representation of the Hamiltonian to be written as

$$H = \begin{bmatrix} -k_{1+} - k_{3-} & k_{3+} & k_{1-} & 0 \\ k_{3-} & -k_{3+} - k_{1+} - k_{3-} & 0 & k_{1-} \\ k_{1+} & 0 & -k_{1-} - k_{1+} - k_{3-} & k_{3+} \\ 0 & k_{1+} & k_{3-} & -k_{3+} - k_{1-} - k_{1+} - k_{3-} \end{bmatrix} \tag{8.5}$$

We have seen that the general solution of the system is given by

$$|\psi(t)\rangle = \sum_{x_i, y_i} P(x_i, y_i; t) |x_i\, y_i\rangle, \tag{8.6}$$

where $P(x_i, y_i; t)$ is the probability of the system be found in a state with exactly x_i and $y_i$elements at time t, while the sum runs over all vectors in the basis set. However, we can describe the general solution as

$$|\psi(t)\rangle = \exp(-Ht)|\psi(0)\rangle. \tag{8.7}$$

To evaluate e^{-Ht}, we compute the Jordan form of H, which we denote J_H. As we have $J_H = Q^{-1} \cdot H \cdot Q$, we can write $H = Q \cdot J_H \cdot Q^{-1}$, and then find

$$|\psi(t)\rangle = Q \cdot \exp(-J_H t) \cdot Q^{-1} |\psi(0)\rangle. \tag{8.8}$$

As seen in chapter 5, after finding e^{-Ht} we have

$$|\psi(t)\rangle = \psi_1(t)|1\rangle + \psi_2(t)|2\rangle + \psi_3(t)|3\rangle + \psi_4(t)|4\rangle \tag{8.9}$$

and we calculate the averages $\langle X\rangle$ and $\langle Y\rangle$. For evaluate each average, we take the respectively coordinates of each specie in each $|i\rangle$:

$$\begin{aligned} \langle X\rangle &= \psi_1(t)\cdot 0 + \psi_2(t)\cdot 0 + \psi_3(t)\cdot 1 + \psi_4(t)\cdot 1 \\ \langle Y\rangle &= \psi_1(t)\cdot 0 + \psi_2(t)\cdot 1 + \psi_3(t)\cdot 0 + \psi_4(t)\cdot 1 \end{aligned} \tag{8.10}$$

For the case of one particle of each specie, $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $k_{1-} = k_{2-} = 0.1$, we have the averages below. We have $\langle X\rangle$ in red and $\langle Y\rangle$ in blue.

All calculations are writed in Maple code described in Appendix.

8.2 The general case

In this case, we have

$$\begin{cases} A \underset{k_{1_-}}{\overset{k_{1_+}}{\rightleftharpoons}} X \\ X + 2Y \underset{k_{2_-}}{\overset{k_{2_+}}{\rightleftharpoons}} 3Y \\ Y \underset{k_{3_-}}{\overset{k_{3_+}}{\rightleftharpoons}} B \end{cases} \tag{8.11}$$

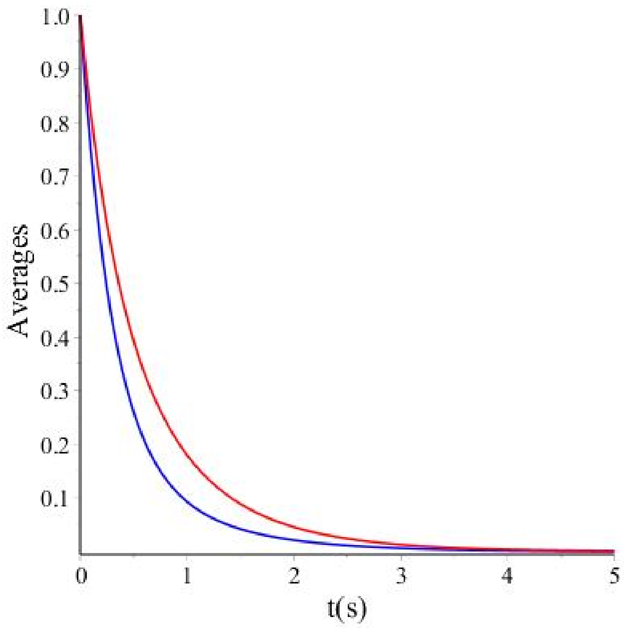

Figure 9 – Solution to the ODE system 8.1 to one particle, $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1, k_{1-} = k_{2-} = 0.1$.

For each of these six reactions, there is a corresponding Hamiltonian. Therefore, in terms of criation and annihilation operators, where a, x, y and b represent the species A, X, Y and B, respectively, we have

$$\begin{aligned}
H_{1_+} &= -k_{1_+}(x^\dagger a - a^\dagger a),\\
H_{1_-} &= -k_{1_-}(a^\dagger x - x^\dagger x),\\
H_{2_+} &= -k_{2_+}((y^\dagger)^3 y^2 x - (y^\dagger)^2 y^2 x^\dagger x),\\
H_{2_-} &= -k_{2_-}((y^\dagger)^2 x^\dagger y^3 - (y^\dagger)^3 y^3),\\
H_{3_+} &= -k_{3_+}(b^\dagger y - y^\dagger y),\\
H_{3_-} &= -k_{3_-}(y^\dagger b - b^\dagger b).
\end{aligned} \tag{8.12}$$

Thus the total Hamiltonian, $H = H_{1_+} + H_{1_-} + H_{2_+} + H_{2_-} + H_{3_+} + H_{3_-}$, is

$$\begin{aligned}
H = \quad & -k_{1_+}(x^\dagger - a^\dagger)a - k_{1_-}(a^\dagger - x^\dagger)x - k_{2_+}((y^\dagger)^3 - (y^\dagger)^2 x^\dagger) y^2 x\\
& -k_{2_-}((y^\dagger)^2 x^\dagger - (y^\dagger)^3) y^3 - k_{3_+}(b^\dagger - y^\dagger)y - k_{3_-}(y^\dagger - b^\dagger)b.
\end{aligned} \tag{8.13}$$

Following the steps described in (29), the Fock space is $F = A \otimes X \otimes Y \otimes B$, and the basis has 16 elements:

$$\begin{aligned}
&|1\rangle = |0\ 0\ 0\ 0\rangle, && |2\rangle = |0\ 0\ 0\ 1\rangle, && |3\rangle = |0\ 0\ 1\ 0\rangle, && |4\rangle = |0\ 0\ 1\ 1\rangle,\\
&|5\rangle = |0\ 1\ 0\ 0\rangle, && |6\rangle = |0\ 1\ 0\ 1\rangle, && |7\rangle = |0\ 1\ 1\ 0\rangle, && |8\rangle = |0\ 1\ 1\ 1\rangle,\\
&|9\rangle = |1\ 0\ 0\ 0\rangle, && |10\rangle = |1\ 0\ 0\ 1\rangle, && |11\rangle = |1\ 0\ 1\ 0\rangle, && |12\rangle = |1\ 0\ 1\ 1\rangle,\\
&|13\rangle = |1\ 1\ 0\ 0\rangle, && |14\rangle = |1\ 1\ 0\ 1\rangle, && |15\rangle = |1\ 1\ 1\ 0\rangle, && |16\rangle = |1\ 1\ 1\ 1\rangle.
\end{aligned} \tag{8.14}$$

For each Hamiltonian, we have a contribution $H_{ij} = \langle i|H|j\rangle$:

1. $H_{1+}: k_{1+}\,\delta_{y_i,y_j}\delta_{b_i,b_j}\left(a_i\,\delta_{a_i,a_j}\delta_{x_i,x_j} - x_i\,\delta_{a_j,a_i+1}\delta_{x_j,x_i-1}\right),$
2. $H_{1-}: -k_{1-}\,\delta_{y_i,y_j}\delta_{b_i,b_j}\left(a_i\,\delta_{a_j,a_i-1}\delta_{x_j,x_i+1} - x_i\,\delta_{a_i,a_j}\delta_{x_i,x_j}\right),$
3. $H_{2+}: \left({y_i}^2 x_i\delta_{x_i,x_j}\delta_{y_i,y_j} - y_i\,x_i\delta_{x_i,x_j}\delta_{y_i,y_j} - y_i\delta_{x_j,x_i+1}\delta_{y_j,y_i-1}\left(y_i-1\right)\left(y_i-2\right)\right)\delta_{a_i,a_j}\delta_{b_i,b_j}k_{2+},$
4. $H_{2-}: -\left(\delta_{x_j,x_i-1}\delta_{y_j,y_i+1}{y_i}^2 x_i - \delta_{x_j,x_i-1}\delta_{y_j,y_i+1}y_i\,x_i - y_i\delta_{x_i,x_j}\delta_{y_i,y_j}\left(y_i-1\right)\left(y_i-2\right)\right)\delta_{a_i,a_j}\delta_{b_i,b_j}k_{2-},$
5. $H_{3+}: -k_{3+}\,\delta_{a_i,a_j}\delta_{x_i,x_j}\left(b_i\,\delta_{b_j,b_i-1}\delta_{y_j,y_i+1} - y_i\,\delta_{b_i,b_j}\delta_{y_i,y_j}\right),$
6. $H_{3-}: k_{3-}\,\delta_{a_i,a_j}\delta_{x_i,x_j}\left(b_i\,\delta_{b_i,b_j}\delta_{y_i,y_j} - y_i\,\delta_{b_j,b_i+1}\delta_{y_j,y_i-1}\right).$

The total nonzero contribution for the Matrix representation are:

$$\begin{gathered}
H_{ij} = -k_{3+}\,y_j\,\delta_{a_i,a_j}\delta_{x_i,x_j}\delta_{y_i,y_j-1}\delta_{b_i,b_j+1} - k_{3-}\,b_j\,\delta_{a_i,a_j}\delta_{x_i,x_j}\delta_{y_i,y_j+1}\delta_{b_i,b_j-1} - \\
k_{2-}\,y_j\,\left(y_j-1\right)\left(y_j-2\right)\delta_{a_i,a_j}\delta_{x_i,x_j+1}\delta_{y_i,y_j-1}\delta_{b_i,b_j} - k_{2+}\,x_j\,y_j\,\left(y_j-1\right)\delta_{a_i,a_j}\delta_{x_i,x_j-1}\delta_{y_i,y_j+1}\delta_{b_i,b_j} \\
+\delta_{x_i,x_j}\left(k_{2-}\,{y_j}^3 + \left(k_{2+}\,x_j - 3\,k_{2-}\right){y_j}^2 + \left(-k_{2+}\,x_j + 2\,k_{2-} + k_{3+}\right)y_j + k_{3-}\,b_j + x_j\,k_{1-} + a_j\,k_{1+}\right)\delta_{a_i,a_j} \\
-a_j\,k_{1+}\,\delta_{a_i,a_j-1}\delta_{x_i,x_j+1} - x_j\,k_{1-}\,\delta_{a_i,a_j+1}\delta_{x_i,x_j-1})\delta_{y_i,y_j}\delta_{b_i,b_j}
\end{gathered}$$

The matrix element of Hamiltonian is of order 16×16. But despite its daunting size (it doesn't fit on this page, to get an idea), this matrix requires a simple treatment; starting with its 4 eigenvalues, each one with degeneracy 4:

$$\begin{array}{ll}
1. & -(k_{3+} + k_{3-} + k_{1+} + k_{1}-) \\
2. & -(k_{3+} + k_{3-}) \\
3. & -(k_{1+} + k_{1}-) \\
4. & 0
\end{array} \tag{8.15}$$

$\exp(-tH)$ and $|\psi(t)\rangle$ are evaluated in the same way of above case. The averages $\langle A\rangle, \langle X\rangle, \langle Y\rangle$ and $\langle B\rangle$ are given by

$$\begin{aligned}
\langle A\rangle = {} & \psi_9(t)\cdot 1 + \psi_{10}(t)\cdot 1 + \psi_{11}(t)\cdot 1 + \psi_{12}(t)\cdot 1 + \psi_{13}(t)\cdot 1 + \psi_{14}(t)\cdot 1 + \psi_{15}(t)\cdot 1 + \psi_{16}(t)\cdot 1, \\
\langle X\rangle = {} & \psi_5(t)\cdot 1 + \psi_6(t)\cdot 1 + \psi_7(t)\cdot 1 + \psi_8(t)\cdot 1 + \psi_{13}(t)\cdot 1 + \psi_{14}(t)\cdot 1 + \psi_{15}(t)\cdot 1 + \psi_{16}(t)\cdot 1, \\
\langle Y\rangle = {} & \psi_3(t)\cdot 1 + \psi_4(t)\cdot 1 + \psi_7(t)\cdot 1 + \psi_8(t)\cdot 1 + \psi_{11}(t)\cdot 1 + \psi_{12}(t)\cdot 1 + \psi_{15}(t)\cdot 1 + \psi_{16}(t)\cdot 1, \\
\langle B\rangle = {} & \psi_2(t)\cdot 1 + \psi_4(t)\cdot 1 + \psi_6(t)\cdot 1 + \psi_8(t)\cdot 1 + \psi_{10}(t)\cdot 1 + \psi_{12}(t)\cdot 1 + \psi_{14}(t)\cdot 1 + \psi_{16}(t)\cdot 1.
\end{aligned} \tag{8.16}$$

When we talk one particle of each specie, $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1$ and $k_{1-} = k_{2-} = 0.1$, we have the averages below:

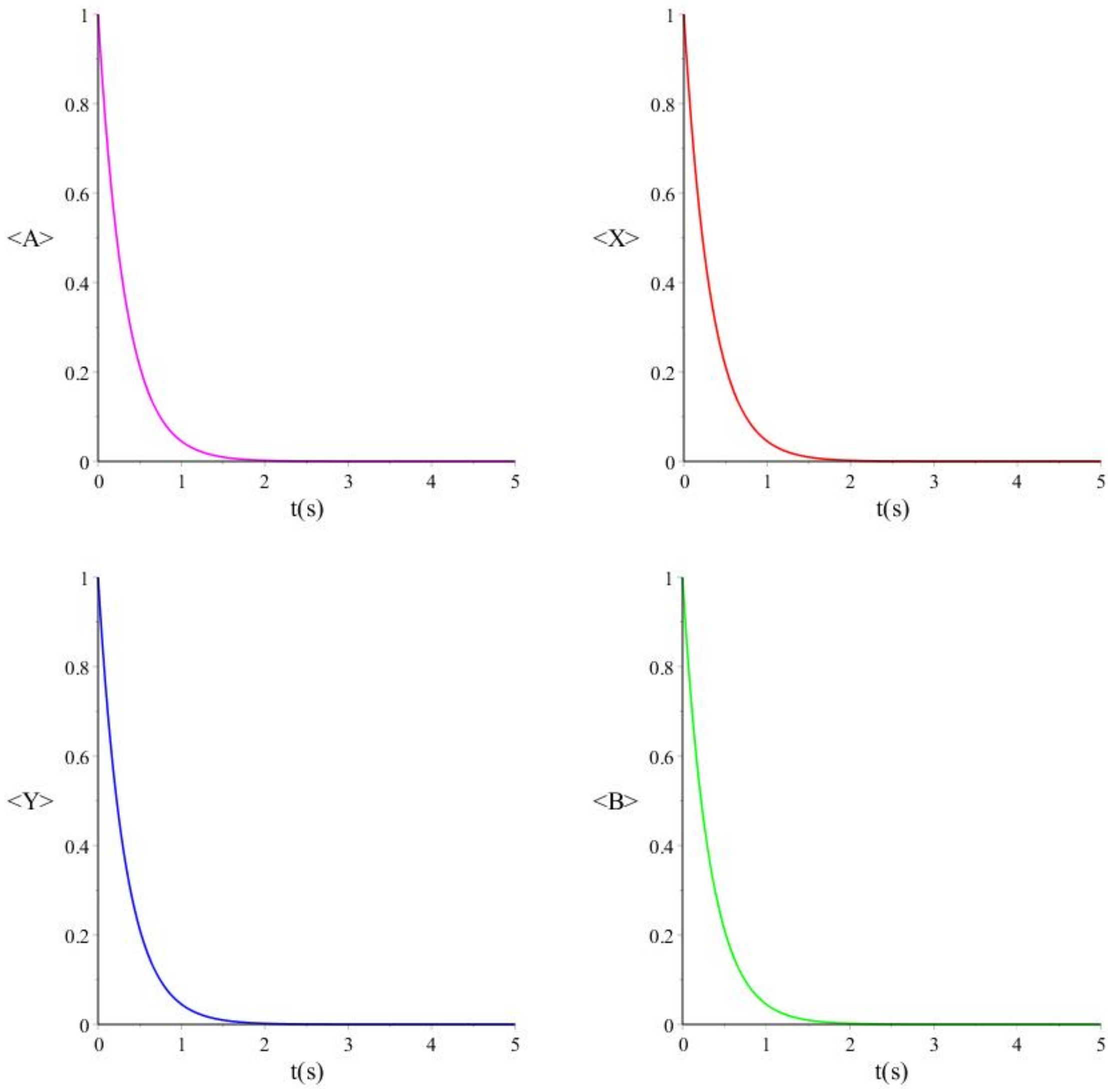

Figure 10 – Graph of averages, to one particle and $k_{1+} = k_{2+} = k_{3+} = k_{3-} = 1, k_{1-} = k_{2-} = 0.1$.

9 Discussion on the results

The quantum method for one particle shows that we have no oscillations or limit cycle for species, in contrast to results of deterministic method. This is a limitation of Fock Space approach: when we increase the number of particles, the complexity of the system does not allow us to find critical reaction constants due to the high dimensionality of the system. Therefore, we need to make some changes in the approach to the study to be more precise.

In our case, we refer to Gillespie Algorithm, which is a probabilistic simulation that generates a possible solution of a stochastic equation, and it is useful to simulate chemical or biochemical systems of reactions efficiently and accurately using limited computational power.

The Gillespie Algorithm is a variety of Monte Carlo methods; more precisely, one of steps is a Monte Carlo simulation. Basically, there are four steps in this algorithm:

1. We put the number of species in the system, the reaction constants and random number generators.

2. We generate random numbers to determine the next reaction to occur as well as the time interval, that is the Monte Carlo simulation in itself. The probability of a given reaction to be chosen is proportional to the number of substrate molecules.

3. Now we increase the time step by the randomly generated time in before step. We update the molecule count based on the reaction that occurred.

4. Go back to Monte Carlo simulation unless the number of reactants is zero or the simulation time has been exceeded.

As an perspective, we want to perform the Gilespie algorithm for reaction mentioned in this text. In fact, the simulation will may clarify the relation between the deterministic and stochastic approach for the Schnackenber model.

Conclusion

The difficulty of being in a wide and interdisciplinary field is that we must take the utmost care in time to take a step forward, just because we need to be consistent with all areas at the same time. Still, the immensity of things to discover and the precision in describing mathematically some biological process becomes necessary the advance in the study.

To avoid contradictions in the work, we took into account several topics, who formed a great prologue. We started, in chapter 1, writing the importance of chemical reactions in the description of biological processes. After, we saw some notions of probability, in chapter 2; rate and master equations, Fock space and its operators later in chapter 3. Moreover we study the occupation number representation, required to describe various chemical reactions, in chapter 4.

In second part of the text, we also explain how to describe biological processes using chemical reactions, Hamiltonians, master equations and quantum operators, in chapter 5, and in chapter 6, we describe the biological oscillators. This is a sign of interaction between various areas of science.

This type of interaction is useful and even common; what happens is that the problems are becoming more complex, and the tools used to study them need to be improved. In our case, where we study the Schnackenberg model, the traditional method of study made by ODE's is too extensive, but even so it was done in this text, which is an advance because it had not been done so far as a four dimensional dinamical system.

With respect to the Fock Space method, at least the species X and Y have no oscillations or limit cycle appears to exist for one particle only; and, since all eigenvalues are negatives, only relaxation (exponential decay) occurs. This results contrast with the deterministic results, where we demonstrated in section that a limit cycle occurs for the parameters determined in Chapter 7. This indicates that oscillations may occur for large size systems, or even in the thermodynamic limit (which actually corresponds to the deterministic approach).

The Fock space approach to chemical reactions has the intrinsic advantage that the solutions for small stochastic chemical systems are analytical in nature; however, a limitation is that, when we increase the number of particles, the complexity of the system does not allow us to find critical reaction constants due to the high dimensionality of the system. That said, a hybrid approach involving numerical and analytical methods is desirable.

As a perspective, in order to confirm that there are neither limit cycle nor oscillations for one particle, we should implement the Gillespie algorithm and perform the stochastic simulation. Once implemented this algorithm, we can find the critical size of the system, in which oscillations may occurs and thus implement the Fock space approach for the desirable parameters and system size. We demonstrated that, for the case of the Schnakenberg model, it is possible to write this reaction in terms of creation and annihilation operators and represent this system as matrix with a basis set created symbolically.

Concerning the problem of more them one particle, since we found a quite general matrix representation for the Hamiltonian, our symbolic approach can also be useful to get information about the system using methods from Linear Algebra. However, to get confident results, at this level of reserach, we should also compare our results with numeric simulations.

We hope that these results may contribute to a proper understanding of how a chemical reaction evolves from small stochastic system size, where the fluctuations are important, into deterministic systems in the thermodynamic limit.

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Appendix

APPENDIX A – Maple Code to Deterministic method (Simplified case)

In this code, we'll describe the process to determine the parameters *a* and *b* which return limit cycle, in case where the system is open. According described in chapter 7, we'll divide the study in four cases.

Before, an important warning: to facilitate the entering the code, we write respectively

$k1c$ and $k1d$

instead of

k_{1+} and k_{1-}

The same goes for the other constants that have subindices.

0. Description of the system

We begin our study write the packages necessary:

```
> with(DETools) : with(VectorCalculus) : with(LinearAlgebra) : with(plots) : with(linalg) : with(student) :
```

Initially, we will write the system of equations, in Maple language, for future reference:

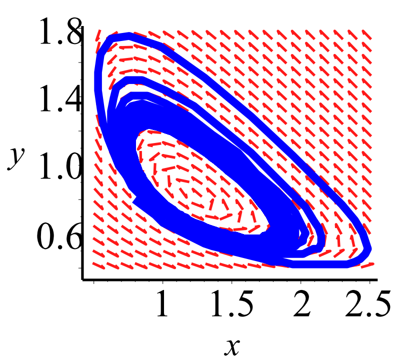
```
> #sis0 := proc(k1c, k1d, k2c, k2d, k3c, k3d, a, b)
  #diff(x(t), t) = k1c·a − k1d·x(t) − k2c·x(t)·y(t)^2 + k2d·y(t)^3,
  #diff(y(t), t) = k2c·x(t)·y(t)^2 − k2d·y(t)^3 − k3c·y(t) + k3d·b;
  # end proc;
```

The code below plots the phase portrait of system, with one initial condition (x0,y0). It will be very useful in our study.

```
> Sol3 :=proc(k1c, k1d, k2c, k2d, k3c, k3d, a, b, x0, y0)
  x4 := diff(x(t), t) = k1c·a − k1d·x(t) − k2c·x(t)·y(t)^2 + k2d·y(t)^3;
  y4 := diff(y(t), t) = k2c·x(t)·y(t)^2 − k2d·y(t)^3 − k3c·y(t) + k3d·b;
  i4 := x(0) = x0, y(0) = y0;
  DEplot({x4, y4}, [x(t), y(t)], t = 0 ..920, [[i4]], linecolor = blue, numpoints = 5000, thickness = 3);
  end proc:
Warning, `x4` is implicitly declared local to procedure `Sol3`
Warning, `y4` is implicitly declared local to procedure `Sol3`
Warning, `i4` is implicitly declared local to procedure `Sol3`
```

To test the code, we will generate the phase portrait of the figure 7.2, with initial condition (0.8,0.8):

```
> Sol3(1, 0.1, 1, 0.1, 1, 1, 0.9, 0.05, 0.8, 0.8)
```



1. The reactions aren't reversible

In this case, we have k1d=k2d=k3d=0, and was studied by Barragán (46). Note that, under this conditions, the system is independent of

b.
The author used the traditional method of study of ODE's, which consists in linearize the system and analyze the fixed points. We found the fixed point and calculate the Jacobian of the system:

> $solve(\{k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0\cdot y^3 - k3c*y + 0*b\}, \{x, y\});$
> $Jacobian([k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0*y^3 - k3c*y + 0*b], [x, y]);$

$$\left\{x = \frac{k3c^2}{k2c\ a\ k1c},\ y = \frac{a\ k1c}{k3c}\right\}$$

$$\begin{bmatrix} -k2c\ y^2 & -2\ k2c\ x\ y \\ k2c\ y^2 & 2\ k2c\ x\ y - k3c \end{bmatrix} \tag{2.1}$$

Now, we apply the fixed point in Jacobian, and calculate the determinant and the trace of matrix:

> $J2 := Jacobian\left([k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0*y^3 - k3c*y + 0*b], [x, y] = \left[\frac{k3c^2}{k2c\ k1c\ a}, \frac{k1c\ a}{k3c}\right]\right);$
> $D2 := Determinant(J2);$
> $T2 := Trace(J2);$

$$J2 := \begin{bmatrix} -\frac{k2c\ a^2\ k1c^2}{k3c^2} & -2\ k3c \\ \frac{k2c\ a^2\ k1c^2}{k3c^2} & k3c \end{bmatrix}$$

$$D2 := \frac{k2c\ a^2\ k1c^2}{k3c}$$

$$T2 := -\frac{k2c\ a^2\ k1c^2}{k3c^2} + k3c \tag{2.2}$$

Note that the determinant of the matrix, D2, is always greater than 0. So, we have limit cycle if the trace of J2 is greater than 0 too, and we managed to get this relationship in terms of a^2 :

> $solve(T2, a^2);$

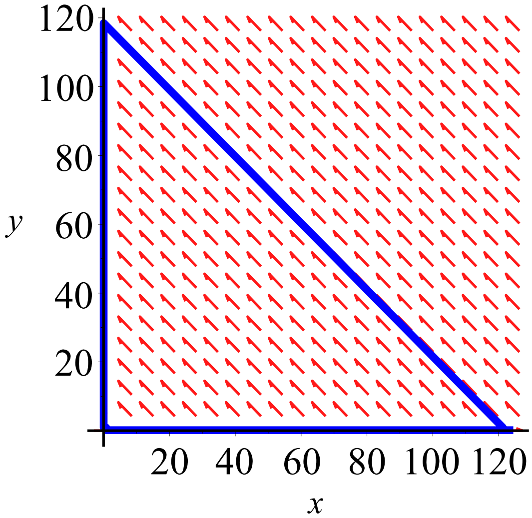
Warning, solving for expressions other than names or functions is not recommended.

$$\frac{k3c^3}{k2c\ k1c^2} \tag{2.3}$$

Thus, if we take values of a such that $a^2 < \frac{k3c^3}{k1c^2\ k2c}$, the system returns a limit cycle. Indeed, it applies to the conditions below, for example:

> $\left(\frac{(0.2)^3}{(0.2)^2\cdot(0.3)}\right);$
> $Sol3(0.2, 0, 0.3, 0, 0.2, 0, \mathrm{sqrt}(0.66) - 0.1, 140, 120, 0.006);$

$$0.6666666666$$



2. The Schnakenberg model

In this case, we have k1d=k2d=0; it was described initially by Schnakenberg (37), and it is used as a teaching model for several authors in the study of biomathematics, among which Murray (41).
Let's study the system using the previous method: find the fixed points, compute the Jacobian, apply to the fixed point and calculate the determinant and the trace of resulting matrix.

```
> solve({k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0·y^3 - k3c*y + k3d*b}, {x, y});

Jacobian([k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0*y^3 - k3c*y + k3d*b], [x, y]);
J3 := Jacobian([k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0*y^3 - k3c*y + k3d*b], [x, y] = [k1c a k3c^2/(k2c (a k1c + b k3d)^2), (a k1c + b k3d)/k3c]);
D3 := Determinant(J3);
T3 := Trace(J3);
```

$$\left\{x = \frac{a\,k1c\,k3c^2}{k2c\,(a\,k1c + b\,k3d)^2},\ y = \frac{a\,k1c + b\,k3d}{k3c}\right\}$$

$$\begin{bmatrix} -k2c\,y^2 & -2\,k2c\,x\,y \\ k2c\,y^2 & 2\,k2c\,x\,y - k3c \end{bmatrix}$$

$$J3 := \begin{bmatrix} -\frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c^2} & -\frac{2\,a\,k1c\,k3c}{a\,k1c + b\,k3d} \\ \frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c^2} & \frac{2\,a\,k1c\,k3c}{a\,k1c + b\,k3d} - k3c \end{bmatrix}$$

$$D3 := \frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c}$$

$$T3 := -\frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c^2} + \frac{2\,a\,k1c\,k3c}{a\,k1c + b\,k3d} - k3c \qquad \mathbf{(3.1)}$$

Note that the study becomes more difficult if we follow this path. Therefore, we adopt the method described in Murray, explained in Chapter 7.

Initially, we'll write x in terms of y. For this, from the fixed point, we isolate k3c

$\left(k3c = \dfrac{a\,k1c + b\,k3d}{y}\right)$ and replace in x:

$$> \frac{k1c\, a \left(\frac{a\, k1c + b\, k3d}{y}\right)^2}{k2c\, (a\, k1c + b\, k3d)^2}$$

$$\frac{a\, k1c}{k2c\, y^2} \tag{3.2}$$

Then, we obtain the point $\left(\dfrac{a\cdot k1c}{k2c\cdot y^2}, y\right)$. Thus, we replace this point in Jacobian of the system, and calculate the determinant and the trace of the matrix:

$$> J32 := Jacobian\left([k1c*a - 0*x - k2c*x*y^2 + 0*y^3, k2c*x*y^2 - 0*y^3 - k3c*y + k3d*b], [x, y] = \left[\frac{a\cdot k1c}{k2c\cdot y^2}, y\right]\right);$$
$Determinant(J32);$
$Trace(J32);$

$$J32 := \begin{bmatrix} -k2c\, y^2 & -\dfrac{2\, a\, k1c}{y} \\ k2c\, y^2 & \dfrac{2\, a\, k1c}{y} - k3c \end{bmatrix}$$

$$k2c\, k3c\, y^2$$

$$-k2c\, y^2 + \frac{2\, a\, k1c}{y} - k3c \tag{3.3}$$

We have a Hopf bifurcation if the trace of the Jacobian is equal to 0. Therefore, solving the equation in terms of a, we get:

$> solve(Trace(J32), a);$

$$\frac{1}{2}\, \frac{(k2c\, y^2 + k3c)\, y}{k1c} \tag{3.4}$$

To find the value of b, we replace the value found in $y = \dfrac{a\, k1c + b\, k3d}{k3c}$ and obtain:

$$> \frac{-\left(\frac{(k2c\, y^2 + k3c)\, y}{2\cdot k1c}\right) k1c + k3c\, y}{k3d}:$$
$normal(\%);$

$$-\frac{1}{2}\, \frac{y\, (k2c\, y^2 - k3c)}{k3d} \tag{3.5}$$

Then, we plot the parametric graph in axis *Oab:*

$> ABC31 :=$ **proc**$(k1c, k1d, k2c, k2d, k3c, k3d, yi, yf)$

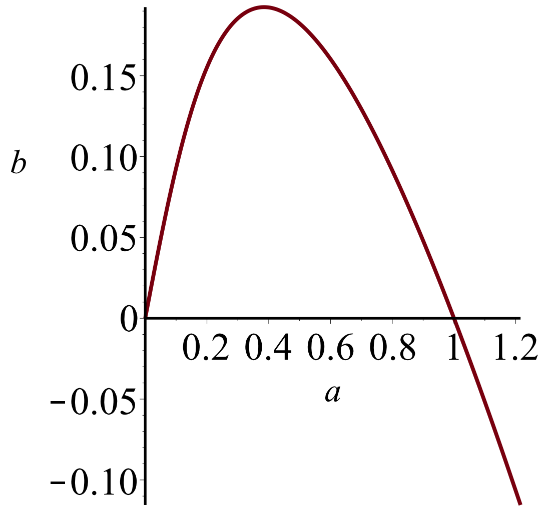
$$g1 := plot\left(\left[\frac{1}{2}\, \frac{(k2c\, y^2 + k3c)\, y}{k1c}, -\frac{1}{2}\, \frac{y\, (k2c\, y^2 - k3c)}{k3d}, \mathrm{y} = \mathrm{yi}\, ..\mathrm{yf}\right], labels = [a, b]\right):$$

end proc :

```
Warning, `g1` is implicitly declared local to procedure `ABC31`
```

For example, take every the non-zero constants equal to 1, we have:

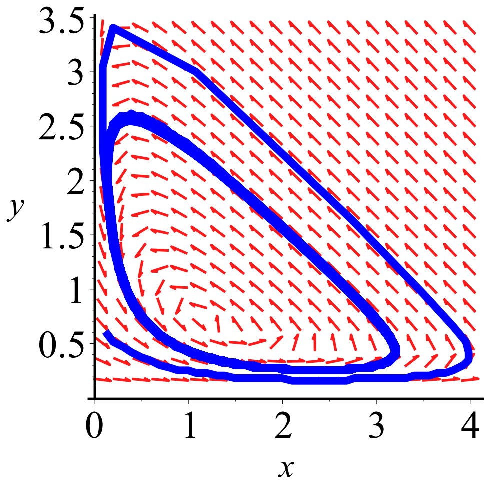
$> ABC31(1, 0, 1, 0, 1, 1, 0, 1.1);$



Really, take *(a,b)=(0.6,0.1)*, we obtain a limit cycle. The initial condition is (0.1,0.6):

> $Sol3(1, 0, 1, 0, 1, 1, 0.6, 0.1, 0.1, 0.6);$

```
Warning, plot may be incomplete, the following errors(s) were issued:
   cannot evaluate the solution further right of 678.16023, maxfun limit exceeded
(see ?dsolve,maxfun for details)
```



3. The intermediate case

In this case, we have k1d=0. We'll follow the same path taken in case 2. First, we analyze the Jacobian from the fixed point found.

> $solve(\{k1c*a - 0*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b\}, \{x, y\});$
> $Jacobian([k1c*a - 0*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b], [x, y]);$
> $J4 := Jacobian\left([k1c*a - 0*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b], [x, y]\right.$
> $= \left[\frac{a^3\ k1c^3\ k2d + 3\ a^2\ b\ k1c^2\ k2d\ k3d + 3\ a\ b^2\ k1c\ k2d\ k3d^2 + b^3\ k2d\ k3d^3 + a\ k1c\ k3c^3}{k3c\ k2c\ (a\ k1c + b\ k3d)^2}, \frac{a\ k1c + b\ k3d}{k3c}\right]\Big)\Big);$
> $D4 := Determinant(J4);$
> $T4 := Trace(J4)$

$$\left\{x = \frac{a^3\ k1c^3\ k2d + 3\ a^2\ b\ k1c^2\ k2d\ k3d + 3\ a\ b^2\ k1c\ k2d\ k3d^2 + b^3\ k2d\ k3d^3 + a\ k1c\ k3c^3}{k3c\ k2c\ (a\ k1c + b\ k3d)^2}, y = \frac{a\ k1c + b\ k3d}{k3c}\right\}$$

$$\begin{bmatrix} -k2c\,y^2 & -2\,k2c\,x\,y + 3\,k2d\,y^2 \\ k2c\,y^2 & 2\,k2c\,x\,y - 3\,k2d\,y^2 - k3c \end{bmatrix}$$

$$J4 := \left[\left[-\frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c^2}, -\frac{2\,(a^3\,k1c^3\,k2d + 3\,a^2\,b\,k1c^2\,k2d\,k3d + 3\,a\,b^2\,k1c\,k2d\,k3d^2 + b^3\,k2d\,k3d^3 + a\,k1c\,k3c^3)}{k3c^2\,(a\,k1c + b\,k3d)} + \frac{3\,k2d\,(a\,k1c + b\,k3d)^2}{k3c^2}\right], \left[\frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c^2}, \frac{2\,(a^3\,k1c^3\,k2d + 3\,a^2\,b\,k1c^2\,k2d\,k3d + 3\,a\,b^2\,k1c\,k2d\,k3d^2 + b^3\,k2d\,k3d^3 + a\,k1c\,k3c^3)}{k3c^2\,(a\,k1c + b\,k3d)} - \frac{3\,k2d\,(a\,k1c + b\,k3d)^2}{k3c^2} - k3c\right]\right]$$

$$D4 := \frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c}$$

$$T4 := -\frac{k2c\,(a\,k1c + b\,k3d)^2}{k3c^2} + \frac{2\,(a^3\,k1c^3\,k2d + 3\,a^2\,b\,k1c^2\,k2d\,k3d + 3\,a\,b^2\,k1c\,k2d\,k3d^2 + b^3\,k2d\,k3d^3 + a\,k1c\,k3c^3)}{k3c^2\,(a\,k1c + b\,k3d)} - \frac{3\,k2d\,(a\,k1c + b\,k3d)^2}{k3c^2} - k3c \qquad \textbf{(4.1)}$$

Note that the fixed point found suggests that there is no easy job to find out the parameters a and b. Then, we apply the method described in Murray; at first, we write x in terms of y, from the fixed point found. Take $k3c = \dfrac{a\,k1c + b\,k3d}{y}$ and substitute in x:

> $\dfrac{a^3\,k1c^3\,k2d + 3\,a^2\,b\,k1c^2\,k2d\,k3d + 3\,a\,b^2\,k1c\,k2d\,k3d^2 + b^3\,k2d\,k3d^3 + a\,k1c\left(\frac{a\,k1c + b\,k3d}{y}\right)^3}{\left(\frac{a\,k1c + b\,k3d}{y}\right)\cdot k2c\,(a\,k1c + b\,k3d)^2}$:
> $normal(\%)$;

$$\frac{k2d\,y^3 + a\,k1c}{k2c\,y^2} \qquad \textbf{(4.2)}$$

We compute the Jacobian in point $\left(\dfrac{k2d\,y^3 + a\,k1c}{k2c\,y^2}, y\right)$:

> $J41 := Jacobian\left([k1c*a - 0*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b], [x, y] = \left[\dfrac{k2d\,y^3 + a\,k1c}{k2c\,y^2}, y\right]\right)$;
> $Determinant(J41)$;
> $Trace(J41)$;

$$J41 := \begin{bmatrix} -k2c\,y^2 & -\frac{2\,(k2d\,y^3 + a\,k1c)}{y} + 3\,k2d\,y^2 \\ k2c\,y^2 & \frac{2\,(k2d\,y^3 + a\,k1c)}{y} - 3\,k2d\,y^2 - k3c \end{bmatrix}$$

$$k2c\,k3c\,y^2$$

$$-k2c\,y^2 + \frac{2\,(k2d\,y^3 + a\,k1c)}{y} - 3\,k2d\,y^2 - k3c \qquad \textbf{(4.3)}$$

We have a Hopf bifurcation when trace of $J41$ is equal to 0. Then, we solve

> $solve(Trace(J41), a)$

$$\frac{1}{2}\frac{(k2c\,y^2 + k2d\,y^2 + k3c)\,y}{k1c} \tag{4.4}$$

and substitute the result in $y = \dfrac{a\,k1c + b\,k3d}{k3c}$:

> $\dfrac{-\left(\frac{1}{2}\frac{(k2c\,y^2 + k2d\,y^2 + k3c)\,y}{k1c}\right)k1c + k3c\,y}{k3d}$:
> $normal(\%);$

$$-\frac{1}{2}\frac{y\,(k2c\,y^2 + k2d\,y^2 - k3c)}{k3d} \tag{4.5}$$

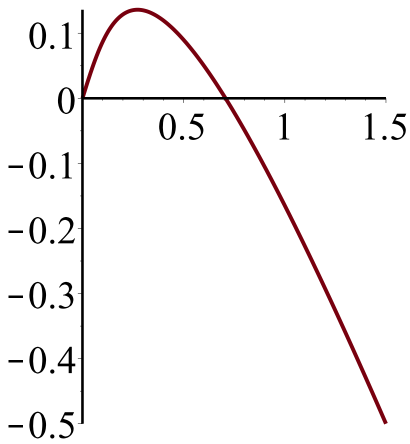
Thus, we plot the parametric graph in axis *Oab:*

> $ABC41 := \mathbf{proc}(k1c, k1d, k2c, k2d, k3c, k3d, yi, yf)$
> $h1 := plot\left(\left[\frac{1}{2}\frac{(k2c\,y^2 + k2d\,y^2 + k3c)\,y}{k1c}, -\frac{1}{2}\frac{y\,(k2c\,y^2 + k2d\,y^2 - k3c)}{k3d}, \mathrm{y} = \mathrm{yi}\,..\mathrm{yf}\right]\right)$:
> **end proc** :

```
Warning, `h1` is implicitly declared local to procedure `ABC41`
```

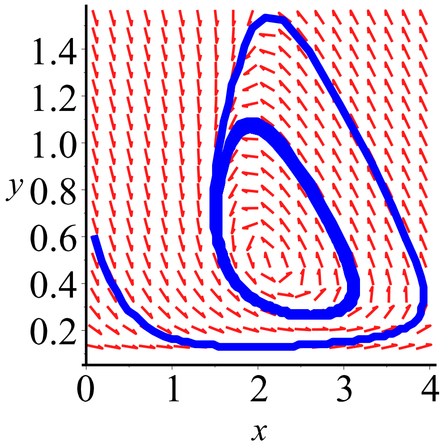
For example, take every the non-zero constants equal to 1, we have:

> $ABC41(1, 0, 1, 1, 1, 1, 0, 1);$



Really, take *(a,b)=(0.4,0.1)*, we obtain a limit cycle. The initial condition is (0.1,0.6):

> $Sol3(1, 0, 1, 1, 1, 1, 0.4, 0.1, 0.1, 0.6);$



4. The general case

This case is more complex than previous, regardless of the way forward. The difficulty starts from the calculation of fixed point:

> $solve(\{k1c*a - k1d*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b\}, \{x, y\});$

$$\{x = (a\,k1c\,k2d\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)^2 + b\,k2d\,k3d\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)^2 - b\,k3c\,k3d + k3c^2\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)) \Big/ ((k1d\,k2d + k2c\,k3c)\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)^2), y = RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)\} \quad \textbf{(5.1)}$$

A quick calculation, using the command *allvalues,* reveals that this result gives us one real fixed point and two complex fixed points.
Then, we consider only the real fixed point.
The programs below estimates numerically the Jacobian and its determinant and trace.

> $abc11 :=$ **proc**(k1c, k1d, k2c, k2d, k3c, k3d, a, b, x0, y0)

$Jacobian([k1c*a - k1d*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b], [x, y] = [(a\,k1c\,k2d\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)^2 + b\,k2d\,k3d\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)^2 - b\,k3c\,k3d + k3c^2\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)) \Big/ ((k1d\,k2d + k2c\,k3c)\,RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)^2), RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1d\,k3d)]);$

end proc:

$abc12 :=$ **proc**(k1c, k1d, k2c, k2d, k3c, k3d, a, b, a0, b0)
[*evalf*(*Determinant*(*abc11*(k1c, k1d, k2c, k2d, k3c, k3d, a, b, x0, y0))), *evalf*(*Trace*(*abc11*(k1c, k1d, k2c, k2d, k3c, k3d, a, b, x0, y0)))]
end proc:

Testing for k1c=k2c=k3c=k3d=1 and k1d=k2d=0.1, a=0.5, b=0.2, x0=0.1, y0=0.6:

> *abc11*(1, 0.1, 1, 0.1, 1, 1, 0.5, 0.2, 0.1, 0.6) :
ABC11 := *evalf*(%);

$$ABC11 := \begin{bmatrix} -0.437968220635514 & -1.27814991516112 \\ 0.337968220635514 & 0.278149915161124 \end{bmatrix} \quad \textbf{(5.2)}$$

> [*Determinant*(*ABC11*), *Trace*(*ABC11*)];
abc12(1, 0.1, 1, 0.1, 1, 1, 0.5, 0.2, 0.1, 0.6);

$$[0.310153229119401, -0.159818305474390]$$
$$[0.310153229142655, -0.159818305474390] \tag{5.3}$$

Note that the results are equal and that, under this conditions, the system returns a stable node.

Applying the artifice of Murray (41), we will try to write x in terms of y. For this, observe the term *RootOf(...)* in coordinate y of fixed point; it is identical to the term *RootOf(...)* described in coordinate x! Then, substitute y in x, we have

$$> \frac{a \cdot k1c \cdot k2d \cdot y^2 + b \cdot k2d \cdot k3d \cdot y^2 - b \cdot k3c \cdot k3d + k3c^2 \cdot y}{(k1d \cdot k2d + k2c \cdot k3c) \cdot y^2} :$$
$simplify(\%, size);$

$$\frac{k2d\,(a\,k1c + b\,k3d)\,y^2 + k3c^2\,y - b\,k3c\,k3d}{(k1d\,k2d + k2c\,k3c)\,y^2} \tag{5.4}$$

Next, we compute the Jacobian in point discovered:

$$> J131 := Jacobian\left([k1c*a - k1d*x - k2c*x*y^2 + k2d*y^3, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b], [x, y] = \left[\frac{k2d\,(a\,k1c + b\,k3d)\,y^2 + k3c^2\,y - b\,k3c\,k3d}{(k1d\,k2d + k2c\,k3c)\,y^2}, y\right]\right);$$
$Determinant(J131);$
$Trace(J131);$

$$J131 := \begin{bmatrix} -k2c\,y^2 - k1d & -\frac{2\,k2c\,(k2d\,(a\,k1c + b\,k3d)\,y^2 + k3c^2\,y - b\,k3c\,k3d)}{(k1d\,k2d + k2c\,k3c)\,y} + 3\,k2d\,y^2 \\ k2c\,y^2 & \frac{2\,k2c\,(k2d\,(a\,k1c + b\,k3d)\,y^2 + k3c^2\,y - b\,k3c\,k3d)}{(k1d\,k2d + k2c\,k3c)\,y} - 3\,k2d\,y^2 - k3c \end{bmatrix}$$

$$-\frac{1}{(k1d\,k2d + k2c\,k3c)\,y}\,(2\,a\,k1c\,k1d\,k2c\,k2d\,y^2 + 2\,b\,k1d\,k2c\,k2d\,k3d\,y^2 - 3\,k1d^2\,k2d^2\,y^3 - 4\,k1d\,k2c\,k2d\,k3c\,y^3 - k2c^2\,k3c^2\,y^3 - 2\,b\,k1d\,k2c\,k3c\,k3d - k1d^2\,k2d\,k3c\,y + k1d\,k2c\,k3c^2\,y)$$

$$-k2c\,y^2 - k1d + \frac{2\,k2c\,(k2d\,(a\,k1c + b\,k3d)\,y^2 + k3c^2\,y - b\,k3c\,k3d)}{(k1d\,k2d + k2c\,k3c)\,y} - 3\,k2d\,y^2 - k3c \tag{5.5}$$

Note that the trace of Jacobian depends on a and b. Then, instead of simply solve Trace(J131)=0, we will add other equation, which is the coordinate y from fixed point. Thus, we have the system:

$$> solve([y = RootOf((k1d\,k2d + k2c\,k3c)\,\_Z^3 + (-a\,k1c\,k2c - b\,k2c\,k3d)\,\_Z^2 + k1d\,k3c\,\_Z - b\,k1dk3d), \mathrm{Trace(J131)}], [a, b])$$

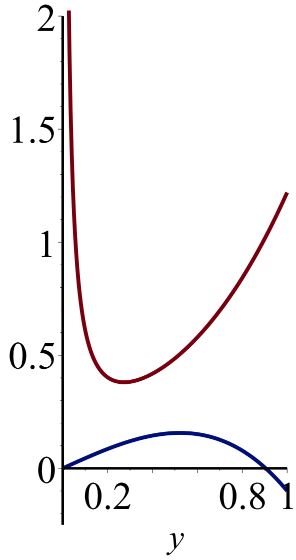
$$\left[\left[a = \frac{1}{2}\,\frac{k2c^2\,y^4 + k2c\,k2d\,y^4 + 2\,k1d\,k2c\,y^2 + 3\,k1d\,k2d\,y^2 + k2c\,k3c\,y^2 + k1d^2 + k1d\,k3c}{y\,k1c\,k2c}, b = -\frac{1}{2}\,\frac{y\,(k2c\,y^2 + k2d\,y^2 + k1d - k3c)}{k3d}\right]\right] \tag{5.6}$$

Now, we can plot the graph in axis *Oab*:

$$> abc150 := \mathbf{proc}(k1c, k1d, k2c, k2d, k3c, k3d)$$
$$plot\left(\left[\frac{1}{2}\,\frac{k2c^2\,y^4 + k2c\,k2d\,y^4 + 2\,k1d\,k2c\,y^2 + 3\,k1d\,k2d\,y^2 + k2c\,k3c\,y^2 + k1d^2 + k1d\,k3c}{y\,k1c\,k2c}, -\frac{1}{2}\,\frac{y\,(k2c\,y^2 + k2d\,y^2 + k1d - k3c)}{k3d}\right], y = 0..1\right)$$
end proc:

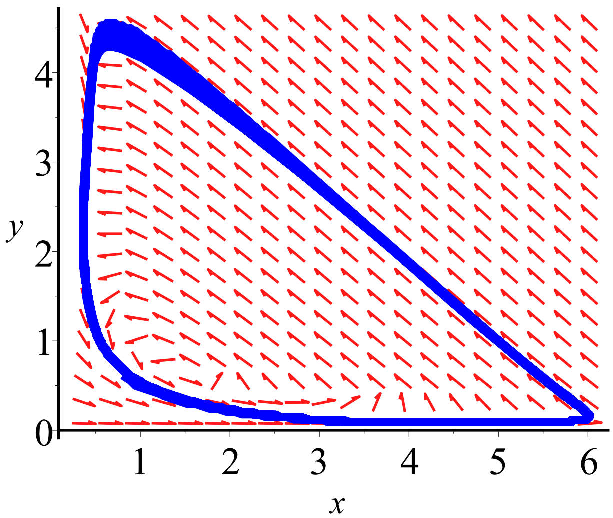
Testing for k1c=k2c=k3c=k3d=1 and k1d=k2d=0.1

> $abc150(1, 0.1, 1, 0.1, 1, 1)$



Note that the graph delineates various regions in plane AB, but there is only one closed region, which is delimited by the blue line.
Then, the region is much smaller than in other cases.
As example, look at k1c=k2c=k3c=k3d=1 and k1d=k2d=0.1, a=0.75,b=0.05 and x0=0.8, y0=0.6:

> $Sol3(1, 0.1, 1, 0.1, 1, 1, 0.75, 0.05, 0.8, 0.6)$



APPENDIX B – Maple Code to Deterministic method (General case)

In this code, we'll study the Schnackenberg model, in case where the system is closed, i.e., the general case.

Before, an important warning: to facilitate the entering the code, we write respectively $k1c$ and $k1d$ instead of k_{1+} and k_{1-}

The same goes for the other constants that have subindices.

1. Description of the system and fixed points

We begin our study write the packages necessary:

```
> with(DETools) : with(VectorCalculus) : with(LinearAlgebra) : with(plots) : with(linalg) : with(student) :
```

Initially, we will write the system of equations, in Maple language, for future reference:

```
> #sis1 := diff(a(t), t) = -k1c*a(t) + k1d*x(t),
  #diff(x(t), t) = k1c*a(t) - k1d*x(t) - k2c*x(t)*y(t)^2 + k2d*y(t)^3,
  #diff(y(t), t) = k2c*x(t)*y(t)^2 - k2d*y(t)^3 - k3c*y(t) + k3d*b(t),
  #diff(b(t), t) = k3c*y(t) - k3d*b(t);
```

We find the fixed points of system:

```
> solve({-k1c*a + k1d*x, -k2c*x*y^2 + k2d*y^3 + k1c*a - k1d*x, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b, k3c*y - k3d*b}, {a, x, y, b});
```

$$\left\{a = \frac{k1d\ x}{k1c},\ b = 0,\ x = x,\ y = 0\right\},\ \left\{a = \frac{k1d\ y\ k2d}{k2c\ k1c},\ b = \frac{k3c\ y}{k3d},\ x = \frac{y\ k2d}{k2c},\ y = y\right\} \tag{1.1}$$

2. Jacobian of the system

We describe the Jacobian of the system:

```
> MM0 := Jacobian([-k1c*a + k1d*x, -k2c*x*y^2 + k2d*y^3 + k1c*a - k1d*x, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b, k3c*y - k3d*b], [a,
  x, y, b]) :
  MM0
```

$$\begin{bmatrix} -k1c & k1d & 0 & 0 \\ k1c & -k2c\ y^2 - k1d & -2\ k2c\ x\ y + 3\ k2d\ y^2 & 0 \\ 0 & k2c\ y^2 & 2\ k2c\ x\ y - 3\ k2d\ y^2 - k3c & k3d \\ 0 & 0 & k3c & -k3d \end{bmatrix} \tag{2.1}$$

and applying the two fixed points found:

- The point $\left(\frac{k_{1+}x(t)}{k_{1-}},\ x(t),\ 0,\ 0\right)$:

```
> MM1 := Jacobian([-k1c*a + k1d*x, -k2c*x*y^2 + k2d*y^3 + k1c*a - k1d*x, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b, k3c*y - k3d*b],
  [a, x, y, b] = [k1d*x/k1c, x, 0, 0]) : MM1;
```

$$\begin{bmatrix} -k1c & k1d & 0 & 0 \\ k1c & -k1d & 0 & 0 \\ 0 & 0 & -k3c & k3d \\ 0 & 0 & k3c & -k3d \end{bmatrix} \tag{2.2}$$

- The point $\left(\frac{k_{1-}k_{2-}}{k_{1+}k_{2+}}y(t),\ \frac{k_{2-}}{k_{2+}},\ y(t),\ \frac{k_{3-}}{k_{3+}}y(t)\right)$:

```
> MM2 := Jacobian([-k1c*a + k1d*x, -k2c*x*y^2 + k2d*y^3 + k1c*a - k1d*x, k2c*x*y^2 - k2d*y^3 - k3c*y + k3d*b, k3c*y - k3d*b], [a,
  x, y, b] = [((k1d*k2d)/(k2c*k1c))*y, (k2d/k2c)*y, y, (k3c/k3d)*y]) : MM2;
```

(2.3)

$$\begin{bmatrix} -k1c & k1d & 0 & 0 \\ k1c & -k2c\ y2 - k1d & k2d\ y2 & 0 \\ 0 & k2c\ y2 & -k2d\ y2 - k3c & k3d \\ 0 & 0 & k3c & -k3d \end{bmatrix} \tag{2.3}$$

3. Study of the Jacobians

The respective traces, determinants and eigenvalues, for each Jacobian, are:

> $Trace(MM1);\ Determinant(MM1);\ eigenvalues(MM1);$

$$-k1c - k1d - k3c - k3d$$

$$0$$

$$0,\ 0,\ -k3c - k3d,\ -k1c - k1d \tag{3.1}$$

> $Trace(MM2);\ Determinant(MM2);$

$$-k2c\ y2 - k2d\ y2 - k1c - k1d - k3c - k3d$$

$$0 \tag{3.2}$$

> $eigenvalues(MM2);$

0, **(3.3)**

$$\frac{1}{6}\Big(12\,\big(-3k1c^{2}k2c^{4}y^{8} - 12k1c^{2}k2c^{3}k2dy^{8} - 18k1c^{2}k2c^{2}k2d^{2}y^{8} - 12k1c^{2}k2ck2d^{3}y^{8} - 3k1c^{2}k2d^{4}y^{8} - 6k1ck1dk2c^{3}k2dy^{8}$$

$$- 18k1ck1dk2c^{2}k2d^{2}y^{8} - 18k1ck1dk2ck2d^{3}y^{8} - 6k1ck1dk2d^{4}y^{8} + 6k1ck2c^{4}k3cy^{8} + 6k1ck2c^{4}k3dy^{8} + 18k1ck2c^{3}k2dk3cy^{8}$$

$$+ 24k1ck2c^{3}k2dk3dy^{8} + 18k1ck2c^{2}k2d^{2}k3cy^{8} + 36k1ck2c^{2}k2d^{2}k3dy^{8} + 6k1ck2ck2d^{3}k3cy^{8} + 24k1ck2ck2d^{3}k3dy^{8} + 6k1ck2d^{4}k3dy^{8}$$

$$- 3k1d^{2}k2c^{2}k2d^{2}y^{8} - 6k1d^{2}k2ck2d^{3}y^{8} - 3k1d^{2}k2d^{4}y^{8} - 6k1dk2c^{3}k2dk3cy^{8} + 6k1dk2c^{3}k2dk3dy^{8} - 12k1dk2c^{2}k2d^{2}k3cy^{8} + 18k1dk2c^{2}k2d^{2}k3dy^{8}$$

$$- 6k1dk2ck2d^{3}k3cy^{8} + 18k1dk2ck2d^{3}k3dy^{8} + 6k1dk2d^{4}k3dy^{8} - 3k2c^{4}k3c^{2}y^{8} - 6k2c^{4}k3ck3dy^{8} - 3k2c^{4}k3d^{2}y^{8} - 6k2c^{3}k2dk3c^{2}y^{8}$$

$$- 18k2c^{3}k2dk3ck3dy^{8} - 12k2c^{3}k2dk3d^{2}y^{8} - 3k2c^{2}k2d^{2}k3c^{2}y^{8} - 18k2c^{2}k2d^{2}k3ck3dy^{8} - 18k2c^{2}k2d^{2}k3d^{2}y^{8} - 6k2ck2d^{3}k3ck3dy^{8}$$

$$- 12k2ck2d^{3}k3d^{2}y^{8} - 3k2d^{4}k3d^{2}y^{8} + 6k1c^{3}k2c^{3}y^{6} + 18k1c^{3}k2c^{2}k2dy^{6} + 18k1c^{3}k2ck2d^{2}y^{6} + 6k1c^{3}k2d^{3}y^{6} - 6k1c^{2}k1dk2c^{3}y^{6} + 6k1c^{2}k1dk2c^{2}k2dy^{6}$$

$$+ 30k1c^{2}k1dk2ck2d^{2}y^{6} + 18k1c^{2}k1dk2d^{3}y^{6} - 6k1c^{2}k2c^{3}k3cy^{6} - 6k1c^{2}k2c^{3}k3dy^{6} - 24k1c^{2}k2c^{2}k2dk3cy^{6} - 18k1c^{2}k2c^{2}k2dk3dy^{6}$$

$$- 30k1c^{2}k2ck2d^{2}k3cy^{6} - 18k1c^{2}k2ck2d^{2}k3dy^{6} - 12k1c^{2}k2d^{3}k3cy^{6} - 6k1c^{2}k2d^{3}k3dy^{6} - 12k1ck1d^{2}k2c^{2}k2dy^{6} + 6k1ck1d^{2}k2ck2d^{2}y^{6}$$

$$+ 18k1ck1d^{2}k2d^{3}y^{6} + 18k1ck1dk2c^{3}k3cy^{6} + 18k1ck1dk2c^{3}k3dy^{6} + 18k1ck1dk2c^{2}k2dk3cy^{6} + 24k1ck1dk2c^{2}k2dk3dy^{6}$$

$$- 24k1ck1dk2ck2d^{2}k3cy^{6} - 6k1ck1dk2ck2d^{2}k3dy^{6} - 24k1ck1dk2d^{3}k3cy^{6} - 12k1ck1dk2d^{3}k3dy^{6} - 6k1ck2c^{3}k3c^{2}y^{6} - 12k1ck2c^{3}k3ck3dy^{6}$$

$$- 6k1ck2c^{3}k3d^{2}y^{6} + 12k1ck2c^{2}k2dk3c^{2}y^{6} - 6k1ck2c^{2}k2dk3ck3dy^{6} - 18k1ck2c^{2}k2dk3d^{2}y^{6} + 18k1ck2ck2d^{2}k3c^{2}y^{6} + 24k1ck2ck2d^{2}k3ck3dy^{6}$$

$$- 18k1ck2ck2d^{2}k3d^{2}y^{6} + 18k1ck2d^{3}k3ck3dy^{6} - 6k1ck2d^{3}k3d^{2}y^{6} - 6k1d^{3}k2ck2d^{2}y^{6} + 6k1d^{3}k2d^{3}y^{6} - 18k1d^{2}k2c^{2}k2dk3cy^{6}$$

$$+ 18k1d^{2}k2c^{2}k2dk3dy^{6} + 6k1d^{2}k2ck2d^{2}k3cy^{6} + 12k1d^{2}k2ck2d^{2}k3dy^{6} - 12k1d^{2}k2d^{3}k3cy^{6} - 6k1d^{2}k2d^{3}k3dy^{6} - 12k1dk2c^{3}k3c^{2}y^{6}$$

$$- 24k1dk2c^{3}k3ck3dy^{6} - 12k1dk2c^{3}k3d^{2}y^{6} + 6k1dk2c^{2}k2dk3c^{2}y^{6} - 24k1dk2c^{2}k2dk3ck3dy^{6} - 30k1dk2c^{2}k2dk3d^{2}y^{6} - 18k1dk2ck2d^{2}k3c^{2}y^{6}$$

$$+ 18k1dk2ck2d^{2}k3ck3dy^{6} - 24k1dk2ck2d^{2}k3d^{2}y^{6} + 18k1dk2d^{3}k3ck3dy^{6} - 6k1dk2d^{3}k3d^{2}y^{6} + 6k2c^{3}k3c^{3}y^{6} + 18k2c^{3}k3c^{2}k3dy^{6}$$

$$+ 18k2c^{3}k3ck3d^{2}y^{6} + 6k2c^{3}k3d^{3}y^{6} - 6k2c^{2}k2dk3c^{3}y^{6} + 6k2c^{2}k2dk3c^{2}k3dy^{6} + 30k2c^{2}k2dk3ck3d^{2}y^{6} + 18k2c^{2}k2dk3d^{3}y^{6} - 12k2ck2d^{2}k3c^{2}k3dy^{6}$$

$$+ 6k2ck2d^{2}k3ck3d^{2}y^{6} + 18k2ck2d^{2}k3d^{3}y^{6} - 6k2d^{3}k3ck3d^{2}y^{6} + 6k2d^{3}k3d^{3}y^{6} - 3k1c^{4}k2c^{2}y^{4} - 6k1c^{4}k2ck2dy^{4} - 3k1c^{4}k2d^{2}y^{4} - 6k1c^{3}k1dk2c^{2}y^{4}$$

$$- 18k1c^{3}k1dk2ck2dy^{4} - 12k1c^{3}k1dk2d^{2}y^{4} - 6k1c^{3}k2c^{2}k3cy^{4} - 6k1c^{3}k2c^{2}k3dy^{4} + 12k1c^{3}k2ck2dk3cy^{4} - 12k1c^{3}k2ck2dk3dy^{4}$$

$$+ 18k1c^{3}k2d^{2}k3cy^{4} - 6k1c^{3}k2d^{2}k3dy^{4} - 3k1c^{2}k1d^{2}k2c^{2}y^{4} - 18k1c^{2}k1d^{2}k2ck2dy^{4} - 18k1c^{2}k1d^{2}k2d^{2}y^{4} + 12k1c^{2}k1dk2c^{2}k3cy^{4}$$

$$+ 12k1c^{2}k1dk2c^{2}k3dy^{4} + 6k1c^{2}k1dk2ck2dk3cy^{4} - 6k1c^{2}k1dk2ck2dk3dy^{4} + 54k1c^{2}k1dk2d^{2}k3cy^{4} - 18k1c^{2}k1dk2d^{2}k3dy^{4} + 18k1c^{2}k2c^{2}k3c^{2}y^{4}$$

$$+ 36k1c^{2}k2c^{2}k3ck3dy^{4} + 18k1c^{2}k2c^{2}k3d^{2}y^{4} - 24k1c^{2}k2ck2dk3c^{2}y^{4} + 12k1c^{2}k2ck2dk3ck3dy^{4} + 36k1c^{2}k2ck2dk3d^{2}y^{4} - 18k1c^{2}k2d^{2}k3c^{2}y^{4}$$

$$- 24k1c^{2}k2d^{2}k3ck3dy^{4} + 18k1c^{2}k2d^{2}k3d^{2}y^{4} - 6k1ck1d^{3}k2ck2dy^{4} - 12k1ck1d^{3}k2d^{2}y^{4} + 18k1ck1d^{2}k2c^{2}k3cy^{4} + 18k1ck1d^{2}k2c^{2}k3dy^{4}$$

$$- 24k1ck1d^{2}k2ck2dk3cy^{4} + 24k1ck1d^{2}k2ck2dk3dy^{4} + 54k1ck1d^{2}k2d^{2}k3cy^{4} - 18k1ck1d^{2}k2d^{2}k3dy^{4} - 24k1ck1dk2c^{2}k3c^{2}y^{4}$$

$$- 48k1ck1dk2c^{2}k3ck3dy^{4} - 24k1ck1dk2c^{2}k3d^{2}y^{4} + 6k1ck1dk2ck2dk3c^{2}y^{4} + 18k1ck1dk2ck2dk3ck3dy^{4} + 12k1ck1dk2ck2dk3d^{2}y^{4}$$

$$- 36k1ck1dk2d^{2}k3c^{2}y^{4} - 48k1ck1dk2d^{2}k3ck3dy^{4} + 36k1ck1dk2d^{2}k3d^{2}y^{4} - 6k1ck2c^{2}k3c^{3}y^{4} - 18k1ck2c^{2}k3c^{2}k3dy^{4} - 18k1ck2c^{2}k3ck3d^{2}y^{4}$$

$$- 6k1ck2c^{2}k3d^{3}y^{4} + 18k1ck2ck2dk3c^{3}y^{4} + 24k1ck2ck2dk3c^{2}k3dy^{4} - 6k1ck2ck2dk3ck3d^{2}y^{4} - 12k1ck2ck2dk3d^{3}y^{4} + 18k1ck2d^{2}k3c^{2}k3dy^{4}$$

$$+ 12k1ck2d^{2}k3ck3d^{2}y^{4} - 6k1ck2d^{2}k3d^{3}y^{4} - 3k1d^{4}k2d^{2}y^{4} - 18k1d^{3}k2ck2dk3cy^{4} + 18k1d^{3}k2ck2dk3dy^{4} + 18k1d^{3}k2d^{2}k3cy^{4} - 6k1d^{3}k2d^{2}k3dy^{4}$$

$$- 18k1d^{2}k2c^{2}k3c^{2}y^{4} - 36k1d^{2}k2c^{2}k3ck3dy^{4} - 18k1d^{2}k2c^{2}k3d^{2}y^{4} + 30k1d^{2}k2ck2dk3c^{2}y^{4} + 6k1d^{2}k2ck2dk3ck3dy^{4} - 24k1d^{2}k2ck2dk3d^{2}y^{4}$$

$$- 18k1d^{2}k2d^{2}k3c^{2}y^{4} - 24k1d^{2}k2d^{2}k3ck3dy^{4} + 18k1d^{2}k2d^{2}k3d^{2}y^{4} + 18k1dk2c^{2}k3c^{3}y^{4} + 54k1dk2c^{2}k3c^{2}k3dy^{4} + 54k1dk2c^{2}k3ck3d^{2}y^{4}$$

$$+ 18k1dk2c^{2}k3d^{3}y^{4} - 18k1dk2ck2dk3c^{3}y^{4} - 24k1dk2ck2dk3c^{2}k3dy^{4} + 6k1dk2ck2dk3ck3d^{2}y^{4} + 12k1dk2ck2dk3d^{3}y^{4} + 18k1dk2d^{2}k3c^{2}k3dy^{4}$$

$$+ 12k1dk2d^{2}k3ck3d^{2}y^{4} - 6k1dk2d^{2}k3d^{3}y^{4} - 3k2c^{2}k3c^{4}y^{4} - 12k2c^{2}k3c^{3}k3dy^{4} - 18k2c^{2}k3c^{2}k3d^{2}y^{4} - 12k2c^{2}k3ck3d^{3}y^{4} - 3k2c^{2}k3d^{4}y^{4}$$

$$- 6k2ck2dk3c^{3}k3dy^{4} - 18k2ck2dk3c^{2}k3d^{2}y^{4} - 18k2ck2dk3ck3d^{3}y^{4} - 6k2ck2dk3d^{4}y^{4} - 3k2d^{2}k3c^{2}k3d^{2}y^{4} - 6k2d^{2}k3ck3d^{3}y^{4} - 3k2d^{2}k3d^{4}y^{4}$$

$$+ 6k1c^{4}k2ck3cy^{2} + 6k1c^{4}k2ck3dy^{2} - 6k1c^{4}k2dk3cy^{2} + 6k1c^{4}k2dk3dy^{2} + 18k1c^{3}k1dk2ck3cy^{2} + 18k1c^{3}k1dk2ck3dy^{2} - 24k1c^{3}k1dk2dk3cy^{2}$$

$$+ 24k1c^{3}k1dk2dk3dy^{2} - 6k1c^{3}k2ck3c^{2}y^{2} - 12k1c^{3}k2ck3ck3dy^{2} - 6k1c^{3}k2ck3d^{2}y^{2} + 18k1c^{3}k2dk3c^{2}y^{2} + 12k1c^{3}k2dk3ck3dy^{2} - 6k1c^{3}k2dk3d^{2}y^{2}$$

$$+ 18k1c^{2}k1d^{2}k2ck3cy^{2} + 18k1c^{2}k1d^{2}k2ck3dy^{2} - 36k1c^{2}k1d^{2}k2dk3cy^{2} + 36k1c^{2}k1d^{2}k2dk3dy^{2} - 24k1c^{2}k1dk2ck3c^{2}y^{2} - 48k1c^{2}k1dk2ck3ck3dy^{2}$$

$$- 24k1c^{2}k1dk2ck3d^{2}y^{2} + 54k1c^{2}k1dk2dk3c^{2}y^{2} + 36k1c^{2}k1dk2dk3ck3dy^{2} - 18k1c^{2}k1dk2dk3d^{2}y^{2} - 6k1c^{2}k2ck3c^{3}y^{2} - 18k1c^{2}k2ck3c^{2}k3dy^{2}$$

$$- 18k1c^{2}k2ck3ck3d^{2}y^{2} - 6k1c^{2}k2ck3d^{3}y^{2} - 12k1c^{2}k2dk3c^{3}y^{2} - 30k1c^{2}k2dk3c^{2}k3dy^{2} - 24k1c^{2}k2dk3ck3d^{2}y^{2} - 6k1c^{2}k2dk3d^{3}y^{2}$$

$$+ 6k1ck1d^{3}k2ck3cy^{2} + 6k1ck1d^{3}k2ck3dy^{2} - 24k1ck1d^{3}k2dk3cy^{2} + 24k1ck1d^{3}k2dk3dy^{2} - 30k1ck1d^{2}k2ck3c^{2}y^{2} - 60k1ck1d^{2}k2ck3ck3dy^{2}$$

$$- 30k1ck1d^{2}k2ck3d^{2}y^{2} + 54k1ck1d^{2}k2dk3c^{2}y^{2} + 36k1ck1d^{2}k2dk3ck3dy^{2} - 18k1ck1d^{2}k2dk3d^{2}y^{2} + 12k1ck1dk2ck3c^{3}y^{2}$$

$$+ 36k1ck1dk2ck3c^{2}k3dy^{2} + 36k1ck1dk2ck3ck3d^{2}y^{2} + 12k1ck1dk2ck3d^{3}y^{2} - 24k1ck1dk2dk3c^{3}y^{2} - 60k1ck1dk2dk3c^{2}k3dy^{2}$$

$$- 48k1ck1dk2dk3ck3d^{2}y^{2} - 12k1ck1dk2dk3d^{3}y^{2} + 6k1ck2ck3c^{4}y^{2} + 24k1ck2ck3c^{3}k3dy^{2} + 36k1ck2ck3c^{2}k3d^{2}y^{2} + 24k1ck2ck3ck3d^{3}y^{2}$$

$$+ 6k1ck2ck3d^{4}y^{2} + 6k1ck2dk3c^{3}k3dy^{2} + 18k1ck2dk3c^{2}k3d^{2}y^{2} + 18k1ck2dk3ck3d^{3}y^{2} + 6k1ck2dk3d^{4}y^{2} - 6k1d^{4}k2dk3cy^{2} + 6k1d^{4}k2dk3dy^{2}$$

$$- 12k1d^{3}k2ck3c^{2}y^{2} - 24k1d^{3}k2ck3ck3dy^{2} - 12k1d^{3}k2ck3d^{2}y^{2} + 18k1d^{3}k2dk3c^{2}y^{2} + 12k1d^{3}k2dk3ck3dy^{2} - 6k1d^{3}k2dk3d^{2}y^{2} + 18k1d^{2}k2ck3c^{3}y^{2}$$

$$+ 54k1d^{2}k2ck3c^{2}k3dy^{2} + 54k1d^{2}k2ck3ck3d^{2}y^{2} + 18k1d^{2}k2ck3d^{3}y^{2} - 12k1d^{2}k2dk3c^{3}y^{2} - 30k1d^{2}k2dk3c^{2}k3dy^{2} - 24k1d^{2}k2dk3ck3d^{2}y^{2}$$

$$- 6k1d^{2}k2dk3d^{3}y^{2} - 6k1dk2ck3c^{4}y^{2} - 24k1dk2ck3c^{3}k3dy^{2} - 36k1dk2ck3c^{2}k3d^{2}y^{2} - 24k1dk2ck3ck3d^{3}y^{2} - 6k1dk2ck3d^{4}y^{2}$$

$$+ 6k1dk2dk3c^{3}k3dy^{2} + 18k1dk2dk3c^{2}k3d^{2}y^{2} + 18k1dk2dk3ck3d^{3}y^{2} + 6k1dk2dk3d^{4}y^{2} - 3k1c^{4}k3c^{2} - 6k1c^{4}k3ck3d - 3k1c^{4}k3d^{2}$$

$$- 12k1c^{3}k1dk3c^{2} - 24k1c^{3}k1dk3ck3d - 12k1c^{3}k1dk3d^{2} + 6k1c^{3}k3c^{3} + 18k1c^{3}k3c^{2}k3d + 18k1c^{3}k3ck3d^{2} + 6k1c^{3}k3d^{3} - 18k1c^{2}k1d^{2}k3c^{2}$$

$$- 36k1c^{2}k1d^{2}k3ck3d - 18k1c^{2}k1d^{2}k3d^{2} + 18k1c^{2}k1dk3c^{3} + 54k1c^{2}k1dk3c^{2}k3d + 54k1c^{2}k1dk3ck3d^{2} + 18k1c^{2}k1dk3d^{3} - 3k1c^{2}k3c^{4}$$

$$- 12k1c^{2}k3c^{3}k3d - 18k1c^{2}k3c^{2}k3d^{2} - 12k1c^{2}k3ck3d^{3} - 3k1c^{2}k3d^{4} - 12k1ck1d^{3}k3c^{2} - 24k1ck1d^{3}k3ck3d - 12k1ck1d^{3}k3d^{2} + 18k1ck1d^{2}k3c^{3}$$

$$+ 54k1ck1d^{2}k3c^{2}k3d + 54k1ck1d^{2}k3ck3d^{2} + 18k1ck1d^{2}k3d^{3} - 6k1ck1dk3c^{4} - 24k1ck1dk3c^{3}k3d - 36k1ck1dk3c^{2}k3d^{2} - 24k1ck1dk3ck3d^{3}$$

$$- 6k1ck1dk3d^{4} - 3k1d^{4}k3c^{2} - 6k1d^{4}k3ck3d - 3k1d^{4}k3d^{2} + 6k1d^{3}k3c^{3} + 18k1d^{3}k3c^{2}k3d + 18k1d^{3}k3ck3d^{2} + 6k1d^{3}k3d^{3} - 3k1d^{2}k3c^{4}$$

$$- 12k1d^{2}k3c^{3}k3d - 18k1d^{2}k3c^{2}k3d^{2} - 12k1d^{2}k3ck3d^{3} - 3k1d^{2}k3d^{4}\Big)^{1/2} - 8k1c^{3} - 8k1d^{3} - 8k3c^{3} - 8k3d^{3} + 12k1d^{2}k3c + 12k1d^{2}k3d$$

$$+ 12k1dk3c^{2} + 12k1dk3d^{2} - 8k2c^{3}y^{6} - 8k2d^{3}y^{6} - 24k1c^{2}k1d - 24k1ck1d^{2} - 24k3c^{2}k3d - 24k3ck3d^{2} + 12k1ck3c^{2} + 12k1ck3d^{2} + 12k1ck2c^{2}y^{4}$$

$$+ 12k1ck2d^{2}y^{4} + 12k1dk2d^{2}y^{4} + 12k2c^{2}k3cy^{4} + 12k2c^{2}k3dy^{4} + 12k2d^{2}k3dy^{4} + 12k1c^{2}k2cy^{2} + 12k1c^{2}k2dy^{2} + 12k1d^{2}k2dy^{2} + 12k2ck3c^{2}y^{2}$$

$$+ 12k2ck3d^{2}y^{2} + 12k2dk3d^{2}y^{2} + 24k1ck1dk3c + 24k1ck1dk3d + 24k1ck3ck3d + 24k1dk3ck3d - 24k2c^{2}k2dy^{6} - 24k2ck2d^{2}y^{6} - 24k1dk2c^{2}y^{4}$$

$$- 24k2d^{2}k3cy^{4} - 24k1d^{2}k2cy^{2} - 24k2dk3c^{2}y^{2} + 24k1dk2dk3cy^{2} + 24k2ck3ck3dy^{2} - 12k2dk3ck3dy^{2} + 24k1ck2ck2dy^{4} - 12k1dk2ck2dy^{4}$$

$$- 12k2ck2dk3cy^{4} - 12k1ck1dk2cy^{2} + 24k1ck1dk2dy^{2} + 24k1ck2dk3cy^{2} + 24k1dk2ck3cy^{2} + 24k1dk2ck3dy^{2} - 48k1ck2ck3cy^{2}$$

$$- 48k1ck2ck3dy^{2} - 48k1ck2dk3dy^{2} + 12k1c^{2}k3c + 12k1c^{2}k3d + 24k2cy^{4}k2dk3d - 48k1dk2dk3dy^{2}\Big)^{1/3} - \Bigg(6\bigg(-\frac{1}{9}k2c^{2}y^{4} - \frac{1}{9}k2d^{2}y^{4}$$

$$- \frac{1}{9}k1d^{2} - \frac{1}{9}k3c^{2} - \frac{1}{9}k3d^{2} + \frac{1}{9}k1ck2cy^{2} + \frac{1}{9}k1ck2dy^{2} + \frac{1}{9}k1dk2dy^{2} + \frac{1}{9}k2ck3cy^{2} + \frac{1}{9}k2ck3dy^{2} - \frac{2}{9}k2cy^{2}k1d - \frac{2}{9}k2dy^{2}k3c - \frac{2}{9}k2cy^{4}k2d$$

$$+\frac{1}{9}k2dy^2k3d-\frac{1}{9}k1c^2+\frac{1}{9}k1ck3d+\frac{1}{9}k1dk3c+\frac{1}{9}k1dk3d+\frac{1}{9}k1ck3c-\frac{2}{9}k1ck1d-\frac{2}{9}k3ck3d\Big)\Big)\Big/$$

$$\Big(12\,\big(-3k1c^2k2c^4y^8-12k1c^2k2c^3k2dy^8-18k1c^2k2c^2k2d^2y^8-12k1c^2k2ck2d^3y^8-3k1c^2k2d^4y^8-6k1ck1dk2c^3k2dy^8$$

$$-18k1ck1dk2c^2k2d^2y^8-18k1ck1dk2ck2d^3y^8-6k1ck1dk2d^4y^8+6k1ck2c^4k3cy^8+6k1ck2c^4k3dy^8+18k1ck2c^3k2dk3cy^8$$

$$+24k1ck2c^3k2dk3dy^8+18k1ck2c^2k2d^2k3cy^8+36k1ck2c^2k2d^2k3dy^8+6k1ck2ck2d^3k3cy^8+24k1ck2ck2d^3k3dy^8+6k1ck2d^4k3dy^8$$

$$-3k1d^2k2c^2k2d^2y^8-6k1d^2k2ck2d^3y^8-3k1d^2k2d^4y^8-6k1dk2c^3k2dk3cy^8+6k1dk2c^3k2dk3dy^8-12k1dk2c^2k2d^2k3cy^8+18k1dk2c^2k2d^2k3dy^8$$

$$-6k1dk2ck2d^3k3cy^8+18k1dk2ck2d^3k3dy^8+6k1dk2d^4k3dy^8-3k2c^4k3c^2y^8-6k2c^4k3ck3dy^8-3k2c^4k3d^2y^8-6k2c^3k2dk3c^2y^8$$

$$-18k2c^3k2dk3ck3dy^8-12k2c^3k2dk3d^2y^8-3k2c^2k2d^2k3c^2y^8-18k2c^2k2d^2k3ck3dy^8-18k2c^2k2d^2k3d^2y^8-6k2ck2d^3k3ck3dy^8$$

$$-12k2ck2d^3k3d^2y^8-3k2d^4k3d^2y^8+6k1c^3k2c^3y^6+18k1c^3k2c^2k2dy^6+18k1c^3k2ck2d^2y^6+6k1c^3k2d^3y^6-6k1c^2k1dk2c^3y^6+6k1c^2k1dk2c^2k2dy^6$$

$$+30k1c^2k1dk2ck2d^2y^6+18k1c^2k1dk2d^3y^6-6k1c^2k2c^3k3cy^6-6k1c^2k2c^3k3dy^6-24k1c^2k2c^2k2dk3cy^6-18k1c^2k2c^2k2dk3dy^6$$

$$-30k1c^2k2ck2d^2k3cy^6-18k1c^2k2ck2d^2k3dy^6-12k1c^2k2d^3k3cy^6-6k1c^2k2d^3k3dy^6-12k1ck1d^2k2c^2k2dy^6+6k1ck1d^2k2ck2d^2y^6$$

$$+18k1ck1d^2k2d^3y^6+18k1ck1dk2c^3k3cy^6+18k1ck1dk2c^3k3dy^6+18k1ck1dk2c^2k2dk3cy^6+24k1ck1dk2c^2k2dk3dy^6$$

$$-24k1ck1dk2ck2d^2k3cy^6-6k1ck1dk2ck2d^2k3dy^6-24k1ck1dk2d^3k3cy^6-12k1ck1dk2d^3k3dy^6-6k1ck2c^3k3c^2y^6-12k1ck2c^3k3ck3dy^6$$

$$-6k1ck2c^3k3d^2y^6+12k1ck2c^2k2dk3c^2y^6-6k1ck2c^2k2dk3ck3dy^6-18k1ck2c^2k2dk3d^2y^6+18k1ck2ck2d^2k3c^2y^6+24k1ck2ck2d^2k3ck3dy^6$$

$$-18k1ck2ck2d^2k3d^2y^6+18k1ck2d^3k3ck3dy^6-6k1ck2d^3k3d^2y^6-6k1d^3k2ck2d^2y^6+6k1d^3k2d^3y^6-18k1d^2k2c^2k2dk3cy^6$$

$$+18k1d^2k2c^2k2dk3dy^6+6k1d^2k2ck2d^2k3cy^6+12k1d^2k2ck2d^2k3dy^6-12k1d^2k2d^3k3cy^6-6k1d^2k2d^3k3dy^6-12k1dk2c^3k3c^2y^6$$

$$-24k1dk2c^3k3ck3dy^6-12k1dk2c^3k3d^2y^6+6k1dk2c^2k2dk3c^2y^6-24k1dk2c^2k2dk3ck3dy^6-30k1dk2c^2k2dk3d^2y^6-18k1dk2ck2d^2k3c^2y^6$$

$$+18k1dk2ck2d^2k3ck3dy^6-24k1dk2ck2d^2k3d^2y^6+18k1dk2d^3k3ck3dy^6-6k1dk2d^3k3d^2y^6+6k2c^3k3c^3y^6+18k2c^3k3c^2k3dy^6$$

$$+18k2c^3k3ck3d^2y^6+6k2c^3k3d^3y^6-6k2c^2k2dk3c^3y^6+6k2c^2k2dk3c^2k3dy^6+30k2c^2k2dk3ck3d^2y^6+18k2c^2k2dk3d^3y^6-12k2ck2d^2k3c^2k3dy^6$$

$$+6k2ck2d^2k3ck3d^2y^6+18k2ck2d^2k3d^3y^6-6k2d^3k3ck3d^2y^6+6k2d^3k3d^3y^6-3k1c^4k2c^2y^4-6k1c^4k2ck2dy^4-3k1c^4k2d^2y^4-6k1c^3k1dk2c^2y^4$$

$$-18k1c^3k1dk2ck2dy^4-12k1c^3k1dk2d^2y^4-6k1c^3k2c^2k3cy^4-6k1c^3k2c^2k3dy^4+12k1c^3k2ck2dk3cy^4-12k1c^3k2ck2dk3dy^4$$

$$+18k1c^3k2d^2k3cy^4-6k1c^3k2d^2k3dy^4-3k1c^2k1d^2k2c^2y^4-18k1c^2k1d^2k2ck2dy^4-18k1c^2k1d^2k2d^2y^4+12k1c^2k1dk2c^2k3cy^4$$

$$+12k1c^2k1dk2c^2k3dy^4+6k1c^2k1dk2ck2dk3cy^4-6k1c^2k1dk2ck2dk3dy^4+54k1c^2k1dk2d^2k3cy^4-18k1c^2k1dk2d^2k3dy^4+18k1c^2k2c^2k3c^2y^4$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36k1ck1dk2ck3c^2k3dy^2+36k1ck1dk2ck3ck3d^2y^2+12k1ck1dk2ck3d^3y^2-24k1ck1dk2dk3c^3y^2-60k1ck1dk2dk3c^2k3dy^2$$

$$-48k1ck1dk2dk3ck3d^2y^2-12k1ck1dk2dk3d^3y^2+6k1ck2ck3c^4y^2+24k1ck2ck3c^3k3dy^2+36k1ck2ck3c^2k3d^2y^2+24k1ck2ck3ck3d^3y^2$$

$$+6k1ck2ck3d^4y^2+6k1ck2dk3c^3k3dy^2+18k1ck2dk3c^2k3d^2y^2+18k1ck2dk3ck3d^3y^2+6k1ck2dk3d^4y^2-6k1d^4k2dk3cy^2+6k1d^4k2dk3dy^2$$

$$-12k1d^3k2ck3c^2y^2-24k1d^3k2ck3ck3dy^2-12k1d^3k2ck3d^2y^2+18k1d^3k2dk3c^2y^2+12k1d^3k2dk3ck3dy^2-6k1d^3k2dk3d^2y^2+18k1d^2k2ck3c^3y^2$$

$$+54k1d^2k2ck3c^2k3dy^2+54k1d^2k2ck3ck3d^2y^2+18k1d^2k2ck3d^3y^2-12k1d^2k2dk3c^3y^2-30k1d^2k2dk3c^2k3dy^2-24k1d^2k2dk3ck3d^2y^2$$

$$-6k1d^2k2dk3d^3y^2-6k1dk2ck3c^4y^2-24k1dk2ck3c^3k3dy^2-36k1dk2ck3c^2k3d^2y^2-24k1dk2ck3ck3d^3y^2-6k1dk2ck3d^4y^2$$

$$+6k1dk2dk3c^3k3dy^2+18k1dk2dk3c^2k3d^2y^2+18k1dk2dk3ck3d^3y^2+6k1dk2dk3d^4y^2-3k1c^4k3c^2-6k1c^4k3ck3d-3k1c^4k3d^2$$

$$-12k1c^3k1dk3c^2-24k1c^3k1dk3ck3d-12k1c^3k1dk3d^2+6k1c^3k3c^3+18k1c^3k3c^2k3d+18k1c^3k3ck3d^2+6k1c^3k3d^3-18k1c^2k1d^2k3c^2$$

$$-36k1c^2k1d^2k3ck3d-18k1c^2k1d^2k3d^2+18k1c^2k1dk3c^3+54k1c^2k1dk3c^2k3d+54k1c^2k1dk3ck3d^2+18k1c^2k1dk3d^3-3k1c^2k3c^4$$

$$-12k1c^2k3c^3k3d-18k1c^2k3c^2k3d^2-12k1c^2k3ck3d^3-3k1c^2k3d^4-12k1ck1d^3k3c^2-24k1ck1d^3k3ck3d-12k1ck1d^3k3d^2+18k1ck1d^2k3c^3$$

$$+54k1ck1d^2k3c^2k3d+54k1ck1d^2k3ck3d^2+18k1ck1d^2k3d^3-6k1ck1dk3c^4-24k1ck1dk3c^3k3d-36k1ck1dk3c^2k3d^2-24k1ck1dk3ck3d^3$$

$$-6k1ck1dk3d^4-3k1d^4k3c^2-6k1d^4k3ck3d-3k1d^4k3d^2+6k1d^3k3c^3+18k1d^3k3c^2k3d+18k1d^3k3ck3d^2+6k1d^3k3d^3-3k1d^2k3c^4$$

$$-12k1d^2k3c^3k3d-18k1d^2k3c^2k3d^2-12k1d^2k3ck3d^3-3k1d^2k3d^4)^{1/2}-8k1c^3-8k1d^3-8k3c^3-8k3d^3+12k1d^2k3c+12k1d^2k3d$$

$$+12k1dk3c^2+12k1dk3d^2-8k2c^3y^6-8k2d^3y^6-24k1c^2k1d-24k1ck1d^2-24k3c^2k3d-24k3ck3d^2+12k1ck3c^2+12k1ck3d^2+12k1ck2c^2y^4$$

$$+12k1ck2d^2y^4+12k1dk2d^2y^4+12k2c^2k3cy^4+12k2c^2k3dy^4+12k2d^2k3dy^4+12k1c^2k2cy^2+12k1c^2k2dy^2+12k1d^2k2dy^2+12k2ck3c^2y^2$$

$$+12k2ck3d^2y^2+12k2dk3d^2y^2+24k1ck1dk3c+24k1ck1dk3d+24k1ck3ck3d+24k1dk3ck3d-24k2c^2k2dy^6-24k2ck2d^2y^6-24k1dk2c^2y^4$$

$$-24k2d^2k3cy^4-24k1d^2k2cy^2-24k2dk3c^2y^2+24k1dk2dk3cy^2+24k2ck3ck3dy^2-12k2dk3ck3dy^2+24k1ck2ck2dy^4-12k1dk2ck2dy^4$$

$$-12k2ck2dk3cy^4-12k1ck1dk2cy^2+24k1ck1dk2dy^2+24k1ck2dk3cy^2+24k1dk2ck3cy^2+24k1dk2ck3dy^2-48k1ck2ck3cy^2$$

$$-48k1ck2ck3dy^2-48k1ck2dk3dy^2+12k1c^2k3c+12k1c^2k3d+24k2cy^4k2dk3d-48k1dk2dk3dy^2\Big)^{1/3}-\frac{1}{3}k2cy^2-\frac{1}{3}k2dy^2-\frac{1}{3}k1c-\frac{1}{3}k1d$$

$$-\frac{1}{3}k3c-\frac{1}{3}k3d,$$

$$-\frac{1}{12}\Big(12\,(-3k1c^2k2c^4y^8-12k1c^2k2c^3k2dy^8-18k1c^2k2c^2k2d^2y^8-12k1c^2k2ck2d^3y^8-3k1c^2k2d^4y^8-6k1ck1dk2c^3k2dy^8$$

$$-18k1ck1dk2c^2k2d^2y^8-18k1ck1dk2ck2d^3y^8-6k1ck1dk2d^4y^8+6k1ck2c^4k3cy^8+6k1ck2c^4k3dy^8+18k1ck2c^3k2dk3cy^8$$

$$+24k1ck2c^3k2dk3dy^8+18k1ck2c^2k2d^2k3cy^8+36k1ck2c^2k2d^2k3dy^8+6k1ck2ck2d^3k3cy^8+24k1ck2ck2d^3k3dy^8+6k1ck2d^4k3dy^8$$

$$-3k1d^2k2c^2k2d^2y^8-6k1d^2k2ck2d^3y^8-3k1d^2k2d^4y^8-6k1dk2c^3k2dk3cy^8+6k1dk2c^3k2dk3dy^8-12k1dk2c^2k2d^2k3cy^8+18k1dk2c^2k2d^2k3dy^8$$

$$-6k1dk2ck2d^3k3cy^8+18k1dk2ck2d^3k3dy^8+6k1dk2d^4k3dy^8-3k2c^4k3c^2y^8-6k2c^4k3ck3dy^8-3k2c^4k3d^2y^8-6k2c^3k2dk3c^2y^8$$

$$-18k2c^3k2dk3ck3dy^8-12k2c^3k2dk3d^2y^8-3k2c^2k2d^2k3c^2y^8-18k2c^2k2d^2k3ck3dy^8-18k2c^2k2d^2k3d^2y^8-6k2ck2d^3k3ck3dy^8$$

$$-12k2ck2d^3k3d^2y^8-3k2d^4k3d^2y^8+6k1c^3k2c^3y^6+18k1c^3k2c^2k2dy^6+18k1c^3k2ck2d^2y^6+6k1c^3k2d^3y^6-6k1c^2k1dk2c^3y^6+6k1c^2k1dk2c^2k2dy^6$$

$$+30k1c^2k1dk2ck2d^2y^6+18k1c^2k1dk2d^3y^6-6k1c^2k2c^3k3cy^6-6k1c^2k2c^3k3dy^6-24k1c^2k2c^2k2dk3cy^6-18k1c^2k2c^2k2dk3dy^6$$

$$-30k1c^2k2ck2d^2k3cy^6-18k1c^2k2ck2d^2k3dy^6-12k1c^2k2d^3k3cy^6-6k1c^2k2d^3k3dy^6-12k1ck1d^2k2c^2k2dy^6+6k1ck1d^2k2ck2d^2y^6$$

$$+18k1ck1d^2k2d^3y^6+18k1ck1dk2c^3k3cy^6+18k1ck1dk2c^3k3dy^6+18k1ck1dk2c^2k2dk3cy^6+24k1ck1dk2c^2k2dk3dy^6$$

$$-24k1ck1dk2ck2d^2k3cy^6-6k1ck1dk2ck2d^2k3dy^6-24k1ck1dk2d^3k3cy^6-12k1ck1dk2d^3k3dy^6-6k1ck2c^3k3c^2y^6-12k1ck2c^3k3ck3dy^6$$

$$-6k1ck2c^3k3d^2y^6+12k1ck2c^2k2dk3c^2y^6-6k1ck2c^2k2dk3ck3dy^6-18k1ck2c^2k2dk3d^2y^6+18k1ck2ck2d^2k3c^2y^6+24k1ck2ck2d^2k3ck3dy^6$$

$$-18k1ck2ck2d^2k3d^2y^6+18k1ck2d^3k3ck3dy^6-6k1ck2d^3k3d^2y^6-6k1d^3k2ck2d^2y^6+6k1d^3k2d^3y^6-18k1d^2k2c^2k2dk3cy^6$$

$$+18k1d^2k2c^2k2dk3dy^6+6k1d^2k2ck2d^2k3cy^6+12k1d^2k2ck2d^2k3dy^6-12k1d^2k2d^3k3cy^6-6k1d^2k2d^3k3dy^6-12k1dk2c^3k3c^2y^6$$

$$-24k1dk2c^3k3ck3dy^6-12k1dk2c^3k3d^2y^6+6k1dk2c^2k2dk3c^2y^6-24k1dk2c^2k2dk3ck3dy^6-30k1dk2c^2k2dk3d^2y^6-18k1dk2ck2d^2k3c^2y^6$$

$$+18k1dk2ck2d^2k3ck3dy^6-24k1dk2ck2d^2k3d^2y^6+18k1dk2d^3k3ck3dy^6-6k1dk2d^3k3d^2y^6+6k2c^3k3c^3y^6+18k2c^3k3c^2k3dy^6$$

$$+18k2c^3k3ck3d^2y^6+6k2c^3k3d^3y^6-6k2c^2k2dk3c^3y^6+6k2c^2k2dk3c^2k3dy^6+30k2c^2k2dk3ck3d^2y^6+18k2c^2k2dk3d^3y^6-12k2ck2d^2k3c^2k3dy^6$$

$$+6k2ck2d^2k3ck3d^2y^6+18k2ck2d^2k3d^3y^6-6k2d^3k3ck3d^2y^6+6k2d^3k3d^3y^6-3k1c^4k2c^2y^4-6k1c^4k2ck2dy^4-3k1c^4k2d^2y^4-6k1c^3k1dk2c^2y^4$$

$$-18k1c^3k1dk2ck2dy^4-12k1c^3k1dk2d^2y^4-6k1c^3k2c^2k3cy^4-6k1c^3k2c^2k3dy^4+12k1c^3k2ck2dk3cy^4-12k1c^3k2ck2dk3dy^4$$

$$+18k1c^3k2d^2k3cy^4-6k1c^3k2d^2k3dy^4-3k1c^2k1d^2k2c^2y^4-18k1c^2k1d^2k2ck2dy^4-18k1c^2k1d^2k2d^2y^4+12k1c^2k1dk2c^2k3cy^4$$

$$+12k1c^2k1dk2c^2k3dy^4+6k1c^2k1dk2ck2dk3cy^4-6k1c^2k1dk2ck2dk3dy^4+54k1c^2k1dk2d^2k3cy^4-18k1c^2k1dk2d^2k3dy^4+18k1c^2k2c^2k3c^2y^4$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36k1ck1dk2ck3c^2k3dy^2+36k1ck1dk2ck3ck3d^2y^2+12k1ck1dk2ck3d^3y^2-24k1ck1dk2dk3c^3y^2-60k1ck1dk2dk3c^2k3dy^2$$

$$-48k1ck1dk2dk3ck3d^2y^2-12k1ck1dk2dk3d^3y^2+6k1ck2ck3c^4y^2+24k1ck2ck3c^3k3dy^2+36k1ck2ck3c^2k3d^2y^2+24k1ck2ck3ck3d^3y^2$$

$$+6k1ck2ck3d^4y^2+6k1ck2dk3c^3k3dy^2+18k1ck2dk3c^2k3d^2y^2+18k1ck2dk3ck3d^3y^2+6k1ck2dk3d^4y^2-6k1d^4k2dk3cy^2+6k1d^4k2dk3dy^2$$

$$-12k1d^3k2ck3c^2y^2-24k1d^3k2ck3ck3dy^2-12k1d^3k2ck3d^2y^2+18k1d^3k2dk3c^2y^2+12k1d^3k2dk3ck3dy^2-6k1d^3k2dk3d^2y^2+18k1d^2k2ck3c^3y^2$$

$$+54k1d^2k2ck3c^2k3dy^2+54k1d^2k2ck3ck3d^2y^2+18k1d^2k2ck3d^3y^2-12k1d^2k2dk3c^3y^2-30k1d^2k2dk3c^2k3dy^2-24k1d^2k2dk3ck3d^2y^2$$

$$-6k1d^2k2dk3d^3y^2-6k1dk2ck3c^4y^2-24k1dk2ck3c^3k3dy^2-36k1dk2ck3c^2k3d^2y^2-24k1dk2ck3ck3d^3y^2-6k1dk2ck3d^4y^2$$

$$+6k1dk2dk3c^3k3dy^2+18k1dk2dk3c^2k3d^2y^2+18k1dk2dk3ck3d^3y^2+6k1dk2dk3d^4y^2-3k1c^4k3c^2-6k1c^4k3ck3d-3k1c^4k3d^2$$

$$-12k1c^3k1dk3c^2-24k1c^3k1dk3ck3d-12k1c^3k1dk3d^2+6k1c^3k3c^3+18k1c^3k3c^2k3d+18k1c^3k3ck3d^2+6k1c^3k3d^3-18k1c^2k1d^2k3c^2$$

$$-36k1c^2k1d^2k3ck3d-18k1c^2k1d^2k3d^2+18k1c^2k1dk3c^3+54k1c^2k1dk3c^2k3d+54k1c^2k1dk3ck3d^2+18k1c^2k1dk3d^3-3k1c^2k3c^4$$

$$-12k1c^2k3c^3k3d-18k1c^2k3c^2k3d^2-12k1c^2k3ck3d^3-3k1c^2k3d^4-12k1ck1d^3k3c^2-24k1ck1d^3k3ck3d-12k1ck1d^3k3d^2+18k1ck1d^2k3c^3$$

$$+54k1ck1d^2k3c^2k3d+54k1ck1d^2k3ck3d^2+18k1ck1d^2k3d^3-6k1ck1dk3c^4-24k1ck1dk3c^3k3d-36k1ck1dk3c^2k3d^2-24k1ck1dk3ck3d^3$$

$$- 6k1ck1dk3d^4 - 3k1d^4k3c^2 - 6k1d^4k3ck3d - 3k1d^4k3d^2 + 6k1d^3k3c^3 + 18k1d^3k3c^2k3d + 18k1d^3k3ck3d^2 + 6k1d^3k3d^3 - 3k1d^2k3c^4$$

$$- 12k1d^2k3c^3k3d - 18k1d^2k3c^2k3d^2 - 12k1d^2k3ck3d^3 - 3k1d^2k3d^4)^{1/2} - 8k1c^3 - 8k1d^3 - 8k3c^3 - 8k3d^3 + 12k1d^2k3c + 12k1d^2k3d$$

$$+ 12k1dk3c^2 + 12k1dk3d^2 - 8k2c^3y^6 - 8k2d^3y^6 - 24k1c^2k1d - 24k1ck1d^2 - 24k3c^2k3d - 24k3ck3d^2 + 12k1ck3c^2 + 12k1ck3d^2 + 12k1ck2c^2y^4$$

$$+ 12k1ck2d^2y^4 + 12k1dk2d^2y^4 + 12k2c^2k3cy^4 + 12k2c^2k3dy^4 + 12k2d^2k3dy^4 + 12k1c^2k2cy^2 + 12k1c^2k2dy^2 + 12k1d^2k2dy^2 + 12k2ck3c^2y^2$$

$$+ 12k2ck3d^2y^2 + 12k2dk3d^2y^2 + 24k1ck1dk3c + 24k1ck1dk3d + 24k1ck3ck3d + 24k1dk3ck3d - 24k2c^2k2dy^6 - 24k2ck2d^2y^6 - 24k1dk2c^2y^4$$

$$- 24k2d^2k3cy^4 - 24k1d^2k2cy^2 - 24k2dk3c^2y^2 + 24k1dk2dk3cy^2 + 24k2ck3ck3dy^2 - 12k2dk3ck3dy^2 + 24k1ck2ck2dy^4 - 12k1dk2ck2dy^4$$

$$- 12k2ck2dk3cy^4 - 12k1ck1dk2cy^2 + 24k1ck1dk2dy^2 + 24k1ck2dk3cy^2 + 24k1dk2ck3cy^2 + 24k1dk2ck3dy^2 - 48k1ck2ck3cy^2$$

$$- 48k1ck2ck3dy^2 - 48k1ck2dk3dy^2 + 12k1c^2k3c + 12k1c^2k3d + 24k2cy^4k2dk3d - 48k1dk2dk3dy^2\Big)^{1/3} + \Big(3\Big(-\frac{1}{9}k2c^2y^4 - \frac{1}{9}k2d^2y^4$$

$$- \frac{1}{9}k1d^2 - \frac{1}{9}k3c^2 - \frac{1}{9}k3d^2 + \frac{1}{9}k1ck2cy^2 + \frac{1}{9}k1ck2dy^2 + \frac{1}{9}k1dk2dy^2 + \frac{1}{9}k2ck3cy^2 + \frac{1}{9}k2ck3dy^2 - \frac{2}{9}k2cy^2k1d - \frac{2}{9}k2dy^2k3c - \frac{2}{9}k2cy^4k2d$$

$$+ \frac{1}{9}k2dy^2k3d - \frac{1}{9}k1c^2 + \frac{1}{9}k1ck3d + \frac{1}{9}k1dk3c + \frac{1}{9}k1dk3d + \frac{1}{9}k1ck3c - \frac{2}{9}k1ck1d - \frac{2}{9}k3ck3d\Big)\Big) \Big/$$

$$\Big(12\,(-3k1c^2k2c^4y^8 - 12k1c^2k2c^3k2dy^8 - 18k1c^2k2c^2k2d^2y^8 - 12k1c^2k2ck2d^3y^8 - 3k1c^2k2d^4y^8 - 6k1ck1dk2c^3k2dy^8$$

$$- 18k1ck1dk2c^2k2d^2y^8 - 18k1ck1dk2ck2d^3y^8 - 6k1ck1dk2d^4y^8 + 6k1ck2c^4k3cy^8 + 6k1ck2c^4k3dy^8 + 18k1ck2c^3k2dk3cy^8$$

$$+ 24k1ck2c^3k2dk3dy^8 + 18k1ck2c^2k2d^2k3cy^8 + 36k1ck2c^2k2d^2k3dy^8 + 6k1ck2ck2d^3k3cy^8 + 24k1ck2ck2d^3k3dy^8 + 6k1ck2d^4k3dy^8$$

$$- 3k1d^2k2c^2k2d^2y^8 - 6k1d^2k2ck2d^3y^8 - 3k1d^2k2d^4y^8 - 6k1dk2c^3k2dk3cy^8 + 6k1dk2c^3k2dk3dy^8 - 12k1dk2c^2k2d^2k3cy^8 + 18k1dk2c^2k2d^2k3dy^8$$

$$- 6k1dk2ck2d^3k3cy^8 + 18k1dk2ck2d^3k3dy^8 + 6k1dk2d^4k3dy^8 - 3k2c^4k3c^2y^8 - 6k2c^4k3ck3dy^8 - 3k2c^4k3d^2y^8 - 6k2c^3k2dk3c^2y^8$$

$$- 18k2c^3k2dk3ck3dy^8 - 12k2c^3k2dk3d^2y^8 - 3k2c^2k2d^2k3c^2y^8 - 18k2c^2k2d^2k3ck3dy^8 - 18k2c^2k2d^2k3d^2y^8 - 6k2ck2d^3k3ck3dy^8$$

$$- 12k2ck2d^3k3d^2y^8 - 3k2d^4k3d^2y^8 + 6k1c^3k2c^3y^6 + 18k1c^3k2c^2k2dy^6 + 18k1c^3k2ck2d^2y^6 + 6k1c^3k2d^3y^6 - 6k1c^2k1dk2c^3y^6 + 6k1c^2k1dk2c^2k2dy^6$$

$$+ 30k1c^2k1dk2ck2d^2y^6 + 18k1c^2k1dk2d^3y^6 - 6k1c^2k2c^3k3cy^6 - 6k1c^2k2c^3k3dy^6 - 24k1c^2k2c^2k2dk3cy^6 - 18k1c^2k2c^2k2dk3dy^6$$

$$- 30k1c^2k2ck2d^2k3cy^6 - 18k1c^2k2ck2d^2k3dy^6 - 12k1c^2k2d^3k3cy^6 - 6k1c^2k2d^3k3dy^6 - 12k1ck1d^2k2c^2k2dy^6 + 6k1ck1d^2k2ck2d^2y^6$$

$$+ 18k1ck1d^2k2d^3y^6 + 18k1ck1dk2c^3k3cy^6 + 18k1ck1dk2c^3k3dy^6 + 18k1ck1dk2c^2k2dk3cy^6 + 24k1ck1dk2c^2k2dk3dy^6$$

$$- 24k1ck1dk2ck2d^2k3cy^6 - 6k1ck1dk2ck2d^2k3dy^6 - 24k1ck1dk2d^3k3cy^6 - 12k1ck1dk2d^3k3dy^6 - 6k1ck2c^3k3c^2y^6 - 12k1ck2c^3k3ck3dy^6$$

$$- 6k1ck2c^3k3d^2y^6 + 12k1ck2c^2k2dk3c^2y^6 - 6k1ck2c^2k2dk3ck3dy^6 - 18k1ck2c^2k2dk3d^2y^6 + 18k1ck2ck2d^2k3c^2y^6 + 24k1ck2ck2d^2k3ck3dy^6$$

$$- 18k1ck2ck2d^2k3d^2y^6 + 18k1ck2d^3k3ck3dy^6 - 6k1ck2d^3k3d^2y^6 - 6k1d^3k2ck2d^2y^6 + 6k1d^3k2d^3y^6 - 18k1d^2k2c^2k2dk3cy^6$$

$$+ 18k1d^2k2c^2k2dk3dy^6 + 6k1d^2k2ck2d^2k3cy^6 + 12k1d^2k2ck2d^2k3dy^6 - 12k1d^2k2d^3k3cy^6 - 6k1d^2k2d^3k3dy^6 - 12k1dk2c^3k3c^2y^6$$

$$- 24k1dk2c^3k3ck3dy^6 - 12k1dk2c^3k3d^2y^6 + 6k1dk2c^2k2dk3c^2y^6 - 24k1dk2c^2k2dk3ck3dy^6 - 30k1dk2c^2k2dk3d^2y^6 - 18k1dk2ck2d^2k3c^2y^6$$

$$+ 18k1dk2ck2d^2k3ck3dy^6 - 24k1dk2ck2d^2k3d^2y^6 + 18k1dk2d^3k3ck3dy^6 - 6k1dk2d^3k3d^2y^6 + 6k2c^3k3c^3y^6 + 18k2c^3k3c^2k3dy^6$$

$$+ 18k2c^3k3ck3d^2y^6 + 6k2c^3k3d^3y^6 - 6k2c^2k2dk3c^3y^6 + 6k2c^2k2dk3c^2k3dy^6 + 30k2c^2k2dk3ck3d^2y^6 + 18k2c^2k2dk3d^3y^6 - 12k2ck2d^2k3c^2k3dy^6$$

$$+ 6k2ck2d^2k3ck3d^2y^6 + 18k2ck2d^2k3d^3y^6 - 6k2d^3k3ck3d^2y^6 + 6k2d^3k3d^3y^6 - 3k1c^4k2c^2y^4 - 6k1c^4k2ck2dy^4 - 3k1c^4k2d^2y^4 - 6k1c^3k1dk2c^2y^4$$

$$- 18k1c^3k1dk2ck2dy^4 - 12k1c^3k1dk2d^2y^4 - 6k1c^3k2c^2k3cy^4 - 6k1c^3k2c^2k3dy^4 + 12k1c^3k2ck2dk3cy^4 - 12k1c^3k2ck2dk3dy^4$$

$$+ 18k1c^3k2d^2k3cy^4 - 6k1c^3k2d^2k3dy^4 - 3k1c^2k1d^2k2c^2y^4 - 18k1c^2k1d^2k2ck2dy^4 - 18k1c^2k1d^2k2d^2y^4 + 12k1c^2k1dk2c^2k3cy^4$$

$$+ 12k1c^2k1dk2c^2k3dy^4 + 6k1c^2k1dk2ck2dk3cy^4 - 6k1c^2k1dk2ck2dk3dy^4 + 54k1c^2k1dk2d^2k3cy^4 - 18k1c^2k1dk2d^2k3dy^4 + 18k1c^2k2c^2k3c^2y^4$$

$$+ 36k1c^2k2c^2k3ck3dy^4 + 18k1c^2k2c^2k3d^2y^4 - 24k1c^2k2ck2dk3c^2y^4 + 12k1c^2k2ck2dk3ck3dy^4 + 36k1c^2k2ck2dk3d^2y^4 - 18k1c^2k2d^2k3c^2y^4$$

$$- 24k1c^2k2d^2k3ck3dy^4 + 18k1c^2k2d^2k3d^2y^4 - 6k1ck1d^3k2ck2dy^4 - 12k1ck1d^3k2d^2y^4 + 18k1ck1d^2k2c^2k3cy^4 + 18k1ck1d^2k2c^2k3dy^4$$

$$- 24k1ck1d^2k2ck2dk3cy^4 + 24k1ck1d^2k2ck2dk3dy^4 + 54k1ck1d^2k2d^2k3cy^4 - 18k1ck1d^2k2d^2k3dy^4 - 24k1ck1dk2c^2k3c^2y^4$$

$$- 48k1ck1dk2c^2k3ck3dy^4 - 24k1ck1dk2c^2k3d^2y^4 + 6k1ck1dk2ck2dk3c^2y^4 + 18k1ck1dk2ck2dk3ck3dy^4 + 12k1ck1dk2ck2dk3d^2y^4$$

$$- 36k1ck1dk2d^2k3c^2y^4 - 48k1ck1dk2d^2k3ck3dy^4 + 36k1ck1dk2d^2k3d^2y^4 - 6k1ck2c^2k3c^3y^4 - 18k1ck2c^2k3c^2k3dy^4 - 18k1ck2c^2k3ck3d^2y^4$$

$$- 6k1ck2c^2k3d^3y^4 + 18k1ck2ck2dk3c^3y^4 + 24k1ck2ck2dk3c^2k3dy^4 - 6k1ck2ck2dk3ck3d^2y^4 - 12k1ck2ck2dk3d^3y^4 + 18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36k1ck1dk2ck3c^2k3dy^2+36k1ck1dk2ck3ck3d^2y^2+12k1ck1dk2ck3d^3y^2-24k1ck1dk2dk3c^3y^2-60k1ck1dk2dk3c^2k3dy^2$$

$$-48k1ck1dk2dk3ck3d^2y^2-12k1ck1dk2dk3d^3y^2+6k1ck2ck3c^4y^2+24k1ck2ck3c^3k3dy^2+36k1ck2ck3c^2k3d^2y^2+24k1ck2ck3ck3d^3y^2$$

$$+6k1ck2ck3d^4y^2+6k1ck2dk3c^3k3dy^2+18k1ck2dk3c^2k3d^2y^2+18k1ck2dk3ck3d^3y^2+6k1ck2dk3d^4y^2-6k1d^4k2dk3cy^2+6k1d^4k2dk3dy^2$$

$$-12k1d^3k2ck3c^2y^2-24k1d^3k2ck3ck3dy^2-12k1d^3k2ck3d^2y^2+18k1d^3k2dk3c^2y^2+12k1d^3k2dk3ck3dy^2-6k1d^3k2dk3d^2y^2+18k1d^2k2ck3c^3y^2$$

$$+54k1d^2k2ck3c^2k3dy^2+54k1d^2k2ck3ck3d^2y^2+18k1d^2k2ck3d^3y^2-12k1d^2k2dk3c^3y^2-30k1d^2k2dk3c^2k3dy^2-24k1d^2k2dk3ck3d^2y^2$$

$$-6k1d^2k2dk3d^3y^2-6k1dk2ck3c^4y^2-24k1dk2ck3c^3k3dy^2-36k1dk2ck3c^2k3d^2y^2-24k1dk2ck3ck3d^3y^2-6k1dk2ck3d^4y^2$$

$$+6k1dk2dk3c^3k3dy^2+18k1dk2dk3c^2k3d^2y^2+18k1dk2dk3ck3d^3y^2+6k1dk2dk3d^4y^2-3k1c^4k3c^2-6k1c^4k3ck3d-3k1c^4k3d^2$$

$$-12k1c^3k1dk3c^2-24k1c^3k1dk3ck3d-12k1c^3k1dk3d^2+6k1c^3k3c^3+18k1c^3k3c^2k3d+18k1c^3k3ck3d^2+6k1c^3k3d^3-18k1c^2k1d^2k3c^2$$

$$-36k1c^2k1d^2k3ck3d-18k1c^2k1d^2k3d^2+18k1c^2k1dk3c^3+54k1c^2k1dk3c^2k3d+54k1c^2k1dk3ck3d^2+18k1c^2k1dk3d^3-3k1c^2k3c^4$$

$$-12k1c^2k3c^3k3d-18k1c^2k3c^2k3d^2-12k1c^2k3ck3d^3-3k1c^2k3d^4-12k1ck1d^3k3c^2-24k1ck1d^3k3ck3d-12k1ck1d^3k3d^2+18k1ck1d^2k3c^3$$

$$+54k1ck1d^2k3c^2k3d+54k1ck1d^2k3ck3d^2+18k1ck1d^2k3d^3-6k1ck1dk3c^4-24k1ck1dk3c^3k3d-36k1ck1dk3c^2k3d^2-24k1ck1dk3ck3d^3$$

$$-6k1ck1dk3d^4-3k1d^4k3c^2-6k1d^4k3ck3d-3k1d^4k3d^2+6k1d^3k3c^3+18k1d^3k3c^2k3d+18k1d^3k3ck3d^2+6k1d^3k3d^3-3k1d^2k3c^4$$

$$-12k1d^2k3c^3k3d-18k1d^2k3c^2k3d^2-12k1d^2k3ck3d^3-3k1d^2k3d^4)^{1/2}-8k1c^3-8k1d^3-8k3c^3-8k3d^3+12k1d^2k3c+12k1d^2k3d$$

$$+12k1dk3c^2+12k1dk3d^2-8k2c^3y^6-8k2d^3y^6-24k1c^2k1d-24k1ck1d^2-24k3c^2k3d-24k3ck3d^2+12k1ck3c^2+12k1ck3d^2+12k1ck2c^2y^4$$

$$+12k1ck2d^2y^4+12k1dk2d^2y^4+12k2c^2k3cy^4+12k2c^2k3dy^4+12k2d^2k3dy^4+12k1c^2k2cy^2+12k1c^2k2dy^2+12k1d^2k2dy^2+12k2ck3c^2y^2$$

$$+12k2ck3d^2y^2+12k2dk3d^2y^2+24k1ck1dk3c+24k1ck1dk3d+24k1ck3ck3d+24k1dk3ck3d-24k2c^2k2dy^6-24k2ck2d^2y^6-24k1dk2c^2y^4$$

$$-24k2d^2k3cy^4-24k1d^2k2cy^2-24k2dk3c^2y^2+24k1dk2dk3cy^2+24k2ck3ck3dy^2-12k2dk3ck3dy^2+24k1ck2ck2dy^4-12k1dk2ck2dy^4$$

$$-12k2ck2dk3cy^4-12k1ck1dk2cy^2+24k1ck1dk2dy^2+24k1ck2dk3cy^2+24k1dk2ck3cy^2+24k1dk2ck3dy^2-48k1ck2ck3cy^2$$

$$-48k1ck2ck3dy^2-48k1ck2dk3dy^2+12k1c^2k3c+12k1c^2k3d+24k2cy^4k2dk3d-48k1dk2dk3dy^2\Big)\Big)^{1/3}-\frac{1}{3}k2cy^2-\frac{1}{3}k2dy^2-\frac{1}{3}k1c-\frac{1}{3}k1d$$

$$-\frac{1}{3}k3c-\frac{1}{3}k3d$$

$$+\frac{1}{2}I\sqrt{3}\Bigg(\frac{1}{6}\Big(12\big(-3k1c^2k2c^4y^8-12k1c^2k2c^3k2dy^8-18k1c^2k2c^2k2d^2y^8-12k1c^2k2ck2d^3y^8-3k1c^2k2d^4y^8$$

$$-6k1ck1dk2c^3k2dy^8-18k1ck1dk2c^2k2d^2y^8-18k1ck1dk2ck2d^3y^8-6k1ck1dk2d^4y^8+6k1ck2c^4k3cy^8+6k1ck2c^4k3dy^8+18k1ck2c^3k2dk3cy^8$$

$$+24k1ck2c^{3}k2dk3dy^{8}+18k1ck2c^{2}k2d^{2}k3cy^{8}+36k1ck2c^{2}k2d^{2}k3dy^{8}+6k1ck2ck2d^{3}k3cy^{8}+24k1ck2ck2d^{3}k3dy^{8}+6k1ck2d^{4}k3dy^{8}$$

$$-3k1d^{2}k2c^{2}k2d^{2}y^{8}-6k1d^{2}k2ck2d^{3}y^{8}-3k1d^{2}k2d^{4}y^{8}-6k1dk2c^{3}k2dk3cy^{8}+6k1dk2c^{3}k2dk3dy^{8}-12k1dk2c^{2}k2d^{2}k3cy^{8}+18k1dk2c^{2}k2d^{2}k3dy^{8}$$

$$-6k1dk2ck2d^{3}k3cy^{8}+18k1dk2ck2d^{3}k3dy^{8}+6k1dk2d^{4}k3dy^{8}-3k2c^{4}k3c^{2}y^{8}-6k2c^{4}k3ck3dy^{8}-3k2c^{4}k3d^{2}y^{8}-6k2c^{3}k2dk3c^{2}y^{8}$$

$$-18k2c^{3}k2dk3ck3dy^{8}-12k2c^{3}k2dk3d^{2}y^{8}-3k2c^{2}k2d^{2}k3c^{2}y^{8}-18k2c^{2}k2d^{2}k3ck3dy^{8}-18k2c^{2}k2d^{2}k3d^{2}y^{8}-6k2ck2d^{3}k3ck3dy^{8}$$

$$-12k2ck2d^{3}k3d^{2}y^{8}-3k2d^{4}k3d^{2}y^{8}+6k1c^{3}k2c^{3}y^{6}+18k1c^{3}k2c^{2}k2dy^{6}+18k1c^{3}k2ck2d^{2}y^{6}+6k1c^{3}k2d^{3}y^{6}-6k1c^{2}k1dk2c^{3}y^{6}+6k1c^{2}k1dk2c^{2}k2dy^{6}$$

$$+30k1c^{2}k1dk2ck2d^{2}y^{6}+18k1c^{2}k1dk2d^{3}y^{6}-6k1c^{2}k2c^{3}k3cy^{6}-6k1c^{2}k2c^{3}k3dy^{6}-24k1c^{2}k2c^{2}k2dk3cy^{6}-18k1c^{2}k2c^{2}k2dk3dy^{6}$$

$$-30k1c^{2}k2ck2d^{2}k3cy^{6}-18k1c^{2}k2ck2d^{2}k3dy^{6}-12k1c^{2}k2d^{3}k3cy^{6}-6k1c^{2}k2d^{3}k3dy^{6}-12k1ck1d^{2}k2c^{2}k2dy^{6}+6k1ck1d^{2}k2ck2d^{2}y^{6}$$

$$+18k1ck1d^{2}k2d^{3}y^{6}+18k1ck1dk2c^{3}k3cy^{6}+18k1ck1dk2c^{3}k3dy^{6}+18k1ck1dk2c^{2}k2dk3cy^{6}+24k1ck1dk2c^{2}k2dk3dy^{6}$$

$$-24k1ck1dk2ck2d^{2}k3cy^{6}-6k1ck1dk2ck2d^{2}k3dy^{6}-24k1ck1dk2d^{3}k3cy^{6}-12k1ck1dk2d^{3}k3dy^{6}-6k1ck2c^{3}k3c^{2}y^{6}-12k1ck2c^{3}k3ck3dy^{6}$$

$$-6k1ck2c^{3}k3d^{2}y^{6}+12k1ck2c^{2}k2dk3c^{2}y^{6}-6k1ck2c^{2}k2dk3ck3dy^{6}-18k1ck2c^{2}k2dk3d^{2}y^{6}+18k1ck2ck2d^{2}k3c^{2}y^{6}+24k1ck2ck2d^{2}k3ck3dy^{6}$$

$$-18k1ck2ck2d^{2}k3d^{2}y^{6}+18k1ck2d^{3}k3ck3dy^{6}-6k1ck2d^{3}k3d^{2}y^{6}-6k1d^{3}k2ck2d^{2}y^{6}+6k1d^{3}k2d^{3}y^{6}-18k1d^{2}k2c^{2}k2dk3cy^{6}$$

$$+18k1d^{2}k2c^{2}k2dk3dy^{6}+6k1d^{2}k2ck2d^{2}k3cy^{6}+12k1d^{2}k2ck2d^{2}k3dy^{6}-12k1d^{2}k2d^{3}k3cy^{6}-6k1d^{2}k2d^{3}k3dy^{6}-12k1dk2c^{3}k3c^{2}y^{6}$$

$$-24k1dk2c^{3}k3ck3dy^{6}-12k1dk2c^{3}k3d^{2}y^{6}+6k1dk2c^{2}k2dk3c^{2}y^{6}-24k1dk2c^{2}k2dk3ck3dy^{6}-30k1dk2c^{2}k2dk3d^{2}y^{6}-18k1dk2ck2d^{2}k3c^{2}y^{6}$$

$$+18k1dk2ck2d^{2}k3ck3dy^{6}-24k1dk2ck2d^{2}k3d^{2}y^{6}+18k1dk2d^{3}k3ck3dy^{6}-6k1dk2d^{3}k3d^{2}y^{6}+6k2c^{3}k3c^{3}y^{6}+18k2c^{3}k3c^{2}k3dy^{6}$$

$$+18k2c^{3}k3ck3d^{2}y^{6}+6k2c^{3}k3d^{3}y^{6}-6k2c^{2}k2dk3c^{3}y^{6}+6k2c^{2}k2dk3c^{2}k3dy^{6}+30k2c^{2}k2dk3ck3d^{2}y^{6}+18k2c^{2}k2dk3d^{3}y^{6}-12k2ck2d^{2}k3c^{2}k3dy^{6}$$

$$+6k2ck2d^{2}k3ck3d^{2}y^{6}+18k2ck2d^{2}k3d^{3}y^{6}-6k2d^{3}k3ck3d^{2}y^{6}+6k2d^{3}k3d^{3}y^{6}-3k1c^{4}k2c^{2}y^{4}-6k1c^{4}k2ck2dy^{4}-3k1c^{4}k2d^{2}y^{4}-6k1c^{3}k1dk2c^{2}y^{4}$$

$$-18k1c^{3}k1dk2ck2dy^{4}-12k1c^{3}k1dk2d^{2}y^{4}-6k1c^{3}k2c^{2}k3cy^{4}-6k1c^{3}k2c^{2}k3dy^{4}+12k1c^{3}k2ck2dk3cy^{4}-12k1c^{3}k2ck2dk3dy^{4}$$

$$+18k1c^{3}k2d^{2}k3cy^{4}-6k1c^{3}k2d^{2}k3dy^{4}-3k1c^{2}k1d^{2}k2c^{2}y^{4}-18k1c^{2}k1d^{2}k2ck2dy^{4}-18k1c^{2}k1d^{2}k2d^{2}y^{4}+12k1c^{2}k1dk2c^{2}k3cy^{4}$$

$$+12k1c^{2}k1dk2c^{2}k3dy^{4}+6k1c^{2}k1dk2ck2dk3cy^{4}-6k1c^{2}k1dk2ck2dk3dy^{4}+54k1c^{2}k1dk2d^{2}k3cy^{4}-18k1c^{2}k1dk2d^{2}k3dy^{4}+18k1c^{2}k2c^{2}k3c^{2}y^{4}$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36k1ck1dk2ck3c^2k3dy^2+36k1ck1dk2ck3ck3d^2y^2+12k1ck1dk2ck3d^3y^2-24k1ck1dk2dk3c^3y^2-60k1ck1dk2dk3c^2k3dy^2$$

$$-48k1ck1dk2dk3ck3d^2y^2-12k1ck1dk2dk3d^3y^2+6k1ck2ck3c^4y^2+24k1ck2ck3c^3k3dy^2+36k1ck2ck3c^2k3d^2y^2+24k1ck2ck3ck3d^3y^2$$

$$+6k1ck2ck3d^4y^2+6k1ck2dk3c^3k3dy^2+18k1ck2dk3c^2k3d^2y^2+18k1ck2dk3ck3d^3y^2+6k1ck2dk3d^4y^2-6k1d^4k2dk3cy^2+6k1d^4k2dk3dy^2$$

$$-12k1d^3k2ck3c^2y^2-24k1d^3k2ck3ck3dy^2-12k1d^3k2ck3d^2y^2+18k1d^3k2dk3c^2y^2+12k1d^3k2dk3ck3dy^2-6k1d^3k2dk3d^2y^2+18k1d^2k2ck3c^3y^2$$

$$+54k1d^2k2ck3c^2k3dy^2+54k1d^2k2ck3ck3d^2y^2+18k1d^2k2ck3d^3y^2-12k1d^2k2dk3c^3y^2-30k1d^2k2dk3c^2k3dy^2-24k1d^2k2dk3ck3d^2y^2$$

$$-6k1d^2k2dk3d^3y^2-6k1dk2ck3c^4y^2-24k1dk2ck3c^3k3dy^2-36k1dk2ck3c^2k3d^2y^2-24k1dk2ck3ck3d^3y^2-6k1dk2ck3d^4y^2$$

$$+6k1dk2dk3c^3k3dy^2+18k1dk2dk3c^2k3d^2y^2+18k1dk2dk3ck3d^3y^2+6k1dk2dk3d^4y^2-3k1c^4k3c^2-6k1c^4k3ck3d-3k1c^4k3d^2$$

$$-12k1c^3k1dk3c^2-24k1c^3k1dk3ck3d-12k1c^3k1dk3d^2+6k1c^3k3c^3+18k1c^3k3c^2k3d+18k1c^3k3ck3d^2+6k1c^3k3d^3-18k1c^2k1d^2k3c^2$$

$$-36k1c^2k1d^2k3ck3d-18k1c^2k1d^2k3d^2+18k1c^2k1dk3c^3+54k1c^2k1dk3c^2k3d+54k1c^2k1dk3ck3d^2+18k1c^2k1dk3d^3-3k1c^2k3c^4$$

$$-12k1c^2k3c^3k3d-18k1c^2k3c^2k3d^2-12k1c^2k3ck3d^3-3k1c^2k3d^4-12k1ck1d^3k3c^2-24k1ck1d^3k3ck3d-12k1ck1d^3k3d^2+18k1ck1d^2k3c^3$$

$$+54k1ck1d^2k3c^2k3d+54k1ck1d^2k3ck3d^2+18k1ck1d^2k3d^3-6k1ck1dk3c^4-24k1ck1dk3c^3k3d-36k1ck1dk3c^2k3d^2-24k1ck1dk3ck3d^3$$

$$-6k1ck1dk3d^4-3k1d^4k3c^2-6k1d^4k3ck3d-3k1d^4k3d^2+6k1d^3k3c^3+18k1d^3k3c^2k3d+18k1d^3k3ck3d^2+6k1d^3k3d^3-3k1d^2k3c^4$$

$$-12k1d^2k3c^3k3d-18k1d^2k3c^2k3d^2-12k1d^2k3ck3d^3-3k1d^2k3d^4\Big)^{1/2}-8k1c^3-8k1d^3-8k3c^3-8k3d^3+12k1d^2k3c+12k1d^2k3d$$

$$+12k1dk3c^2+12k1dk3d^2-8k2c^3y^6-8k2d^3y^6-24k1c^2k1d-24k1ck1d^2-24k3c^2k3d-24k3ck3d^2+12k1ck3c^2+12k1ck3d^2+12k1ck2c^2y^4$$

$$+12k1ck2d^2y^4+12k1dk2d^2y^4+12k2c^2k3cy^4+12k2c^2k3dy^4+12k2d^2k3dy^4+12k1c^2k2cy^2+12k1c^2k2dy^2+12k1d^2k2dy^2+12k2ck3c^2y^2$$

$$+12k2ck3d^2y^2+12k2dk3d^2y^2+24k1ck1dk3c+24k1ck1dk3d+24k1ck3ck3d+24k1dk3ck3d-24k2c^2k2dy^6-24k2ck2d^2y^6-24k1dk2c^2y^4$$

$$-24k2d^2k3cy^4-24k1d^2k2cy^2-24k2dk3c^2y^2+24k1dk2dk3cy^2+24k2ck3ck3dy^2-12k2dk3ck3dy^2+24k1ck2ck2dy^4-12k1dk2ck2dy^4$$

$$-12k2ck2dk3cy^4-12k1ck1dk2cy^2+24k1ck1dk2dy^2+24k1ck2dk3cy^2+24k1dk2ck3cy^2+24k1dk2ck3dy^2-48k1ck2ck3cy^2$$

$$-48k1ck2ck3dy^2-48k1ck2dk3dy^2+12k1c^2k3c+12k1c^2k3d+24k2cy^4k2dk3d-48k1dk2dk3dy^2\Big)^{1/3}+\Bigg(6\bigg(-\frac{1}{9}k2c^2y^4-\frac{1}{9}k2d^2y^4$$

$$-\frac{1}{9}k1d^2-\frac{1}{9}k3c^2-\frac{1}{9}k3d^2+\frac{1}{9}k1ck2cy^2+\frac{1}{9}k1ck2dy^2+\frac{1}{9}k1dk2dy^2+\frac{1}{9}k2ck3cy^2+\frac{1}{9}k2ck3dy^2-\frac{2}{9}k2cy^2k1d-\frac{2}{9}k2dy^2k3c-\frac{2}{9}k2cy^4k2d$$

$$+\frac{1}{9}k2dy^2k3d-\frac{1}{9}k1c^2+\frac{1}{9}k1ck3d+\frac{1}{9}k1dk3c+\frac{1}{9}k1dk3d+\frac{1}{9}k1ck3c-\frac{2}{9}k1ck1d-\frac{2}{9}k3ck3d\Big)\Big)\Big/$$

$$\Big(12\Big(-3k1c^2k2c^4y^8-12k1c^2k2c^3k2dy^8-18k1c^2k2c^2k2d^2y^8-12k1c^2k2ck2d^3y^8-3k1c^2k2d^4y^8-6k1ck1dk2c^3k2dy^8$$

$$-18k1ck1dk2c^2k2d^2y^8-18k1ck1dk2ck2d^3y^8-6k1ck1dk2d^4y^8+6k1ck2c^4k3cy^8+6k1ck2c^4k3dy^8+18k1ck2c^3k2dk3cy^8$$

$$+24k1ck2c^3k2dk3dy^8+18k1ck2c^2k2d^2k3cy^8+36k1ck2c^2k2d^2k3dy^8+6k1ck2ck2d^3k3cy^8+24k1ck2ck2d^3k3dy^8+6k1ck2d^4k3dy^8$$

$$-3k1d^2k2c^2k2d^2y^8-6k1d^2k2ck2d^3y^8-3k1d^2k2d^4y^8-6k1dk2c^3k2dk3cy^8+6k1dk2c^3k2dk3dy^8-12k1dk2c^2k2d^2k3cy^8+18k1dk2c^2k2d^2k3dy^8$$

$$-6k1dk2ck2d^3k3cy^8+18k1dk2ck2d^3k3dy^8+6k1dk2d^4k3dy^8-3k2c^4k3c^2y^8-6k2c^4k3ck3dy^8-3k2c^4k3d^2y^8-6k2c^3k2dk3c^2y^8$$

$$-18k2c^3k2dk3ck3dy^8-12k2c^3k2dk3d^2y^8-3k2c^2k2d^2k3c^2y^8-18k2c^2k2d^2k3ck3dy^8-18k2c^2k2d^2k3d^2y^8-6k2ck2d^3k3ck3dy^8$$

$$-12k2ck2d^3k3d^2y^8-3k2d^4k3d^2y^8+6k1c^3k2c^3y^6+18k1c^3k2c^2k2dy^6+18k1c^3k2ck2d^2y^6+6k1c^3k2d^3y^6-6k1c^2k1dk2c^3y^6+6k1c^2k1dk2c^2k2dy^6$$

$$+30k1c^2k1dk2ck2d^2y^6+18k1c^2k1dk2d^3y^6-6k1c^2k2c^3k3cy^6-6k1c^2k2c^3k3dy^6-24k1c^2k2c^2k2dk3cy^6-18k1c^2k2c^2k2dk3dy^6$$

$$-30k1c^2k2ck2d^2k3cy^6-18k1c^2k2ck2d^2k3dy^6-12k1c^2k2d^3k3cy^6-6k1c^2k2d^3k3dy^6-12k1ck1d^2k2c^2k2dy^6+6k1ck1d^2k2ck2d^2y^6$$

$$+18k1ck1d^2k2d^3y^6+18k1ck1dk2c^3k3cy^6+18k1ck1dk2c^3k3dy^6+18k1ck1dk2c^2k2dk3cy^6+24k1ck1dk2c^2k2dk3dy^6$$

$$-24k1ck1dk2ck2d^2k3cy^6-6k1ck1dk2ck2d^2k3dy^6-24k1ck1dk2d^3k3cy^6-12k1ck1dk2d^3k3dy^6-6k1ck2c^3k3c^2y^6-12k1ck2c^3k3ck3dy^6$$

$$-6k1ck2c^3k3d^2y^6+12k1ck2c^2k2dk3c^2y^6-6k1ck2c^2k2dk3ck3dy^6-18k1ck2c^2k2dk3d^2y^6+18k1ck2ck2d^2k3c^2y^6+24k1ck2ck2d^2k3ck3dy^6$$

$$-18k1ck2ck2d^2k3d^2y^6+18k1ck2d^3k3ck3dy^6-6k1ck2d^3k3d^2y^6-6k1d^3k2ck2d^2y^6+6k1d^3k2d^3y^6-18k1d^2k2c^2k2dk3cy^6$$

$$+18k1d^2k2c^2k2dk3dy^6+6k1d^2k2ck2d^2k3cy^6+12k1d^2k2ck2d^2k3dy^6-12k1d^2k2d^3k3cy^6-6k1d^2k2d^3k3dy^6-12k1dk2c^3k3c^2y^6$$

$$-24k1dk2c^3k3ck3dy^6-12k1dk2c^3k3d^2y^6+6k1dk2c^2k2dk3c^2y^6-24k1dk2c^2k2dk3ck3dy^6-30k1dk2c^2k2dk3d^2y^6-18k1dk2ck2d^2k3c^2y^6$$

$$+18k1dk2ck2d^2k3ck3dy^6-24k1dk2ck2d^2k3d^2y^6+18k1dk2d^3k3ck3dy^6-6k1dk2d^3k3d^2y^6+6k2c^3k3c^3y^6+18k2c^3k3c^2k3dy^6$$

$$+18k2c^3k3ck3d^2y^6+6k2c^3k3d^3y^6-6k2c^2k2dk3c^3y^6+6k2c^2k2dk3c^2k3dy^6+30k2c^2k2dk3ck3d^2y^6+18k2c^2k2dk3d^3y^6-12k2ck2d^2k3c^2k3dy^6$$

$$+6k2ck2d^2k3ck3d^2y^6+18k2ck2d^2k3d^3y^6-6k2d^3k3ck3d^2y^6+6k2d^3k3d^3y^6-3k1c^4k2c^2y^4-6k1c^4k2ck2dy^4-3k1c^4k2d^2y^4-6k1c^3k1dk2c^2y^4$$

$$-18k1c^3k1dk2ck2dy^4-12k1c^3k1dk2d^2y^4-6k1c^3k2c^2k3cy^4-6k1c^3k2c^2k3dy^4+12k1c^3k2ck2dk3cy^4-12k1c^3k2ck2dk3dy^4$$

$$+18k1c^3k2d^2k3cy^4-6k1c^3k2d^2k3dy^4-3k1c^2k1d^2k2c^2y^4-18k1c^2k1d^2k2ck2dy^4-18k1c^2k1d^2k2d^2y^4+12k1c^2k1dk2c^2k3cy^4$$

$$+12k1c^2k1dk2c^2k3dy^4+6k1c^2k1dk2ck2dk3cy^4-6k1c^2k1dk2ck2dk3dy^4+54k1c^2k1dk2d^2k3cy^4-18k1c^2k1dk2d^2k3dy^4+18k1c^2k2c^2k3c^2y^4$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36k1ck1dk2ck3c^2k3dy^2+36k1ck1dk2ck3ck3d^2y^2+12k1ck1dk2ck3d^3y^2-24k1ck1dk2dk3c^3y^2-60k1ck1dk2dk3c^2k3dy^2$$

$$-48k1ck1dk2dk3ck3d^2y^2-12k1ck1dk2dk3d^3y^2+6k1ck2ck3c^4y^2+24k1ck2ck3c^3k3dy^2+36k1ck2ck3c^2k3d^2y^2+24k1ck2ck3ck3d^3y^2$$

$$+6k1ck2ck3d^4y^2+6k1ck2dk3c^3k3dy^2+18k1ck2dk3c^2k3d^2y^2+18k1ck2dk3ck3d^3y^2+6k1ck2dk3d^4y^2-6k1d^4k2dk3cy^2+6k1d^4k2dk3dy^2$$

$$-12k1d^3k2ck3c^2y^2-24k1d^3k2ck3ck3dy^2-12k1d^3k2ck3d^2y^2+18k1d^3k2dk3c^2y^2+12k1d^3k2dk3ck3dy^2-6k1d^3k2dk3d^2y^2+18k1d^2k2ck3c^3y^2$$

$$+54k1d^2k2ck3c^2k3dy^2+54k1d^2k2ck3ck3d^2y^2+18k1d^2k2ck3d^3y^2-12k1d^2k2dk3c^3y^2-30k1d^2k2dk3c^2k3dy^2-24k1d^2k2dk3ck3d^2y^2$$

$$-6k1d^2k2dk3d^3y^2-6k1dk2ck3c^4y^2-24k1dk2ck3c^3k3dy^2-36k1dk2ck3c^2k3d^2y^2-24k1dk2ck3ck3d^3y^2-6k1dk2ck3d^4y^2$$

$$+6k1dk2dk3c^3k3dy^2+18k1dk2dk3c^2k3d^2y^2+18k1dk2dk3ck3d^3y^2+6k1dk2dk3d^4y^2-3k1c^4k3c^2-6k1c^4k3ck3d-3k1c^4k3d^2$$

$$-12k1c^3k1dk3c^2-24k1c^3k1dk3ck3d-12k1c^3k1dk3d^2+6k1c^3k3c^3+18k1c^3k3c^2k3d+18k1c^3k3ck3d^2+6k1c^3k3d^3-18k1c^2k1d^2k3c^2$$

$$-36k1c^2k1d^2k3ck3d-18k1c^2k1d^2k3d^2+18k1c^2k1dk3c^3+54k1c^2k1dk3c^2k3d+54k1c^2k1dk3ck3d^2+18k1c^2k1dk3d^3-3k1c^2k3c^4$$

$$-12k1c^2k3c^3k3d-18k1c^2k3c^2k3d^2-12k1c^2k3ck3d^3-3k1c^2k3d^4-12k1ck1d^3k3c^2-24k1ck1d^3k3ck3d-12k1ck1d^3k3d^2+18k1ck1d^2k3c^3$$

$$+54k1ck1d^2k3c^2k3d+54k1ck1d^2k3ck3d^2+18k1ck1d^2k3d^3-6k1ck1dk3c^4-24k1ck1dk3c^3k3d-36k1ck1dk3c^2k3d^2-24k1ck1dk3ck3d^3$$

$$-6k1ck1dk3d^4-3k1d^4k3c^2-6k1d^4k3ck3d-3k1d^4k3d^2+6k1d^3k3c^3+18k1d^3k3c^2k3d+18k1d^3k3ck3d^2+6k1d^3k3d^3-3k1d^2k3c^4$$

$$-12k1d^2k3c^3k3d-18k1d^2k3c^2k3d^2-12k1d^2k3ck3d^3-3k1d^2k3d^4\Big)^{1/2}-8k1c^3-8k1d^3-8k3c^3-8k3d^3+12k1d^2k3c+12k1d^2k3d$$

$$+12k1dk3c^2+12k1dk3d^2-8k2c^3y^6-8k2d^3y^6-24k1c^2k1d-24k1ck1d^2-24k3c^2k3d-24k3ck3d^2+12k1ck3c^2+12k1ck3d^2+12k1ck2c^2y^4$$

$$+12k1ck2d^2y^4+12k1dk2d^2y^4+12k2c^2k3cy^4+12k2c^2k3dy^4+12k2d^2k3dy^4+12k1c^2k2cy^2+12k1c^2k2dy^2+12k1d^2k2dy^2+12k2ck3c^2y^2$$

$$+12k2ck3d^2y^2+12k2dk3d^2y^2+24k1ck1dk3c+24k1ck1dk3d+24k1ck3ck3d+24k1dk3ck3d-24k2c^2k2dy^6-24k2ck2d^2y^6-24k1dk2c^2y^4$$

$$-24k2d^2k3cy^4-24k1d^2k2cy^2-24k2dk3c^2y^2+24k1dk2dk3cy^2+24k2ck3ck3dy^2-12k2dk3ck3dy^2+24k1ck2ck2dy^4-12k1dk2ck2dy^4$$

$$-12k2ck2dk3cy^4-12k1ck1dk2cy^2+24k1ck1dk2dy^2+24k1ck2dk3cy^2+24k1dk2ck3cy^2+24k1dk2ck3dy^2-48k1ck2ck3cy^2$$

$$-48k1ck2ck3dy^2-48k1ck2dk3dy^2+12k1c^2k3c+12k1c^2k3d+24k2cy^4k2dk3d-48k1dk2dk3dy^2\Big)^{1/3}\Big),$$

$$-\frac{1}{12}\Big(12\Big(-3k1c^2k2c^4y^8-12k1c^2k2c^3k2dy^8-18k1c^2k2c^2k2d^2y^8-12k1c^2k2ck2d^3y^8-3k1c^2k2d^4y^8-6k1ck1dk2c^3k2dy^8$$

$$-18k1ck1dk2c^2k2d^2y^8-18k1ck1dk2ck2d^3y^8-6k1ck1dk2d^4y^8+6k1ck2c^4k3cy^8+6k1ck2c^4k3dy^8+18k1ck2c^3k2dk3cy^8$$

$$+24k1ck2c^3k2dk3dy^8+18k1ck2c^2k2d^2k3cy^8+36k1ck2c^2k2d^2k3dy^8+6k1ck2ck2d^3k3cy^8+24k1ck2ck2d^3k3dy^8+6k1ck2d^4k3dy^8$$

$$-3k1d^2k2c^2k2d^2y^8-6k1d^2k2ck2d^3y^8-3k1d^2k2d^4y^8-6k1dk2c^3k2dk3cy^8+6k1dk2c^3k2dk3dy^8-12k1dk2c^2k2d^2k3cy^8+18k1dk2c^2k2d^2k3dy^8$$

$$-6k1dk2ck2d^3k3cy^8+18k1dk2ck2d^3k3dy^8+6k1dk2d^4k3dy^8-3k2c^4k3c^2y^8-6k2c^4k3ck3dy^8-3k2c^4k3d^2y^8-6k2c^3k2dk3c^2y^8$$

$$-18k2c^3k2dk3ck3dy^8-12k2c^3k2dk3d^2y^8-3k2c^2k2d^2k3c^2y^8-18k2c^2k2d^2k3ck3dy^8-18k2c^2k2d^2k3d^2y^8-6k2ck2d^3k3ck3dy^8$$

$$-12k2ck2d^3k3d^2y^8-3k2d^4k3d^2y^8+6k1c^3k2c^3y^6+18k1c^3k2c^2k2dy^6+18k1c^3k2ck2d^2y^6+6k1c^3k2d^3y^6-6k1c^2k1dk2c^3y^6+6k1c^2k1dk2c^2k2dy^6$$

$$+30k1c^2k1dk2ck2d^2y^6+18k1c^2k1dk2d^3y^6-6k1c^2k2c^3k3cy^6-6k1c^2k2c^3k3dy^6-24k1c^2k2c^2k2dk3cy^6-18k1c^2k2c^2k2dk3dy^6$$

$$-30k1c^2k2ck2d^2k3cy^6-18k1c^2k2ck2d^2k3dy^6-12k1c^2k2d^3k3cy^6-6k1c^2k2d^3k3dy^6-12k1ck1d^2k2c^2k2dy^6+6k1ck1d^2k2ck2d^2y^6$$

$$+18k1ck1d^2k2d^3y^6+18k1ck1dk2c^3k3cy^6+18k1ck1dk2c^3k3dy^6+18k1ck1dk2c^2k2dk3cy^6+24k1ck1dk2c^2k2dk3dy^6$$

$$-24k1ck1dk2ck2d^2k3cy^6-6k1ck1dk2ck2d^2k3dy^6-24k1ck1dk2d^3k3cy^6-12k1ck1dk2d^3k3dy^6-6k1ck2c^3k3c^2y^6-12k1ck2c^3k3ck3dy^6$$

$$-6k1ck2c^3k3d^2y^6+12k1ck2c^2k2dk3c^2y^6-6k1ck2c^2k2dk3ck3dy^6-18k1ck2c^2k2dk3d^2y^6+18k1ck2ck2d^2k3c^2y^6+24k1ck2ck2d^2k3ck3dy^6$$

$$-18k1ck2ck2d^2k3d^2y^6+18k1ck2d^3k3ck3dy^6-6k1ck2d^3k3d^2y^6-6k1d^3k2ck2d^2y^6+6k1d^3k2d^3y^6-18k1d^2k2c^2k2dk3cy^6$$

$$+18k1d^2k2c^2k2dk3dy^6+6k1d^2k2ck2d^2k3cy^6+12k1d^2k2ck2d^2k3dy^6-12k1d^2k2d^3k3cy^6-6k1d^2k2d^3k3dy^6-12k1dk2c^3k3c^2y^6$$

$$-24k1dk2c^3k3ck3dy^6-12k1dk2c^3k3d^2y^6+6k1dk2c^2k2dk3c^2y^6-24k1dk2c^2k2dk3ck3dy^6-30k1dk2c^2k2dk3d^2y^6-18k1dk2ck2d^2k3c^2y^6$$

$$+18k1dk2ck2d^2k3ck3dy^6-24k1dk2ck2d^2k3d^2y^6+18k1dk2d^3k3ck3dy^6-6k1dk2d^3k3d^2y^6+6k2c^3k3c^3y^6+18k2c^3k3c^2k3dy^6$$

$$+18k2c^3k3ck3d^2y^6+6k2c^3k3d^3y^6-6k2c^2k2dk3c^3y^6+6k2c^2k2dk3c^2k3dy^6+30k2c^2k2dk3ck3d^2y^6+18k2c^2k2dk3d^3y^6-12k2ck2d^2k3c^2k3dy^6$$

$$+6k2ck2d^2k3ck3d^2y^6+18k2ck2d^2k3d^3y^6-6k2d^3k3ck3d^2y^6+6k2d^3k3d^3y^6-3k1c^4k2c^2y^4-6k1c^4k2ck2dy^4-3k1c^4k2d^2y^4-6k1c^3k1dk2c^2y^4$$

$$-18k1c^3k1dk2ck2dy^4-12k1c^3k1dk2d^2y^4-6k1c^3k2c^2k3cy^4-6k1c^3k2c^2k3dy^4+12k1c^3k2ck2dk3cy^4-12k1c^3k2ck2dk3dy^4$$

$$+18k1c^3k2d^2k3cy^4-6k1c^3k2d^2k3dy^4-3k1c^2k1d^2k2c^2y^4-18k1c^2k1d^2k2ck2dy^4-18k1c^2k1d^2k2d^2y^4+12k1c^2k1dk2c^2k3cy^4$$

$$+12k1c^2k1dk2c^2k3dy^4+6k1c^2k1dk2ck2dk3cy^4-6k1c^2k1dk2ck2dk3dy^4+54k1c^2k1dk2d^2k3cy^4-18k1c^2k1dk2d^2k3dy^4+18k1c^2k2c^2k3c^2y^4$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36k1ck1dk2ck3c^2k3dy^2+36k1ck1dk2ck3ck3d^2y^2+12k1ck1dk2ck3d^3y^2-24k1ck1dk2dk3c^3y^2-60k1ck1dk2dk3c^2k3dy^2$$

$$-48k1ck1dk2dk3ck3d^2y^2-12k1ck1dk2dk3d^3y^2+6k1ck2ck3c^4y^2+24k1ck2ck3c^3k3dy^2+36k1ck2ck3c^2k3d^2y^2+24k1ck2ck3ck3d^3y^2$$

$$+6k1ck2ck3d^4y^2+6k1ck2dk3c^3k3dy^2+18k1ck2dk3c^2k3d^2y^2+18k1ck2dk3ck3d^3y^2+6k1ck2dk3d^4y^2-6k1d^4k2dk3cy^2+6k1d^4k2dk3dy^2$$

$$-12k1d^3k2ck3c^2y^2-24k1d^3k2ck3ck3dy^2-12k1d^3k2ck3d^2y^2+18k1d^3k2dk3c^2y^2+12k1d^3k2dk3ck3dy^2-6k1d^3k2dk3d^2y^2+18k1d^2k2ck3c^3y^2$$

$$+54k1d^2k2ck3c^2k3dy^2+54k1d^2k2ck3ck3d^2y^2+18k1d^2k2ck3d^3y^2-12k1d^2k2dk3c^3y^2-30k1d^2k2dk3c^2k3dy^2-24k1d^2k2dk3ck3d^2y^2$$

$$-6k1d^2k2dk3d^3y^2-6k1dk2ck3c^4y^2-24k1dk2ck3c^3k3dy^2-36k1dk2ck3c^2k3d^2y^2-24k1dk2ck3ck3d^3y^2-6k1dk2ck3d^4y^2$$

$$+6k1dk2dk3c^3k3dy^2+18k1dk2dk3c^2k3d^2y^2+18k1dk2dk3ck3d^3y^2+6k1dk2dk3d^4y^2-3k1c^4k3c^2-6k1c^4k3ck3d-3k1c^4k3d^2$$

$$-12k1c^3k1dk3c^2-24k1c^3k1dk3ck3d-12k1c^3k1dk3d^2+6k1c^3k3c^3+18k1c^3k3c^2k3d+18k1c^3k3ck3d^2+6k1c^3k3d^3-18k1c^2k1d^2k3c^2$$

$$-36k1c^2k1d^2k3ck3d-18k1c^2k1d^2k3d^2+18k1c^2k1dk3c^3+54k1c^2k1dk3c^2k3d+54k1c^2k1dk3ck3d^2+18k1c^2k1dk3d^3-3k1c^2k3c^4$$

$$-12k1c^2k3c^3k3d-18k1c^2k3c^2k3d^2-12k1c^2k3ck3d^3-3k1c^2k3d^4-12k1ck1d^3k3c^2-24k1ck1d^3k3ck3d-12k1ck1d^3k3d^2+18k1ck1d^2k3c^3$$

$$+54k1ck1d^2k3c^2k3d+54k1ck1d^2k3ck3d^2+18k1ck1d^2k3d^3-6k1ck1dk3c^4-24k1ck1dk3c^3k3d-36k1ck1dk3c^2k3d^2-24k1ck1dk3ck3d^3$$

$$-6k1ck1dk3d^4-3k1d^4k3c^2-6k1d^4k3ck3d-3k1d^4k3d^2+6k1d^3k3c^3+18k1d^3k3c^2k3d+18k1d^3k3ck3d^2+6k1d^3k3d^3-3k1d^2k3c^4$$

$$- 12k1d^2k3c^3k3d - 18k1d^2k3c^2k3d^2 - 12k1d^2k3ck3d^3 - 3k1d^2k3d^4)^{1/2} - 8k1c^3 - 8k1d^3 - 8k3c^3 - 8k3d^3 + 12k1d^2k3c + 12k1d^2k3d$$

$$+ 12k1dk3c^2 + 12k1dk3d^2 - 8k2c^3y^6 - 8k2d^3y^6 - 24k1c^2k1d - 24k1ck1d^2 - 24k3c^2k3d - 24k3ck3d^2 + 12k1ck3c^2 + 12k1ck3d^2 + 12k1ck2c^2y^4$$

$$+ 12k1ck2d^2y^4 + 12k1dk2d^2y^4 + 12k2c^2k3cy^4 + 12k2c^2k3dy^4 + 12k2d^2k3dy^4 + 12k1c^2k2cy^2 + 12k1c^2k2dy^2 + 12k1d^2k2dy^2 + 12k2ck3c^2y^2$$

$$+ 12k2ck3d^2y^2 + 12k2dk3d^2y^2 + 24k1ck1dk3c + 24k1ck1dk3d + 24k1ck3ck3d + 24k1dk3ck3d - 24k2c^2k2dy^6 - 24k2ck2d^2y^6 - 24k1dk2c^2y^4$$

$$- 24k2d^2k3cy^4 - 24k1d^2k2cy^2 - 24k2dk3c^2y^2 + 24k1dk2dk3cy^2 + 24k2ck3ck3dy^2 - 12k2dk3ck3dy^2 + 24k1ck2ck2dy^4 - 12k1dk2ck2dy^4$$

$$- 12k2ck2dk3cy^4 - 12k1ck1dk2cy^2 + 24k1ck1dk2dy^2 + 24k1ck2dk3cy^2 + 24k1dk2ck3cy^2 + 24k1dk2ck3dy^2 - 48k1ck2ck3cy^2$$

$$- 48k1ck2ck3dy^2 - 48k1ck2dk3dy^2 + 12k1c^2k3c + 12k1c^2k3d + 24k2cy^4k2dk3d - 48k1dk2dk3dy^2)^{1/3} + \Big(3 \Big(-\frac{1}{9} k2c^2y^4 - \frac{1}{9} k2d^2y^4$$

$$- \frac{1}{9} k1d^2 - \frac{1}{9} k3c^2 - \frac{1}{9} k3d^2 + \frac{1}{9} k1ck2cy^2 + \frac{1}{9} k1ck2dy^2 + \frac{1}{9} k1dk2dy^2 + \frac{1}{9} k2ck3cy^2 + \frac{1}{9} k2ck3dy^2 - \frac{2}{9} k2cy^2k1d - \frac{2}{9} k2dy^2k3c - \frac{2}{9} k2cy^4k2d$$

$$+ \frac{1}{9} k2dy^2k3d - \frac{1}{9} k1c^2 + \frac{1}{9} k1ck3d + \frac{1}{9} k1dk3c + \frac{1}{9} k1dk3d + \frac{1}{9} k1ck3c - \frac{2}{9} k1ck1d - \frac{2}{9} k3ck3d \Big) \Big) \Big/$$

$$\Big(12 \Big(-3k1c^2k2c^4y^8 - 12k1c^2k2c^3k2dy^8 - 18k1c^2k2c^2k2d^2y^8 - 12k1c^2k2ck2d^3y^8 - 3k1c^2k2d^4y^8 - 6k1ck1dk2c^3k2dy^8$$

$$- 18k1ck1dk2c^2k2d^2y^8 - 18k1ck1dk2ck2d^3y^8 - 6k1ck1dk2d^4y^8 + 6k1ck2c^4k3cy^8 + 6k1ck2c^4k3dy^8 + 18k1ck2c^3k2dk3cy^8$$

$$+ 24k1ck2c^3k2dk3dy^8 + 18k1ck2c^2k2d^2k3cy^8 + 36k1ck2c^2k2d^2k3dy^8 + 6k1ck2ck2d^3k3cy^8 + 24k1ck2ck2d^3k3dy^8 + 6k1ck2d^4k3dy^8$$

$$- 3k1d^2k2c^2k2d^2y^8 - 6k1d^2k2ck2d^3y^8 - 3k1d^2k2d^4y^8 - 6k1dk2c^3k2dk3cy^8 + 6k1dk2c^3k2dk3dy^8 - 12k1dk2c^2k2d^2k3cy^8 + 18k1dk2c^2k2d^2k3dy^8$$

$$- 6k1dk2ck2d^3k3cy^8 + 18k1dk2ck2d^3k3dy^8 + 6k1dk2d^4k3dy^8 - 3k2c^4k3c^2y^8 - 6k2c^4k3ck3dy^8 - 3k2c^4k3d^2y^8 - 6k2c^3k2dk3c^2y^8$$

$$- 18k2c^3k2dk3ck3dy^8 - 12k2c^3k2dk3d^2y^8 - 3k2c^2k2d^2k3c^2y^8 - 18k2c^2k2d^2k3ck3dy^8 - 18k2c^2k2d^2k3d^2y^8 - 6k2ck2d^3k3ck3dy^8$$

$$- 12k2ck2d^3k3d^2y^8 - 3k2d^4k3d^2y^8 + 6k1c^3k2c^3y^6 + 18k1c^3k2c^2k2dy^6 + 18k1c^3k2ck2d^2y^6 + 6k1c^3k2d^3y^6 - 6k1c^2k1dk2c^3y^6 + 6k1c^2k1dk2c^2k2dy^6$$

$$+ 30k1c^2k1dk2ck2d^2y^6 + 18k1c^2k1dk2d^3y^6 - 6k1c^2k2c^3k3cy^6 - 6k1c^2k2c^3k3dy^6 - 24k1c^2k2c^2k2dk3cy^6 - 18k1c^2k2c^2k2dk3dy^6$$

$$- 30k1c^2k2ck2d^2k3cy^6 - 18k1c^2k2ck2d^2k3dy^6 - 12k1c^2k2d^3k3cy^6 - 6k1c^2k2d^3k3dy^6 - 12k1ck1d^2k2c^2k2dy^6 + 6k1ck1d^2k2ck2d^2y^6$$

$$+ 18k1ck1d^2k2d^3y^6 + 18k1ck1dk2c^3k3cy^6 + 18k1ck1dk2c^3k3dy^6 + 18k1ck1dk2c^2k2dk3cy^6 + 24k1ck1dk2c^2k2dk3dy^6$$

$$- 24k1ck1dk2ck2d^2k3cy^6 - 6k1ck1dk2ck2d^2k3dy^6 - 24k1ck1dk2d^3k3cy^6 - 12k1ck1dk2d^3k3dy^6 - 6k1ck2c^3k3c^2y^6 - 12k1ck2c^3k3ck3dy^6$$

$$- 6k1ck2c^3k3d^2y^6 + 12k1ck2c^2k2dk3c^2y^6 - 6k1ck2c^2k2dk3ck3dy^6 - 18k1ck2c^2k2dk3d^2y^6 + 18k1ck2ck2d^2k3c^2y^6 + 24k1ck2ck2d^2k3ck3dy^6$$

$$- 18k1ck2ck2d^2k3d^2y^6 + 18k1ck2d^3k3ck3dy^6 - 6k1ck2d^3k3d^2y^6 - 6k1d^3k2ck2d^2y^6 + 6k1d^3k2d^3y^6 - 18k1d^2k2c^2k2dk3cy^6$$

$$+ 18k1d^2k2c^2k2dk3dy^6 + 6k1d^2k2ck2d^2k3cy^6 + 12k1d^2k2ck2d^2k3dy^6 - 12k1d^2k2d^3k3cy^6 - 6k1d^2k2d^3k3dy^6 - 12k1dk2c^3k3c^2y^6$$

$$- 24k1dk2c^3k3ck3dy^6 - 12k1dk2c^3k3d^2y^6 + 6k1dk2c^2k2dk3c^2y^6 - 24k1dk2c^2k2dk3ck3dy^6 - 30k1dk2c^2k2dk3d^2y^6 - 18k1dk2ck2d^2k3c^2y^6$$

$$+ 18k1dk2ck2d^2k3ck3dy^6 - 24k1dk2ck2d^2k3d^2y^6 + 18k1dk2d^3k3ck3dy^6 - 6k1dk2d^3k3d^2y^6 + 6k2c^3k3c^3y^6 + 18k2c^3k3c^2k3dy^6$$

$$+ 18k2c^3k3ck3d^2y^6 + 6k2c^3k3d^3y^6 - 6k2c^2k2dk3c^3y^6 + 6k2c^2k2dk3c^2k3dy^6 + 30k2c^2k2dk3ck3d^2y^6 + 18k2c^2k2dk3d^3y^6 - 12k2ck2d^2k3c^2k3dy^6$$

$$+ 6k2ck2d^2k3ck3d^2y^6 + 18k2ck2d^2k3d^3y^6 - 6k2d^3k3ck3d^2y^6 + 6k2d^3k3d^3y^6 - 3k1c^4k2c^2y^4 - 6k1c^4k2ck2dy^4 - 3k1c^4k2d^2y^4 - 6k1c^3k1dk2c^2y^4$$

$$- 18k1c^3k1dk2ck2dy^4 - 12k1c^3k1dk2d^2y^4 - 6k1c^3k2c^2k3cy^4 - 6k1c^3k2c^2k3dy^4 + 12k1c^3k2ck2dk3cy^4 - 12k1c^3k2ck2dk3dy^4$$

$$+ 18k1c^3k2d^2k3cy^4 - 6k1c^3k2d^2k3dy^4 - 3k1c^2k1d^2k2c^2y^4 - 18k1c^2k1d^2k2ck2dy^4 - 18k1c^2k1d^2k2d^2y^4 + 12k1c^2k1dk2c^2k3cy^4$$

$$+ 12k1c^2k1dk2c^2k3dy^4 + 6k1c^2k1dk2ck2dk3cy^4 - 6k1c^2k1dk2ck2dk3dy^4 + 54k1c^2k1dk2d^2k3cy^4 - 18k1c^2k1dk2d^2k3dy^4 + 18k1c^2k2c^2k3c^2y^4$$

$$+ 36k1c^2k2c^2k3ck3dy^4 + 18k1c^2k2c^2k3d^2y^4 - 24k1c^2k2ck2dk3c^2y^4 + 12k1c^2k2ck2dk3ck3dy^4 + 36k1c^2k2ck2dk3d^2y^4 - 18k1c^2k2d^2k3c^2y^4$$

$$- 24k1c^2k2d^2k3ck3dy^4 + 18k1c^2k2d^2k3d^2y^4 - 6k1ck1d^3k2ck2dy^4 - 12k1ck1d^3k2d^2y^4 + 18k1ck1d^2k2c^2k3cy^4 + 18k1ck1d^2k2c^2k3dy^4$$

$$- 24k1ck1d^2k2ck2dk3cy^4 + 24k1ck1d^2k2ck2dk3dy^4 + 54k1ck1d^2k2d^2k3cy^4 - 18k1ck1d^2k2d^2k3dy^4 - 24k1ck1dk2c^2k3c^2y^4$$

$$- 48k1ck1dk2c^2k3ck3dy^4 - 24k1ck1dk2c^2k3d^2y^4 + 6k1ck1dk2ck2dk3c^2y^4 + 18k1ck1dk2ck2dk3ck3dy^4 + 12k1ck1dk2ck2dk3d^2y^4$$

$$- 36k1ck1dk2d^2k3c^2y^4 - 48k1ck1dk2d^2k3ck3dy^4 + 36k1ck1dk2d^2k3d^2y^4 - 6k1ck2c^2k3c^3y^4 - 18k1ck2c^2k3c^2k3dy^4 - 18k1ck2c^2k3ck3d^2y^4$$

$$- 6k1ck2c^2k3d^3y^4 + 18k1ck2ck2dk3c^3y^4 + 24k1ck2ck2dk3c^2k3dy^4 - 6k1ck2ck2dk3ck3d^2y^4 - 12k1ck2ck2dk3d^3y^4 + 18k1ck2d^2k3c^2k3dy^4$$

$$+ 12k1ck2d^2k3ck3d^2y^4 - 6k1ck2d^2k3d^3y^4 - 3k1d^4k2d^2y^4 - 18k1d^3k2ck2dk3cy^4 + 18k1d^3k2ck2dk3dy^4 + 18k1d^3k2d^2k3cy^4 - 6k1d^3k2d^2k3dy^4$$

$$- 18k1d^{2}k2c^{2}k3c^{2}y^{4} - 36k1d^{2}k2c^{2}k3ck3dy^{4} - 18k1d^{2}k2c^{2}k3d^{2}y^{4} + 30k1d^{2}k2ck2dk3c^{2}y^{4} + 6k1d^{2}k2ck2dk3ck3dy^{4} - 24k1d^{2}k2ck2dk3d^{2}y^{4}$$

$$- 18k1d^{2}k2d^{2}k3c^{2}y^{4} - 24k1d^{2}k2d^{2}k3ck3dy^{4} + 18k1d^{2}k2d^{2}k3d^{2}y^{4} + 18k1dk2c^{2}k3c^{3}y^{4} + 54k1dk2c^{2}k3c^{2}k3dy^{4} + 54k1dk2c^{2}k3ck3d^{2}y^{4}$$

$$+ 18k1dk2c^{2}k3d^{3}y^{4} - 18k1dk2ck2dk3c^{3}y^{4} - 24k1dk2ck2dk3c^{2}k3dy^{4} + 6k1dk2ck2dk3ck3d^{2}y^{4} + 12k1dk2ck2dk3d^{3}y^{4} + 18k1dk2d^{2}k3c^{2}k3dy^{4}$$

$$+ 12k1dk2d^{2}k3ck3d^{2}y^{4} - 6k1dk2d^{2}k3d^{3}y^{4} - 3k2c^{2}k3c^{4}y^{4} - 12k2c^{2}k3c^{3}k3dy^{4} - 18k2c^{2}k3c^{2}k3d^{2}y^{4} - 12k2c^{2}k3ck3d^{3}y^{4} - 3k2c^{2}k3d^{4}y^{4}$$

$$- 6k2ck2dk3c^{3}k3dy^{4} - 18k2ck2dk3c^{2}k3d^{2}y^{4} - 18k2ck2dk3ck3d^{3}y^{4} - 6k2ck2dk3d^{4}y^{4} - 3k2d^{2}k3c^{2}k3d^{2}y^{4} - 6k2d^{2}k3ck3d^{3}y^{4} - 3k2d^{2}k3d^{4}y^{4}$$

$$+ 6k1c^{4}k2ck3cy^{2} + 6k1c^{4}k2ck3dy^{2} - 6k1c^{4}k2dk3cy^{2} + 6k1c^{4}k2dk3dy^{2} + 18k1c^{3}k1dk2ck3cy^{2} + 18k1c^{3}k1dk2ck3dy^{2} - 24k1c^{3}k1dk2dk3cy^{2}$$

$$+ 24k1c^{3}k1dk2dk3dy^{2} - 6k1c^{3}k2ck3c^{2}y^{2} - 12k1c^{3}k2ck3ck3dy^{2} - 6k1c^{3}k2ck3d^{2}y^{2} + 18k1c^{3}k2dk3c^{2}y^{2} + 12k1c^{3}k2dk3ck3dy^{2} - 6k1c^{3}k2dk3d^{2}y^{2}$$

$$+ 18k1c^{2}k1d^{2}k2ck3cy^{2} + 18k1c^{2}k1d^{2}k2ck3dy^{2} - 36k1c^{2}k1d^{2}k2dk3cy^{2} + 36k1c^{2}k1d^{2}k2dk3dy^{2} - 24k1c^{2}k1dk2ck3c^{2}y^{2} - 48k1c^{2}k1dk2ck3ck3dy^{2}$$

$$- 24k1c^{2}k1dk2ck3d^{2}y^{2} + 54k1c^{2}k1dk2dk3c^{2}y^{2} + 36k1c^{2}k1dk2dk3ck3dy^{2} - 18k1c^{2}k1dk2dk3d^{2}y^{2} - 6k1c^{2}k2ck3c^{3}y^{2} - 18k1c^{2}k2ck3c^{2}k3dy^{2}$$

$$- 18k1c^{2}k2ck3ck3d^{2}y^{2} - 6k1c^{2}k2ck3d^{3}y^{2} - 12k1c^{2}k2dk3c^{3}y^{2} - 30k1c^{2}k2dk3c^{2}k3dy^{2} - 24k1c^{2}k2dk3ck3d^{2}y^{2} - 6k1c^{2}k2dk3d^{3}y^{2}$$

$$+ 6k1ck1d^{3}k2ck3cy^{2} + 6k1ck1d^{3}k2ck3dy^{2} - 24k1ck1d^{3}k2dk3cy^{2} + 24k1ck1d^{3}k2dk3dy^{2} - 30k1ck1d^{2}k2ck3c^{2}y^{2} - 60k1ck1d^{2}k2ck3ck3dy^{2}$$

$$- 30k1ck1d^{2}k2ck3d^{2}y^{2} + 54k1ck1d^{2}k2dk3c^{2}y^{2} + 36k1ck1d^{2}k2dk3ck3dy^{2} - 18k1ck1d^{2}k2dk3d^{2}y^{2} + 12k1ck1dk2ck3c^{3}y^{2}$$

$$+ 36k1ck1dk2ck3c^{2}k3dy^{2} + 36k1ck1dk2ck3ck3d^{2}y^{2} + 12k1ck1dk2ck3d^{3}y^{2} - 24k1ck1dk2dk3c^{3}y^{2} - 60k1ck1dk2dk3c^{2}k3dy^{2}$$

$$- 48k1ck1dk2dk3ck3d^{2}y^{2} - 12k1ck1dk2dk3d^{3}y^{2} + 6k1ck2ck3c^{4}y^{2} + 24k1ck2ck3c^{3}k3dy^{2} + 36k1ck2ck3c^{2}k3d^{2}y^{2} + 24k1ck2ck3ck3d^{3}y^{2}$$

$$+ 6k1ck2ck3d^{4}y^{2} + 6k1ck2dk3c^{3}k3dy^{2} + 18k1ck2dk3c^{2}k3d^{2}y^{2} + 18k1ck2dk3ck3d^{3}y^{2} + 6k1ck2dk3d^{4}y^{2} - 6k1d^{4}k2dk3cy^{2} + 6k1d^{4}k2dk3dy^{2}$$

$$- 12k1d^{3}k2ck3c^{2}y^{2} - 24k1d^{3}k2ck3ck3dy^{2} - 12k1d^{3}k2ck3d^{2}y^{2} + 18k1d^{3}k2dk3c^{2}y^{2} + 12k1d^{3}k2dk3ck3dy^{2} - 6k1d^{3}k2dk3d^{2}y^{2} + 18k1d^{2}k2ck3c^{3}y^{2}$$

$$+ 54k1d^{2}k2ck3c^{2}k3dy^{2} + 54k1d^{2}k2ck3ck3d^{2}y^{2} + 18k1d^{2}k2ck3d^{3}y^{2} - 12k1d^{2}k2dk3c^{3}y^{2} - 30k1d^{2}k2dk3c^{2}k3dy^{2} - 24k1d^{2}k2dk3ck3d^{2}y^{2}$$

$$- 6k1d^{2}k2dk3d^{3}y^{2} - 6k1dk2ck3c^{4}y^{2} - 24k1dk2ck3c^{3}k3dy^{2} - 36k1dk2ck3c^{2}k3d^{2}y^{2} - 24k1dk2ck3ck3d^{3}y^{2} - 6k1dk2ck3d^{4}y^{2}$$

$$+ 6k1dk2dk3c^{3}k3dy^{2} + 18k1dk2dk3c^{2}k3d^{2}y^{2} + 18k1dk2dk3ck3d^{3}y^{2} + 6k1dk2dk3d^{4}y^{2} - 3k1c^{4}k3c^{2} - 6k1c^{4}k3ck3d - 3k1c^{4}k3d^{2}$$

$$- 12k1c^{3}k1dk3c^{2} - 24k1c^{3}k1dk3ck3d - 12k1c^{3}k1dk3d^{2} + 6k1c^{3}k3c^{3} + 18k1c^{3}k3c^{2}k3d + 18k1c^{3}k3ck3d^{2} + 6k1c^{3}k3d^{3} - 18k1c^{2}k1d^{2}k3c^{2}$$

$$- 36k1c^{2}k1d^{2}k3ck3d - 18k1c^{2}k1d^{2}k3d^{2} + 18k1c^{2}k1dk3c^{3} + 54k1c^{2}k1dk3c^{2}k3d + 54k1c^{2}k1dk3ck3d^{2} + 18k1c^{2}k1dk3d^{3} - 3k1c^{2}k3c^{4}$$

$$- 12k1c^{2}k3c^{3}k3d - 18k1c^{2}k3c^{2}k3d^{2} - 12k1c^{2}k3ck3d^{3} - 3k1c^{2}k3d^{4} - 12k1ck1d^{3}k3c^{2} - 24k1ck1d^{3}k3ck3d - 12k1ck1d^{3}k3d^{2} + 18k1ck1d^{2}k3c^{3}$$

$$+ 54k1ck1d^{2}k3c^{2}k3d + 54k1ck1d^{2}k3ck3d^{2} + 18k1ck1d^{2}k3d^{3} - 6k1ck1dk3c^{4} - 24k1ck1dk3c^{3}k3d - 36k1ck1dk3c^{2}k3d^{2} - 24k1ck1dk3ck3d^{3}$$

$$- 6k1ck1dk3d^{4} - 3k1d^{4}k3c^{2} - 6k1d^{4}k3ck3d - 3k1d^{4}k3d^{2} + 6k1d^{3}k3c^{3} + 18k1d^{3}k3c^{2}k3d + 18k1d^{3}k3ck3d^{2} + 6k1d^{3}k3d^{3} - 3k1d^{2}k3c^{4}$$

$$- 12k1d^{2}k3c^{3}k3d - 18k1d^{2}k3c^{2}k3d^{2} - 12k1d^{2}k3ck3d^{3} - 3k1d^{2}k3d^{4})^{1/2} - 8k1c^{3} - 8k1d^{3} - 8k3c^{3} - 8k3d^{3} + 12k1d^{2}k3c + 12k1d^{2}k3d$$

$$+ 12k1dk3c^{2} + 12k1dk3d^{2} - 8k2c^{3}y^{6} - 8k2d^{3}y^{6} - 24k1c^{2}k1d - 24k1ck1d^{2} - 24k3c^{2}k3d - 24k3ck3d^{2} + 12k1ck3c^{2} + 12k1ck3d^{2} + 12k1ck2c^{2}y^{4}$$

$$+ 12k1ck2d^{2}y^{4} + 12k1dk2d^{2}y^{4} + 12k2c^{2}k3cy^{4} + 12k2c^{2}k3dy^{4} + 12k2d^{2}k3dy^{4} + 12k1c^{2}k2cy^{2} + 12k1c^{2}k2dy^{2} + 12k1d^{2}k2dy^{2} + 12k2ck3c^{2}y^{2}$$

$$+ 12k2ck3d^{2}y^{2} + 12k2dk3d^{2}y^{2} + 24k1ck1dk3c + 24k1ck1dk3d + 24k1ck3ck3d + 24k1dk3ck3d - 24k2c^{2}k2dy^{6} - 24k2ck2d^{2}y^{6} - 24k1dk2c^{2}y^{4}$$

$$- 24k2d^{2}k3cy^{4} - 24k1d^{2}k2cy^{2} - 24k2dk3c^{2}y^{2} + 24k1dk2dk3cy^{2} + 24k2ck3ck3dy^{2} - 12k2dk3ck3dy^{2} + 24k1ck2ck2dy^{4} - 12k1dk2ck2dy^{4}$$

$$- 12k2ck2dk3cy^{4} - 12k1ck1dk2cy^{2} + 24k1ck1dk2dy^{2} + 24k1ck2dk3cy^{2} + 24k1dk2ck3cy^{2} + 24k1dk2ck3dy^{2} - 48k1ck2ck3cy^{2}$$

$$- 48k1ck2ck3dy^{2} - 48k1ck2dk3dy^{2} + 12k1c^{2}k3c + 12k1c^{2}k3d + 24k2cy^{4}k2dk3d - 48k1dk2dk3dy^{2} \Big)^{1/3} - \frac{1}{3}k2cy^{2} - \frac{1}{3}k2dy^{2} - \frac{1}{3}k1c - \frac{1}{3}k1d$$

$$- \frac{1}{3}k3c - \frac{1}{3}k3d$$

$$- \frac{1}{2}I\sqrt{3}\left(\frac{1}{6}\Big(12\,(-3k1c^{2}k2c^{4}y^{8} - 12k1c^{2}k2c^{3}k2dy^{8} - 18k1c^{2}k2c^{2}k2d^{2}y^{8} - 12k1c^{2}k2ck2d^{3}y^{8} - 3k1c^{2}k2d^{4}y^{8}\right.$$

$$- 6k1ck1dk2c^{3}k2dy^{8} - 18k1ck1dk2c^{2}k2d^{2}y^{8} - 18k1ck1dk2ck2d^{3}y^{8} - 6k1ck1dk2d^{4}y^{8} + 6k1ck2c^{4}k3cy^{8} + 6k1ck2c^{4}k3dy^{8} + 18k1ck2c^{3}k2dk3cy^{8}$$

$$+24k1ck2c^3k2dk3dy^8+18k1ck2c^2k2d^2k3cy^8+36k1ck2c^2k2d^2k3dy^8+6k1ck2ck2d^3k3cy^8+24k1ck2ck2d^3k3dy^8+6k1ck2d^4k3dy^8$$

$$-3k1d^2k2c^2k2d^2y^8-6k1d^2k2ck2d^3y^8-3k1d^2k2d^4y^8-6k1dk2c^3k2dk3cy^8+6k1dk2c^3k2dk3dy^8-12k1dk2c^2k2d^2k3cy^8+18k1dk2c^2k2d^2k3dy^8$$

$$-6k1dk2ck2d^3k3cy^8+18k1dk2ck2d^3k3dy^8+6k1dk2d^4k3dy^8-3k2c^4k3c^2y^8-6k2c^4k3ck3dy^8-3k2c^4k3d^2y^8-6k2c^3k2dk3c^2y^8$$

$$-18k2c^3k2dk3ck3dy^8-12k2c^3k2dk3d^2y^8-3k2c^2k2d^2k3c^2y^8-18k2c^2k2d^2k3ck3dy^8-18k2c^2k2d^2k3d^2y^8-6k2ck2d^3k3ck3dy^8$$

$$-12k2ck2d^3k3d^2y^8-3k2d^4k3d^2y^8+6k1c^3k2c^3y^6+18k1c^3k2c^2k2dy^6+18k1c^3k2ck2d^2y^6+6k1c^3k2d^3y^6-6k1c^2k1dk2c^3y^6+6k1c^2k1dk2c^2k2dy^6$$

$$+30k1c^2k1dk2ck2d^2y^6+18k1c^2k1dk2d^3y^6-6k1c^2k2c^3k3cy^6-6k1c^2k2c^3k3dy^6-24k1c^2k2c^2k2dk3cy^6-18k1c^2k2c^2k2dk3dy^6$$

$$-30k1c^2k2ck2d^2k3cy^6-18k1c^2k2ck2d^2k3dy^6-12k1c^2k2d^3k3cy^6-6k1c^2k2d^3k3dy^6-12k1ck1d^2k2c^2k2dy^6+6k1ck1d^2k2ck2d^2y^6$$

$$+18k1ck1d^2k2d^3y^6+18k1ck1dk2c^3k3cy^6+18k1ck1dk2c^3k3dy^6+18k1ck1dk2c^2k2dk3cy^6+24k1ck1dk2c^2k2dk3dy^6$$

$$-24k1ck1dk2ck2d^2k3cy^6-6k1ck1dk2ck2d^2k3dy^6-24k1ck1dk2d^3k3cy^6-12k1ck1dk2d^3k3dy^6-6k1ck2c^3k3c^2y^6-12k1ck2c^3k3ck3dy^6$$

$$-6k1ck2c^3k3d^2y^6+12k1ck2c^2k2dk3c^2y^6-6k1ck2c^2k2dk3ck3dy^6-18k1ck2c^2k2dk3d^2y^6+18k1ck2ck2d^2k3c^2y^6+24k1ck2ck2d^2k3ck3dy^6$$

$$-18k1ck2ck2d^2k3d^2y^6+18k1ck2d^3k3ck3dy^6-6k1ck2d^3k3d^2y^6-6k1d^3k2ck2d^2y^6+6k1d^3k2d^3y^6-18k1d^2k2c^2k2dk3cy^6$$

$$+18k1d^2k2c^2k2dk3dy^6+6k1d^2k2ck2d^2k3cy^6+12k1d^2k2ck2d^2k3dy^6-12k1d^2k2d^3k3cy^6-6k1d^2k2d^3k3dy^6-12k1dk2c^3k3c^2y^6$$

$$-24k1dk2c^3k3ck3dy^6-12k1dk2c^3k3d^2y^6+6k1dk2c^2k2dk3c^2y^6-24k1dk2c^2k2dk3ck3dy^6-30k1dk2c^2k2dk3d^2y^6-18k1dk2ck2d^2k3c^2y^6$$

$$+18k1dk2ck2d^2k3ck3dy^6-24k1dk2ck2d^2k3d^2y^6+18k1dk2d^3k3ck3dy^6-6k1dk2d^3k3d^2y^6+6k2c^3k3c^3y^6+18k2c^3k3c^2k3dy^6$$

$$+18k2c^3k3ck3d^2y^6+6k2c^3k3d^3y^6-6k2c^2k2dk3c^3y^6+6k2c^2k2dk3c^2k3dy^6+30k2c^2k2dk3ck3d^2y^6+18k2c^2k2dk3d^3y^6-12k2ck2d^2k3c^2k3dy^6$$

$$+6k2ck2d^2k3ck3d^2y^6+18k2ck2d^2k3d^3y^6-6k2d^3k3ck3d^2y^6+6k2d^3k3d^3y^6-3k1c^4k2c^2y^4-6k1c^4k2ck2dy^4-3k1c^4k2d^2y^4-6k1c^3k1dk2c^2y^4$$

$$-18k1c^3k1dk2ck2dy^4-12k1c^3k1dk2d^2y^4-6k1c^3k2c^2k3cy^4-6k1c^3k2c^2k3dy^4+12k1c^3k2ck2dk3cy^4-12k1c^3k2ck2dk3dy^4$$

$$+18k1c^3k2d^2k3cy^4-6k1c^3k2d^2k3dy^4-3k1c^2k1d^2k2c^2y^4-18k1c^2k1d^2k2ck2dy^4-18k1c^2k1d^2k2d^2y^4+12k1c^2k1dk2c^2k3cy^4$$

$$+12k1c^2k1dk2c^2k3dy^4+6k1c^2k1dk2ck2dk3cy^4-6k1c^2k1dk2ck2dk3dy^4+54k1c^2k1dk2d^2k3cy^4-18k1c^2k1dk2d^2k3dy^4+18k1c^2k2c^2k3c^2y^4$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$-24k1c^2k1dk2ck3d^2y^2+54k1c^2k1dk2dk3c^2y^2+36k1c^2k1dk2dk3ck3dy^2-18k1c^2k1dk2dk3d^2y^2-6k1c^2k2ck3c^3y^2-18k1c^2k2ck3c^2k3dy^2$$

$$-18k1c^2k2ck3ck3d^2y^2-6k1c^2k2ck3d^3y^2-12k1c^2k2dk3c^3y^2-30k1c^2k2dk3c^2k3dy^2-24k1c^2k2dk3ck3d^2y^2-6k1c^2k2dk3d^3y^2$$

$$+6k1ck1d^3k2ck3cy^2+6k1ck1d^3k2ck3dy^2-24k1ck1d^3k2dk3cy^2+24k1ck1d^3k2dk3dy^2-30k1ck1d^2k2ck3c^2y^2-60k1ck1d^2k2ck3ck3dy^2$$

$$-30k1ck1d^2k2ck3d^2y^2+54k1ck1d^2k2dk3c^2y^2+36k1ck1d^2k2dk3ck3dy^2-18k1ck1d^2k2dk3d^2y^2+12k1ck1dk2ck3c^3y^2$$

$$+36 k1ck1dk2ck3c^{2}k3dy^{2}+36 k1ck1dk2ck3ck3d^{2}y^{2}+12 k1ck1dk2ck3d^{3}y^{2}-24 k1ck1dk2dk3c^{3}y^{2}-60 k1ck1dk2dk3c^{2}k3dy^{2}$$

$$-48 k1ck1dk2dk3ck3d^{2}y^{2}-12 k1ck1dk2dk3d^{3}y^{2}+6 k1ck2ck3c^{4}y^{2}+24 k1ck2ck3c^{3}k3dy^{2}+36 k1ck2ck3c^{2}k3d^{2}y^{2}+24 k1ck2ck3ck3d^{3}y^{2}$$

$$+6 k1ck2ck3d^{4}y^{2}+6 k1ck2dk3c^{3}k3dy^{2}+18 k1ck2dk3c^{2}k3d^{2}y^{2}+18 k1ck2dk3ck3d^{3}y^{2}+6 k1ck2dk3d^{4}y^{2}-6 k1d^{4}k2dk3cy^{2}+6 k1d^{4}k2dk3dy^{2}$$

$$-12 k1d^{3}k2ck3c^{2}y^{2}-24 k1d^{3}k2ck3ck3dy^{2}-12 k1d^{3}k2ck3d^{2}y^{2}+18 k1d^{3}k2dk3c^{2}y^{2}+12 k1d^{3}k2dk3ck3dy^{2}-6 k1d^{3}k2dk3d^{2}y^{2}+18 k1d^{2}k2ck3c^{3}y^{2}$$

$$+54 k1d^{2}k2ck3c^{2}k3dy^{2}+54 k1d^{2}k2ck3ck3d^{2}y^{2}+18 k1d^{2}k2ck3d^{3}y^{2}-12 k1d^{2}k2dk3c^{3}y^{2}-30 k1d^{2}k2dk3c^{2}k3dy^{2}-24 k1d^{2}k2dk3ck3d^{2}y^{2}$$

$$-6 k1d^{2}k2dk3d^{3}y^{2}-6 k1dk2ck3c^{4}y^{2}-24 k1dk2ck3c^{3}k3dy^{2}-36 k1dk2ck3c^{2}k3d^{2}y^{2}-24 k1dk2ck3ck3d^{3}y^{2}-6 k1dk2ck3d^{4}y^{2}$$

$$+6 k1dk2dk3c^{3}k3dy^{2}+18 k1dk2dk3c^{2}k3d^{2}y^{2}+18 k1dk2dk3ck3d^{3}y^{2}+6 k1dk2dk3d^{4}y^{2}-3 k1c^{4}k3c^{2}-6 k1c^{4}k3ck3d-3 k1c^{4}k3d^{2}$$

$$-12 k1c^{3}k1dk3c^{2}-24 k1c^{3}k1dk3ck3d-12 k1c^{3}k1dk3d^{2}+6 k1c^{3}k3c^{3}+18 k1c^{3}k3c^{2}k3d+18 k1c^{3}k3ck3d^{2}+6 k1c^{3}k3d^{3}-18 k1c^{2}k1d^{2}k3c^{2}$$

$$-36 k1c^{2}k1d^{2}k3ck3d-18 k1c^{2}k1d^{2}k3d^{2}+18 k1c^{2}k1dk3c^{3}+54 k1c^{2}k1dk3c^{2}k3d+54 k1c^{2}k1dk3ck3d^{2}+18 k1c^{2}k1dk3d^{3}-3 k1c^{2}k3c^{4}$$

$$-12 k1c^{2}k3c^{3}k3d-18 k1c^{2}k3c^{2}k3d^{2}-12 k1c^{2}k3ck3d^{3}-3 k1c^{2}k3d^{4}-12 k1ck1d^{3}k3c^{2}-24 k1ck1d^{3}k3ck3d-12 k1ck1d^{3}k3d^{2}+18 k1ck1d^{2}k3c^{3}$$

$$+54 k1ck1d^{2}k3c^{2}k3d+54 k1ck1d^{2}k3ck3d^{2}+18 k1ck1d^{2}k3d^{3}-6 k1ck1dk3c^{4}-24 k1ck1dk3c^{3}k3d-36 k1ck1dk3c^{2}k3d^{2}-24 k1ck1dk3ck3d^{3}$$

$$-6 k1ck1dk3d^{4}-3 k1d^{4}k3c^{2}-6 k1d^{4}k3ck3d-3 k1d^{4}k3d^{2}+6 k1d^{3}k3c^{3}+18 k1d^{3}k3c^{2}k3d+18 k1d^{3}k3ck3d^{2}+6 k1d^{3}k3d^{3}-3 k1d^{2}k3c^{4}$$

$$-12 k1d^{2}k3c^{3}k3d-18 k1d^{2}k3c^{2}k3d^{2}-12 k1d^{2}k3ck3d^{3}-3 k1d^{2}k3d^{4}\Big)^{1/2}-8 k1c^{3}-8 k1d^{3}-8 k3c^{3}-8 k3d^{3}+12 k1d^{2}k3c+12 k1d^{2}k3d$$

$$+12 k1dk3c^{2}+12 k1dk3d^{2}-8 k2c^{3}y^{6}-8 k2d^{3}y^{6}-24 k1c^{2}k1d-24 k1ck1d^{2}-24 k3c^{2}k3d-24 k3ck3d^{2}+12 k1ck3c^{2}+12 k1ck3d^{2}+12 k1ck2c^{2}y^{4}$$

$$+12 k1ck2d^{2}y^{4}+12 k1dk2d^{2}y^{4}+12 k2c^{2}k3cy^{4}+12 k2c^{2}k3dy^{4}+12 k2d^{2}k3dy^{4}+12 k1c^{2}k2cy^{2}+12 k1c^{2}k2dy^{2}+12 k1d^{2}k2dy^{2}+12 k2ck3c^{2}y^{2}$$

$$+12 k2ck3d^{2}y^{2}+12 k2dk3d^{2}y^{2}+24 k1ck1dk3c+24 k1ck1dk3d+24 k1ck3ck3d+24 k1dk3ck3d-24 k2c^{2}k2dy^{6}-24 k2ck2d^{2}y^{6}-24 k1dk2c^{2}y^{4}$$

$$-24 k2d^{2}k3cy^{4}-24 k1d^{2}k2cy^{2}-24 k2dk3c^{2}y^{2}+24 k1dk2dk3cy^{2}+24 k2ck3ck3dy^{2}-12 k2dk3ck3dy^{2}+24 k1ck2ck2dy^{4}-12 k1dk2ck2dy^{4}$$

$$-12 k2ck2dk3cy^{4}-12 k1ck1dk2cy^{2}+24 k1ck1dk2dy^{2}+24 k1ck2dk3cy^{2}+24 k1dk2ck3cy^{2}+24 k1dk2ck3dy^{2}-48 k1ck2ck3cy^{2}$$

$$-48 k1ck2ck3dy^{2}-48 k1ck2dk3dy^{2}+12 k1c^{2}k3c+12 k1c^{2}k3d+24 k2cy^{4}k2dk3d-48 k1dk2dk3dy^{2}\Big)^{1/3}+\Big(6\Big(-\frac{1}{9}k2c^{2}y^{4}-\frac{1}{9}k2d^{2}y^{4}$$

$$-\frac{1}{9}k1d^{2}-\frac{1}{9}k3c^{2}-\frac{1}{9}k3d^{2}+\frac{1}{9}k1ck2cy^{2}+\frac{1}{9}k1ck2dy^{2}+\frac{1}{9}k1dk2dy^{2}+\frac{1}{9}k2ck3cy^{2}+\frac{1}{9}k2ck3dy^{2}-\frac{2}{9}k2cy^{2}k1d-\frac{2}{9}k2dy^{2}k3c-\frac{2}{9}k2cy^{4}k2d$$

$$+\frac{1}{9}\,k2dy^2k3d-\frac{1}{9}\,k1c^2+\frac{1}{9}\,k1ck3d+\frac{1}{9}\,k1dk3c+\frac{1}{9}\,k1dk3d+\frac{1}{9}\,k1ck3c-\frac{2}{9}\,k1ck1d-\frac{2}{9}\,k3ck3d\Big)\Big)\Big/$$

$$\Big(12\,\big(-3k1c^2k2c^4y^8-12k1c^2k2c^3k2dy^8-18k1c^2k2c^2k2d^2y^8-12k1c^2k2ck2d^3y^8-3k1c^2k2d^4y^8-6k1ck1dk2c^3k2dy^8$$

$$-18k1ck1dk2c^2k2d^2y^8-18k1ck1dk2ck2d^3y^8-6k1ck1dk2d^4y^8+6k1ck2c^4k3cy^8+6k1ck2c^4k3dy^8+18k1ck2c^3k2dk3cy^8$$

$$+24k1ck2c^3k2dk3dy^8+18k1ck2c^2k2d^2k3cy^8+36k1ck2c^2k2d^2k3dy^8+6k1ck2ck2d^3k3cy^8+24k1ck2ck2d^3k3dy^8+6k1ck2d^4k3dy^8$$

$$-3k1d^2k2c^2k2d^2y^8-6k1d^2k2ck2d^3y^8-3k1d^2k2d^4y^8-6k1dk2c^3k2dk3cy^8+6k1dk2c^3k2dk3dy^8-12k1dk2c^2k2d^2k3cy^8+18k1dk2c^2k2d^2k3dy^8$$

$$-6k1dk2ck2d^3k3cy^8+18k1dk2ck2d^3k3dy^8+6k1dk2d^4k3dy^8-3k2c^4k3c^2y^8-6k2c^4k3ck3dy^8-3k2c^4k3d^2y^8-6k2c^3k2dk3c^2y^8$$

$$-18k2c^3k2dk3ck3dy^8-12k2c^3k2dk3d^2y^8-3k2c^2k2d^2k3c^2y^8-18k2c^2k2d^2k3ck3dy^8-18k2c^2k2d^2k3d^2y^8-6k2ck2d^3k3ck3dy^8$$

$$-12k2ck2d^3k3d^2y^8-3k2d^4k3d^2y^8+6k1c^3k2c^3y^6+18k1c^3k2c^2k2dy^6+18k1c^3k2ck2d^2y^6+6k1c^3k2d^3y^6-6k1c^2k1dk2c^3y^6+6k1c^2k1dk2c^2k2dy^6$$

$$+30k1c^2k1dk2ck2d^2y^6+18k1c^2k1dk2d^3y^6-6k1c^2k2c^3k3cy^6-6k1c^2k2c^3k3dy^6-24k1c^2k2c^2k2dk3cy^6-18k1c^2k2c^2k2dk3dy^6$$

$$-30k1c^2k2ck2d^2k3cy^6-18k1c^2k2ck2d^2k3dy^6-12k1c^2k2d^3k3cy^6-6k1c^2k2d^3k3dy^6-12k1ck1d^2k2c^2k2dy^6+6k1ck1d^2k2ck2d^2y^6$$

$$+18k1ck1d^2k2d^3y^6+18k1ck1dk2c^3k3cy^6+18k1ck1dk2c^3k3dy^6+18k1ck1dk2c^2k2dk3cy^6+24k1ck1dk2c^2k2dk3dy^6$$

$$-24k1ck1dk2ck2d^2k3cy^6-6k1ck1dk2ck2d^2k3dy^6-24k1ck1dk2d^3k3cy^6-12k1ck1dk2d^3k3dy^6-6k1ck2c^3k3c^2y^6-12k1ck2c^3k3ck3dy^6$$

$$-6k1ck2c^3k3d^2y^6+12k1ck2c^2k2dk3c^2y^6-6k1ck2c^2k2dk3ck3dy^6-18k1ck2c^2k2dk3d^2y^6+18k1ck2ck2d^2k3c^2y^6+24k1ck2ck2d^2k3ck3dy^6$$

$$-18k1ck2ck2d^2k3d^2y^6+18k1ck2d^3k3ck3dy^6-6k1ck2d^3k3d^2y^6-6k1d^3k2ck2d^2y^6+6k1d^3k2d^3y^6-18k1d^2k2c^2k2dk3cy^6$$

$$+18k1d^2k2c^2k2dk3dy^6+6k1d^2k2ck2d^2k3cy^6+12k1d^2k2ck2d^2k3dy^6-12k1d^2k2d^3k3cy^6-6k1d^2k2d^3k3dy^6-12k1dk2c^3k3c^2y^6$$

$$-24k1dk2c^3k3ck3dy^6-12k1dk2c^3k3d^2y^6+6k1dk2c^2k2dk3c^2y^6-24k1dk2c^2k2dk3ck3dy^6-30k1dk2c^2k2dk3d^2y^6-18k1dk2ck2d^2k3c^2y^6$$

$$+18k1dk2ck2d^2k3ck3dy^6-24k1dk2ck2d^2k3d^2y^6+18k1dk2d^3k3ck3dy^6-6k1dk2d^3k3d^2y^6+6k2c^3k3c^3y^6+18k2c^3k3c^2k3dy^6$$

$$+18k2c^3k3ck3d^2y^6+6k2c^3k3d^3y^6-6k2c^2k2dk3c^3y^6+6k2c^2k2dk3c^2k3dy^6+30k2c^2k2dk3ck3d^2y^6+18k2c^2k2dk3d^3y^6-12k2ck2d^2k3c^2k3dy^6$$

$$+6k2ck2d^2k3ck3d^2y^6+18k2ck2d^2k3d^3y^6-6k2d^3k3ck3d^2y^6+6k2d^3k3d^3y^6-3k1c^4k2c^2y^4-6k1c^4k2ck2dy^4-3k1c^4k2d^2y^4-6k1c^3k1dk2c^2y^4$$

$$-18k1c^3k1dk2ck2dy^4-12k1c^3k1dk2d^2y^4-6k1c^3k2c^2k3cy^4-6k1c^3k2c^2k3dy^4+12k1c^3k2ck2dk3cy^4-12k1c^3k2ck2dk3dy^4$$

$$+18k1c^3k2d^2k3cy^4-6k1c^3k2d^2k3dy^4-3k1c^2k1d^2k2c^2y^4-18k1c^2k1d^2k2ck2dy^4-18k1c^2k1d^2k2d^2y^4+12k1c^2k1dk2c^2k3cy^4$$

$$+12k1c^2k1dk2c^2k3dy^4+6k1c^2k1dk2ck2dk3cy^4-6k1c^2k1dk2ck2dk3dy^4+54k1c^2k1dk2d^2k3cy^4-18k1c^2k1dk2d^2k3dy^4+18k1c^2k2c^2k3c^2y^4$$

$$+36k1c^2k2c^2k3ck3dy^4+18k1c^2k2c^2k3d^2y^4-24k1c^2k2ck2dk3c^2y^4+12k1c^2k2ck2dk3ck3dy^4+36k1c^2k2ck2dk3d^2y^4-18k1c^2k2d^2k3c^2y^4$$

$$-24k1c^2k2d^2k3ck3dy^4+18k1c^2k2d^2k3d^2y^4-6k1ck1d^3k2ck2dy^4-12k1ck1d^3k2d^2y^4+18k1ck1d^2k2c^2k3cy^4+18k1ck1d^2k2c^2k3dy^4$$

$$-24k1ck1d^2k2ck2dk3cy^4+24k1ck1d^2k2ck2dk3dy^4+54k1ck1d^2k2d^2k3cy^4-18k1ck1d^2k2d^2k3dy^4-24k1ck1dk2c^2k3c^2y^4$$

$$-48k1ck1dk2c^2k3ck3dy^4-24k1ck1dk2c^2k3d^2y^4+6k1ck1dk2ck2dk3c^2y^4+18k1ck1dk2ck2dk3ck3dy^4+12k1ck1dk2ck2dk3d^2y^4$$

$$-36k1ck1dk2d^2k3c^2y^4-48k1ck1dk2d^2k3ck3dy^4+36k1ck1dk2d^2k3d^2y^4-6k1ck2c^2k3c^3y^4-18k1ck2c^2k3c^2k3dy^4-18k1ck2c^2k3ck3d^2y^4$$

$$-6k1ck2c^2k3d^3y^4+18k1ck2ck2dk3c^3y^4+24k1ck2ck2dk3c^2k3dy^4-6k1ck2ck2dk3ck3d^2y^4-12k1ck2ck2dk3d^3y^4+18k1ck2d^2k3c^2k3dy^4$$

$$+12k1ck2d^2k3ck3d^2y^4-6k1ck2d^2k3d^3y^4-3k1d^4k2d^2y^4-18k1d^3k2ck2dk3cy^4+18k1d^3k2ck2dk3dy^4+18k1d^3k2d^2k3cy^4-6k1d^3k2d^2k3dy^4$$

$$-18k1d^2k2c^2k3c^2y^4-36k1d^2k2c^2k3ck3dy^4-18k1d^2k2c^2k3d^2y^4+30k1d^2k2ck2dk3c^2y^4+6k1d^2k2ck2dk3ck3dy^4-24k1d^2k2ck2dk3d^2y^4$$

$$-18k1d^2k2d^2k3c^2y^4-24k1d^2k2d^2k3ck3dy^4+18k1d^2k2d^2k3d^2y^4+18k1dk2c^2k3c^3y^4+54k1dk2c^2k3c^2k3dy^4+54k1dk2c^2k3ck3d^2y^4$$

$$+18k1dk2c^2k3d^3y^4-18k1dk2ck2dk3c^3y^4-24k1dk2ck2dk3c^2k3dy^4+6k1dk2ck2dk3ck3d^2y^4+12k1dk2ck2dk3d^3y^4+18k1dk2d^2k3c^2k3dy^4$$

$$+12k1dk2d^2k3ck3d^2y^4-6k1dk2d^2k3d^3y^4-3k2c^2k3c^4y^4-12k2c^2k3c^3k3dy^4-18k2c^2k3c^2k3d^2y^4-12k2c^2k3ck3d^3y^4-3k2c^2k3d^4y^4$$

$$-6k2ck2dk3c^3k3dy^4-18k2ck2dk3c^2k3d^2y^4-18k2ck2dk3ck3d^3y^4-6k2ck2dk3d^4y^4-3k2d^2k3c^2k3d^2y^4-6k2d^2k3ck3d^3y^4-3k2d^2k3d^4y^4$$

$$+6k1c^4k2ck3cy^2+6k1c^4k2ck3dy^2-6k1c^4k2dk3cy^2+6k1c^4k2dk3dy^2+18k1c^3k1dk2ck3cy^2+18k1c^3k1dk2ck3dy^2-24k1c^3k1dk2dk3cy^2$$

$$+24k1c^3k1dk2dk3dy^2-6k1c^3k2ck3c^2y^2-12k1c^3k2ck3ck3dy^2-6k1c^3k2ck3d^2y^2+18k1c^3k2dk3c^2y^2+12k1c^3k2dk3ck3dy^2-6k1c^3k2dk3d^2y^2$$

$$+18k1c^2k1d^2k2ck3cy^2+18k1c^2k1d^2k2ck3dy^2-36k1c^2k1d^2k2dk3cy^2+36k1c^2k1d^2k2dk3dy^2-24k1c^2k1dk2ck3c^2y^2-48k1c^2k1dk2ck3ck3dy^2$$

$$
\begin{aligned}
&-24k1c^{2}k1dk2ck3d^{2}y^{2}+54k1c^{2}k1dk2dk3c^{2}y^{2}+36k1c^{2}k1dk2dk3ck3dy^{2}-18k1c^{2}k1dk2dk3d^{2}y^{2}-6k1c^{2}k2ck3c^{3}y^{2}-18k1c^{2}k2ck3c^{2}k3dy^{2}\\
&-18k1c^{2}k2ck3ck3d^{2}y^{2}-6k1c^{2}k2ck3d^{3}y^{2}-12k1c^{2}k2dk3c^{3}y^{2}-30k1c^{2}k2dk3c^{2}k3dy^{2}-24k1c^{2}k2dk3ck3d^{2}y^{2}-6k1c^{2}k2dk3d^{3}y^{2}\\
&+6k1ck1d^{3}k2ck3cy^{2}+6k1ck1d^{3}k2ck3dy^{2}-24k1ck1d^{3}k2dk3cy^{2}+24k1ck1d^{3}k2dk3dy^{2}-30k1ck1d^{2}k2ck3c^{2}y^{2}-60k1ck1d^{2}k2ck3ck3dy^{2}\\
&-30k1ck1d^{2}k2ck3d^{2}y^{2}+54k1ck1d^{2}k2dk3c^{2}y^{2}+36k1ck1d^{2}k2dk3ck3dy^{2}-18k1ck1d^{2}k2dk3d^{2}y^{2}+12k1ck1dk2ck3c^{3}y^{2}\\
&+36k1ck1dk2ck3c^{2}k3dy^{2}+36k1ck1dk2ck3ck3d^{2}y^{2}+12k1ck1dk2ck3d^{3}y^{2}-24k1ck1dk2dk3c^{3}y^{2}-60k1ck1dk2dk3c^{2}k3dy^{2}\\
&-48k1ck1dk2dk3ck3d^{2}y^{2}-12k1ck1dk2dk3d^{3}y^{2}+6k1ck2ck3c^{4}y^{2}+24k1ck2ck3c^{3}k3dy^{2}+36k1ck2ck3c^{2}k3d^{2}y^{2}+24k1ck2ck3ck3d^{3}y^{2}\\
&+6k1ck2ck3d^{4}y^{2}+6k1ck2dk3c^{3}k3dy^{2}+18k1ck2dk3c^{2}k3d^{2}y^{2}+18k1ck2dk3ck3d^{3}y^{2}+6k1ck2dk3d^{4}y^{2}-6k1d^{4}k2dk3cy^{2}+6k1d^{4}k2dk3dy^{2}\\
&-12k1d^{3}k2ck3c^{2}y^{2}-24k1d^{3}k2ck3ck3dy^{2}-12k1d^{3}k2ck3d^{2}y^{2}+18k1d^{3}k2dk3c^{2}y^{2}+12k1d^{3}k2dk3ck3dy^{2}-6k1d^{3}k2dk3d^{2}y^{2}+18k1d^{2}k2ck3c^{3}y^{2}\\
&+54k1d^{2}k2ck3c^{2}k3dy^{2}+54k1d^{2}k2ck3ck3d^{2}y^{2}+18k1d^{2}k2ck3d^{3}y^{2}-12k1d^{2}k2dk3c^{3}y^{2}-30k1d^{2}k2dk3c^{2}k3dy^{2}-24k1d^{2}k2dk3ck3d^{2}y^{2}\\
&-6k1d^{2}k2dk3d^{3}y^{2}-6k1dk2ck3c^{4}y^{2}-24k1dk2ck3c^{3}k3dy^{2}-36k1dk2ck3c^{2}k3d^{2}y^{2}-24k1dk2ck3ck3d^{3}y^{2}-6k1dk2ck3d^{4}y^{2}\\
&+6k1dk2dk3c^{3}k3dy^{2}+18k1dk2dk3c^{2}k3d^{2}y^{2}+18k1dk2dk3ck3d^{3}y^{2}+6k1dk2dk3d^{4}y^{2}-3k1c^{4}k3c^{2}-6k1c^{4}k3ck3d-3k1c^{4}k3d^{2}\\
&-12k1c^{3}k1dk3c^{2}-24k1c^{3}k1dk3ck3d-12k1c^{3}k1dk3d^{2}+6k1c^{3}k3c^{3}+18k1c^{3}k3c^{2}k3d+18k1c^{3}k3ck3d^{2}+6k1c^{3}k3d^{3}-18k1c^{2}k1d^{2}k3c^{2}\\
&-36k1c^{2}k1d^{2}k3ck3d-18k1c^{2}k1d^{2}k3d^{2}+18k1c^{2}k1dk3c^{3}+54k1c^{2}k1dk3c^{2}k3d+54k1c^{2}k1dk3ck3d^{2}+18k1c^{2}k1dk3d^{3}-3k1c^{2}k3c^{4}\\
&-12k1c^{2}k3c^{3}k3d-18k1c^{2}k3c^{2}k3d^{2}-12k1c^{2}k3ck3d^{3}-3k1c^{2}k3d^{4}-12k1ck1d^{3}k3c^{2}-24k1ck1d^{3}k3ck3d-12k1ck1d^{3}k3d^{2}+18k1ck1d^{2}k3c^{3}\\
&+54k1ck1d^{2}k3c^{2}k3d+54k1ck1d^{2}k3ck3d^{2}+18k1ck1d^{2}k3d^{3}-6k1ck1dk3c^{4}-24k1ck1dk3c^{3}k3d-36k1ck1dk3c^{2}k3d^{2}-24k1ck1dk3ck3d^{3}\\
&-6k1ck1dk3d^{4}-3k1d^{4}k3c^{2}-6k1d^{4}k3ck3d-3k1d^{4}k3d^{2}+6k1d^{3}k3c^{3}+18k1d^{3}k3c^{2}k3d+18k1d^{3}k3ck3d^{2}+6k1d^{3}k3d^{3}-3k1d^{2}k3c^{4}\\
&-12k1d^{2}k3c^{3}k3d-18k1d^{2}k3c^{2}k3d^{2}-12k1d^{2}k3ck3d^{3}-3k1d^{2}k3d^{4}\Big)^{1/2}-8k1c^{3}-8k1d^{3}-8k3c^{3}-8k3d^{3}+12k1d^{2}k3c+12k1d^{2}k3d\\
&+12k1dk3c^{2}+12k1dk3d^{2}-8k2c^{3}y^{6}-8k2d^{3}y^{6}-24k1c^{2}k1d-24k1ck1d^{2}-24k3c^{2}k3d-24k3ck3d^{2}+12k1ck3c^{2}+12k1ck3d^{2}+12k1ck2c^{2}y^{4}\\
&+12k1ck2d^{2}y^{4}+12k1dk2d^{2}y^{4}+12k2c^{2}k3cy^{4}+12k2c^{2}k3dy^{4}+12k2d^{2}k3dy^{4}+12k1c^{2}k2cy^{2}+12k1c^{2}k2dy^{2}+12k1d^{2}k2dy^{2}+12k2ck3c^{2}y^{2}\\
&+12k2ck3d^{2}y^{2}+12k2dk3d^{2}y^{2}+24k1ck1dk3c+24k1ck1dk3d+24k1ck3ck3d+24k1dk3ck3d-24k2c^{2}k2dy^{6}-24k2ck2d^{2}y^{6}-24k1dk2c^{2}y^{4}\\
&-24k2d^{2}k3cy^{4}-24k1d^{2}k2cy^{2}-24k2dk3c^{2}y^{2}+24k1dk2dk3cy^{2}+24k2ck3ck3dy^{2}-12k2dk3ck3dy^{2}+24k1ck2ck2dy^{4}-12k1dk2ck2dy^{4}\\
&-12k2ck2dk3cy^{4}-12k1ck1dk2cy^{2}+24k1ck1dk2dy^{2}+24k1ck2dk3cy^{2}+24k1dk2ck3cy^{2}+24k1dk2ck3dy^{2}-48k1ck2ck3cy^{2}\\
&-48k1ck2ck3dy^{2}-48k1ck2dk3dy^{2}+12k1c^{2}k3c+12k1c^{2}k3d+24k2cy^{4}k2dk3d-48k1dk2dk3dy^{2}\Big)^{1/3}\Big)
\end{aligned}
$$

Note that one of these eigenvalues is 0.

The programs below compute the eigenvalues according the constants of reactions of the system. For Jacobian 1:

```
> ei1 :=proc(k1c, k1d, k2c, k2d, k3c, k3d)
   MM11 := Jacobian([-k1c*a+k1d*x, -k2c*x*y^2+k2d*y^3+k1c*a-k1d*x, k2c*x*y^2-k2d*y^3-k3c*y+k3d*b, k3c*y-k3d*b],
        [a, x, y, b] = [k1d*x/k1c, x, 0, 0]);
  eigenvalues(MM11);
   end proc:
Warning, `MM11` is implicitly declared local to procedure `ei1`
```

For every constants equal to 1, we have:

```
> ei1(1, 1, 1, 1, 1, 1)
```

$$-2, -2, 0, 0 \tag{3.4}$$

For Jacobian 2:

```
> ei2 :=proc(k1c, k1d, k2c, k2d, k3c, k3d)
   MM22 := Jacobian([-k1c*a+k1d*x, -k2c*x*y^2+k2d*y^3+k1c*a-k1d*x, k2c*x*y^2-k2d*y^3-k3c*y+k3d*b, k3c*y-k3d*b],
        [a, x, y, b] = [((k1d*k2d)/(k2c*k1c))*y, (k2d/k2c)*y, y, (k3c/k3d)*y]);
   eigenvalues(MM22);
   end proc:
Warning, `MM22` is implicitly declared local to procedure `ei2`
```

For every constants equal to 1, we have:

```
> ei2(1, 1, 1, 1, 1, 1)
```

$$0,\ -2,\ -y^2-1+\sqrt{y^4+1},\ -y^2-1-\sqrt{y^4+1} \qquad \textbf{(3.5)}$$

The study of the eigenvalues in specific cases can generate interesting results, as some of those described in Chapter 7.

APPENDIX C – Maple Code to Fock Space Method (Simplified case)

In this code, we'll describe the algorithm to study the simplified case of Schnackenberg model, as described in Chapter 8.

Before, an important warning: to facilitate the entering the code, we write respectively

$k1c$ and $k1d$

instead of

k_{1+} **and** k_{1-}

The same goes for the other constants that have subindices.

Another important note: for the correct functioning of the codes, check if they are written in language "Maple imput". Otherwise, some commands may fail or give wrong results.

1. Description of Fock Space

We begin our study write the packages necessary.

The Maple has a specific package to describe quantum operators, which is the package *physics*. Make sure that you are using the latest version of the package (or at least the version *2014, February 10, 21:29 hours*), otherwise some commands may not work properly. If necessary, download the package at http://www.maplesoft.com/products/maple/features/physicsresearch.aspx.

The other packages are in Maple.

```
> restart;
with(Physics):with(MTM):with(LinearAlgebra):with(linalg):with(plots):
Physics:-Version();
```

"C:\Program Files\Maple 2015\lib\update.mla", *2015, May 14, 11:23 hours* **(1.1)**

Below write a command to generate large matrices in the code:

```
> interface(rtablesize=301);
```

10 **(1.2)**

Now, we write the Fock space in which we are going work. Note that, because *a* and *b* are fixed, the Fock space only consists of the direct product between X and Y.

```
> Setup(op = X,Y);
```

** Partial match of 'op' against keyword 'quantumoperators'*

** Partial match of 'Y' against keyword 'keywords'*

[Dgammarepresentation, abbreviations, additionally, advanced, algebrarules, anticommutativecolor, anticommutativeprefix, automaticsimplification, bracketbasis, bracketrules, clear, combinepowersofsamebase, conventions, coordinatesystems, default, deletesavedsetup, differentiationvariables, dimension, gaugeindices, geometricdifferentiation, hermitianoperators, keywords, levicivita, mathematicalnotation, metric, noncommutativecolor, noncommutativeprefix, normusesconjugate, quantumbasisdimension, quantumcontinuousbasis, quantumdiscretebasis, quantumoperators, query, quiet, readusersetup, realobjects, redefinesum, redo, savesetup, signature, spaceindices, spacetimeindices, spinorindices, tensors, tetrad, tetradindices, tetradmetric, traceonlymatrices, unitaryoperators, unitvectordisplay, usephysicsevaluator, usewirtingerderivatives, vectordisplay, vectorpostfix] **(1.3)**

The codes below define the sets of creation and annihilation operators, and ajusting them for the suitable phase. For X:

```
> N:=1;
for i from 1 to N do
Xp[i]:= Creation(X,i,phaseconvention= proc(n) 1 end proc,notation = explicit);
```

```
Xm[i]:=Annihilation(X,i,phaseconvention= proc(n) n end proc,notation = explicit);
end do;
```

$$N := 1$$
$$Xp_1 := a+_{X_1}$$
$$Xm_1 := a-_{X_1} \quad (1.4)$$

For *Y*:

```
> N:=1;
for i from 1 to N do
Yp[i]:= Creation(Y,i,phaseconvention= proc(n) 1 end proc,notation = explicit);
Ym[i]:=Annihilation(Y,i,phaseconvention= proc(n) n end proc,notation = explicit);
end do;
```

$$N := 1$$
$$Yp_1 := a+_{Y_1}$$
$$Ym_1 := a-_{Y_1} \quad (1.5)$$

2. The Hamiltonian of the system

We will describe the reactions of the system and and their Hamiltonians, according the section 2 of Chapter 8. In every cases, the *r* indicates the back part of the reaction.

First reaction, ∅ <-> *X:*

```
> H1:=proc(k1p) -Expand(k1p*(Xp[1]*1-1*1)); end proc;
H1r:=proc(k1m) -Expand(k1m*(1*Xm[1]-Xp[1]*Xm[1])); end proc;
```

H1 := **proc**(*k1p*) *Physics:-Expand*(*k1p* * (*Xp*[1] * 1 − 1 * 1)) * (−1) **end proc**

H1r := **proc**(*k1m*) *Physics:-Expand*(*k1m* * (1 * *Xm*[1] − *Xp*[1] * *Xm*[1])) * (−1) **end proc** (2.1)

Second reaction, *X+2Y* <-> *3Y*:

```
> H2:=proc(k2p) -Expand(k2p*(Yp[1]*Yp[1]*Yp[1]*Ym[1]*Ym[1]*Xm[1]-Yp[1]*Yp[1]*Ym[1]*Ym[1]*Xp[1]*Xm
[1])); end proc;
H2r:=proc(k2m) -Expand(k2m*(Yp[1]*Yp[1]*Xp[1]*Ym[1]*Ym[1]*Ym[1]-Yp[1]*Yp[1]*Yp[1]*Ym[1]*Ym[1]*Ym
[1])); end proc;
```

H2 := **proc**(*k2p*)

Physics:-Expand(*k2p* * (*Yp*[1] * *Yp*[1] * *Yp*[1] * *Ym*[1] * *Ym*[1] * *Xm*[1] − *Yp*[1] * *Yp*[1] * *Ym*[1] * *Ym*[1] * *Xp*[1] * *Xm*[1])) * (−1)

end proc

H2r := **proc**(*k2m*) (2.2)

Physics:-Expand(*k2m* * (*Yp*[1] * *Yp*[1] * *Xp*[1] * *Ym*[1] * *Ym*[1] * *Ym*[1] − *Yp*[1] * *Yp*[1] * *Yp*[1] * *Ym*[1] * *Ym*[1] * *Ym*[1])) * (
−1)

end proc

Third reaction, *Y*<->∅:

```
> H3:=proc(k3p) -Expand(k3p*(1*Ym[1]-Yp[1]*Ym[1])); end proc;
H3r:=proc(k3m) -Expand(k3m*(Yp[1]*1-1*1)); end proc;
```

H3 := **proc**(*k3p*) *Physics:-Expand*(*k3p* * (1 * *Ym*[1] − *Yp*[1] * *Ym*[1])) * (−1) **end proc**

H3r := **proc**(*k3m*) *Physics:-Expand*(*k3m* * (*Yp*[1] * 1 − 1 * 1)) * (−1) **end proc** (2.3)

Then, we compute the total Hamiltonian:

```
> H:=proc(k1p,k1m,k2p,k2m,k3p,k3m) H1(k1p)+H1r(k1m)+H2(k2p)+H2r(k2m)+H3(k3p)+H3r(k3m); end proc;
> H(k1p,k1m,k2p,k2m,k3p,k3m);
```

H := **proc**(*k1p*, *k1m*, *k2p*, *k2m*, *k3p*, *k3m*) *H1*(*k1p*) + *H1r*(*k1m*) + *H2*(*k2p*) + *H2r*(*k2m*) + *H3*(*k3p*) + *H3r*(*k3m*) **end proc**

$$-k1p\left(a+_{X_1}-1\right)-k1m\,a-_{X_1}+k1m\ `*`\left(a+_{X_1},a-_{X_1}\right)-k2p\ `*`\left(`\wedge`\left(a+_{Y_1},3\right),`\wedge`\left(a-_{Y_1},2\right),a-_{X_1}\right)+k2p\ `*`\left(`\wedge`\left(a+_{Y_1},2\right),`\wedge`\left(a-_{Y_1},2\right),\right. \quad (2.4)$$

$$a+_{X_1}, a-_{X_1}\Big) - k2m \text{`*`}\Big(\text{`^`}\big(a+_{Y_1}, 2\big), a+_{X_1}, \text{`^`}\big(a-_{Y_1}, 3\big)\Big) + k2m \text{`*`}\Big(\text{`^`}\big(a+_{Y_1}, 3\big), \text{`^`}\big(a-_{Y_1}, 3\big)\Big) - k3p\, a-_{Y_1} + k3p \text{`*`}\big(a+_{Y_1}, a-_{Y_1}\big)$$
$$- k3m\, \big(a+_{Y_1} - 1\big)$$

The nonzero contributions for the Hamiltonian, i.e. the averages, are given in Eq. 8.16 of the text, and can be found as follows:

```
> (Bra(Y,yi).Bra(X,xri)).(H(k1p,k1m,k2p,k2m,k3p,k3m)).(Ket(X,xrj).Ket(Y,yj));
```

$$-\delta_{yi, yj-1}\, yj\, \big(k2m\, (yj-1)\, (yj-2)\, \delta_{xri, xrj+1} + k3p\, \delta_{xri, xrj}\big) - \big(yj\, k2p\, xrj\, (yj-1)\, \delta_{xri, xrj-1} + k3m\, \delta_{xri, xrj}\big)\, \delta_{yi, yj+1} + \Big(\big(k2m\, yj^3 + \big(k2p\, xrj - 3\, k2m\big)\, yj^2 + \big(-k2p\, xrj + 2\, k2m + k3p\big)\, yj + k1m\, xrj + k1p + k3m\big)\, \delta_{xri, xrj} - k1m\, xrj\, \delta_{xri, xrj-1} - k1p\, \delta_{xri, xrj+1}\Big)\, \delta_{yi, yj} \quad \textbf{(2.5)}$$

3. The basis of Fock space

To enumerate the elements of the basis of Fock space, we compute the code below:

```
> Baseset :=proc(xm, ym) global B; global ket; global bra; global Bdim;
  i := 1;

        for xri from 0 to xm
            do
               for yi from 0 to ym
                  do
                        B[i] := (xri, yi);
                        ket[i] := Ket(X, xri).Ket(Y, yi);
                        bra[i] := Bra(Y, yi).Bra(X, xri);
                        print(i, B[i] = ket[i]);
                        i := i+1;
                  end do;
               end do;
         Bdim := i-1;
   end proc:
```

```
Warning, `i` is implicitly declared local to procedure `Baseset`
Warning, `xri` is implicitly declared local to procedure `Baseset`
Warning, `yi` is implicitly declared local to procedure `Baseset`
```

If we have xm=ym=1, then we obtain the basis described in (8.4):

```
> Baseset(1, 1);
```

$$1, (0, 0) = \left|X_0\right\rangle \left|Y_0\right\rangle$$
$$2, (0, 1) = \left|X_0\right\rangle \left|Y_1\right\rangle$$
$$3, (1, 0) = \left|X_1\right\rangle \left|Y_0\right\rangle$$
$$4, (1, 1) = \left|X_1\right\rangle \left|Y_1\right\rangle$$
$$4 \quad \textbf{(3.1)}$$

4. The matrix element of Hamiltonian

To describe the matrix element of Hamiltonian, we compute the code below. Note that the Matrix Element (*ME*, in code) is the contributions computed in section 2 of this Appendix.

```
> Mat :=proc(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m)
  delta :=proc(a, b) piecewise(a=b, 1, 0); end proc;
  Baseset :=proc(xm, ym) global B; global Bdim;
  i := 1;
```

```
        for xri from 0 to xm
           do
              for yi from 0 to ym
                 do
                       B[i] := (xri, yi) :
                       i := i + 1;
                 end do;
        end do;
    Bdim := i-1;
end proc;
Baseset(xm, ym) :
ME :=proc(xri, xrj, yi, yj, k1p, k1m, k2p, k2m, k3p, k3m)
 - delta(yi, yj-1)*(k2m*(yj-1)*(yj-2)*delta(xri, xrj + 1) + k3p*delta(xri, xrj))*yj-(yj*k2p*xrj*(yj-1)
     *delta(xri, xrj-1) + k3m*delta(xri, xrj))*delta(yi, yj + 1) + ((k2m*yj^3 + (k2p*xrj-3*k2m)*yj^2 + (
     -k2p*xrj + 2*k2m + k3p)*yj + k1m*xrj + k1p + k3m)*delta(xri, xrj)-k1m*xrj*delta(xri, xrj-1)-k1p
     *delta(xri, xrj + 1))*delta(yi, yj); end proc;

element := proc(i, j, k1p, k1m, k2p, k2m, k3p, k3m) -ME(B[i][1], B[j][1], B[i][2], B[j][2], k1p, k1m, k2p, k2m,
     k3p, k3m); end proc;

   for i from 1 to Bdim do
      for j from 1 to Bdim do
      A[i, j] := element(i, j, k1p, k1m, k2p, k2m, k3p, k3m);
      end do;
   end do;
Mt := Array(1..Bdim, 1..Bdim, (i, j) → A[i, j]);
 end proc:
```

For $xm=ym=1$, we obtain the matrix $4x4$ described in the text:

```
> G := Mat(1, 1, k1p, k1m, k2p, k2m, k3p, k3m) :
  G
```

$$\begin{bmatrix} -k1p-k3m & k3p & k1m & 0 \\ k3m & -k3p-k1p-k3m & 0 & k1m \\ k1p & 0 & -k1m-k1p-k3m & k3p \\ 0 & k1p & k3m & -k3p-k1m-k1p-k3m \end{bmatrix} \quad (4.1)$$

whose the eigenvalues are given by

```
> Eigenvalues(G)
```

$$\Bigg[\bigg[-\frac{1}{2}\,k3p-\frac{1}{2}\,k1m-k1p-k3m+\frac{1}{2}\sqrt{k1m^2+4\,k1p\,k1m+4\,k3m\,k3p+k3p^2+2\sqrt{4\,k1m^2\,k3m\,k3p+k1m^2\,k3p^2+16\,k1m\,k1p\,k3m\,k3p+4\,k1m\,k1p\,k3p^2}}\bigg], \quad (4.2)$$

$$\bigg[-\frac{1}{2}\,k3p-\frac{1}{2}\,k1m-k1p-k3m-\frac{1}{2}\sqrt{k1m^2+4\,k1p\,k1m+4\,k3m\,k3p+k3p^2+2\sqrt{4\,k1m^2\,k3m\,k3p+k1m^2\,k3p^2+16\,k1m\,k1p\,k3m\,k3p+4\,k1m\,k1p\,k3p^2}}\bigg],$$

$$\bigg[-\frac{1}{2}\,k3p-\frac{1}{2}\,k1m-k1p-k3m+\frac{1}{2}\sqrt{k1m^2+4\,k1p\,k1m+4\,k3m\,k3p+k3p^2-2\sqrt{4\,k1m^2\,k3m\,k3p+k1m^2\,k3p^2+16\,k1m\,k1p\,k3m\,k3p+4\,k1m\,k1p\,k3p^2}}$$

$$\Bigg],$$

$$\Bigg[-\frac{1}{2}\,k3p-\frac{1}{2}\,k1m-k1p-k3m$$

$$-\frac{1}{2}\sqrt{k1m^2+4\,k1p\,k1m+4\,k3m\,k3p+k3p^2-2\sqrt{4\,k1m^2\,k3m\,k3p+k1m^2\,k3p^2+16\,k1m\,k1p\,k3m\,k3p+4\,k1m\,k1p\,k3p^2}}$$

$$\Bigg]\Bigg]$$

The exponential of matrix G is defined by the code below:

```
> ExpHt := proc(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t)
  M := Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m);
  MatrixExponential(M*t); end proc;
```

```
ExpHt := proc(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t)
    local M;
    M := Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m); LinearAlgebra:-MatrixExponential(M*t)
end proc
```
(4.3)

Make every the constants of reaction equals a 1, the matrix is

```
> ExpHt(1, 1, 1, 1, 1, 1, 1, 1, 1);
```

$$\Big[\Big[\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}+3\,e^{-\sqrt{5}}+3\,e^{\sqrt{5}}+4\right)e^{-3},\ \frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}+e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},$$
$$\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}+e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},\ \frac{1}{5}\left(e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3}\Big],$$
$$\Big[\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}+e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},\ \frac{1}{5}\left(e^{-\sqrt{5}}+e^{\sqrt{5}}+3\right)e^{-3},\ \frac{1}{5}\left(e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},$$
$$\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}-e^{-\sqrt{5}}-e^{\sqrt{5}}+2\right)e^{-3}\Big],$$
$$\Big[\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}+e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},\ \frac{1}{5}\left(e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},\ \frac{1}{5}\left(e^{-\sqrt{5}}+e^{\sqrt{5}}+3\right)e^{-3},$$
$$\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}-e^{-\sqrt{5}}-e^{\sqrt{5}}+2\right)e^{-3}\Big],$$
$$\Big[\frac{1}{5}\left(e^{-\sqrt{5}}+e^{\sqrt{5}}-2\right)e^{-3},\ \frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}-e^{-\sqrt{5}}-e^{\sqrt{5}}+2\right)e^{-3},\ \frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}\right.$$
$$\left.-e^{-\sqrt{5}}-e^{\sqrt{5}}+2\right)e^{-3},\ -\frac{1}{10}\left(-\sqrt{5}\,e^{-\sqrt{5}}+\sqrt{5}\,e^{\sqrt{5}}-3\,e^{-\sqrt{5}}-3\,e^{\sqrt{5}}-4\right)e^{-3}\Big]\Big] \tag{4.4}$$

5. Plots

To plot the averages of species, we use the sequence of codes below, as described in reference (29):

```
> Expi :=proc(L, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t)
  Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m) :
  evalf(ExpHt(xm, ym, 1.0*k1p, 1.0*k1m, 1.0*k2p, 1.0*k2m, 1.0*k3p, 1.0*k3m, t)[L][Bdim]);
  end proc;
```

```
Expi := proc(L, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t)
    Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m); evalf(ExpHt(xm, ym, 1.0*k1p, 1.0*k1m, 1.0*k2p, 1.0*k2m, 1.0*k3p, 1.0*k3m, t)[L]
    [Bdim])
end proc
```
(5.1)

```
> Vexp :=proc(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t)
  Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m) :
```

```
⟨seq(Expi(i, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t), i=1..Bdim)⟩ : end proc;
```

Vexp := **proc**(*xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t*)

Mat(*xm, ym, k1p, k1m, k2p, k2m, k3p, k3m*); $\langle seq(Expi(i, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t), i = 1 ..Bdim)\rangle$

end proc **(5.2)**

```
> Vx :=proc(k, xm, ym)
  Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m) :
  ⟨seq(1.0*B[i][1]**k, i=1..Bdim)⟩ : end proc;

  Vy :=proc(k, xm, ym)
  Mat(xm, ym, k1p, k1m, k2p, k2m, k3p, k3m) :
  ⟨seq(1.0*B[i][2]**k, i=1..Bdim)⟩ : end proc;
```

Vx := **proc**(*k, xm, ym*) *Mat*(*xm, ym, k1p, k1m, k2p, k2m, k3p, k3m*); $\langle seq(1.0 * B[i][1] \hat{} k, i = 1 ..Bdim)\rangle$ **end proc**

Vy := **proc**(*k, xm, ym*) *Mat*(*xm, ym, k1p, k1m, k2p, k2m, k3p, k3m*); $\langle seq(1.0 * B[i][2] \hat{} k, i = 1 ..Bdim)\rangle$ **end proc** **(5.3)**

```
> Xk :=proc(k, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t) DotProduct(Vx(k, xm, ym), Vexp(xm, ym, k1p, k1m, k2p, k2m,
      k3p, k3m, t)); end proc;
  Yk :=proc(k, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t) DotProduct(Vy(k, xm, ym), Vexp(xm, ym, k1p, k1m, k2p, k2m,
      k3p, k3m, t)); end proc;
```

Xk := **proc**(*k, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t*)

LinearAlgebra:-DotProduct(*Vx*(*k, xm, ym*), *Vexp*(*xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t*))

end proc

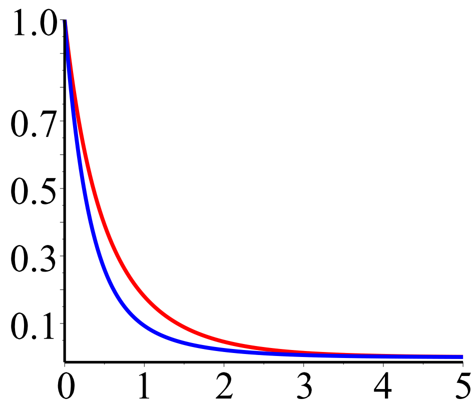
Yk := **proc**(*k, xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t*) **(5.4)**

LinearAlgebra:-DotProduct(*Vy*(*k, xm, ym*), *Vexp*(*xm, ym, k1p, k1m, k2p, k2m, k3p, k3m, t*))

end proc

Take *xm=ym=1, k1p=k2p=k3p=k3m=1* and *k1m=k2m=0.1*, we have:

```
> Xp := pointplot([seq([t, evalf(Xk(1, 1, 1, 1, .1, 1, .1, 1, 1, t))], t=0..5, 0.01)], color=red, connect=true) :
  Yp := pointplot([seq([t, evalf(Yk(1, 1, 1, 1, .1, 1, .1, 1, 1, t))], t=0..5, 0.01)], color=blue, connect=true) :
  display(Xp, Yp);
```




```
>
```

APPENDIX D – Maple Code to Fock Space Method (General case)

In this code, we'll describe the algorithm to study the general case of Schnackenberg model, as described in Chapter 8.

Before, an important warning: to facilitate the entering the code, we write respectively $k1c$ and $k1d$ instead of k_{1+} and k_{1-}

The same goes for the other constants that have subindices.

Another important note: for the correct functioning of the codes, check if they are written in language "Maple imput". Otherwise, some commands may fail or give wrong results.

1. Description of Fock Space

We begin our study write the packages necessary.

The Maple has a specific package to describe quantum operators, which is the package *physics.* Make sure that you are using the latest version of the package (or at least the version *2014, February 10, 21:29 hours*), otherwise some commands may not work properly. If necessary, download the package at http://www.maplesoft.com/products/maple/features/physicsresearch.aspx.

The other packages are in Maple.

```
> restart:
  with(Physics) : with(MTM) : with(LinearAlgebra) : with(plots) :
  Physics:-Version();
```

"C:\Program Files\Maple 2015\lib\update.mla", *2015, May 14, 11:23 hours* **(1.1)**

Below write a command to generate large matrices in the code:

```
> interface(rtablesize = 301);
```

$$10 \tag{1.2}$$

Now, we write the Fock space in which we are going work:

```
> Setup(op = A,X,Y,B);
```

** Partial match of 'op' against keyword 'quantumoperators'*

** Partial match of 'X' against keyword 'vectorpostfix'*

** Partial match of 'Y' against keyword 'keywords'*

** Partial or misspelled keyword matches more than one possible keyword. Please select the correct one from below and try again.*

bracketbasis, bracketrules **(1.3)**

The codes below define the sets of creation and annihilation operators, and ajusting them for the suitable phase. For *A*:

```
> N:=1;
  for i from 1 to N do
  Ap[i]:= Creation(A,i,phaseconvention= proc(n) 1 end proc,notation = explicit);
  Am[i]:=Annihilation(A,i,phaseconvention= proc(n) n end proc,notation = explicit);
  end do;
```

$$N := 1$$

$$Ap_1 := a^{+}_{A_1}$$

$$Am_1 := a^{-}_{A_1} \tag{1.4}$$

For *X*:

```
> N:=1;
```

```
for i from 1 to N do
Xp[i]:= Creation(X,i,phaseconvention= proc(n) 1 end proc,notation = explicit);
Xm[i]:=Annihilation(X,i,phaseconvention= proc(n) n end proc,notation = explicit);
end do;
```

$$N := 1$$
$$Xp_1 := a+_{X_1}$$
$$Xm_1 := a-_{X_1} \tag{1.5}$$

For *Y*:

```
> N:=1;
for i from 1 to N do
Yp[i]:= Creation(Y,i,phaseconvention= proc(n) 1 end proc,notation = explicit);
Ym[i]:=Annihilation(Y,i,phaseconvention= proc(n) n end proc,notation = explicit);
end do;
```

$$N := 1$$
$$Yp_1 := a+_{Y_1}$$
$$Ym_1 := a-_{Y_1} \tag{1.6}$$

For *B*:

```
> N:=1;
for i from 1 to N do
Bp[i]:= Creation(B,i,phaseconvention= proc(n) 1 end proc,notation = explicit);
Bm[i]:=Annihilation(B,i,phaseconvention= proc(n) n end proc,notation = explicit);
end do;
```

$$N := 1$$
$$Bp_1 := a+_{B_1}$$
$$Bm_1 := a-_{B_1} \tag{1.7}$$

2. The Hamiltonian of the system

We will describe the reactions of the system and and their Hamiltonians, according the section 2 of Chapter 8. In every cases, the *r* indicates the back part of the reaction.

First reaction, *A <-> X:*

```
> H1:=proc(k1p) -Expand(k1p*(Xp[1]*(Am[1])-(Ap[1])*(Am[1]))); end proc;
H1r:=proc(k1m) -Expand(k1m*((Ap[1])*Xm[1]-Xp[1]*Xm[1])); end proc;
```

$$H1 := \textbf{proc}(k1p)\ \ Physics\text{:-}Expand(k1p * (Xp[1] * Am[1] - Ap[1] * Am[1])) * (-1)\ \ \textbf{end proc}$$

$$H1r := \textbf{proc}(k1m)\ \ Physics\text{:-}Expand(k1m * (Ap[1] * Xm[1] - Xp[1] * Xm[1])) * (-1)\ \ \textbf{end proc} \tag{2.1}$$

Second reaction, *X+2Y <-> 3Y*:

```
> H2:=proc(k2p) -Expand(k2p*(Yp[1]*Yp[1]*Yp[1]*Ym[1]*Ym[1]*Xm[1]-Yp[1]*Yp[1]*Ym[1]*Ym[1]*Xp[1]*Xm
[1])); end proc;
H2r:=proc(k2m) -Expand(k2m*(Yp[1]*Yp[1]*Xp[1]*Ym[1]*Ym[1]*Ym[1]-Yp[1]*Yp[1]*Yp[1]*Ym[1]*Ym[1]*Ym
[1])); end proc;
```

$H2 := \textbf{proc}(k2p)$

$$Physics\text{:-}Expand(k2p * (Yp[1] * Yp[1] * Yp[1] * Ym[1] * Ym[1] * Xm[1] - Yp[1] * Yp[1] * Ym[1] * Ym[1] * Xp[1] * Xm[1])) * (-1)$$

end proc

$H2r := \textbf{proc}(k2m)$ **(2.2)**

$$Physics\text{:-}Expand(k2m * (Yp[1] * Yp[1] * Xp[1] * Ym[1] * Ym[1] * Ym[1] - Yp[1] * Yp[1] * Yp[1] * Ym[1] * Ym[1] * Ym[1])) * (-1)$$

end proc

Third reaction, *Y<->B*:

```
> H3:=proc(k3p) -Expand(k3p*((Bp[1])*Ym[1]-Yp[1]*Ym[1])); end proc;
H3r:=proc(k3m) -Expand(k3m*(Yp[1]*(Bm[1])-(Bp[1])*(Bm[1]))); end proc;
```

$$H3 := \mathbf{proc}(k3p)\ \ Physics{:}\text{-}Expand(k3p*(Bp[1]*Ym[1] - Yp[1]*Ym[1]))*(-1)\ \ \mathbf{end\ proc}$$

$$H3r := \mathbf{proc}(k3m)\ \ Physics{:}\text{-}Expand(k3m*(Yp[1]*Bm[1] - Bp[1]*Bm[1]))*(-1)\ \ \mathbf{end\ proc} \tag{2.3}$$

Then, we compute the total Hamiltonian:

```
> H:=proc(k1p,k1m,k2p,k2m,k3p,k3m) H1(k1p)+H1r(k1m)+H2(k2p)+H2r(k2m)+H3(k3p)+H3r(k3m); end proc;
> H(k1p,k1m,k2p,k2m,k3p,k3m);
```

$$H := \mathbf{proc}(k1p, k1m, k2p, k2m, k3p, k3m)\ \ H1(k1p) + H1r(k1m) + H2(k2p) + H2r(k2m) + H3(k3p) + H3r(k3m)\ \ \mathbf{end\ proc}$$

$$-k1p\ `*`\left(a+_{X_1}, a-_{A_1}\right) + k1p\ `*`\left(a+_{A_1}, a-_{A_1}\right) - k1m\ `*`\left(a+_{A_1}, a-_{X_1}\right) + k1m\ `*`\left(a+_{X_1}, a-_{X_1}\right) - k2p\ `*`\left(`\wedge`\left(a+_{Y_1}, 3\right), `\wedge`\left(a-_{Y_1}, 2\right), a-_{X_1}\right) + k2p\ `*`\left(`\wedge`\left(a+_{Y_1}, 2\right), `\wedge`\left(a-_{Y_1}, 2\right), a+_{X_1}, a-_{X_1}\right) - k2m\ `*`\left(`\wedge`\left(a+_{Y_1}, 2\right), a+_{X_1}, `\wedge`\left(a-_{Y_1}, 3\right)\right) + k2m\ `*`\left(`\wedge`\left(a+_{Y_1}, 3\right), `\wedge`\left(a-_{Y_1}, 3\right)\right) - k3p\ `*`\left(a+_{B_1}, a-_{Y_1}\right) + k3p\ `*`\left(a+_{Y_1}, a-_{Y_1}\right) - k3m\ `*`\left(a+_{Y_1}, a-_{B_1}\right) + k3m\ `*`\left(a+_{B_1}, a-_{B_1}\right) \tag{2.4}$$

The nonzero contributions for each Hamiltonian is:

H1:

```
> (Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai)).(H1(k1p)).(Ket(A, aj).Ket(X, xrj).Ket(Y, yj).Ket(B, bj));
```

$$k1p\ \delta_{yi, yj}\ \delta_{bi, bj}\left(ai\ \delta_{ai, aj}\ \delta_{xri, xrj} - xri\ \delta_{aj, ai+1}\ \delta_{xrj, xri-1}\right) \tag{2.5}$$

H1r:

```
> (Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai)).(H1r(k1m)).(Ket(A, aj).Ket(X, xrj).Ket(Y, yj).Ket(B, bj));
```

$$-k1m\ \delta_{yi, yj}\ \delta_{bi, bj}\left(ai\ \delta_{aj, ai-1}\ \delta_{xrj, xri+1} - xri\ \delta_{ai, aj}\ \delta_{xri, xrj}\right) \tag{2.6}$$

H2:

```
> (Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai)).(H2(k2p)).(Ket(A, aj).Ket(X, xrj).Ket(Y, yj).Ket(B, bj));
```

$$\left(\overline{yi^2\ xri}\ \delta_{xri, xrj}\ \delta_{yi, yj} - \overline{yi\ xri}\ \delta_{xri, xrj}\ \delta_{yi, yj} - \overline{yi}\ \delta_{xrj, xri+1}\ \delta_{yj, yi-1}\ (\overline{yi}-1)\ (\overline{yi}-2)\right)\ \delta_{ai, aj}\ \delta_{bi, bj}\ k2p \tag{2.7}$$

H2r:

```
> (Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai)).(H2r(k2m)).(Ket(A, aj).Ket(X, xrj).Ket(Y, yj).Ket(B, bj));
```

$$-\left(\delta_{xrj, xri-1}\ \delta_{yj, yi+1}\ \overline{yi^2\ xri} - \delta_{xrj, xri-1}\ \delta_{yj, yi+1}\ \overline{yi\ xri} - \overline{yi}\ \delta_{xri, xrj}\ \delta_{yi, yj}\ (\overline{yi}-1)\ (\overline{yi}-2)\right)\ \delta_{ai, aj}\ \delta_{bi, bj}\ k2m \tag{2.8}$$

H3:

```
> (Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai)).(H3(k3p)).(Ket(A, aj).Ket(X, xrj).Ket(Y, yj).Ket(B, bj));
```

$$-k3p\ \delta_{ai, aj}\ \delta_{xri, xrj}\left(bi\ \delta_{bj, bi-1}\ \delta_{yj, yi+1} - yi\ \delta_{bi, bj}\ \delta_{yi, yj}\right) \tag{2.9}$$

H3r:

```
> (Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai)).(H3r(k3m)).(Ket(A, aj).Ket(X, xrj).Ket(Y, yj).Ket(B, bj));
```

$$k3m\ \delta_{ai, aj}\ \delta_{xri, xrj}\left(bi\ \delta_{bi, bj}\ \delta_{yi, yj} - yi\ \delta_{bj, bi+1}\ \delta_{yj, yi-1}\right) \tag{2.10}$$

The total nonzero contribution can be found as follows:

```
> (Bra(B,bi).Bra(Y,yi).Bra(X,xri).Bra(A,ai)).(H(k1p,k1m,k2p,k2m,k3p,k3m)).(Ket(A,aj).Ket(X,xrj).Ket
  (Y,yj).Ket(B,bj));
```

$$-k3p\ yj\ \delta_{ai, aj}\ \delta_{xri, xrj}\ \delta_{yi, yj-1}\ \delta_{bi, bj+1} - k3m\ bj\ \delta_{ai, aj}\ \delta_{xri, xrj}\ \delta_{yi, yj+1}\ \delta_{bi, bj-1} - k2m\ yj\ (yj-1)\ (yj-2)\ \delta_{ai, aj}\ \delta_{xri, xrj+1}\ \delta_{yi, yj-1}\ \delta_{bi, bj} - k2p\ xrj\ yj\ (yj-1)\ \delta_{ai, aj}\ \delta_{xri, xrj-1}\ \delta_{yi, yj+1}\ \delta_{bi, bj} + \left(\delta_{xri, xrj}\left(k2m\ yj^3 + (k2p\ xrj - 3\ k2m)\ yj^2 + (-k2p\ xrj + 2\ k2m + k3p)\ yj + k3m\ bj + xrj\ k1m + aj\ k1p\right)\ \delta_{ai, aj} - xrj\ k1m\ \delta_{ai, aj+1}\ \delta_{xri, xrj-1} - aj\ k1p\ \delta_{ai, aj-1}\ \delta_{xri, xrj+1}\right)\ \delta_{yi, yj}\ \delta_{bi, bj} \tag{2.11}$$

3. The basis of Fock space

To enumerate the elements of the basis of Fock space, we compute the code below:

```
> Baseset := proc(am, xm, ym, bm) global B; global ket; global bra; global Bdim;
  i := 1;

  for ai from 0 to am
     do
       for xri from 0 to xm
          do
            for yi from 0 to ym
               do
                 for bi from 0 to bm
                    do
                    B[i] := (ai, xri, yi, bi);
                    ket[i] := Ket(A, ai).Ket(X, xri).Ket(Y, yi).Ket(B, bi);
                    bra[i] := Bra(B, bi).Bra(Y, yi).Bra(X, xri).Bra(A, ai);
                    print(i, B[i] = ket[i]);
                    i := i+1;
                    end do;
               end do;
            end do;
        end do;
     Bdim := i-1;
   end proc:
```

If we have am=xm=ym=bm=1, then we obtain the basis described in (8.14):

```
> Baseset(1, 1, 1, 1);
```

$$1, (0, 0, 0, 0) = \left|A_0\right\rangle \left|X_0\right\rangle \left|Y_0\right\rangle \left|B_0\right\rangle$$

$$2, (0, 0, 0, 1) = \left|A_0\right\rangle \left|X_0\right\rangle \left|Y_0\right\rangle \left|B_1\right\rangle$$

$$3, (0, 0, 1, 0) = \left|A_0\right\rangle \left|X_0\right\rangle \left|Y_1\right\rangle \left|B_0\right\rangle$$

$$4, (0, 0, 1, 1) = \left|A_0\right\rangle \left|X_0\right\rangle \left|Y_1\right\rangle \left|B_1\right\rangle$$

$$5, (0, 1, 0, 0) = \left|A_0\right\rangle \left|X_1\right\rangle \left|Y_0\right\rangle \left|B_0\right\rangle$$

$$6, (0, 1, 0, 1) = \left|A_0\right\rangle \left|X_1\right\rangle \left|Y_0\right\rangle \left|B_1\right\rangle$$

$$7, (0, 1, 1, 0) = \left|A_0\right\rangle \left|X_1\right\rangle \left|Y_1\right\rangle \left|B_0\right\rangle$$

$$8, (0, 1, 1, 1) = \left|A_0\right\rangle \left|X_1\right\rangle \left|Y_1\right\rangle \left|B_1\right\rangle$$

$$9, (1, 0, 0, 0) = \left|A_1\right\rangle \left|X_0\right\rangle \left|Y_0\right\rangle \left|B_0\right\rangle$$

$$10, (1, 0, 0, 1) = \left|A_1\right\rangle \left|X_0\right\rangle \left|Y_0\right\rangle \left|B_1\right\rangle$$

$$11, (1, 0, 1, 0) = \left|A_1\right\rangle \left|X_0\right\rangle \left|Y_1\right\rangle \left|B_0\right\rangle$$

$$12, (1, 0, 1, 1) = \left|A_1\right\rangle \left|X_0\right\rangle \left|Y_1\right\rangle \left|B_1\right\rangle$$

$$13, (1, 1, 0, 0) = \left|A_1\right\rangle \left|X_1\right\rangle \left|Y_0\right\rangle \left|B_0\right\rangle$$

$$14, (1, 1, 0, 1) = \left|A_1\right\rangle \left|X_1\right\rangle \left|Y_0\right\rangle \left|B_1\right\rangle$$

$$15, (1, 1, 1, 0) = \left|A_1\right\rangle \left|X_1\right\rangle \left|Y_1\right\rangle \left|B_0\right\rangle$$

$$16, (1, 1, 1, 1) = \left|A_1\right\rangle \left|X_1\right\rangle \left|Y_1\right\rangle \left|B_1\right\rangle$$

$$16 \tag{3.1}$$

4. The matrix element of Hamiltonian

To describe the matrix element of Hamiltonian, we compute the code below. Note that the Matrix Element (*ME*, in code) is the contributions computed in section 2 of this Appendix.

```
> Mat := proc(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m)
  delta := proc(a, b) piecewise(a=b, 1, 0); end proc;
  Baseset := proc(am, xm, ym, bm) global B; global Bdim;
  i := 1;

  for ai from 0 to am
     do
       for xri from 0 to xm
          do
            for yi from 0 to ym
               do
                 for bi from 0 to bm
                    do
                    B[i] := (ai, xri, yi, bi) :
                    i := i+1;
                    end do;
               end do;
            end do;
       end do;
     Bdim := i-1;
  end proc;
  Baseset(am, xm, ym, bm) :
   ME := proc(ai, aj, xri, xrj, yi, yj, bi, bj, k1p, k1m, k2p, k2m, k3p, k3m) -k3p*yj*delta(ai, aj)*delta(xri,
      xrj)*delta(yi, yj-1)*delta(bi, bj+1)-k3m*bj*delta(ai, aj)*delta(xri, xrj)*delta(yi, yj+1)
     *delta(bi, bj-1)-k2m*yj*(yj-1)*(yj-2)*delta(ai, aj)*delta(xri, xrj+1)*delta(yi, yj-1)*delta(bi,
      bj)-k2p*xrj*yj*(yj-1)*delta(ai, aj)*delta(xri, xrj-1)*delta(yi, yj+1)*delta(bi, bj)+(delta(xri,
      xrj)*(k2m*(yj^3)+(k2p*xrj-3*k2m)*(yj^2)+(-k2p*xrj+2*k2m+k3p)*yj+k3m*bj+k1m*xrj+k1p*aj)
     *delta(ai, aj)-k1m*xrj*delta(ai, aj+1)*delta(xri, xrj-1)-k1p*aj*delta(ai, aj-1)*delta(xri, xrj
     +1))*delta(yi, yj)*delta(bi, bj); end proc;

  element := proc(i, j, k1p, k1m, k2p, k2m, k3p, k3m) -ME(B[i][1], B[j][1], B[i][2], B[j][2], B[i][3], B[j][3],
      B[i][4], B[j][4], k1p, k1m, k2p, k2m, k3p, k3m); end proc;

    for i from 1 to Bdim do
       for j from 1 to Bdim do
       A[i, j] := element(i, j, k1p, k1m, k2p, k2m, k3p, k3m);
       end do;
    end do;
  Mt := Array(1..Bdim, 1..Bdim, (i, j) → A[i, j]);
   end proc:
```

For *am=xm=ym=bm=1*, we obtain the matrix *16x16* described in the text:

```
> G := Mat(1, 1, 1, 1, k1p, k1m, k2p, k2m, k3p, k3m) :
   G
```

$$\begin{aligned}&[[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], \\ &\quad [0, -k3m, k3p, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], \\ &\quad [0, k3m, -k3p, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], \\ &\quad [0, 0, 0, -k3p-k3m, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],\end{aligned} \tag{4.1}$$

$$[0, 0, 0, 0, -k1m, 0, 0, 0, k1p, 0, 0, 0, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, -k3m - k1m, k3p, 0, 0, k1p, 0, 0, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, k3m, -k3p - k1m, 0, 0, 0, k1p, 0, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, 0, 0, -k3p - k3m - k1m, 0, 0, 0, k1p, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, k1m, 0, 0, 0, -k1p, 0, 0, 0, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, k1m, 0, 0, 0, -k3m - k1p, k3p, 0, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, 0, k1m, 0, 0, k3m, -k3p - k1p, 0, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, 0, 0, k1m, 0, 0, 0, -k3p - k3m - k1p, 0, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -k1m - k1p, 0, 0, 0],$$
$$[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -k3m - k1m - k1p, k3p, 0],$$
$$[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, k3m, -k3p - k1m - k1p, 0],$$
$$[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -k3p - k3m - k1m - k1p]]$$

whose the eigenvalues are, as described in (8.15), given by

```
> Eigenvalues(G)
```

$$\begin{bmatrix} -k3p - k3m - k1m - k1p \\ -k3p - k3m - k1m - k1p \\ -k3p - k3m - k1m - k1p \\ -k3p - k3m - k1m - k1p \\ -k3p - k3m \\ -k3p - k3m \\ -k3p - k3m \\ -k3p - k3m \\ -k1m - k1p \\ -k1m - k1p \\ -k1m - k1p \\ -k1m - k1p \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{4.2}$$

The exponential of matrix G is defined by the code below:

```
> ExpHt := proc(am, xm, ym, bm, k1m, k1p, k2p, k2m, k3p, k3m, t)
  M := Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m);
  MatrixExponential(M*t); end proc;
ExpHt := proc(am, xm, ym, bm, k1m, k1p, k2p, k2m, k3p, k3m, t)
    local M;
    M := Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m); LinearAlgebra:-MatrixExponential(M* t)
end proc
```
(4.3)

Make every the constants of reaction equals a 1, the matrix is

```
> ExpHt(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1);
```

$$[[1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], \tag{4.4}$$
$$[0, \frac{1}{2} e^{-2} + \frac{1}{2}, -\frac{1}{2} e^{-2} + \frac{1}{2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],$$

$$\left[0,\ -\frac{1}{2}\,e^{-2}+\frac{1}{2},\ \frac{1}{2}\,e^{-2}+\frac{1}{2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ e^{-2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ \frac{1}{2}\,e^{-2}+\frac{1}{2},\ 0,\ 0,\ 0,\ -\frac{1}{2}\,e^{-2}+\frac{1}{2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ \frac{1}{4}\,e^{-4}+\frac{1}{2}\,e^{-2}+\frac{1}{4},\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ 0,\ 0,\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ \frac{1}{4}\,e^{-4}-\frac{1}{2}\,e^{-2}+\frac{1}{4},\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ \frac{1}{4}\,e^{-4}+\frac{1}{2}\,e^{-2}+\frac{1}{4},\ 0,\ 0,\ \frac{1}{4}\,e^{-4}-\frac{1}{2}\,e^{-2}+\frac{1}{4},\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ 0,\ 0,\ 0,\ -\frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ -\frac{1}{2}\,e^{-2}+\frac{1}{2},\ 0,\ 0,\ 0,\ \frac{1}{2}\,e^{-2}+\frac{1}{2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ \frac{1}{4}\,e^{-4}-\frac{1}{2}\,e^{-2}+\frac{1}{4},\ 0,\ 0,\ \frac{1}{4}\,e^{-4}+\frac{1}{2}\,e^{-2}+\frac{1}{4},\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ \frac{1}{4}\,e^{-4}-\frac{1}{2}\,e^{-2}+\frac{1}{4},\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ 0,\ 0,\ -\frac{1}{4}\,e^{-4}+\frac{1}{4},\ \frac{1}{4}\,e^{-4}+\frac{1}{2}\,e^{-2}+\frac{1}{4},\ 0,\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ -\frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ 0,\ 0,\ 0,\ \frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ 0,\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ e^{-2},\ 0,\ 0,\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ -\frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ -\frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ \frac{1}{2}\,e^{-4}+\frac{1}{2}\,e^{-2},\ 0\right],$$

$$\left[0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ e^{-4}\right]\Big]$$

5. Plots

To plot the averages of species, we use the sequence of codes below, as described in reference (29):

```
> Expi :=proc(L, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t)
  Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m) :
  evalf(ExpHt(am, xm, ym, bm, 1.0*k1p, 1.0*k1m, 1.0*k2p, 1.0*k2m, 1.0*k3p, 1.0*k3m, t)[L][Bdim]);
  end proc;
```

Expi := **proc**(*L, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*)

Mat(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m*);

evalf(*ExpHt*(*am, xm, ym, bm,* 1.0 * *k1p,* 1.0 * *k1m,* 1.0 * *k2p,* 1.0 * *k2m,* 1.0 * *k3p,* 1.0 * *k3m, t*)[*L*][*Bdim*])

end proc **(5.1)**

```
> Vexp :=proc(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t)
  Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m) :
  ⟨seq(Expi(i, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t), i=1..Bdim)⟩ : end proc;
```

Vexp := **proc**(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*)

Mat(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m*); ⟨ *seq*(*Expi*(*i, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*), *i* = 1 ..*Bdim*) ⟩

end proc **(5.2)**

```
> Va :=proc(k, am, xm, ym, bm)
  Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m) :
  ⟨seq(1.0*B[i][1]**k, i=1..Bdim)⟩ : end proc;


  Vx :=proc(k, am, xm, ym, bm)
```

```
Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m) :
⟨seq(1.0*B[i][2]**k, i=1..Bdim)⟩ : end proc;

Vy := proc(k, am, xm, ym, bm)
Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m) :
⟨seq(1.0*B[i][3]**k, i=1..Bdim)⟩ : end proc;

Vb := proc(k, am, xm, ym, bm)
Mat(am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m) :
⟨seq(1.0*B[i][4]**k, i=1..Bdim)⟩ : end proc;
```

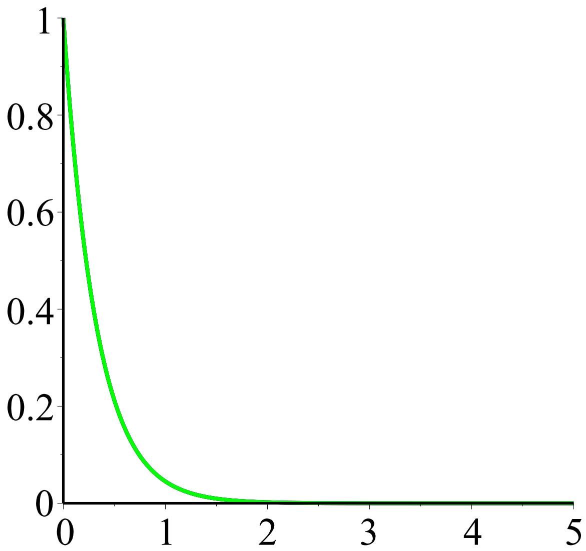
Va := **proc**(*k, am, xm, ym, bm*) *Mat*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m*); < *seq*(1.0 * *B*[*i*] [1] ^*k*, *i* = 1 ..*Bdim*) > **end proc**
Vx := **proc**(*k, am, xm, ym, bm*) *Mat*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m*); < *seq*(1.0 * *B*[*i*] [2] ^*k*, *i* = 1 ..*Bdim*) > **end proc**
Vy := **proc**(*k, am, xm, ym, bm*) *Mat*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m*); < *seq*(1.0 * *B*[*i*] [3] ^*k*, *i* = 1 ..*Bdim*) > **end proc**
Vb := **proc**(*k, am, xm, ym, bm*) *Mat*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m*); < *seq*(1.0 * *B*[*i*] [4] ^*k*, *i* = 1 ..*Bdim*) > **end proc** **(5.3)**

```
> Ak := proc(k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t) DotProduct(Va(k, am, xm, ym, bm), Vexp(am, xm, ym, bm,
      k1p, k1m, k2p, k2m, k3p, k3m, t)); end proc;
  Xk := proc(k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t) DotProduct(Vx(k, am, xm, ym, bm), Vexp(am, xm, ym, bm,
      k1p, k1m, k2p, k2m, k3p, k3m, t)); end proc;
  Yk := proc(k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t) DotProduct(Vy(k, am, xm, ym, bm), Vexp(am, xm, ym, bm,
      k1p, k1m, k2p, k2m, k3p, k3m, t)); end proc;
  Bk := proc(k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t) DotProduct(Vb(k, am, xm, ym, bm), Vexp(am, xm, ym, bm,
      k1p, k1m, k2p, k2m, k3p, k3m, t)); end proc;
```

Ak := **proc**(*k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*)
  LinearAlgebra:-DotProduct(*Va*(*k, am, xm, ym, bm*), *Vexp*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*))
end proc
Xk := **proc**(*k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*)
  LinearAlgebra:-DotProduct(*Vx*(*k, am, xm, ym, bm*), *Vexp*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*))
end proc
Yk := **proc**(*k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*)
  LinearAlgebra:-DotProduct(*Vy*(*k, am, xm, ym, bm*), *Vexp*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*))
end proc
Bk := **proc**(*k, am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*) **(5.4)**
  LinearAlgebra:-DotProduct(*Vb*(*k, am, xm, ym, bm*), *Vexp*(*am, xm, ym, bm, k1p, k1m, k2p, k2m, k3p, k3m, t*))
end proc

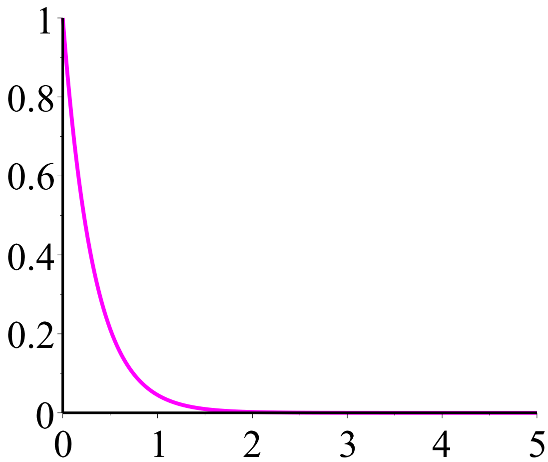
Take *am*=*xm*=*ym*=*bm*=*1* and every the constants of reactions equals to 1, we have:

```
> Ap := pointplot([seq([t, evalf(Ak(1, 1, 1, 1, 1, 1, 0.1, 1, 0.1, 1, 1, t))], t=0..5, 0.01)], color=magenta, connect
      =true) :
  Xp := pointplot([seq([t, evalf(Xk(1, 1, 1, 1, 1, 1, 0.1, 1, 0.1, 1, 1, t))], t=0..5, 0.01)], color=red, connect
      =true) :
  Yp := pointplot([seq([t, evalf(Yk(1, 1, 1, 1, 1, 1, 0.1, 1, 0.1, 1, 1, t))], t=0..5, 0.01)], color=blue, connect
      =true) :
  Bp := pointplot([seq([t, evalf(Bk(1, 1, 1, 1, 1, 1, 0.1, 1, 0.1, 1, 1, t))], t=0..5, 0.01)], color=green, connect
      =true) :
  display(Ap, Xp, Yp, Bp);
```

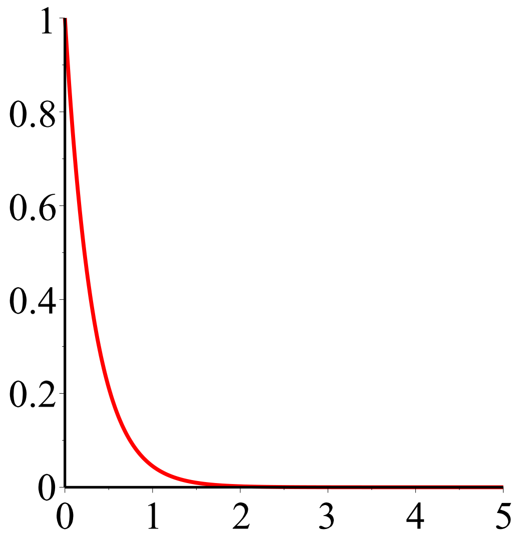


The graphics are identical, changing only the colors:

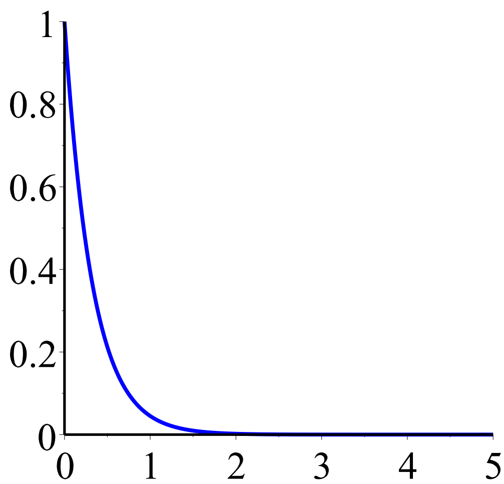
```
> display(Ap)
```



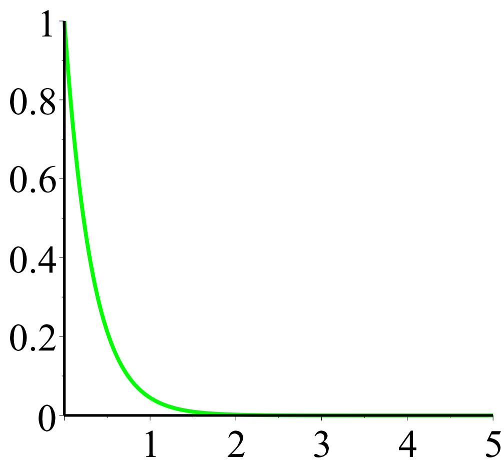

```
> display(Xp)
```




```
> display(Yp)
```




```
> display(Bp)
```




```
>
```