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Analytic Solutions to Stochastic Epidemic Models

Recife

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Dissertation, supervised by Prof. Fernando Nobrega and co-supervised by Prof. Eamonn Andrew Gaffney, presented to the Federal University of Pernambuco, as part of the requirements for the completion of the master's degree in mathematics.

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DANILLO BARROS DE SOUZA

ANALYTIC SOLUTIONS TO STOCHASTIC EPIDEMIC MODELS

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Abstract

Even the simplest outbreaks might not be easily predictable. Fortunately, deterministic and stochastic models, systems differential equations and computational simulations have proved to be useful to a better understanding of the mechanics that leads to an epidemic outbreak. Whilst such systems are regularly studied from a modelling viewpoint using stochastic simulation algorithms, numerous potential analytical tools can be inherited from statistical and quantum physics, replacing randomness due to quantum fluctuations with low copy number stochasticity. Here, the Fock space representation, used in quantum mechanics, is combined with the symbolic algebra of creation and annihilation operators to consider explicit solutions for the master equations describing epidemics represented via the SIR model (Susceptible-Infected-Recovered), originally developed via Kermack and McKendrick's theory. This is illustrated with an exact solution for a short size of population, including a consideration of very short time scales for the next infection, which emphasises when stiffness is present even for small copy numbers. Furthermore, we present a general matrix representation for the SIR model with an arbitrary number of individuals following diagonalization. This leads to the solution of this complex stochastic problem, including an explicit way to express the mean time of epidemic and basic reproduction number depending on the size of population and parameters of infection and recovery. Specifically, the project objective to apply use of the same tools in the approach of system governed by law of mass action, as previously developed for the Michaelis-Menten enzyme kinetics model [Santos et. al. Phys Rev. E 92, 062714 (2015)]. For this, a flexible symbolic Maple code is provided, demonstrating the prospective advantages of this framework compared to Gillespie stochastic simulation algorithms.

Key-words: Fock space. Epidemic models. Exact solutions.

Resumo

Mesmo os surtos mais simples podem não ser facilmente previsíveis. Felizmente, modelos determinísticos e estocásticos, equações diferenciais de sistemas e simulações computacionais provaram ser úteis para uma melhor compreensão da mecânica que leva a um surto epidêmico. Enquanto tais sistemas são regularmente estudados a partir de um ponto de vista de modelagem usando algoritmos de simulação estocástica, inúmeras ferramentas analíticas potenciais podem ser herdadas da física estatística e quântica, substituindo aleatoriedade devido a flutuações quânticas com baixa estocástica de número de cópias. Aqui, a representação do espaço de Fock, usada na mecânica quântica, é combinada com a álgebra simbólica dos operadores de criação e aniquilação para considerar soluções explícitas para as equações mestra que descrevem epidemias representadas via modelo SIR (Suscetível-Infectado-Recuperado), originalmente desenvolvido pela teoria de Kermack e McKendrick. Isto é ilustrado com uma solução exata para um tamanho pequeno de população, considerando escalas de tempo muito curtas para a próxima infecção, que enfatiza quando a rigidez está presente mesmo para números de cópias pequenos. Além disso, apresentamos uma representação matricial geral para o modelo SIR com um número arbitrário de indivíduos após diagonalização. Isto nos leva à solução deste problema estocástico complexo, além de ter uma maneira explícita de expressar o tempo médio de epidemia e o número básico de reprodução, ambos dependendo do tamanho da população e parâmetros de infecção e recuperação. Especificamente, o objetivo é utilizar as mesmas ferramentas na abordagem de um sistema regido por lei de ação das massas, como anteriormente desenvolvido para o modelo de cinética enzimática de Michaelis-Menten [Santos et. Al PRE 2015]. Para isso, é fornecido um código Maple simbólico flexível, demonstrando as vantagens potenciais desta estrutura comparados aos algoritmos de simulação estocástica de Gillespie.

Palavras-chaves: Espaços de Fock. Modelos epidêmicos. Soluções exatas.

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List of symbols

Alpha

 β Beta

γ Gamma

 δ Delta

 ϵ Epsilon

 θ Theta

 λ Lambda

au Tau

 ϕ Phi

 Ω Omega

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1 INTRODUCTION

The SIR model (Susceptible-Infected-Recovered) inaugurated the theory of epidemiology (Kermack and Mc Kendrick in the 1920s) (KERMACK; MCKENDRICK, 1927), proposed to explain the dynamics of infected patients observed in epidemics such as the plague and cholera. This type of model is based on our intuitive understanding of how an epidemic occurs in the real world. In this system, we have three categories of individuals: those who are susceptible to disease (S), those who are infected and can spread the disease to susceptible (I), and those who have recovered from previous infection and can no longer spread or catch the disease (R). Differential equations are used to model the dynamics of each of these subpopulations through the course of an epidemic. Disease transmission occurs by the stochastic infection of a susceptible by a neighboring infective, and spread takes place when infected individuals mix among susceptible (CHEN BERNARD MOULIN, 2015). In fact, an epidemic spread depends of a contact between susceptible and infected individuals, i.e., satisfying the mass action principle of transmission for directly transmitted viral and bacterial infections (ANDERSON, 1991). From this, all the theory used made possible the construction of the mathematical model from differential equations to express its dynamics and further the behavior of the population starting an infection. In both of cases, the approach requires several works on statistics tools and differential equations in order to estimate the minimum understanding of the dynamics. Unfortunately, due to all inherent difficulty in terms of algebra computation of nonlinear differential equations, the analytic solutions of the system of differential equation cannot be found by the methods used until now, even for the deterministic model. Very recently, methods adapted from quantum mechanics have been used to improve the approach of the epidemic dynamics (SANTOS; GADÊLHA; GAFFNEY, 2015).

In this dissertation, we will introduce a new approach to treat epidemic stochastic models using tools inherited from quantum physics that allow us to express an analytical solution for the stochastic SIR model. Furthermore, this technique can be used to express the same statistical results presented by Bailey (BAILEY et al., 1975). All this is now possible due to the quantum operators expressed in the Fock-space and linear algebra results implemented in a Maple software code. The same technique was implemented in the modeling of enzymes interaction and was successful in finding analytical solutions for Michaelis-Menten Enzyme Kinectics (SANTOS; GADÊLHA; GAFFNEY, 2015).

Currently, the Zika-virus has taking a big dimension of the Brazilian territory and spreading to another 46 countries. The same virus is suspected of causing Gillain-Barré syndrome in adults and microcephaly in newborns. Since May 2015, Brasil has been hit by the disease, where we have at least 148905 confirmed cases of Zika-virus, 12612 of this

cases are pregnant. Furthermore, in the State of Pernambuco, has a warning suspect of 1968 new cases of microcephaly whose 359 was confirmed, according to World Health Organization (August 4, 2015 report). Such circumstances give us a motivation to improve our work made in this thesis and adopt some others suitable techniques to make possible a new stochastic epidemic model characterizing this viral behavior via Master equations.

This work is written as follows: We will start our construction of modeling by Petri Nets in the section 1.1 and apply its results to epidemic models either in the deterministic and stochastic versions, in section 2. Important techniques can be shown from (BAILEY et al., 1975), as the control of the percentage of infections and removals according to the intensity of an epidemic in the deterministic model, the total size of epidemic in terms of the rate of infection and the parameter estimation, for the stochastic model. In sections 3 and 4 we will introduce all the tools necessary to search for analytical solution of a general stochastic model from the expression of the quantum operators in the Fock space and show how this techniques can be applied to the SIR. In the same section, we have a didactic example for a small number of individuals and the general expression for the analytic solution in terms of the eigenvalues of the Hamilton operator expressing the dynamics in question. Furthermore, we have the comparison between the numeric Fock space approach and the Gillespie stochastic simulation, for different values of the rates of infection. All the complete discussion can be summarized in the section 5. For future work, we intend to adapt these techniques for study of arbovirus models, as shown is the section 5.1. All the computational tools was made in a Maple code and is presented in the Appendix. Beforehand, we can conclude that the new approach of SIR model enables all the statistical work by Kermack and McKendrick to be considered in a simpler way. A subtle difference between this work and (SANTOS; GADÊLHA; GAFFNEY, 2015) is that this new treatment of SIR model in the Fock-space make it possible to find a direct or a recursive formula to the eigenvalues of the Hamiltonian matrix, which could not be found in the work of the enzyme kinetics treatment. Furthermore, the Fock-space method allows as to compute the stochastic basic reproduction number (\mathcal{R}_0) and the mean time of the epidemic as well.

1.1 PETRI NETS

In order to introduce the population dynamics for deterministic models we will use a very important tool commonly adopted, called *Petri Nets*. Petri Net are visual tools used to symbolic representation that help us to simplify the understanding about the dynamic of modeling. It is often used in Chemistry (GOSS; PECCOUD, 1998) and Engineering (GIRAULT; VALK, 2013). Once applied to population models, in Biology, the approach becomes more clear in sense of obtain the deterministic and stochastic differential equations of the model in question. In general, are diagrams with figures and arrows that

helps to model some dynamics behavior from visual tools. We have some examples bellow:

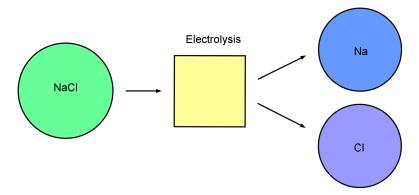


Figure 1: Petri Net model used to show the process of dissociation of Sodium Chloride by electrolysis.

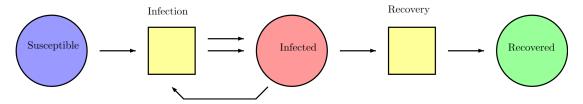


Figure 2: Petri Net model applied in the process of infection and recovery of some species in Biology. This is called SIR model (Susceptible, Infected and Recovered).

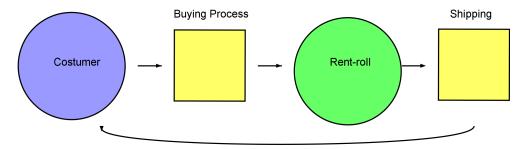
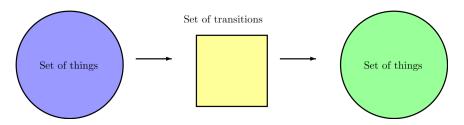


Figure 3: Simplified model of some logistics process.

In general, we will have something like the figure bellow, i.e., we have a set of things as



input that, over a set of actions, becomes a set of other things as output. This set of things will be called *species*, while the set of this actions will be called *transitions*.

Formally, a $Petri\ Net$ is a set of species S and a set of transitions T with a function

$$i: S \times T \to \mathbb{N}$$

that will tell us how many copies of each species appears as *input* for each transition, and a function

$$o: S \times T \to \mathbb{N}$$

that will count how many times they appears as output.

A Stochastic Petri Net is a Petri Net with a fuction

$$r: T \to (0, \infty),$$

where r is a constant rate for each transition. Given a Stochastic Petri Net we are able to obtain a $Rate\ Equation$ and the $Master\ Equation$, that will be discussed in the next sections.

1.2 STOCHASTIC PETRI NET

A Stochastic Petri Net is provided for a set of species and a set of transitions. At first, consider just one transition and k species, $x_1, ..., x_k$, where each species x_i appears m_i times as input and n_i times as output. Suppose also that each transition has a Reaction rate, $r \in (0, \infty)$. Thus, we define the Rate Equation by

$$\frac{dx_i}{dt} = r(n_i - m_i)x_1^{m_1} \cdots x_k^{m_k}.$$
 (1.2.1)

For an example with a transition only, consider the Petri net in the figure 1. We have a dissociation of the sodium chloride (NaCl) in sodium (Na) and chloride (Cl) via electrolysis with reaction rate r. The chemical reaction can be written as

$$NaCl \rightarrow Na^{+} + Cl^{-}$$

Considering the changing rate of sodium, chloride and sodium chloride as $\frac{d[Na]}{dt}$, $\frac{d[Cl]}{dt}$ and $\frac{d[NaCl]}{dt}$, respectively, the rate equation for sodium is given by

$$\frac{d[Na]}{dt} = r(1-0)[Na]^{0}[Cl]^{0}[NaCl]^{1} = r[NaCl].$$

Analogously, we have the rate equations to chloride and sodium chloride as follows

$$\frac{d[Cl]}{dt} = r(1-0)[Na]^{0}[Cl]^{0}[NaCl]^{1} = r[NaCl]$$

$$\frac{d[NaCl]}{dt} = r(0-1)[Na]^{0}[Cl]^{0}[NaCl]^{1} = -r[NaCl].$$

Thus, the rate equation of each species give us the following ODE's system

$$\begin{cases} \frac{d[Na]}{dt} &= r[NaCl] \\ \frac{d[Cl]}{dt} &= r[NaCl] \\ \frac{d[NaCl]}{dt} &= -r[NaCl] \end{cases}$$

Consider now a chemical model with two reactions. The first reaction gives carbon dioxide

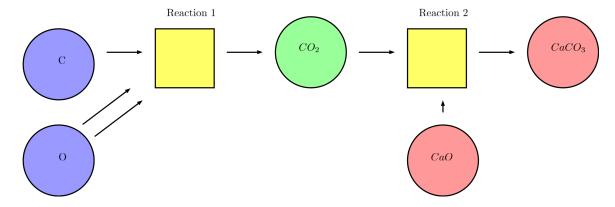


Figure 4: Two chemical reactions represented by a Petri net.

 (CO_2) from Carbon (C) and oxygen (O_2) , while the second reaction between carbon dioxide and calcium oxide (CaO) results in calcium carbonate $(CaCO_3)$. The chemical model is represented by

$$C + O_2 \rightarrow CO_2$$

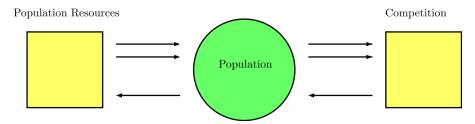
 $CO_2 + CaO \rightarrow CaCO_3.$

Considering the first reaction of the figure 4 has rate α and the second has rate β and each species are represented by $[C],[O],[CO_2],[CaO]$ and $[CaCO_3]$, we are able to obtain the rate equation of each species by the following ODE's sistem:

$$\begin{cases} \frac{d[C]}{dt} &= -\alpha[C][O]^2 \\ \frac{d[O]}{dt} &= -2\alpha[C][O]^2 \end{cases}$$

$$\begin{cases} \frac{d[CO_2]}{dt} &= \alpha[C][O]^2 & -\beta[CO_2][CaO] \\ \frac{d[CaCO_3]}{dt} &= \beta[CO_2][CaO] \end{cases}$$

For a biological example, we have a Petri net modeling the rising of a population due to its natural resources and its decrising due to competition. Considering P as the population



variable, α and β the rate transitions of population resources and competition, respectively. The diagram can be interpreted by

$$P \xrightarrow{\alpha} P + P$$

$$P + P \xrightarrow{\beta} P$$
.

Than its rate equation is written as

$$\frac{dP}{dt} = \alpha P - \beta P^2.$$

This is the Logistic Equation. In general, consider a system with k species. We will use the notation

$$x = (x_1, ..., x_k)$$

to define the vector of species $x_1, x_2, ..., x_i$

$$m = (m_1, ..., m_k)$$

to define the vector of the quantity of elements of each species in input x_i . Analogously, we have

$$n = (n_1, ..., n_k).$$

Also, we will define

$$x^{m} = x_1^{m_1} \cdot x_2^{m_2} \cdot \dots \cdot x_k^{m_k}.$$

Thus, our system of rate equations with constant rate $0 < r < \infty$ can be written as

$$\frac{dx}{dt} = r(n-m)x^m$$

Furthermore, consider T the set of transitions and $r(\tau)$ the rate constant of the transition $\tau \in T$. If $m(\tau)$ and $n(\tau)$ are the input and output vectors of the transition τ then we can write our rate equations of stochastic Petri Net in the form

$$\frac{dx}{dt} = \sum_{\tau \in T} r(\tau)(n(\tau) - m(\tau))x^{m(\tau)}.$$
(1.2.2)

This is the deterministic model for chemical reactions in general. The term for the reaction is proportional to the rate constant $r(\tau)$. Each reaction goes between two complexes, so

we can write it as $m(\tau) \to n(\tau)$. Among chemists the input $m(\tau)$ is called the reactant complex, and the output is called the product complex. The difference $n_i(\tau) - m_i(\tau)$ tells us how many items of species i get created, minus how many get destroyed. So, it's the net amount of this species that gets produced by the reaction τ . The term for the reaction is proportional to this τ . Finally, the law of mass action says that the rate of a reaction is proportional to the product of the concentrations of the species that enter as inputs. More precisely, if we have a reaction τ where the input is the complex $m(\tau)$, then $x^{m(\tau)} = x_1^{m_1(\tau)} \dots x_k^{m_k(\tau)}$. The law of mass action says the term for the reaction is proportional to τ (BAEZ; FONG, 2013). The rate equation in (1.2.2) will be useful to construct the deterministic SI and SIR epidemic models in the next sections. Further, the Petri nets will be crucial to construct the Master equations of the stochastic SIR model from the Hamiltonian built from creation and annihilation operators.

2 EPIDEMIC MODELS

In this section we will treat some known specific epidemic models whose modeling are simple comparing to the reality, but the systematic is enough in order to understanding the population dynamics. At first, in this models, we are considering that every event (contagion, recovery, predation, etc) is always happening, that is, for example, we are not considering that an infection may occur properly just because someone of that species is susceptible. In nature, it does not happens this way. We need to consider the randomness involved. The contagion between individuals may occurs or not according to the circumstances that makes the event probable or not. Otherwise, models that ignores this randomness can be useful to estimate the dynamics involved by a simpler problem, but the approximation to the reality may not be satisfactory. In general, this models are used to express the dynamics of some phenomenal whose actions are well predictable and determined. This kind of model is called deterministic. For example, patients exposed to excessive radiation have a great chance of having its health compromised and the risks are growing larger with the time of exposition. In this case, we can use a deterministic differential equation to model this dynamic. Otherwise, if we are trying to understand the dynamic of contagion between a patient exposed to radiation and another healthy we need to consider that the contact or the intensity of radiation emanated from the infected may not be sufficient to turn the other one sick too. A model that treats this kind of phenomenon are called *stochastic*. The same reasoning is applied to epidemic models in general. Even, sometimes, not being the better way to express its dynamics compared to reality, the study of stochastic processes by a deterministic model can open the mind to a better approach in future. Furthermore, for a large number of population, the deterministic approach may be close to the stochastic dynamics as well. To start our discussion in this section we will pay attention to the Petri net of two classic epidemic models, the SI and SIR, and we will give to them the basic treatment made by (BAILEY et al., 1975).

2.1 DETERMINISTIC SI MODEL

This model can be considered the simplest in epidemiology. We have a population distributed as susceptible (S) and infected or infectious (I), where a susceptible can be infected an infectious over some rate of infection, α . In the simplest deterministic formulation we suppose that the number of individuals are kept constant. In the figure 5 we have the deterministic Petri net used to represent the SI model. Mathematically, we have

$$S + I \xrightarrow{\alpha} 2I,$$
 (2.1.1)

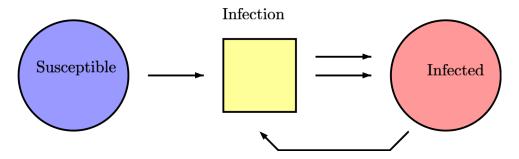


Figure 5: The dynamics of a SI model expressed by a Petri net.

and from this, we have conditions to express our model by

$$\begin{cases}
\frac{dS}{dt} = -\alpha SI \\
\frac{dI}{dt} = \alpha SI
\end{cases}$$
(2.1.2)

Note that the sum of this two differential equations lead us that the population is constant, as we wanted. It is intuitive that if we have a positive number M of total population, then this system must satisfies

$$S + I = M, (2.1.3)$$

and the number of susceptible is decreasing as the infection is rising, respecting some rate of infection α . In fact, we have

$$\frac{dS}{dt} = -\alpha S(M - S),\tag{2.1.4}$$

a Bernoulli's differential equation such that

$$\frac{dW}{dt} - \alpha MW + \alpha = 0, (2.1.5)$$

where W = 1/S. Solving 2.1.5 and considering the initial condition $(S(0), I(0)) = (S_0, I_0)$, we conclude that

$$S(t) = M \left[1 - \frac{1}{1 + (M/I_0 - 1)e^{-\alpha Mt}} \right]$$
 (2.1.6)

and using 2.1,

$$I(t) = \frac{M}{1 + (M/I_0 - 1)e^{-\alpha Mt}},$$
(2.1.7)

where I_0 might be replaced by $M - S_0$. Suppose now that we have M susceptible population and I_0 infected at t = 0, it.e,

$$S + I = M + I_0 (2.1.8)$$

such that $(S(0), I(0)) = (M, I_0)$. The equations 2.1.6 and 2.1.7 will be expressed by

$$\begin{cases}
S(t) = \frac{M(M+I_0)}{M+I_0e^{\alpha(M+I_0)t}} \\
I(t) = \frac{I_0(M+I_0)}{I_0+Me^{-\alpha(M+I_0)t}}
\end{cases} (2.1.9)$$

The product of the equations in 2.1.9 give us a new expression to $\frac{dI}{dt}$, given by

$$\frac{dI}{dt} = \frac{\alpha I_0 M (M + I_0)^2}{(M + I_0 e^{\alpha (M + I_0)t})(I_0 + M e^{-\alpha (M + I_0)t})}$$

$$= \frac{\alpha I_0 M (M + I_0)^2 e^{\alpha (M + I_0)t}}{(M + I_0 e^{\alpha (M + I_0)t})^2}.$$
 (2.1.10)

If we had taken $\tau = \alpha t$, this parameter should have done the α vanishes as we had considered $\alpha = 1$, and this way we have

$$\frac{dI}{d\tau} = \frac{I_0 M (M + I_0)^2 e^{(M+I_0)\tau}}{(M + I_0 e^{(M+I_0)\tau})^2}$$
(2.1.11)

This equation will be called the *epidemic curve*. In particular, considering that the epidemic started with one only infected $(I_0 = 1)$ this formula becomes

$$\frac{dI}{d\tau} = \frac{M(M+1)^2 e^{(M+1)\tau}}{(M+e^{(M+1)\tau})^2}.$$
(2.1.12)

A simple analysis gives us that 2.1.12 has a maximum at $\tau_0 = (\log(M))/(M+1)$. Either, we have $S(\tau_0) = I(\tau_0) = \frac{1}{2}(M+1)$, and clearly $\frac{dI}{d\tau}\big|_{\tau=\tau_0} = \frac{1}{4}(M+1)^2$. For example, taking M=20 we have a epidemic curve of the figure above. In general, it is clear that there is no mathematical difficulty to obtain the analytic results for this model. In (BAILEY et al., 1975), section 5.2 we have easily all the approach made to acquire the comparison between stochastic and deterministic forms. Different from SI model, the approaches made over SIR deterministic model was not sufficient to give all expected results. It is explicit how difficult the modelling becomes by taking one other new variable on SI model. The next sections shows the approach developed by Bailey on SIR deterministic and stochastic models.

2.2 DETERMINISTIC SIR MODEL

This model is also well known from epidemiology (KERMACK; MCKENDRICK, 1927). In this system, we have three categories of individuals: those who are susceptible to disease (S), those who are infected and can spread the disease to susceptible (I), and those who have recovered from previous infection and can no longer spread or catch the disease

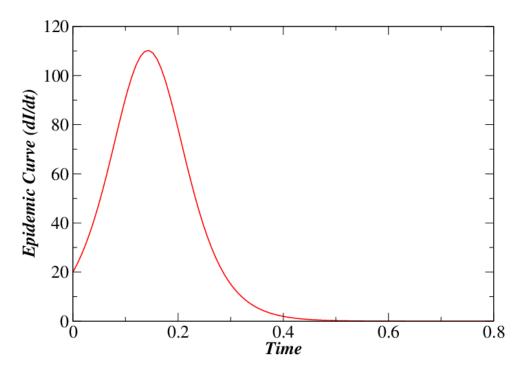


Figure 6: Epidemic curve of the SI model with initial conditions $S_0 = 20$ and $I_0 = 1$.

(R). In this model, we still have a contagion of suceptible from an infected over some rate of infection, just like in the SI model. The difference is on the possibility of an infected becomes recovered of the infection, that we will assume occurring over same recovery rate either. The idea is include one more variable to make this model consistent to its epidemic reality. We still assuming that there are no changing on the total number of population, so this is kept constant. The dynamics can be expressed visually by the following Petri net:

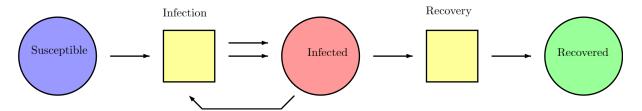


Figure 7: Petri Net model applied in the process of infection and recovery of some species in Biology.

Suppose now that we have an infection and a recovery whose rates are α and β , respectively. As we saw in preview section, this Petri net can be expressed in style of chemical equations as follows:

$$S + I \xrightarrow{\alpha} 2I,$$
$$I \xrightarrow{\beta} R.$$

From that, we are able to express it's dynamic by the rate equations bellow:

$$\begin{cases} \frac{dS}{dt} = -\alpha SI \\ \frac{dI}{dt} = \alpha SI - \beta I \\ \frac{dR}{dt} = \beta I \end{cases}$$
 (2.2.1)

We are supposing the total population is N, *i.e.*,

$$S + I + R = N. (2.2.2)$$

The new variable R tell us the number of cases of immune/recovered or isolated people. It is clear that 2.2.1 satisfies this condition. Furthermore, this model is a generalization of 2.1.2. We can obtain the SI model just supposing that the number of recovered people does not changes as the times goes by. It means that $\frac{dR}{dt} = 0$ and we have all we had before. Even this model seems simple at first, we don't have tools to express an explicit solution to 2.2.1. What we have until then is a way to see the system's behavior just manipulating the equations.

To make our analysis simpler, we will consider $\rho = \frac{\beta}{\alpha}$, the relative removal-rate. At first, we are considering that our population has no one recovered yet, so the initial condition is kind of

$$(S(t_0), I(t_0), R(t_0)) = (S_0, I_0, 0). (2.2.3)$$

Dividing the third equation by the first,

$$\frac{dR}{dS} := \frac{\frac{dR}{dt}}{\frac{dS}{dt}} = -\frac{\rho}{S}.$$
 (2.2.4)

Using 2.2.2 and considering the initial condition 2.2.3, then

$$S = S_0 e^{-\frac{R}{\rho}},\tag{2.2.5}$$

and we can use this on 2.2.2 to express the third equation of 2.2.1 depending only of R. This will lead us

$$\frac{dR}{dt} = \beta \left(N - R - S_0 e^{-\frac{R}{\rho}} \right). \tag{2.2.6}$$

Definitely, solve 2.2.6 is not an easy work. Actually, it may not be possible. An alternative way is express this expression in a series expansion. It is enough to us express it until second order. This way we have

$$\frac{dR}{dt} = \beta \left[N - S_0 + \left(\frac{S_0}{\rho} - 1 \right) R - \frac{S_0 R^2}{2\rho^2} \right]. \tag{2.2.7}$$

That is an example of a *Riccati equation*. To solve this is enough to take a particular solution \bar{R} of 2.2.7 and solve the system

$$\frac{dR}{dt} = -\left[\frac{S_0}{\rho} - 1 + \frac{S_0\bar{R}}{\rho^2}\right] + \frac{S_0}{2\rho^2}.$$
 (2.2.8)

Other standard methods can be applied in 2.2.7 to give us a explicit solution. In (BAILEY et al., 1975), this solution is expressed in the form

$$R(t) = \frac{\rho^2}{S_0} \left[\frac{S_0}{\rho} - 1 + \gamma \tanh\left(\frac{1}{2}\beta\gamma t - \phi\right) \right], \tag{2.2.9}$$

where γ and ϕ are constants given by

$$\gamma = \left\{ \left(\frac{S_0}{\rho} - 1 \right)^2 + \frac{2S_0 I_0}{\rho^2} \right\}^{1/2}, \tag{2.2.10}$$

and

$$\phi = \tanh^{-1} \left(\frac{1}{\gamma} \left[\frac{S_0}{\rho} - 1 \right] \right). \tag{2.2.11}$$

Substituting on 2.2.8 we have easily that

$$\frac{dR}{dt} = \frac{\beta \rho^2 \gamma^2}{2s_0} \operatorname{sech}^2 \left(\frac{1}{2} \beta \gamma t - \phi \right). \tag{2.2.12}$$

This equation will be our *epidemic curve* for the SIR deterministic model.

If we plot a sample graphic of R(t) and $\frac{dR}{dt}$ we will see that, in general, they are S-shaped and a bell-shaped, respectively. The number of infection cases reported has a peak, and than, decreases until vanish. Taking a look at figure 8 we can see that the behavior matches with the rate of recovery growing, once that the rising has a limit, due to population growth being bounded, but, compared to the numerical solution, we see a hard difference of the total number of recovered population after a long time. It means that the approach made in (KERMACK; MCKENDRICK, 1927) by taking an polynomial approximation is sufficient to just show the shape of the curve and model the behavior during a short time from the start of the epidemic. The same can be said about the approximate solution and numerical approximation of the epidemic curve dR/dt, as shown in the figure 9. Returning to equation 2.2.9 and taking $t \longrightarrow \infty$ we can see that R(t) is limited. In fact,

$$R_{\infty} := \lim_{t \to \infty} R(t)$$

$$= \frac{\rho^2}{S_0} \left[\frac{S_0}{\rho} - 1 + \gamma \right]. \tag{2.2.13}$$

This number give us the *total size of epidemic*, *i.e.*, the total number of removals after a long period of time. Considering that $\left(\frac{S_0}{\rho}-1\right)^2 >> \frac{2S_0I_0}{\rho^2}$, and supposing $\gamma \simeq \frac{S_0}{\rho}-1$, than

$$R_{\infty} \simeq \frac{2\rho^2}{S_0} \left[\frac{S_0}{\rho} - 1 \right] = 2\rho \left[1 - \frac{\rho}{S_0} \right]$$
 (2.2.14)

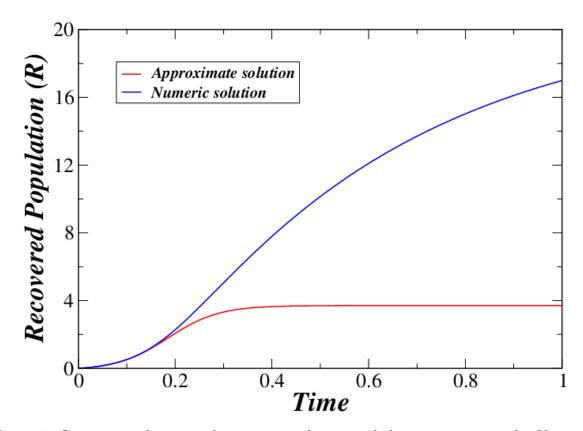


Figure 8: Comparison between the numeric solution and the approximation by Kermark and McKendrick (KERMACK; MCKENDRICK, 1927) of the recovered population R(t), when $S_0 = 20$, $I_0 = 1$, $\alpha = 1$ and $\beta = 2$. In general are S-shaped curves.

Notice that, if $S_0 < \rho$, than R_{∞} is a negative number, so it does not make sense as epidemic model. Suppose $S_0 > \rho$. There is a positive number ϵ such that

$$S_0 = \rho + \epsilon \tag{2.2.15}$$

Using 2.2.15 in 2.2.14 than we conclude

$$R_{\infty} \simeq 2\rho \left[1 - \frac{\rho}{\rho + \epsilon} \right] = 2 \frac{\rho \epsilon}{\rho + \epsilon} = \frac{2\epsilon}{1 - \epsilon/\rho}.$$
 (2.2.16)

Considering ϵ too small comparing to ρ , than

$$R_{\infty} \simeq 2\epsilon.$$
 (2.2.17)

When we say 2.2.15 happens for a small ϵ , than it is reasonable to expect that the initial condition I_0 does not have a significant changing. Let consider S_0^{∞} the final susceptible population after a long time (when $t \longrightarrow \infty$). We still have S + I + R = N.

In this case,

$$S_0^{\infty} + I_0 + 2\epsilon = N, \tag{2.2.18}$$

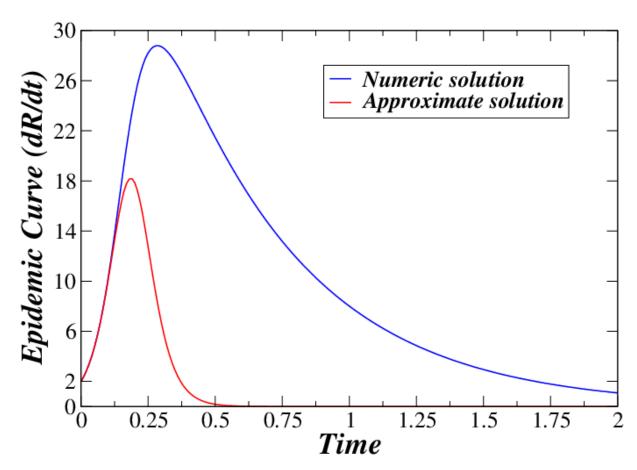


Figure 9: Comparison between the numeric solution and the approximation by Kermark and McKendrick (KERMACK; MCKENDRICK, 1927) of the epidemic curve, dR/dt, when $S_0=20,\ I_0=1,\ \alpha=1$ and $\beta=2$. In general are bell-shaped curves.

but, from the initial conditions,

$$S_0 + I_0 + R_0 = (\rho + \epsilon) + I_0 + 0 = N. \tag{2.2.19}$$

From 2.2.18 and 2.2.19, we conclude that

$$S_0^{\infty} = \rho - \epsilon. \tag{2.2.20}$$

It means that, over the condition 2.2.15, when the initial population of susceptible exceeds ρ the final population is above the threshold, ρ . This phenomenon is the *Kermack* and *McKendrick's Threshold Theorem*. More precisely, defining the *effective reproductive* number as

$$\mathcal{R}_e = S_0/\rho \tag{2.2.21}$$

and the basic reproduction number,

$$\mathcal{R}_0 = N/\rho, \tag{2.2.22}$$

we have that if $\mathcal{R}_e \leq 1$, then the number of infectives decreases monotonically to zero as $t \to \infty$. If $\mathcal{R}_e > 1$, then the number of infectives increases until reach the maximum and decreases to zero as $t \to \infty$. In other words, the infection reaches all the susceptible population if $\mathcal{R}_0 > 1$, or, alternatively, if $N > \rho$. This important result can be easily proved. For the all details, see (WEISS, 2013). Now, will be interesting assume that the rate of infection is no more constant. This next approach was made by Kendall (KENDALL, 1956) and is more precise and elegant. In the case of α is a function of R, the equation 2.2.4 becomes

$$\frac{dR}{dS} = -\frac{\beta}{\alpha(R)} \frac{1}{S}.$$
 (2.2.23)

Performing the separations of variables and integrating, we have a similar equation

$$S = S_0 \exp\left\{ \left(-\frac{1}{\beta} \int_0^R \alpha(u) du \right) \right\}, \tag{2.2.24}$$

then, over the same conditions imposed before,

$$\frac{dR}{dt} = \beta \left[N - R - S_0 \exp\left\{ \left(-\frac{1}{\beta} \int_0^R \alpha(u) du \right) \right\} \right]. \tag{2.2.25}$$

Using this equation it is possible to find an explicit expression for $\alpha(R)$. Substituting $\frac{dR}{dt}$ expressed in 2.2.7 in the expression 2.2.25 we have

$$\exp\left[-\frac{1}{\beta} \int_0^R \alpha(u) du\right] = 1 - \frac{R}{\rho} + \frac{R^2}{2\rho^2},$$
 (2.2.26)

i.e.,

$$\frac{1}{\beta} \int_0^R \alpha(u) du = -\log \left[1 - \frac{R}{\rho} + \frac{R^2}{2\rho^2} \right]$$
 (2.2.27)

Derivating this expression with respect to R, we have

$$\alpha(R) = \beta \left[\frac{1/\rho - R/\rho^2}{1 - R/\rho + R^2/2\rho^2} \right]. \tag{2.2.28}$$

Multiplying the expression before by ρ , we have

$$\alpha(R) = \beta \left[\frac{1 - R/\rho}{\rho - R + R^2/2\rho} \right] \tag{2.2.29}$$

$$= \alpha \left[\frac{1 - R/\rho}{\rho (1 - R/\rho + R^2/2\rho^2)} \right]$$
 (2.2.30)

$$= \alpha \left[\frac{1 - R/\rho}{1 - R/\rho + R^2/2\rho^2} \right]$$
 (2.2.31)

$$= 2\alpha \left[\frac{1 - R/\rho}{2 - 2R/\rho + R^2/2\rho^2} \right]$$
 (2.2.32)

$$= 2\alpha \left[\frac{1 - R/\rho}{\left(1 - R/\rho\right)^2 + 1} \right]. \tag{2.2.33}$$

Dividing this last expression by $1 - R/\rho$ we finally have

$$\alpha(R) = \frac{2\alpha}{(1 - R/\rho) + (1 - R/\rho)^{-1}}.$$
 (2.2.34)

Notice that $\alpha(0) = \alpha$, the same constant originally in the system 2.1.2. Also, we have that $\alpha(R) > 0$ if $0 < R < \rho$ and $\alpha(R) < 0$ if $R > \rho$. This second condition turns the model non realistic, because $\alpha(R)$ needs to be a positive parameter. This approximation by Kermark and McKendrick underestimates the infection rate of the system and the total size of epidemic as well.

Now we will consider the points where $\frac{dR}{dt} = 0$, *i.e.*,

$$N - R - S_0 e^{-\frac{R}{\rho}} = 0. (2.2.35)$$

Taking $F(R) := \frac{dR}{dt}$ restrict to the interval [0, N], we have that $F(0) = \beta \left[N - S_0\right] = 0$, if $N = S_0$ or F(0) > 0, if $N < S_0$. The first case give us clearly a root to 2.2.35. Suppose that the second condition is the only possible. Yet, $F(N) = -S_0 e^{-\frac{N}{\rho}} < 0$. The Intermediate Value Theorem guarantees a positive root η_+ . Repeat the same analysis to the interval $(-\infty, 0]$. There is a negative root to 2.2.35, defined by η_- . Note that $\frac{dF}{dR}$ changes the signal just once, so F(R) has two only roots.

Integrating 2.2.1 we have a formal expression to the time t, given by

$$t = \frac{1}{\beta} \int_0^R \left[N - \tau - S_0 e^{-\frac{\tau}{\rho}} \right]^{-1} d\tau, \tag{2.2.36}$$

for $0 \le R < \eta_+$.

From this expression and 2.2.6 we are able to find a formal solution to the epidemic curve $\frac{dR}{dt}$ by some parametric method. The parameter t runs in the interval $(0, \infty)$ since the integral 2.2.36 diverges when R is near to the root η_+ , and then, $R_{\infty} = \eta_+$. But, unfortunately, the integral also diverges when $S_0 \longrightarrow N$. It means that a infinite times elapses before the epidemic starts.

We have another defy trying to change the initial point to some point which $S_0 = \rho$. This will be called the *centre* of the epidemic. Using the approach we made for $\frac{dR}{dt}$, we will recall the equation

$$\frac{dR}{dt} = \beta(N - R - S). \tag{2.2.37}$$

Differentiating this equation with respect to t and using 2.1.2 we have that

$$\frac{d}{dt} \left(\frac{dR}{dt} \right) = \beta \left(-\frac{dR}{dt} - \frac{dS}{dt} \right)
= \beta \left(-\beta I + \alpha S I \right)
= \beta^2 I \left(\frac{\alpha}{\beta} S - 1 \right)
= \beta^2 I \left(\frac{S}{\rho} - 1 \right).$$
(2.2.38)

It is easy to see that the epidemic has a peak in the centre $S_0 = \rho$. By the third equation of 2.2.1, the number of infected has a maximum at the same time. Considering now that ρ is the initial number of susceptible and that still there is no population recovered as initial conditions, we have that

$$S_0 + I_0 + R_0 = \rho + I_0 = N. (2.2.39)$$

From this, the new expression for $\frac{dR}{dt}$ is given by

$$\frac{dR}{dt} = \beta \left[I_0 - R + \rho (1 - e^{-\frac{R}{\rho}}) \right]. \tag{2.2.40}$$

The importance of this new equation is that we can find explicitly formal expression to t by integrating without caring about its convergence and, this way, having a parametric solution to the number of recovered population, R(t).

Indeed, integrating 2.2.40, we have

$$t = \frac{1}{\beta} \int_0^R \left[I_0 - \tau + \rho (1 - e^{-\frac{\tau}{\rho}}) \right]^{-1} d\tau, \quad -\xi_- < R < \xi_+, \tag{2.2.41}$$

where $-\xi_{-}$ and ξ_{+} are the only negative and positive roots of

$$I_0 - R + \rho(1 - e^{-\frac{R}{\rho}}) = 0. {(2.2.42)}$$

The existence of those roots is guaranteed since we define again $F(R) := \frac{dR}{dt}$ and verify that $F(0) = I_0 > 0$ and $\frac{dF}{dR}$ goes to -1 as $R \longrightarrow \infty$, giving us the only positive root. Also, we have that F(R) goes to $-\infty$ as $R \longrightarrow -\infty$, giving us the other negative root $-\xi_-$. Using this approach we have t a parameter for our equations such that the numerical value of R(t) is the number of removals in the interval (0,t), for t>0 and (t,0) for t<0. Thus, the parametric solution is given by

$$\begin{cases}
t = \frac{1}{\beta} \int_0^R \left[I_0 - \tau + \rho (1 - e^{-\frac{\tau}{\rho}}) \right]^{-1} d\tau \\
\frac{dR}{dt} = \beta \left[I_0 - R + \rho (1 - e^{-\frac{R}{\rho}}) \right]
\end{cases} (2.2.43)$$

where $-\infty < t < \infty$, $-\xi_- < R < \xi_+$ and $-\xi_-,\xi_+$ are the roots of 2.2.42. Thus, from 2.2.43 we have $R_{-\infty} := \lim_{t \to -\infty} R(t) = -\xi_-$ and $R_{\infty} := \lim_{t \to +\infty} R(t) = \xi_+$. This way we are not thinking about an epidemic starting in at initial point, but treating it like an entity running during all the time $-\infty < 0 < \infty$. The numbers $-\xi_-$ and ξ_+ are the number of removals before and after the central point. Thus, $\xi_- + \xi_+$ is the total size of the epidemic for this new approach. Notice that

$$\lim_{t \to -\infty} \frac{dR}{dt} = F(-\xi_{-}) = 0 \tag{2.2.44}$$

and than

$$\lim_{t \to -\infty} I(t) = \frac{1}{\beta} \frac{dR}{dt} = 0. \tag{2.2.45}$$

It says that we do not have infected during a long time before the epidemic starts. Supposing we still have $t \to -\infty$, define as n the total number of susceptible population. We have that

$$n = \rho + I_0 + \xi_-. \tag{2.2.46}$$

This quantity may also be called the total size of the population. We can conclude that, if $t \to -\infty$, than $(S, I, R) \to (n, 0, -\xi_-)$. Either, if $t \to \infty$, we have the quantities $(S, I, R) \to (n - \xi_- - \xi_+, 0, \xi_+)$. Lets define i, the *intensity* of the epidemic, i.e, the proportion of the total number of susceptible that contract the disease. It is given by

$$i = \frac{\xi_- + \xi_+}{n}.$$
 (2.2.47)

Using this equation we can write

$$(S, I, R) = (n - ni, 0, ni - \xi_{-}),$$
 (2.2.48)

when $t \to \infty$. Regarding 2.2.5 and keeping $S_0 = n$ as initial condition and 2.2.48 we have that

$$S = ne^{-(R+\xi_{-})/\rho}, \tag{2.2.49}$$

i.e.,

$$n - n\mathbf{i} = ne^{-n\mathbf{i}/\rho}. (2.2.50)$$

Simplifying this expression we conclude that

$$\frac{n}{\rho} = -\frac{\log(1-i)}{i}.\tag{2.2.51}$$

We are able to show explicit formulations to some constants in terms of the initial condition, when t = 0, i.e.,

$$(S_0, I_0, R_0) = (\rho, I_0, 0). \tag{2.2.52}$$

Using again 2.2.5,

$$\rho = ne^{-\xi_{-}/\rho},\tag{2.2.53}$$

i.e.,

$$\log \frac{n}{\rho} = \frac{\xi_-}{\rho}.\tag{2.2.54}$$

This way we have

$$\xi_{-} = \rho \log \frac{n}{\rho}.\tag{2.2.55}$$

The equation 2.2.47 give us

$$\frac{\xi_{-}}{\xi_{-} + \xi_{+}} = \frac{\rho}{ni} \log \frac{n}{\rho} \tag{2.2.56}$$

and we can express the quantity of infected at t = 0, given by

$$I_0 = n - \rho - \rho \log \frac{n}{\rho},\tag{2.2.57}$$

and then

$$\frac{I_0}{n} = 1 - \frac{\rho}{n} \Big[1 + \log(n/\rho) \Big]. \tag{2.2.58}$$

Finally we are able to know what happens to the ratio of population, $\frac{n}{\rho}$, the percentage of infection at the central epoch, $\frac{I_0}{n}$, and the percentage of removals before central epoch, $\frac{\xi_-}{\xi_- + \xi_+}$, in terms of the intensity of the epidemic, i. Taking the intensity i as a variable, whe can see by 2.2.51 that $\frac{n}{\rho} \to 1$ as i $\to 0$, and then $\frac{I_0}{n} \to 0$ by 2.2.58. We have also that $\frac{\xi_-}{\xi_- + \xi_+} \to \frac{1}{2}$ by 2.2.56. This way, the values of each function at i = 0 can be well defined. The table 1 displays numerically this behavior for the intensity i varying form 0 to around 0.98.

Looking at the table 1 we are able to do our analysis without difficulty. For example, if we take the total size of population n=102 and $\rho=100$ we have a population with ratio $n/\rho=1.05$ and then, an epidemic whose intensity is near to 0.1, i.e, 10% of population has been affected by the disease, and the number of susceptible is reduced about 95. When n/ρ is about 4, we have 50% of population reached by the disease at the central epoch. This techniques adopted in (BAILEY et al., 1975) was the best way to obtain the results of the deterministic model without trying to solve the differential equation or using numeric methods to approximate solutions, that was not possible due to limitations of computational tools until then. The following subsection gives continuity of the Bailey approach (BAILEY et al., 1975) to the SIR stochastic model, whose have such interesting methods as limitations, as in the deterministic model.

2.3 STOCHASTIC SIR MODEL

The previous section evidenced all the difficulty on the treatment about the deterministic version of the SIR model. Even so, the rough approximation in the adopted

Table 1: Epidemic	behavior from	the intensity	(adapted from	table 6.1 of	(BAILEY	et al.,
1975)).						

Intensity	Ratio	Percentage of infected	Percentage of removals
of the	of the population	population	occurring
epidemic	to thershold	at central epoch	before the central epoch
(i)	$\left(\frac{n}{-}\right)$	$\left(\frac{I_0}{n}\right)$	$\left(\underbrace{\xi_{-}}\right)$
	(ρ)		$\left(\xi_{-}+\xi_{+}\right)$
0.00	1.00000	0.0000	50.000
0.05	1.02587	0.0321	49.786
0.10	1.05361	0.1317	49.561
0.15	1.08346	0.3046	49.323
0.20	1.11572	0.5575	49.071
0.25	1.15073	0.8980	48.802
0.30	1.18892	1.3352	48.515
0.35	1.23081	1.8798	48.208
0.40	1.27706	2.5449	47.876
0.45	1.32853	3.3463	47.516
0.50	1.38629	4.3036	47.123
0.55	1.45183	5.4418	46.690
0.60	1.52715	6.7935	46.208
0.65	1.61511	8.4024	45.665
0.70	1.71996	10.329	45.043
0.75	1.84839	12.664	44.314
0.8	2.01180	15.547	43.433
0.85	2.23191	19.223	43.320
0.8	2.55843	24.196	40.797
0.95	3.15340	31.868	38.337
0.98	3.99186	40.272	35.385

methods became the approach less realistic than the expected. In order to obtain a better approach of the dynamics, in this subsection we study the stochastic version of the SIR model. Just like the deterministic model, we still have susceptible S and infected I whose rate of infection and recovering at the time interval Δt are $\alpha SI\Delta t$ and $\beta I\Delta t$, respectively. As before, we are considering that the sum of all population is always a constant number. In this modeling we are considering time intervals sufficiently small to make possible an infection or a recovering at a time. We will define $\omega_{(a,b)\to(c,d)}$ the rate which the number of susceptible and infected are changing from (a,b) to (c,d), respectively. The idea here is consider use the Markov assumption to our approach, i.e., the transitions rate from one state to the other in the interval $(t, t + \Delta t)$ does not depend of the previous time t. Either, we will define $P_{jk}(t)$ as the probability of having j susceptible and k infected population at the time t. Suppose that the total number of susceptible and infected at t = 0 are S_0 and I_0 , respectively. Now, we are able to express the probability of having j susceptible and k infected at the time $t + \Delta t$. Considering that, at each time interval Δt , we may have one individual being infected and/or recovered, than we may have three possible

cases: j+1 susceptible and k-1 infected at the time t, where one susceptible became infected at the time interval $(t, t + \Delta t)$; k+1 infected at the time t, where one infected become recovered at the interval $(t, t + \Delta t)$; no infected and no recovered in the whole interval $(t, t + \Delta t)$. In order to simplify the approach, we will keep the notation $\rho = \beta/\alpha$ and treat the new time as $\tau = \alpha t$, and then $\Delta \tau = \alpha \Delta t$. Thus, we have that

Mathematically,

$$P_{jk}(\tau + \Delta \tau) = \omega_{(j+1,k-1)\to(j,k)} \cdot P_{j+1,k-1}(\tau) + \omega_{(j,k+1)\to(j,k)} \cdot P_{j,k+1}(\tau) + \omega_{(j,k)\to(j,k)} \cdot P_{j,k}(\tau),$$
(2.3.1)

where $\omega_{(j+1,k-1)\to(j,k)}$, $\omega_{(j,k+1)\to(j,k)}$ and $\omega_{(j,k)\to(j,k)}$ are described in the items 1., 2. and 3., respectively. Furthermore,

$$P_{jk}(\tau + \Delta \tau) = (j+1)(k-1)\Delta \tau \cdot P_{j+1,k-1}(\tau)$$

$$+\rho(k+1)\Delta \tau \cdot P_{j,k+1}(\tau)$$

$$+[1-jk\Delta \tau - \rho k\Delta \tau] \cdot P_{jk}(\tau), \qquad (2.3.2)$$

i.e.,

$$\frac{P_{jk}(\tau + \Delta \tau) - P_{jk}(\tau)}{\Delta \tau} = (j+1)(k-1) \cdot P_{j+1,k-1}(\tau)
+ \rho(k+1) \cdot P_{j,k+1}(\tau)
- k(j+\rho) \cdot P_{jk}(\tau).$$
(2.3.3)

From this, taking $\tau \to 0$, we finally have the differential equation

$$\frac{dP_{jk}}{d\tau} = (j+1)(k-1)P_{j+1,k-1} - k(j+\rho)P_{jk} + \rho(k+1)P_{j,k+1}$$
 (2.3.4)

Considering the particular case j = M and k = N we have that the only way of having $(S, I) = (S_0, I_0)$ at the time $\tau + \Delta \tau$ is no one getting recovered or infected, *i.e.*,

$$P_{S_0I_0}(\tau + \Delta \tau) = [1 - S_0I_0\Delta \tau - \rho I_0\Delta \tau] \cdot P_{S_0I_0}(\tau), \qquad (2.3.5)$$

thus, we have the differential equation

$$\frac{dP_{S_0I_0}}{d\tau} = -I_0(S_0 + \rho)P_{S_0I_0}.$$
(2.3.6)

The union of 2.3.4 and 2.3.6 give us

$$\begin{cases}
\frac{dP_{jk}}{d\tau} = (j+1)(k-1)P_{j+1,k-1} - k(j+\rho)P_{jk} + \rho(k+1)P_{j,k+1} \\
\frac{dP_{S_0I_0}}{d\tau} = -I_0(S_0 + \rho)P_{S_0I_0},
\end{cases} (2.3.7)$$

where $0 \le j + k \le S_0 + I_0$, $0 \le j \le S_0$, $0 \le k \le S_0 + I_0$ and $P_{S_0I_0}(0) = 1$, as initial condition. Now, we will introduce the *probability-generating function*, given by

$$P(z, w, \tau) = \sum_{j,k} P_{jk}(\tau) z^j w^k.$$
 (2.3.8)

This equation satisfies the differential equation

$$\frac{dP}{d\tau} = w(w-z)\frac{d^2P}{dzdw} + \rho(1-w)\frac{dP}{dw}$$
(2.3.9)

with initial conditions

$$P(z, w, 0) = z^{S_0} w^{I_0}. (2.3.10)$$

Whe should work on 2.3.7 using the Laplace transform, given by

$$q_{jk}(s) = \int_0^\infty e^{-s\tau} P_{jk}(\tau) d\tau, \qquad (2.3.11)$$

and acquire all the expected results about the explicit formula of P_{jk} and consequently the probability-generating function and total size of epidemic as well. This approach was made by Siskind (SISKIND, 1965), but all the algebra involved and explicit expression adopted turns the approach exhaustive. An alternative approach was made by Gani ((GANI, 1965b),(GANI, 1965a),(GANI, 1967)) and Siskind (SISKIND, 1965), replacing 2.3.9 by

$$P(z, w, \tau) = \sum_{j=0}^{S_0} z^j f_j(w, \tau), \qquad (2.3.12)$$

where

$$f_j(w,\tau) = \sum_{k=0}^{S_0 + I_0 - j} w^k P_{jk}(\tau).$$
 (2.3.13)

Instead using 2.3.13, we should use the Laplace transform at each f_j given by

$$F_j(w,\lambda) = \int_0^\infty e^{-\lambda \tau} f_j(w,\tau) d\tau, \quad Re(\lambda) > 0.$$
 (2.3.14)

Substituting this equations in 2.3.9 we have the system of differential equations

$$\begin{cases}
\lambda F_{j} = w^{2}(j+1)\frac{\partial F_{j+1}}{\partial w} + [(j+\rho)w - \rho]\frac{\partial F_{j}}{\partial w}, 0 \leq j \leq S_{0} - 1 \\
\lambda F_{S_{0}} = w^{I_{0}} - [(S_{0} + \rho)w - \rho]\frac{\partial F_{S_{0}}}{\partial w}.
\end{cases}$$
(2.3.15)

If we write

$$F = \begin{bmatrix} F_{S_0} \\ F_{S_0-1} \\ \vdots \\ F_0 \end{bmatrix}, \tag{2.3.16}$$

$$E = \begin{bmatrix} 1\\0\\\vdots\\0 \end{bmatrix} \tag{2.3.17}$$

and

$$A = \begin{bmatrix} (S_0) + \rho)w - \rho & 0 & 0 & \dots & 0 & 0 \\ -S_0w^2 & (S_0 - 1 + \rho)w - \rho & 0 & \dots & 0 & 0 \\ 0 & -(S_0 - 1)w^2 & (S_0 - 2 + \rho)w - \rho & \dots & 0 & 0 \\ \vdots & \dots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & -2w^2 & \dots & (1 + \rho)w - \rho & 0 \\ 0 & 0 & 0 & \dots & -w^2 & \rho w - \rho \end{bmatrix}$$

$$(2.3.18)$$

we have a matrix formulation of 2.3.15, given by

$$A\frac{\partial F}{\partial w} + \lambda F = w^N E. \tag{2.3.19}$$

This method was made in (GANI, 1967). Using Taylor's Theorem we can write

$$F(w,\lambda) = \sum_{r=0}^{\infty} F^{(r)}(0,\lambda) \frac{w^r}{r!}$$

$$= \sum_{r=0}^{S_0 + I_0} F^{(r)}(0,\lambda) \frac{w^r}{r!}.$$
(2.3.20)

In fact, this series terminates at $r = S_0 + I_0$, because the term $w^{S_0 + I_0}$ has the highest degree, since quantities of P_{jk} 's are limited by the indexes j and k, i.e., $0 \le j + k \le S_0 + I_0$, $0 \le j \le S_0$, $0 \le k \le S_0 + I_0$. In other words, this equation are limited according to the size of population. After some algebra we conclude that the solution of 2.3.19 can be expressed in the form

$$\begin{bmatrix}
F(w,\lambda) \\
\int_0^w F(v,\lambda) dv
\end{bmatrix} = \sum_{i=0}^{I_0 + S_0 + 1} \frac{w^i}{i!} \left\{ \prod_{j=0}^{i-1} B_j \right\} G - \sum_{i=I_0 + 1}^{S_0 + I_0 + 1} \frac{w^i}{i!} \frac{S_0!}{\rho} \left\{ \prod_{j=I_0 + 1}^{i-1} B_j \right\} E,$$
(2.3.21)

where

$$B_{j} \equiv \begin{bmatrix} \frac{1}{\rho} \{ j \mathbf{A}^{(1)}(0) + \lambda \mathbf{I} \} & \frac{j(j-1)}{2\rho} \mathbf{A}^{(2)}(0) \\ \mathbf{I} & \mathbf{O} \end{bmatrix}, \qquad (2.3.22)$$

$$G \equiv \begin{bmatrix} F(0,\lambda) \\ O \end{bmatrix}, \qquad (2.3.23)$$

$$F(0,\lambda) = \left\{ \prod_{j=0}^{S_0 + I_0} \right\}_{S_0 + 1}^{-1} \left[\frac{S_0!}{\rho} \left\{ \prod_{j=I_0 + 1}^{S_0 + I_0} B_j \right\} E \right], \tag{2.3.24}$$

I is an $(S_0 + 1) \times (S_0 + 1)$ unit matrix, **O** is the zero vector or matrix of appropriate dimensions, **E** is a column vector of $2S_0 + 2$ elements of which the first is unity and the rest zero. the suffix $S_0 + 1$ indicates a truncated matrix involving the first $S_0 + 1$ rows and columns only. Conventionally, we will say that

$$\prod_{j=h}^{k} B_{j} = \begin{cases}
I, & h = k+1 \\
B_{k}B_{k-1} \dots B_{h}, & h \leq k,
\end{cases}$$
(2.3.25)

and the matrix multiplications being carried out in the order shown. Is is not difficult to see that the matrix is triangular with non-zero eigenvalues for $Re(\lambda) > 0$. The algorithm becomes quite efficient only if I_0 and S_0 are small. Gani (GANI, 1967) gives an example for $I_0 = 1$ and $S_0 = 1$. In order to obtain explicitly the expressions of each $f_j(w,\tau)$ we must apply the Laplace transforms, and then 2.3.13, 2.3.12, and 2.3.8. This way, we are able to obtain the probability generating function and individual probabilities.

2.3.1 TOTAL SIZE OF EPIDEMIC

As seen, due to the difficult of treating the stochastic SIR system we have an alternative way to obtain useful information about the epidemic in terms of ρ and the initial patients over infection. Recalling the results of the previous section, we are able to define the probability of total size of an epidemic, P_w , *i.e.*, the probability of having w as total number of infected after epidemic, without counting the initial number of infectives. Following Bailey (BAILEY et al., 1975), we have explicitly

$$P_{w} = \lim_{t \to \infty} P_{S_{0}-w,0}(t),$$

$$0 \le w \le S_{0}.$$
(2.3.26)

Analyzing this definition, it is reasonable observe the number of susceptible population left long time after the epidemic, (or making $t \to \infty$). In fact, this results clearly converges due to the exponential terms with negative sings in P_{jk} . In this section, we will follow the approach made by Gani (GANI, 1967) to expand the results about P_w . From the equations 2.3.14, 2.3.13, and 2.3.11, respectively, we have that

$$F_{j}(0,\lambda) = \int_{0}^{\infty} e^{-\lambda \tau} f_{j}(0,\tau) d\tau$$

$$= \int_{0}^{\infty} e^{-\lambda \tau} P_{j0}(0,\tau) d\tau$$

$$= q_{j0}(\lambda). \qquad (2.3.27)$$

Hence, using 2.3.27 and Laplace transform propriety, we see that

$$P_{w} = \lim_{t \to \infty} P_{S_{0}-w,0}$$

$$= \lim_{\lambda \to 0} \lambda q_{S_{0}-w,0}$$

$$= \lim_{\lambda \to 0} \lambda F_{S_{0}-w}(0,\lambda), \qquad (2.3.28)$$

(2.3.29)

for $0 \le w \le S_0$. Considering

$$\mathbf{P} = \begin{bmatrix} P_0 \\ P_1 \\ \vdots \\ P_{S_0} \end{bmatrix}, \tag{2.3.30}$$

and the equations 2.3.28 and 2.3.16 we have

$$\mathbf{P} = \lim_{\lambda \to \infty} F(0, \lambda)$$

$$= S_0! \left\{ \prod_{j=1}^{S_0 + I_0} \mathbf{B}_j(0) \right\}_{S_0 + 1}^{-1} \left\{ \prod_{j=I_0 + 1}^{S_0 + I_0} \mathbf{B}_j(0) \right\}_{S_0 + 1} \mathbf{E}, \qquad (2.3.31)$$

such that

$$B_{j} = \begin{bmatrix} \frac{\lambda}{\rho} & O \\ \rho & I & O \end{bmatrix}, \tag{2.3.32}$$

An alternative way to obtain an expression of P_w was made by Bailey ((BAILEY, 1953a),(BAILEY, 1953b)) and can be consulted according to interest of the reader in (BAILEY et al., 1975), section 6.4, but this method followed by Gani makes the approach easier for large values of total population. In (BAILEY et al., 1975), table 6.2 has some calculated values of P_w as function of ρ and different sizes of population.

2.3.2 ESTIMATION OF PARAMETERS

After getting the probability of the epidemic process we have to concern about the estimation of the parameter ρ . This is an important step on trying to predict the epidemic behavior. For this, is necessary to use a very useful technique from statistics, the *Maximum-likelihood estimation*. The idea here is to find a way of estimate ρ from the number of households that keep touch to the disease. In general, we don't know when a susceptible individual becomes infected and even when becomes recovered. Thus, it is reasonable trying to observe the number of infectives per households after a sufficient long time to have no more infections. The risk is to take a too long time and overlap with a new epidemic outbreak and get confused with to the first one. However, this approach can be easily done by using the P_w 's found in the previous subsection. Suppose we have the data of K households, each containing S_0 susceptible besides the initial case introducing the disease. Let h_w be the number of households with w new cases after the first, for $0 \le w \le S_0$. Then, the *Maximum-likelihood score* of ρ is

$$Sc(\rho) = \sum_{w=0}^{S_0} h_w Sc_w(\rho),$$
 (2.3.33)

where

$$Sc_w(\rho) = \frac{1}{P_w} \frac{\partial P_w}{\partial \rho}.$$
 (2.3.34)

The estimate $\hat{\rho}$ is given by finding a positive root of $Sc(\hat{\rho}) = 0$, while the standard error is given by $(Inf(\rho))^{-1/2}$, where the information $Inf(\rho)$ is approximately

$$Inf(\rho) \approx \frac{Sc(\rho_{-}) - Sc(\rho_{+})}{\rho_{+} - \rho_{-}},$$
 (2.3.35)

where ρ_{-} and ρ_{+} are values sufficiently close to ρ with opposites signs. For instance, suppose we have 93 households that was not reached by the infection, 45 cases of households with one infected and 96 with two infected, tantalizing 234 households in question. By (BAILEY et al., 1975), table 6.2, we can see that the expression of $Sr(\rho)$ for $S_0 = 2$ is given explicitly by

$$Sc(\rho) = \frac{h_0 + 2h_1}{\rho} + 2\frac{h_2}{2\rho + 1} - \frac{2h_1 + 2h_2}{\rho + 1} - \frac{K}{\rho + 2}.$$
 (2.3.36)

Substituting the values given we find that $Sc(\rho) = 93S_0 + 45S_1 + 96S_2$ and $\rho = 1.30936$ is the positive root. Furthermore, Sc(1.29) = 1.22303 and Sc(1.31) = -0.03950, thus Inf = 63.12404 and finally we have the estimation

$$\hat{\rho} = 1.31 \pm 0.13.$$

The table 2 shows the comparison between the real and estimated values of households.

Table 2: Sample of observed and expected numbers for an epidemic in households starting with one infected and reaching at most two individuals, for $\rho = 1.31$.

Number	Number	Probality	Number
of	of households	of	of households
secundary cases	observed	infection	expected
(w)	(h_w)	(P_w)	(KP_w)
0	93	39.6%	92.6
1	45	19.4%	45.5
2	96	41.0%	95.9
Total (K)	234	100%	234.0

2.3.3 STOCHASTIC THRESHOLD THEOREM

As we saw in the subsection 2.2, the control of an epidemic can be estimated from the its intensity and the ratio of infection and recovery. The Kermack and Mckendrick Threshold Theorem was fundamental to predict the epidemic behavior from the initial number of susceptible exposed to infection. We have similar results for stochastic models due to the approach made by Whittle (WHITTLE, 1955) and can also be called the Whittle's Stochastic Threshold Theorem. In his approach, it is considered the treatment for a large number of susceptible population (or total population, N). This way, we have that

the population of infectives can be compared to a birth-and-death process whose rates of birth-and-death are respectively αS_0 and β . The results will be shown at the end of this subsection. For this, consider the *intensity of epidemic*, i. Calling π_i the chance of an epidemic reach at most the proportion i of the S_0 initial susceptible. Then, we have

$$\pi_i(\rho) = \sum_{w=0}^{i \cdot S_0} P_w(\rho),$$
(2.3.37)

where $i = \frac{1}{S_0}, \frac{2}{S_0}, \dots, \frac{S_0-1}{S_0}$ (BAILEY et al., 1975; REINERT, 1992) and all the P_w 's are defined as in the section 2.3 and can be obtained by all the methods presented in (BAILEY et al., 1975), section 6.2. Comparing the chance of a new infection in the interval Δt given by $\alpha SI\Delta t$, as before, with te other two processes whose chance of infection is give by $\alpha S_0 I \Delta t$ and $\alpha S_0 (1-i) I \Delta t$, respectively, we can see that, since the epidemic cannot attain a larger number than $i \cdot S_0$, the true process lies uniformly between the other two, i.e., the probabilities of reach some number of infectives are an intermediate of this other two. This way, the two new procedures can characterize birth-and-death processes whose solutions are known. The next step is consider a process for wich the chance of have a new infection in Δt is $AI\Delta t$, where A can assume the previous values, αS_0 or $\alpha S_0(1-i)$. This way, we are considering a birth-and-death process for the infective population whose constant rates are A and β , respectively. Now, we must restrict to the case in that there are no new births in a cumulative population size, i.e., the total number of infected individuals reaches at most $S_0 + I_0$. Taking $w = u - I_0$, when $t \to \infty$, where u in the cumulative population size, we have the total size of epidemic, as already defined. It is easily seen that so far as epidemic sizes, given by a $S_0 \leq u_\infty \leq S_0 + I_0 - 1$, are concerned, the probabilities for these states of the restricted process are exactly the same as those for the corresponding states in the unrestricted process, for which u may take any value. The balance of probability, to make up a total of unity, is then assigned to the state $u_{\infty} = S_0 + I_0$. We now can obtain the expected results by considering the approach for the unrestricted process and than apply the results to the restriction of population. The entire approach for this birth-and-death process was made by Kendall (KENDALL, 1948), leading us the partial differential equation of the probability-generating function and its initial conditions. The analytic solutions of this differential equation make possible the expression of P_w in terms of β , I_0 and w, given by

$$P_w(A) = \frac{I_0(2w + I_0 - 1)!}{w!(w + I_0)!} \frac{A^w \beta^{w + I_0}}{(A + \beta)^{2w + I_0}},$$
(2.3.38)

for $0 \le w \le S_0 - 1$, and

$$P_{S_0}(A) = 1 - \sum_{w=0}^{S_0 - 1} P_w(A). \tag{2.3.39}$$

The details can be shown in (BAILEY et al., 1975), section 6.5. Finally, substituting the respective values of A we have that the approach lead us to the inequality

$$\sum_{w=0}^{i \cdot S_0} P_w(\alpha S_0) \le \pi_i \le \sum_{w=0}^{i \cdot S_0} P_w(\alpha S_0(1-i)). \tag{2.3.40}$$

Using 2.3.38 and 2.3.39 we can conclude that the sum $\sum_{w=0}^{\infty} P_w(A)$ is convergent by the ratio test. Furthermore,

$$\sum_{w=0}^{\infty} P_w(A) = \left(\frac{A + \beta - |A - \beta|}{2A}\right)^{I_0}$$

$$= \min\{\beta/A, 1\}^{I_0}.$$
(2.3.41)

For a sufficient large number of susceptible, we have π_i close to 2.3.41. Applying the result to 2.3.40 we have

$$\min\{\rho/S_0, 1\}^{I_0} \le \pi_i \le \min\{\rho/S_0(1-i), 1\}^{I_0}, \tag{2.3.42}$$

for S_0 sufficiently large. From 2.3.42 we have three faces to be considered:

If
$$\rho < S_0(1-i)$$
 then $\left(\frac{\rho}{s_0}\right)^{I_0} \le \pi_i \le \left(\frac{\rho}{S_0(1-i)}\right)^{I_0}$; If $S_0(1-i) \le \rho < S_0$, then $\left(\frac{\rho}{S_0}\right) \le \pi_i \le 1$; If $S_0 \le \rho$, then $\pi_i = 1$.

These conditions lead us the interpretation for the probability of the epidemic do not exceed the intensity i is zero, if $\rho \geq S_0$ and $1 - (\rho/S_0)^{I_0}$, if $\rho < S_0$, for small intensity i. This results can also be obtained by using the approach of a random walk, as in (ALLEN, 2008) and lead us

$$Prob\{Have\ an\ outbreak\} \approx \begin{cases} 0, & if \quad \rho \ge S_0 \\ 1 - \left(\frac{\rho}{S_0}\right)^{I_0} & if \quad \rho < S_0 \end{cases}$$
 (2.3.43)

for a sufficiently large S_0 and small I_0 . Usually, we set $I_0 = 1$ and make all the rest of population as susceptible to estimate the epidemic due to the initial infected, called the patient zero. All this approach has similar result compared to the Kermark and McKendrick Threshold theorem, in the deterministic version. Unfortunately, the results, in general, are reasonable since we have a very large population to guaranteeing the values of partial sums closer to the convergence value of 2.3.40. The next sections will be dedicated to construct a new method for SIR stochastic model that turns the approach simpler and more efficient, where will be possible to obtain the same results of this section. Furthermore, we will be able to employ quantum techniques constantly used to study reaction-diffusion systems applied to a Fock-space and make possible the analytic expressions for the epidemic model, besides having the grand result of estimation the mean time and stochastic basic reproduction number (\mathcal{R}_0) of an epidemic in terms of the initial state and the constant

rates, α and β , as will be shown in the next part of this work. For this, we will introduce some notations and results of linear algebra necessary to understand the application of the this quantum techniques.

3 BASICS OF LINEAR ALGEBRA

This section recalls all some important results of linear algebra that will be useful to implement the quantum operators adopted to build our stochastic approach in a Fock space. In this section, we want to introduce Basics of Linear Algebra using Dirac notation, most used by physicists, which will be useful in our approach for finding analytical solutions to the SIR model. We are not concerned with the demonstrations of the results of this section, once that all the algebra linear results can be easily found in any known linear algebra book. For this approach, in special, we adopted (DIRAC, 1981). All we need to recall in this section is the fundamental concepts of vector spaces, orthogonal basis, linear transformations, eigenvalues and characteristic polynomial using the Dirac notation. A linear vector space $\mathbb V$ is a collection of objects called vectors respecting some operations of sum and scalar multiplication. We will denote this vectors by $|1\rangle, |2\rangle, \ldots, |V\rangle, \ldots$, etc. The symbolic representation $|V\rangle$ is called $|V\rangle$ and all $|V\rangle, |W\rangle \in \mathbb V$, $|V\rangle$, scalars, need to satisfy:

- $|V\rangle + |W\rangle \in \mathbb{V}$;
- $a|V\rangle \in \mathbb{V}$;
- $a(|V\rangle + |W\rangle) = a|V\rangle + a|V\rangle;$
- $a(b|V\rangle) = ab|V\rangle$;
- $|V\rangle + |W\rangle = |W\rangle + |V\rangle$;
- $|V\rangle + (|W\rangle + |Z\rangle) = (|V\rangle + |W\rangle) + |Z\rangle;$
- For all vector $|V\rangle \in \mathbb{V}$ there exists an inverse under addition $|-V\rangle$ such that $|V\rangle + |-V\rangle = |0\rangle$.

From this properties we are able to understand that there is a unique null vector $|0\rangle$ satisfying $0 \cdot |V\rangle = |0\rangle$, for all $|V\rangle \in \mathbb{V}$. Furthermore, $-|V\rangle = |-V\rangle$ and the uniqueness of the inverse under addition.

We say that $|W\rangle$ is a linear combination of the vectors $|1\rangle, |2\rangle, \ldots, |n\rangle, \ldots$ if there exists $a_1, a_2, \ldots, a_n, \ldots$ scalars such that $|W\rangle = \sum_i a_i |i\rangle$. In general, the scalars a_i are called the field over which the vector space is defined.

The collection of vectors $|1\rangle, |2\rangle, \dots, |n\rangle, \dots$ is said *linearly independent* if the only linear combination resulting the null vector is the trivial combination, i.e., if $\sum_{i} a_{i} |i\rangle = |0\rangle$, than $a_{i} = 0$ for all i.

If there is a scalar $a_j \neq 0$ such that $\sum_{i=1}^{\infty} a_i |i\rangle = |0\rangle$ whe say that this collection is linearly dependent.

A vector space has dimension n if we have at least n linearly independent vectors. In fact, any vector $|V\rangle$ in a n-dimensional space can be written as a linear combination of n linearly independent vectors $|1\rangle, |2\rangle, \dots, |n\rangle$. This collection is called basis for this n-dimensional vector space and every vector $|V\rangle$ can be expressed uniquely in that basis, i.e, there are unique scalars v_1, v_2, \ldots, v_n such that $|V\rangle = \sum_{i=1}^n v_i |i\rangle$. In this work, we are going to write symbolically a basis that will represent all possible configuration for a possible epidemic involving n individuals.

For example, considering the set of $n \times n$ matrices with real entrances and take

$$|1\rangle = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix}, |2\rangle = \begin{bmatrix} 0 & 1 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix}, \dots, |n^2\rangle = \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}.$$
Than we have

that $|1\rangle, |2\rangle, \ldots, |n^2\rangle$ is a basis to this space and every $n \times n$ matrix $M = [a_{ij}]$ can be expressed by $M = a_{11}|1\rangle + a_{12}|2\rangle + ... + a_{nn}|n^2\rangle$.

3.0.1 THE INNER PRODUCT

Given a vector space defined over a field K, if we are able to define a function $\langle \cdot | \cdot \rangle : \mathbb{V} \times \mathbb{V} \to \mathbb{K}$, satisfying:

- $\bullet \langle V|W\rangle = \langle W|V\rangle^*;$
- $\langle V|V\rangle \ge 0$, $\langle V|V\rangle = 0$ if and only if V = 0; $\langle V|(a|W\rangle + b|Z\rangle)\rangle = a\langle V|W\rangle + b\langle V|W\rangle$,

than we say that \mathbb{V} is a vector space with an inner product, i.e., a inner product space. We may also call scalar product or dot product.

Notice that we did not give a meaning to the symbol * yet, but to make sense in the second item we need to say that $\langle V|V\rangle$ is always a positive real number (or zero). All this rules above defines the linearity in the first entrance. To make some similar in the second entrance we define that

$$\langle aW + bZ|V \rangle = \langle V|aW + bZ \rangle^* = (a\langle V|W \rangle + b\langle V|w \rangle)^*$$
$$= a^* \langle V|W \rangle^* + b^* \langle V|W \rangle^* = a^* \langle W|V \rangle + b^* \langle W|V \rangle,$$
(3.0.1)

whatever * means. For example, in the real case, we have the symmetry in each entrance, so $\langle V|W\rangle = \langle W|V\rangle$. In complex case we need a different condition to make sense the second item. So, * means the complex conjugate.

We say that two vectors are *orthogonal* if their inner product is zero. Also, we will use the notation $|V| = \sqrt{\langle V, V \rangle}$ to define the *norm* of the vector. A set of basis vectors whose norm is one and which are pairwise orthogonal will be called *orthonormal* basis.

Now we are able to define a explicit formula for the inner product between two vector in terms of its components. Given $|V\rangle = \sum_i v_i |i\rangle$ and $|W\rangle = \sum_i w_i |i\rangle$ expressed in a basis, we can use the axioms of inner product to have the following result:

$$\langle V|W\rangle = \sum_{i} \sum_{j} v_{i}^{*} w_{j} \langle i|j\rangle. \tag{3.0.2}$$

Now, it is enough to know the value of $\langle i|j\rangle$, the inner between each basis vector. Of course, it depends of the basis vectors. In fact, it is easy to work over orthonormal basis and we have a theorem (Gram-Schmidt) which guarantees a linear orthonormal basis from any vector basis. Suppose that we already have a orthonormal basis to the vector space. Thus, we have

$$\langle i|j\rangle = \delta_{ij} = \begin{cases} 1 & for \ i=j \\ 0 & for \ i \neq j \end{cases}$$

where δ_{ij} is the Kronecker delta symbol. So, in a orthonormal basis we have

$$\langle V|W\rangle = \sum_{i} v_i^* w_i. \tag{3.0.3}$$

From now on, we will assume that every vector basis is orthonormal. Suppose, as before, $|V\rangle = \sum_{i} v_{i}|i\rangle$ and $|W\rangle = \sum_{i} w_{i}|i\rangle$ are two vectors expressed in a basis. We have a representation of this vectors (in this basis) in a matrix form like column vectors:

$$|V\rangle \rightarrow \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix},$$
 (3.0.4)

$$|W\rangle \to \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}. \tag{3.0.5}$$

We also define

$$\langle V| \rightarrow \left[\begin{array}{cccc} v_1^* & v_2^* & \dots & v_n^* \end{array} \right], \tag{3.0.6}$$

and we will call the symbolic representation $\langle V|$ by bra V. This way, the inner product expressed in 3.0.3 can be written as

$$\langle V|W\rangle = \begin{bmatrix} v_1^* & v_2^* & \dots & v_n^* \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}. \tag{3.0.7}$$

3.0.2 DIRAC NOTATION

We saw in the previous section a way to represent a vector V by $ket\ V\ (|V\rangle,$ a column vector), in an orthonormal basis of a vector space. But, if we want a number generated by an inner product of two vectors, $|V\rangle$ and $|W\rangle$ we need to have a way to represent one of this vector as a row to make sense the matrix product between them and respect all the axioms showed before. In particular, what can we say about $\langle V|W\rangle$ and $\langle W|V\rangle$? What is the relationship between them? To solve this problem we will consider that every $|V\rangle$ in this vector space $\mathbb V$ is associated to another vector $\langle V|$ defined by the transpose conjugate of the vector column $\langle V|$. Of course, $\langle V|$ is a row vector and the vector space generated by all of them will be called the dual space of $\mathbb V$, which notation is $\mathbb V^*$. In this way, the definition of inner product is consistent.

Notice that, by this previous definition, both spaces have the same dimension and we can establish a basis to \mathbb{V}^* given a basis of \mathbb{V} . If $|i\rangle$ is a vector basis to \mathbb{V} , a column vector, we can just take $\langle i|$ to give a vector basis for \mathbb{V}^* . All this representation can be expressed as follows:

$$|V\rangle \leftrightarrow \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \leftrightarrow \begin{bmatrix} v_1^* & v_2^* & \dots & v_n^* \end{bmatrix} \leftrightarrow \langle V|, \tag{3.0.8}$$

where the symbol \leftrightarrow means within a basis. Taking $|V\rangle$ expressed in an orthonormal basis $|i\rangle$, we have again that $|V\rangle = \sum_{i} v_{i}|i\rangle$, so that $v_{j} = \langle j|V\rangle$ and then $|V\rangle = \sum_{i} |i\rangle\langle i|V\rangle$. This way we have that $\langle V| = \sum_{i} \langle i|v_{i}^{*}$ and $v_{i}^{*} = \langle V|j\rangle$, where $|i\rangle$ is a basis to the dual space.

Setting a a constant we have that

$$a|V\rangle \rightarrow \begin{bmatrix} av_1 \\ av_2 \\ \vdots \\ av_n \end{bmatrix} \rightarrow \begin{bmatrix} a^*v_1^* & a^*v_2^* & \dots & a^*v_n^* \end{bmatrix} \rightarrow \langle V|a^*.$$
 (3.0.9)

Using linearity we know that $|aV\rangle = a|V\rangle$. We have a similar rule for bras: $\langle aV| = \langle V|a^*$. This way we have

$$a|V\rangle = b|W\rangle + c|Z\rangle \dots \Leftrightarrow \langle V|a^* = \langle W|b^* + \langle Z|c^* \dots$$
 (3.0.10)

These two equations are said to be *adjoints of each other*, and we are able to obtain both of them just taking the complex conjugate of the respective bra (ket).

We can extend this rules for a general vector $|V\rangle = \sum_{i=1} v_i |i\rangle$. The adjoint of $|V\rangle$ is

$$|V\rangle = \sum_{i=1} \langle i| v_i^*. \tag{3.0.11}$$

Recalling that $v_i = \langle i|V\rangle$ and $v_i^* = \langle V|i\rangle$, it follows that the adjoint of

$$|V\rangle = \sum_{i=1} |i\rangle \langle i| V\rangle \tag{3.0.12}$$

is

$$\langle V| = \sum_{i=1}^{\infty} \langle V|i\rangle \langle i|. \tag{3.0.13}$$

3.0.3 SUBSPACES

Given a vector space \mathbb{V} , a subset of its elements that form a vector space among themselves is called *subspace*. Here, we will assume that the reader is able to understand all about basics of subspaces results and bring them to all results about the previous sections.

3.0.4 LINEAR OPERATORS

An operator Ω is a function defined over a vector space into itself that carries information from a vector $|V\rangle$ to another $|V'\rangle$, represented symbolically by

$$\Omega |V\rangle = |V'\rangle, \qquad (3.0.14)$$

i.e., the operator Ω has transformed the ket $|V\rangle$ into the ket $|V'\rangle$. Operators can act on bras by

$$\langle V' | \Omega = \langle V'' | . \tag{3.0.15}$$

An operator is said *linear* if, for every $|V_i\rangle, |V_j\rangle$ vectors and α, β scalars, the following rules are respected:

- $\Omega \alpha |V_i\rangle = \alpha \Omega |V_i\rangle;$
- $\Omega(\alpha | V_i \rangle + \beta | V_j \rangle) = \alpha \Omega | V_i \rangle + \beta \Omega | V_j \rangle;$
- $\langle V_i | \alpha \Omega = \langle V_i | \Omega \alpha;$
- $(\langle V_i | \alpha + \langle V_j | \beta)\Omega = \alpha \langle V_i | \Omega + \beta \langle V_j | \Omega$. As known from linear operators, given a basis $|1\rangle, |2\rangle, \dots |n\rangle$ for the vector space we have that, if

$$\Omega |i\rangle = |i'\rangle \,, \tag{3.0.16}$$

then for any vector $|V\rangle = \sum v_i |i\rangle$ we have

$$\Omega |V\rangle = \sum_{i} \Omega v_{i} |i\rangle = \sum_{i} v_{i} \Omega |i\rangle = \sum_{i} v_{i} |i'\rangle.$$
 (3.0.17)

The product of two operators can be done as follows:

$$\Lambda\Omega |V\rangle = \Lambda(\Omega |V\rangle) = \Lambda |\Omega V\rangle, \qquad (3.0.18)$$

where $|\Omega V\rangle$ is the vector obtained by the action of Ω on V. In general, the order of action of this operators is important. We define de *commutator* of this two operators by

$$[\Omega, \Lambda] = \Omega \Lambda - \Lambda \Omega. \tag{3.0.19}$$

In general, the commutator is not zero. The *inverse* of an operator Ω is denoted by Ω^{-1} and satisfies

$$\Omega\Omega^{-1} = \Omega^{-1}\Omega = I. \tag{3.0.20}$$

The inverse of a product of two operators satisfies

$$(\Omega\Lambda)^{-1} = \Omega^{-1}\Lambda^{-1}. (3.0.21)$$

From this, we have

$$(\Omega\Lambda)(\Omega\Lambda)^{-1} = (\Omega\Lambda)(\Lambda^{-1}\Omega^{-1}) = \Omega(\Lambda\Lambda^{-1})\Omega^{-1} = \Omega\Omega^{-1} = I. \tag{3.0.22}$$

3.0.5 MATRIX ELEMENT OF LINEAR OPERATORS

From the tools given until now, we are able to express the matrix element of a linear operator in therms of coefficients of a vector expressed in a basis. Taking the results of expressions 3.0.16 and 3.0.17 we have that, when $|i'\rangle$ is known, we mean that its components in the original basis

$$\langle j|i'\rangle = \langle j|\Omega|i\rangle = \Omega_{ji},$$
 (3.0.23)

are known. All the n^2 numbers, Ω_{ji} , are the matrix elements of Ω in this basis. If 3.0.14, then the components of the transformed ket $|V'\rangle$ are expressible in terms of the matrix elements and the components of $|V'\rangle$ are

$$v_i' = \langle i | V' \rangle = \langle i | \Omega | V \rangle = \sum_j v_j \langle i | \Omega | j \rangle = \sum_j \Omega_{ij} v_j, \qquad (3.0.24)$$

or, in the matrix form

$$\begin{bmatrix} v_1' \\ v_2' \\ \vdots \\ v_n' \end{bmatrix} = \begin{bmatrix} \langle 1 | \Omega | 1 \rangle & \dots & \langle 1 | \Omega | n \rangle \\ \vdots & \langle i | \Omega | j \rangle & \vdots \\ \langle n | \Omega | 1 \rangle & \dots & \langle n | \Omega | n \rangle \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$
(3.0.25)

3.0.6 MATRICES AND PRODUCTS OF OPERATORS

Considering, again, the linear operators Ω and Λ , we can express the matrix element of the product operator,

$$(\Omega \Lambda)_{ij} = \langle i | \Omega \Lambda | j \rangle = \langle i | \Omega I \Lambda | j \rangle = \sum_{k} \langle i | \Omega | k \rangle \langle k | \Lambda | j \rangle = \sum_{k} \Omega_{ik} \Lambda_{kj}.$$
 (3.0.26)

3.0.7 EIGENVALUES OF AN LINEAR OPERATOR

Let Ω be a linear operator over a vector space and a nonzero vector ket, $|V\rangle$. We say that the number ω is an eigenvalue of Ω when

$$\Omega |V\rangle = \omega |V\rangle. \tag{3.0.27}$$

If this equation is satisfied we say that $|V\rangle$ is an eigenket. This previous equation can be rewritten as

$$(\Omega - \omega I) |V\rangle = |0\rangle. \tag{3.0.28}$$

We know from results of linear algebra (DIRAC, 1981) that the condition to nonzero eigenvectors is

$$\det(\Omega - \omega I) = 0. \tag{3.0.29}$$

This equation gives us the eigenvalues ω . To find them, consider a basis $\langle i|$. We get that

$$\langle i | \Omega - \omega I | V \rangle = 0, \tag{3.0.30}$$

i.e.,

$$\sum_{j} (\Omega_{ij} - \omega \delta_{ij}) v_j = 0. \tag{3.0.31}$$

Setting the determinant to zero will give us an expression of the form

$$\sum_{m=0}^{n} c_m \omega^m = 0, (3.0.32)$$

where c_m are scalars. This equation is called *characteristic equation* and

$$P^{n}(\omega) = \sum_{m=0}^{n} c_{m} \omega^{m}, \qquad (3.0.33)$$

is called the *characteristic polynomial*.

All this results of linear algebra will be very useful to be applied on the construction of quantum operators in a Fock space, witch will be treated in the next section.

4 FOCK SPACE APPROACH TO EPI-DEMIC MODELS

The Fock space approach has been used recently to represent the interaction of particles by the law of mass-action, whose dynamics is represented from quantum operators. More precisely, the Fock space inherits the structure of Hilbert spaces (YOUNG, 1988; SANTOS; GADELHA; GAFFNEY, 2015) and is an algebraic construction used in quantum mechanics to construct quantum states space of particles. The dynamics involved between particle can be expressed in terms of creation and annihilation operators and identified in a vector space using the Dirac notation, presented in the previous section. In general, this representation can be done even for a infinite number of particles involved, although symbolically we can only achieve a finite number. Other Fock space approaches were used to obtain analytic results about stochastic epidemic models. In (SCHÜTZ; BRANDAUT; TRIMPER, 2008) was possible to obtain the exact solutions for the density population, compared to stochastic simulation algorithms for a large number of individuals. The work in (MONDAINI, 2015) was possible to obtain numeric solutions for the improved SIR model applied to Hepatitis C dynamics population from the moment generating function. The idea is adopt the same techniques applied in the work of chemical reactions as a finite and closed population respecting the dynamic imposed by an epidemic model. Suppose we have a closed distinct population doted of k species N_1, N_2, \cdots, N_k , totaling N individuals, $(i.e.,\sum_{i=1}^{\kappa}N_j=N)$ respecting some kind of interaction τ between them that occurs at rates $r(\tau)$. At each interaction, each species N_j begins with a certain number of individuals, $m_j(\tau)$, and after interaction, results in an updated number, $n_j(\tau)$, of this species.

This dynamics can be described via

$$\sum_{j=1}^{k} m_j N_j(t) \xrightarrow{r(\tau)} \sum_{j=1}^{k} n_j N_j(t) , \qquad (4.0.1)$$

where T is the set of interactions, $\tau \in T$.

Furthermore, the probability of finding the system in a given state

$$\mathbf{N}(t) = (N_1(t), \dots, N_k(t))$$

at time t is denoted by $\mathcal{P}(\mathbf{N}, t)$. Considering $\tau_{\mathbf{N}' \to \mathbf{N}}$ the transition rates in witch the system jumps from the state \mathbf{N}' to \mathbf{N} and a sufficiently small time interval $(t + \Delta t)$ we have clearly that

$$\mathcal{P}(\mathbf{N}, t + \Delta t) = \left[1 - \sum_{\mathbf{N}'} \tau_{\mathbf{N} \to \mathbf{N}'} \Delta t\right] \mathcal{P}(\mathbf{N}, t) + \sum_{\mathbf{N}'} \tau_{\mathbf{N}' \to \mathbf{N}} \mathcal{P}(\mathbf{N}, t) \Delta t + O(\Delta t^2), \quad (4.0.2)$$

or, equivalently,

$$\frac{\mathcal{P}(\mathbf{N}, t + \Delta t) - \mathcal{P}(\mathbf{N}, t)}{\Delta t} = \sum_{\mathbf{N}'} \left[\tau_{\mathbf{N}' \to \mathbf{N}} \mathcal{P}(\mathbf{N}', t) - \tau_{\mathbf{N} \to \mathbf{N}'} \mathcal{P}(\mathbf{N}, t) \right] + O(\Delta t). \tag{4.0.3}$$

Taking $\Delta t \to 0$ we have

$$\frac{\partial \mathcal{P}(\mathbf{N}, t)}{\partial t} = \sum_{\mathbf{N}'} \left[\tau_{\mathbf{N}' \to \mathbf{N}} \mathcal{P}(\mathbf{N}', t) - \tau_{\mathbf{N} \to \mathbf{N}'} \mathcal{P}(\mathbf{N}, t) \right], \tag{4.0.4}$$

where the transition rates, $\tau_{\mathbf{N}'\to\mathbf{N}}$, between the configurations \mathbf{N}' and \mathbf{N} are independent of the time. To start exploiting Fock space tools, a given configuration state of the system is represented in the Fock space by a direct product of the Hilbert space \mathcal{S}_j for each species N_j in the population. Symbolically we have $\mathcal{S}_i = \{1, \ldots, N\}$, where N is the maximal number of individuals and our Fock space is defined by $\mathcal{F} = \mathcal{S}_{N_1} \otimes \ldots \otimes \mathcal{S}_{N_k}$. Hence with $s_j \in \mathcal{S}_j$, a state with s_j individuals from species $N_j \in \{N_1, \ldots, N_k\}$ is an element of the Fock space and can be represented in Dirac's bra-ket notation via $|n\rangle = |s_1 \ldots s_k\rangle$, and is referred to as a pure Fock state, with the set of all pure Fock states providing a basis for the Fock space. With the probability of being in a state \mathbf{N} at time t, from the master equation, $\mathcal{P}(\mathbf{N},t)$, rewritten in the new notation as P(n,t), the stochastic system at time t can be fully characterized by $|\Psi(t)\rangle$, which is defined via the linear summation of pure Fock states

$$|\Psi(t)\rangle := \sum_{n} P(n;t) |n\rangle.$$

We introduce the creation and annihilation operators for each species, which act on the pure Fock states via

$$\gamma_j^{\dagger} | n \rangle = | s_1 \dots (s_j + 1) \dots s_k \rangle$$

$$\gamma_j | n \rangle = s_j | s_1 \dots (s_j - 1) \dots s_k \rangle, \qquad (4.0.5)$$

with linearity determining how γ_j^{\dagger} , and γ_j operate on a general element of the Fock space. It is straightforward to confirm that the commutation rule $[\gamma_j, \gamma_k^{\dagger}] = \delta_{jk}$ is satisfied, whence the Master equation can be recast as a Schrödinger equation, with $i\hbar = 1$,

$$\frac{\partial |\Psi(t)\rangle}{\partial t} = -H(\gamma_1^{\dagger}, \gamma_1, \dots, \gamma_k^{\dagger}, \gamma_k) |\Psi(t)\rangle. \tag{4.0.6}$$

The resulting solution is explicitly given in terms of the quasi-Hamiltonian H

$$|\Psi(t)\rangle = \exp\left(-H(\gamma_1^{\dagger}, \gamma_1, \dots, \gamma_k^{\dagger}, \gamma_k)t\right)|\Psi(0)\rangle.$$
 (4.0.7)

With γ_j^{\dagger} , and γ_j respectively denoting the creation and annihilation operators for the species S_j for the individual populations in (4.0.1), the contribution to the quasi-Hamiltonian, H, from the forward population interaction can be written as (BAEZ; FONG, 2013)

$$H = -\sum_{\tau \in T} r(\tau) \left[\gamma^{\dagger n(\tau)} - \gamma^{\dagger m(\tau)} \right] \gamma^{m(\tau)}. \tag{4.0.8}$$

All this representation is made symbolically in a vector space, and the basis vectors are identified with the possible states on the Fock space. This way, we use symbolic algebra to calculate the matrices representing the general dynamics of the pseudo - Hamiltonian and, using methods of symbolic and numeric linear algebra we can find solutions for the stochastic problem.

4.0.1 FOCK SPACE APPROACH TO SIR STOCHASTIC MODEL

In this subsection, we will restrict the Fock space approach to continue our study of SIR model. It is useful recall the same expression of SIR stochastic model expressed in 2.3.7 which, using Fock space techniques, can be presented easily when written in terms of quantum operators. We will show the explicit Hamiltonian for this epidemic model and compare the symbolic and numerical solutions obtained using the Fock space approach with Gillespie simulations. Furthermore, our approach can open the possibility of new analytical results for the SIR model, like the mean time of an epidemic and a simpler way to obtain the stochastic basic reproduction number, which corresponds to \mathcal{R}_0 in the deterministic version of the SIR model. All the algebraic implementation was made in a Maple code. Taking as reference the model in the previous subsection, the dynamics that rules these three species are

$$S(t) + I(t) \xrightarrow{\alpha} 2I(t)$$
, (4.0.9)

$$I(t) \xrightarrow{\beta} R(t)$$
, (4.0.10)

with constant population

$$S(t) + I(t) + R(t) = N, (4.0.11)$$

as before. The quantum operators can be reformulated as

$$s^{\dagger} |n\rangle = |(s+1) \ i \ r\rangle$$

 $s |n\rangle = s |(s-1) \ i \ r\rangle$, (4.0.12)

$$i^{\dagger} | n \rangle = | s (i+1) r \rangle$$

 $i | n \rangle = i | s (i-1) r \rangle,$ (4.0.13)

$$r^{\dagger} |n\rangle = |s \ i \ (r+1)\rangle$$

 $r |n\rangle = r |s \ i \ (r-1)\rangle$. (4.0.14)

The quasi-Hamiltonian, written in terms of creation and annihilation operators as in Eq. [4.0.14], is given by

$$H = -\alpha((i^{\dagger})^2 - s^{\dagger}i^{\dagger})si - \beta(r^{\dagger} - i^{\dagger})i. \tag{4.0.15}$$

Furthermore, the ket $|sir\rangle$ represents a state with s susceptible, i infected and r recovered people. The Fock Space associated can be write as

$$\mathcal{F} = \mathcal{S} \otimes \mathcal{I} \otimes \mathcal{R}. \tag{4.0.16}$$

In general, a basis for 4.0.16 is constituted by all kets $|s_j i_j r_j\rangle$ with $s_j \in \mathcal{S}, i_j \in \mathcal{I}$, and $r_j \in \mathcal{R}$, respectively such that $s_j + i_j + r_j = N$ are fixed, representing the conservation of

the total number of population. This way, the matrix element of 4.0.15 can be expressed as

$$h_{jk} = -i_k \left(\left(-\delta_{i_j, i_k} \left(\alpha \, s_k + \beta \right) \, \delta_{s_j, s_k} + s_k \, \delta_{s_j, s_k - 1} \alpha \, \delta_{i_j, i_k + 1} \right) \delta_{r_j, r_k} + \beta \, \delta_{s_j, s_k} \delta_{i_j, i_k - 1} \delta_{r_j, r_k + 1} \right). \tag{4.0.17}$$

A general state of the system can be written as

$$|\Psi(t)\rangle = \sum_{s_j, i_j, r_j} P(s_j, i_j, r_j; t) |s_j i_j r_j\rangle,$$
 (4.0.18)

or, alternatively,

$$|\Psi(t)\rangle = \sum_{s_j + i_j + r_j = N} P(s_j, i_j, r_j; t) |s_j i_j r_j\rangle,$$
 (4.0.19)

where $P(s_j, i_j, r_j; t)$ is the probability of the system be found in a state with s_j susceptible, i_j infected and r_j recovered at time t, respectively, while the sum runs over all $\frac{(N+1)(N+2)}{2}$ vectors in the Basis set. Eq. [4.0.19] corresponds to the solution of the Schrodinger's equation

$$|\Psi(t)\rangle = \exp(-Ht) |\Psi(0)\rangle, \qquad (4.0.20)$$

where $|\Psi(0)\rangle$ is the initial condition of the system, corresponding to some vector of the Basis set. The latter further provides a straightforward manner to evaluate all the moments for the system via

$$<\gamma^{l}> = \sum_{s_{j},i_{j},r_{j}} \gamma_{j}^{l} P(s_{j},i_{j},r_{j};t)$$

 $= \sum_{s_{j}+i_{j}+r_{j}=N} \gamma_{j}^{l} P(s_{j},i_{j},r_{j};t),$ (4.0.21)

with l > 0, $\gamma \in \{S, I, R\}$ and $\gamma_j \in \{s_j, i_j, r_j\}$

The characteristic polynomial of H is

$$p(\lambda) = \lambda^{N+1} \prod_{r=1}^{N} p_r(\lambda), \tag{4.0.22}$$

where

$$p_r(\lambda) = \prod_{k=0}^{r-1} (\lambda - \lambda_k^r), \ r = N, (N-1), \dots, 3, \tag{4.0.23}$$

$$p_2(\lambda) = (\lambda - (\alpha + \beta))(\lambda - 2\beta), \ p_1(\lambda) = \lambda - \beta \tag{4.0.24}$$

and

$$\lambda_k^r = a_k^r \cdot \alpha + b_k^r \cdot \beta, \tag{4.0.25}$$

here, a_k^r and b_k^r are indexed sequences with r terms, each one, satisfying the recurrent formulas

$$a_k^r = 3a_{k-1}^r - 3a_{k-2}^r + a_{k-3}^r,$$
 $a_0^r = r - 1,$
 $a_1^r = 2(r - 2),$
 $a_2^r = 3(r - 3),$
(4.0.26)

for r = N, (N - 1), ..., 1 and $0 \le k \le r - 1, N \ge 3$, and

$$b_k^r = b_{k-1}^r + 1,$$

 $b_0^r = 1,$ (4.0.27)

for $r=N,(N-1),\ldots,1$ and $0\leq k\leq r-1$ and $N\geq 1$. The equations 4.0.26 and 4.0.27 can be reformulated as

$$a_k^r = -k^2 + (r-2)k + r - 1, (4.0.28)$$

and

$$b_k^r = k + 1, (4.0.29)$$

both for $r = N, (N - 1), \ldots, 1$ and $0 \le k \le r - 1, N \ge 1$. Here, r is an upper index, not an exponent. In fact, the eigenspace whose eigenvalue is zero has dimension N + 1. This is explained by the fact the vectors in basis set of the form $|(N - j) \ 0 \ j\rangle$, $0 \le j \le N$ generates this space. In order to evaluate $\exp(-Ht)$, we compute the Jordan normal form of H, J_H , a matrix whose order is $\frac{(N+1)(N+2)}{2}$, and write $H = Q.J_H.Q^{-1}$ to find $|\Psi(t)\rangle = Q \exp(-J_H t)Q^{-1} |\Psi(0)\rangle$. Choosing an appropriate basis (i.e, an ordinate basis set whose the firsts N + 1 vectors has null eigenvalues) we are able to find a matrix Q so that the solution can be simplified by

$$\exp(-J_H t) = \begin{bmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{O} & e^{-Dt} \end{bmatrix}, \tag{4.0.30}$$

where **I** is the identity matrix of order N+1, e^{-Dt} is the matrix exponential of -Dt, the matrix of order $\frac{N(N+1)}{2}$ corresponding to the eigenspace whose eigenvalues are all the λ_k^r and **O** are null matrices of appropriated sizes. The expression of J_h in the diagonal form in (4.0.30) is not guaranteed, once that the operator H may not be diagonalizable. For example, taking $\alpha = \beta = 1$ the operator has 1 and 2 as nonzero eigenvalues, but $\{[-1\,1\,0\,0\,0\,0], [1-2\,1\,0\,0\,0]\}$ as eigenspace (a 2-dimentional space, instead of three). Otherwise, the expression in 4.0.30 can be obtained by the Jordan's algorithm. Another efficient alternative way to obtain the analytic results is using Laplace transform, defined via

$$\mathcal{L}[f(t)] := \int_0^\infty f(t)e^{-pt}dt,\tag{4.0.31}$$

and thus we obtain

$$\mathcal{L}[|\Psi(t)\rangle] = (p I_n - H)^{-1} |\Psi(0)\rangle. \tag{4.0.32}$$

Assuming a representation of the Fock-space, and thus the Hamiltonian H, in terms of matrices, $|\Psi(t)\rangle$ can also be written in terms of the inverse Laplace transform

$$|\Psi(t)\rangle = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} dp \ e^{pt} \frac{\operatorname{adj}(p I_n - H) |\Psi(0)\rangle}{\det(p I_n - H)}, \tag{4.0.33}$$

where $\operatorname{adj}(M)$ denotes the adjugate of the matrix M and this integral can be evaluated by a sum of residues indexed by the eigenvalues of H. Following the same steps of Bailey (BAILEY et al., 1975), we can redefine the total size of an epidemic from the exacts solutions. Considering the states whose the number of susceptible are zero, the Probability, P_w , of an epidemic of total size w, not counting the initial quantity of infected, taking the limit when $t \to \infty$ from each row of the vector in the equation 4.0.20 satisfying I = 0. The probability P_w is given by the formula

$$P_{w} = \lim_{t \to \infty} P(S_{0} - w, 0, w; t)$$

$$= \lim_{t \to \infty} \langle S_{0} - w \, 0 \, w | \, e^{-Ht} \, | \Psi(0) \rangle ,$$

$$0 \le w \le S_{0}, \tag{4.0.34}$$

where S_0 is the initial number of susceptible population. Note that P_w changes according to the initial state chosen.

Furthermore, the results about analytic expression give us a way to estimate the mean time of an epidemic, inherited from the approach of the first-passage time problem (GILLESPIE; SEITARIDOU, 2012). Suppose η_0 a state whose number of infectives are zero. The probability of the system does not reach the state η_0 at the time t is given by

$$P(\eta \neq \eta_0, t) = 1 - \sum_{\eta = \eta_0} \langle \eta | e^{-Ht} | \Psi(0) \rangle.$$
 (4.0.35)

Let T be the duration time of the epidemic. The cumulative distribution for this time is given by

$$F(t) = P(\eta = \eta_0, t \le T) = \sum_{n=n_0} \langle \eta | e^{-Ht} | \Psi(0) \rangle, \qquad (4.0.36)$$

and thus, the probability distribution of the random variable T is

$$f(t) = \frac{\partial}{\partial t} \sum_{\eta = \eta_0} \langle \eta | e^{-Ht} | \Psi(0) \rangle$$

$$= \frac{\partial}{\partial t} \sum_{j=0}^{N} \langle N - j 0 j | e^{-Ht} | \Psi(0) \rangle. \qquad (4.0.37)$$

All the moments of the epidemic time can be calculated by the formula

$$\langle T^l \rangle = \int_0^\infty t^l f(t) dt. \tag{4.0.38}$$

Explicitly, we have

$$\langle T^{l} \rangle = \int_{0}^{\infty} t^{l} \frac{\partial}{\partial t} \sum_{j=0}^{N} \langle N - j \, 0 \, j | \, e^{-Ht} \, | \Psi(0) \rangle \, \mathrm{d}t. \tag{4.0.39}$$

We can also introduce the stochastic basic reproduction number, \mathcal{R}_0 , from the results in terms of the mean of susceptible population and its rates of infection and recovery. We

define \mathcal{R}_0 by the mean of the number of infectious due to the first infectious case, called the *patient zero*. Using the braket notation,

$$\mathcal{R}_0 = \langle \# \text{ infectious cases due to patient zero} \rangle.$$
 (4.0.40)

To help our approach, consider z(t) the mean number of infectious cases due to patient zero at time t. The supposed events that can happens in a small space of time Δt are that (A_1) the patient zero does not infect any susceptible at the interval $(t, t + \Delta t)$, (A_2) we have the infection of one susceptible only at this interval or (A_3) more than one. Remember that in our approach we are considering time intervals small enough that there at most one infection in the interval. Considering Y as the number of infected by the patient zero at the interval $(t, t + \Delta t)$ we have that

$$z(t + \Delta t) = \sum_{j=1}^{3} \langle Y; A_j \rangle P(A_j)$$

= $\langle Y; A_1 \rangle P(A_1) + \langle Y; A_2 \rangle P(A_2) + o(\Delta t).$ (4.0.41)

One should add the meaning of this terms is not that bra-ket notation. Analyzing $\langle Y; A_1 \rangle$ we have by the definition

$$\langle Y; A_1 \rangle = z(t). \tag{4.0.42}$$

 $\langle Y; A_2 \rangle$ is simplified by observing that we have one more infected so that

$$\langle Y; A_2 \rangle = \langle \# \text{ of infectives at time } t, +1 \rangle$$

= $\langle \# \text{ of infectives at time } t \rangle + 1$
= $z(t) + 1$, (4.0.43)

where the second equality is possible due to the properties of random variables. The events A_1 , A_2 and A_3 are independents, so we have that

$$P(A_1) + P(A_2) + P(A_3) = P(A_1 \cup A_2 \cup A_3) = 1.$$
(4.0.44)

Thus, it is sufficient to know about one of this probabilities. The probability $P(A_2)$ can be estimated by the law of total probabilities. More specifically, suppose we have j susceptible at the time interval $[t, t + \Delta t]$. The possibility of A_2 depends on the probability of having j susceptible at time t, the probability of the patient zero not be removed at this time and infects some of the j susceptible at the time interval. This last one, obviously, depends directly of the rate of infection and number of susceptible and infected. Denoting $P_1(t)$ the probability of not removing the patient zero at time t we have that

$$P(A_2) = \sum_{j} P(S = j; t) \cdot P_1(t) \cdot \alpha \cdot j \cdot 1 \cdot \Delta t$$

$$= \alpha P_1(t) \Delta t \left(\sum_{j} j P(S = j; t) \right)$$

$$= \alpha P_1(t) \Delta t \langle S(t) \rangle. \tag{4.0.45}$$

The $P_1(t)$ is estimated as follows: On fact, the probability of not having the patient zero removed at time interval $[t, t + \Delta t]$ depends on the probability of not being removed at time t and not removed at the interval $(t, t + \Delta t)$. Explicitly,

$$P_1(t + \Delta t) = P_1(t)(1 - \beta \Delta t),$$
 (4.0.46)

i.e.,

$$\frac{P_1(t + \Delta t) - P_1(t)}{\Delta t} = -\beta P_1(t). \tag{4.0.47}$$

Taking $\Delta t \to 0$ we have

$$\frac{dP_1}{dt} = -\beta P_1,\tag{4.0.48}$$

whose solution for initial condition $P_1(0) = 1$ is trivially

$$P_1(t) = e^{-\beta t}. (4.0.49)$$

Substituting on 4.0.45,

$$P(A_2) = \alpha e^{-\beta t} \langle S(t) \rangle \Delta t, \qquad (4.0.50)$$

and thus,

$$P(A_1) = 1 - \alpha e^{-\beta t} \langle S(t) \rangle \Delta t. \tag{4.0.51}$$

substituting 4.0.42, 4.0.43, 4.0.45 and 4.0.51 on 4.0.41 we have

$$z(t + \Delta t) = \left[1 - \alpha e^{-\beta t} \left\langle S(t) \right\rangle \Delta t\right] z(t) + \alpha e^{-\beta t} \left\langle S(t) \right\rangle \Delta t \left[z(t) + 1\right]. \tag{4.0.52}$$

Expanding and taking $\Delta t \to 0$ we have

$$\frac{dz}{dt} = -\alpha e^{-\beta t} \langle S(t) \rangle z(t) + \alpha e^{-\beta t} \langle S(t) \rangle [z(t) + 1]$$

$$= \alpha e^{-\beta t} \langle S(t) \rangle.$$
(4.0.53)

Considering that the only infected at time t = 0 is the patient zero, we have the initial condition z(0) = 0 and, by integration,

$$z(t) = \alpha \int_0^t e^{-\beta \tau} \langle S(\tau) \rangle d\tau, \qquad (4.0.54)$$

thus, by the initial definition of \mathcal{R}_0 in 4.0.40 we finally have

$$\mathcal{R}_0 = \alpha \int_0^\infty e^{-\beta \tau} \langle S(\tau) \rangle d\tau. \tag{4.0.55}$$

In general, the stochastic basic reproduction number will depend on the parameters α, β and the total size of population, N, once that the mean number of susceptible has this

dependence. The convergence of 4.0.55 is guaranteed because of all the dominant terms in the equation of $\langle S(t) \rangle$ are exponential with negative signs. Clearly, the analytic expression for \mathcal{R}_0 has a direct dependence with the deterministic basic reproduction number, ρ .

To see explicitly example, consider a situation when N=2, where we have one infected as initial condition. By 4.0.11, we have that all possible kets are

$$|1\rangle = |0\,0\,2\rangle \,, \quad |2\rangle = |0\,1\,1\rangle \,, \quad |3\rangle = |0\,2\,0\rangle \,,$$

 $|4\rangle = |1\,0\,1\rangle \,, \quad |5\rangle = |1\,1\,0\rangle \,, \quad |6\rangle = |2\,0\,0\rangle \,.$

Explaining the master equation by Bailey in 2.3.7 we have

$$\begin{cases}
\frac{dP_{00}}{dt} = \rho P_{01} \\
\frac{dP_{01}}{dt} = -\rho P_{01} + 2\rho P_{02} \\
\frac{dP_{02}}{dt} = -2\rho P_{02} + P_{11} \\
\frac{dP_{10}}{dt} = \rho P_{11} \\
\frac{dP_{11}}{dt} = -(1+\rho)P_{11} \\
\frac{dP_{20}}{dt} = 0
\end{cases} (4.0.56)$$

with initial condition $P_{11}(0) = 1$. We can obtain the same expression by the Fock space approach just taking the identifications $\alpha = 1$, $\beta = \rho$, $P_{jk}(t) = P(j, k, N - j - k; t)$ and setting the information in vector form, as in 4.0.6.

The matrix element of the quasi-Hamiltonian is given by $H_{jk} = \langle j | H | k \rangle$, where H is specified in Eq. [4.0.15], allowing its matrix representation to be written as

$$H = \begin{bmatrix} 0 & -\beta & 0 & 0 & 0 & 0 \\ 0 & \beta & -2\beta & 0 & 0 & 0 \\ 0 & 0 & 2\beta & 0 & -\alpha & 0 \\ 0 & 0 & 0 & 0 & -\beta & 0 \\ 0 & 0 & 0 & 0 & \alpha + \beta & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$
(4.0.57)

The general solution is $|\Psi(t)\rangle = \exp(-Ht) |\Psi(0)\rangle$, where $|\Psi(0)\rangle = |5\rangle$, while the characteristic polynomial of H is

$$p(\lambda) = \lambda^{3}(\lambda - (\alpha + \beta))(\lambda - 2\beta)(\lambda - \beta)$$
(4.0.58)

Since $\beta/\alpha \neq 1$, the matrix Q represents the changing basis to the basis of eigenvectors,

that can be expressed in the form

$$Q = \begin{bmatrix} 0 & 0 & 1 & 1 & -1 & -2 \frac{\beta^2}{(\alpha - \beta)(\alpha + \beta)} \\ 0 & 0 & 0 & -2 & 1 & 2 \frac{\beta}{\alpha - \beta} \\ 0 & 0 & 0 & 1 & 0 & -\frac{\alpha}{\alpha - \beta} \\ 0 & 1 & 0 & 0 & 0 & -\frac{\beta}{\alpha + \beta} \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{4.0.59}$$

where the firsts 3 vector basis are $|1\rangle$, $|4\rangle$ and $|6\rangle$, the vectors whose eingenvalues are zero. The remaining eigenvectors can be found by known algebra techniques. This way, it is possible to write $H = Q.J_H.Q^{-1}$ to find $|\Psi(t)\rangle = Q \exp(-J_H t)Q^{-1} |\Psi(0)\rangle$, since

$$\exp(-J_H) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-2\beta} & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-\beta} & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-(\alpha+\beta)} \end{bmatrix}, \tag{4.0.60}$$

where J_H is a 6 by 6 matrix whose diagonal is the eigenvalues of H. With the information embedded in the above matrices, an analytical expression for $|\Psi(t)\rangle$ can be readily determined

$$|\Psi(t)\rangle = P(0,0,2;t) |1\rangle + P(0,1,1;t) |2\rangle + P(0,2,0;t) |3\rangle +P(1,0,1;t) |4\rangle + P(1,1,0;t) |5\rangle + P(2,0,0;t) |6\rangle,$$
(4.0.61)

where P(0,0,2;t), P(1,1,0;t), P(0,2,0;t), P(1,0,1;t), P(1,1,0;t) and P(0,0,2;t) are given by Eqs. [4.0.62]–[4.0.73], respectively.

$$P(0,0,2;t) = \frac{e^{-2\beta t}\alpha^2 + e^{-2\beta t}\alpha \beta - 2e^{-\beta t}\alpha^2 + 2e^{-\beta t}\beta^2}{\alpha^2 - \beta^2} - 2\frac{e^{-(\alpha+\beta)t}\beta^2 + \alpha^2 - \alpha \beta}{\alpha^2 - \beta^2}$$
(4.0.62)

$$P(0,1,1;t) = 2 \frac{-e^{-2\beta t}\alpha + e^{-\beta t}\alpha - e^{-\beta t}\beta + e^{-(\alpha+\beta)t}\beta}{\alpha - \beta}$$
(4.0.63)

$$P(0,2,0;t) = \frac{\alpha \left(-e^{-(\alpha+\beta)t} + e^{-2\beta t} \right)}{\alpha - \beta}$$
 (4.0.64)

$$P(1,0,1;t) = \frac{\beta \left(1 - e^{-(\alpha+\beta)t}\right)}{\alpha + \beta}$$
 (4.0.65)

$$P(1, 1, 0; t) = e^{-(\alpha + \beta)t}$$
(4.0.66)

$$P(2,0,0;t) = 0, (4.0.67)$$

for $\alpha \neq \beta$ and

$$P(0,0,2;t) = e^{-2\beta t} \beta t + 3/2 e^{-2\beta t} - 2 e^{-\beta t} + 1/2$$
(4.0.68)

$$P(0, 1, 1; t) = -2 e^{-2\beta t} \beta t - 2 e^{-2\beta t} + 2 e^{-\beta t}$$
(4.0.69)

$$P(0,2,0;t) = e^{-2\beta t} \beta t$$
 (4.0.70)

$$P(1,0,1;t) = -1/2 e^{-2\beta t} + 1/2$$
(4.0.71)

$$P(1,1,0;t) = e^{-2\beta t}$$
(4.0.72)

$$P(2,0,0;t) = 0, (4.0.73)$$

for $\alpha = \beta$. In particular, for this simple case of two total individuals, we have

$$\langle S^{l} \rangle = P(1,0,1;t) + P(1,1,0;t) + 2^{l}P(2,0,0;t),$$

 $\langle I^{l} \rangle = P(0,1,1;t) + 2^{l}P(0,2,0;t) + P(1,1,0;t),$
 $\langle R^{l} \rangle = 2^{l}P(0,0,2;t) + P(0,1,1;t) + P(1,0,1;t),$ (4.0.74)

for l > 0, $l \in \mathbb{N}$. The P_w 's are given in terms of α and β by

$$P_0 = \frac{\beta}{\alpha + \beta},\tag{4.0.75}$$

$$P_1 = \frac{\alpha}{\alpha + \beta}.\tag{4.0.76}$$

The same analytic results obtained here can be compared to (BAILEY et al., 1975) (table 6.2, section 6.4) by taking $\alpha = 1$ and $\beta = \rho$. This way, we can obtain the parameter

estimation as well, using the likelihood function score in 2.3.33. The figure 10 shows the probability distribution according to the different values of ρ and a fixed population N=35, whose just one is infected and is starting the epidemic. Due to computational limitation, we were not able to obtain the analytic expression for the P_w for large sizes. All the calculus was made numerically, taking an accuracy of 6 digits and taking a very large time ($t=10^{11}$), that still a good approximation to the real values. By simple analysis, we can observe that the probabilities of having an epidemic involving a large number of infection increases the smaller ρ is. Large values of ρ revels lower probability of reaching a large number of infectives.

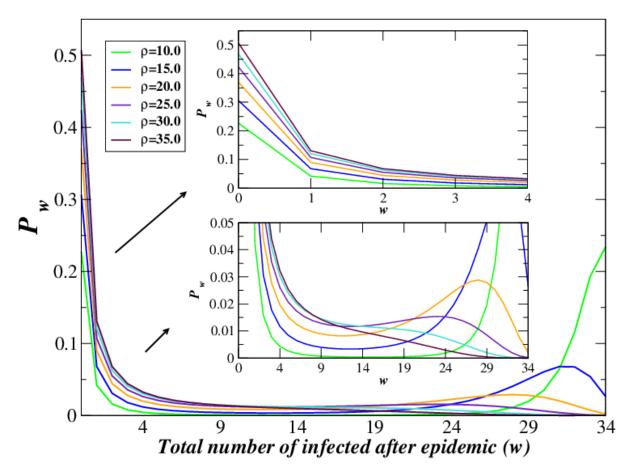


Figure 10: Probability of the final total size of the epidemic for 34 susceptible starting from one infected.

Using 4.0.75 and 4.0.76 we can calculate the mean time of epidemic and the stochastic \mathcal{R}_0 for 2 individuals, one infected as initial condition. It is given by

$$\langle T \rangle = \frac{1}{2\beta (\alpha^2 - \beta^2)} \lim_{t \to \infty} \left[2 \frac{\alpha^2 \beta t}{(e^{\beta t})^2} + 2 \frac{\alpha \beta^2 t}{(e^{\beta t})^2} - 4 \frac{\alpha^2 \beta t}{e^{\beta t}} + 4 \frac{\beta^2}{e^{\beta t}} - 2 \frac{\beta^2}{e^{\alpha t} e^{\beta t}} + 3 \alpha^2 - \alpha \beta - 2 \beta^2 \right],$$

$$(4.0.77)$$

or, explicitly,

$$\langle T \rangle = \frac{3\alpha + 2\beta}{2\beta(\alpha + \beta)},$$
 (4.0.78)

both formulas valid since $\alpha \neq \beta$. If $\alpha = \beta$ then

$$\langle T \rangle = -1/4 \frac{1}{\beta} \lim_{t \to \infty} \left[-4 \frac{\beta^2 t^2}{(e^{\beta t})^2} + 8 \frac{\beta t}{e^{\beta t}} - 6 \frac{\beta t}{(e^{\beta t})^2} + 8 \left(e^{\beta t} \right)^{-1} - 3 \left(e^{\beta t} \right)^{-2} - 5 \right], \tag{4.0.79}$$

i.e.,

$$\langle T \rangle = \frac{5}{4\beta}.\tag{4.0.80}$$

Table 3: Mean time of epidemic for different sizes of population, in fuction of α and β . Here, is considered one infected as initial condition.

Number	Mean time		
of	of		
Individuals	epidemic		
(N)	$(\langle T angle)$		
1	$\frac{1}{eta}$		
2	$rac{3lpha{+}2eta}{2eta(lpha{+}eta)}$		
3	$\frac{11\alpha^3 + 26\alpha^2\beta + 15\alpha\beta^2 + 3\beta^3}{2\beta(2\alpha^3 + 5\alpha^2\beta + 4\alpha\beta^2 + \beta^3)}$		
4	$\frac{50\alpha^{6} + 213\beta\alpha^{5} + 361\alpha^{4}\beta^{2} + 282\alpha^{3}\beta^{3} + 111\alpha^{2}\beta^{4} + 23\alpha\beta^{5} + 2\beta^{6}}{2\beta(12\alpha^{6} + 52\beta\alpha^{5} + 91\alpha^{4}\beta^{2} + 82\alpha^{3}\beta^{3} + 40\alpha^{2}\beta^{4} + 10\alpha\beta^{5} + \beta^{6})}$		
5	$\frac{3288\alpha^{10} + 20948\beta\alpha^{9} + 58424\alpha^{8}\beta^{2} + 93578\alpha^{7}\beta^{3} + 92475\alpha^{6}\beta^{4} + 58110\alpha^{5}\beta^{5} + 23659\alpha^{4}\beta^{6} + 6310\alpha^{3}\beta^{7} + 1085\alpha^{2}\beta^{8} + 110\alpha^{5}\beta^{5} + 23659\alpha^{4}\beta^{6} + 8310\alpha^{3}\beta^{7} + 1085\alpha^{2}\beta^{8} + 110\alpha^{5}\beta^{5} + 2835\alpha^{4}\beta^{6} + 882\alpha^{3}\beta^{7} + 175\alpha^{2}\beta^{8} + 20\alpha^{3}\beta^{7} + 1085\alpha^{2}\beta^{8} + 1085\alpha^{2}\beta^{8$		

Using the equation 4.0.55 we have

$$\mathcal{R}_{0} = \alpha \lim_{\tau \to \infty} -\frac{e^{-\alpha \tau - \beta \tau} e^{-\beta \tau} \alpha + e^{-\beta \tau} \alpha + 2\beta e^{-\beta \tau} - 2\alpha - 2\beta}{(\alpha + 2\beta)(\alpha + \beta)},$$
(4.0.81)

or, explicitly

$$\mathcal{R}_0 = \frac{2\,\alpha}{\alpha + 2\,\beta}.\tag{4.0.82}$$

The tables 3 and 4 shows the Mean time of the epidemic and \mathcal{R}_0 , respectively, for $N \in \{1, 2, 3, 4, 5\}$. Considering $\alpha = \lambda \beta$ it is possible to understand the dynamics of infection from the patient zero and the duration of the epidemic for different sizes of population, as shown in the figure 11.

Table 4: Stochastic basic reproduction number for different sizes of population, in fuction of α and β .

Number	Stochastic	
of	basic reproduction	
Individuals	number	
(N)	(\mathcal{R}_0)	
1	0	
2	$rac{2lpha}{2eta+lpha}$	
3	$\frac{\alpha \left(5 \alpha^2 + 20 \beta \alpha + 12 \beta^2\right)}{2 \alpha^3 + 9 \beta \alpha^2 + 13 \beta^2 \alpha + 6 \beta^3}$	
4	$\frac{6\alpha \left(34 \alpha ^5+232 \beta \alpha ^4+628 \beta ^2 \alpha ^3+739 \beta ^3 \alpha ^2+378 \beta ^4 \alpha +72 \beta ^5\right)}{72 \alpha ^6+522 \alpha ^5 \beta +1531 \alpha ^4 \beta ^2+2325 \alpha ^3 \beta ^3+1928 \alpha ^2 \beta ^4+828 \alpha \beta ^5+144 \beta ^6}$	
5	$\frac{2\alpha \left(1776 \alpha ^8+16244 \alpha ^7 \beta +63580 \alpha ^6 \beta ^2+139751 \alpha ^5 \beta ^3+181371 \alpha ^4 \beta ^4+138806 \alpha ^3 \beta ^5+61076 \alpha ^2 \beta ^6+14472 \alpha \beta ^7+1440 \beta ^8\right)}{1152 \alpha ^9+10944 \alpha ^8 \beta +45016 \alpha ^7 \beta ^2+105204 \beta ^3 \alpha ^6+153902 \alpha ^5 \beta ^4+146111 \beta ^5 \alpha ^4+90009 \alpha ^3 \beta ^6+34696 \beta ^7 \alpha ^2+7596 \alpha \beta ^8+720}$	

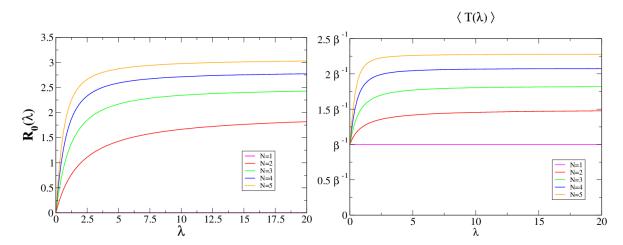


Figure 11: Graphs of the stochastic basic reproduction number (\mathcal{R}_0) and the mean time of epidemic in terms of λ (for fixed values of β), for different sizes of population.

Even being a powerful tool in terms of explaining all the algebraic results in a simple way, our Maple code was not optimized do express analytic results to large populations, once that the internal computational methods of calculating $\exp(-Ht)$ may not be efficient. Furthermore, our hardware limitations did not allow us to compute numeric results in a acceptable time processing. Perhaps, the actual method can be improved from computational techniques that uses known results of sparse matrices (MOLER; LOAN, 1978). Even so, the actual numerical method via Fock space make possible to express graph results to the approach. Some of this results was compared to useful stochastic simulation algorithm (ERBAN; CHAPMAN; MAINI, 2007).

The figure 12 shows an example of the epidemic graph starting with one infected for N=35, $\alpha=1.0$ and $\beta=5.0$. The graph was plotted using the same technique adopted by the approach in the Fock-space, but was obtained numerically due to hardware limitations, and then, the excessive time of expressing an analytic formula.

In this case, the rate $\beta=5.0$ was enough to give a power of infection around 86% of all population. It can be seen by analyzing the total number on recovered population at the end of epidemic or looking at the remaining susceptible population, which is around 15% of the initial susceptible population. The centre of the epidemic occurs right after the initial condition for the epidemic. Considering the time scale in weeks, this graph shows that we have the biggest number of infected in a single day after starting the epidemic.

4.0.1.1 THE SIR STOCHASTIC SIMULATION

To compare the obtained results about the epidemic model we adopted the Gillespie's first reaction method, described as follows:

• Set
$$t = 0$$
, $S(0) = S_0$, $I(0) = I_0$, $R(0) = R_0$;

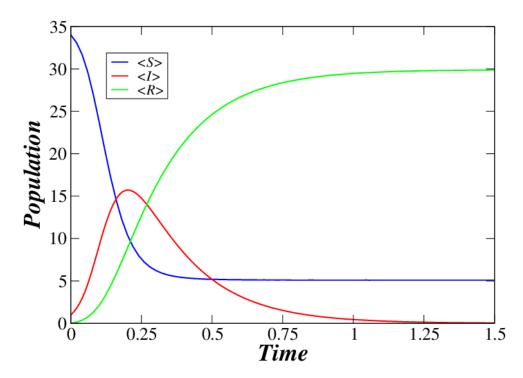


Figure 12: A sample of the SIR dynamic population.

- Generate $r_1, r_2 \in (0, 1)$ two random variables uniformly distributed;
- Calculate the propensities: $\alpha_1 = \alpha S(t)I(t)$, $\alpha_2 = \beta I(t)$, $\alpha_0 = \alpha_1 + \alpha_2$;
- Take $\tau = 1/\alpha_0 \log(1/r_1)$;
- Update the time: $t + \tau$;
- Update the population:

$$S(t+\tau) = \begin{cases} S(t) - 1, & if \quad r_2 \ge \alpha_1/\alpha_0 \\ S(t), & if \quad r_2 < \alpha_1/\alpha_0 \end{cases},$$

$$I(t+\tau) = \begin{cases} I(t) + 1, & if \quad r_2 \ge \alpha_1/\alpha_0 \\ I(t) - 1, & if \quad r_2 < \alpha_1/\alpha_0 \end{cases},$$

$$R(t+\tau) = \begin{cases} R(t), & if \ r_2 \ge \alpha_1/\alpha_0 \\ R(t) + 1, & if \ r_2 < \alpha_1/\alpha_0 \end{cases};$$

• Repeat steps 2-6 until some stop command.

Alternative ways of building stochastic algorithms can be found in (ERBAN; CHAPMAN; MAINI, 2007; TAHERKHANI; PARSAFAR; RAHIMITABAR, 2006). Notice that the manual construction of this algorithm needs caution to avoid bugs and errors when the number of infectives vanishes, once that we have a division by zero in the 4th step. A efficient simulation software, Cain, is provided by Sean Mauch (MAUCH; STALZER, 2011) and available in the link (MAUCH,).

Bellow, the figures 13,14 and 15 show a sample of 10 experiments for N=35, $\alpha=1.0$ and $\beta=5.0$, for each population.

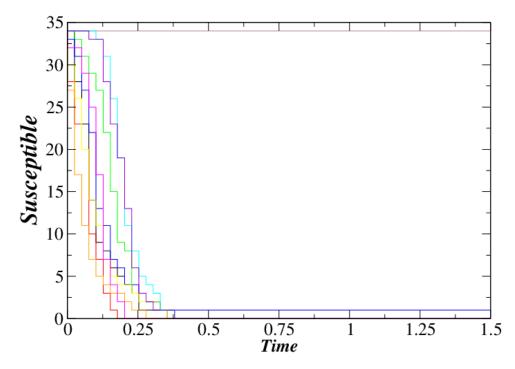


Figure 13: Stochastic simulation of susceptible population for $N=35,~\alpha=1.0$ and $\beta=5.0.$

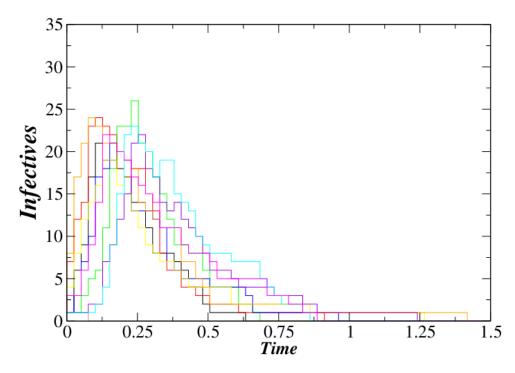


Figure 14: Stochastic simulation of infective population for $N=35, \, \alpha=1.0$ and $\beta=5.0$.

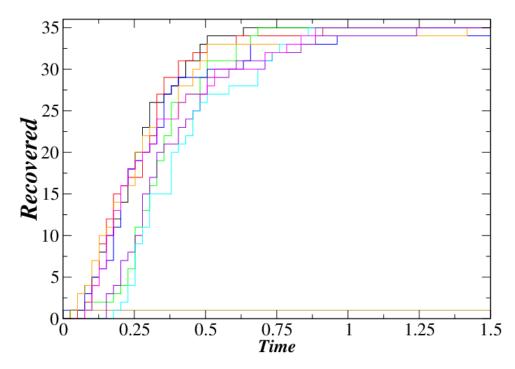


Figure 15: Stochastic simulation of recovered population for $N=35, \alpha=1.0$ and $\beta=5.0$.

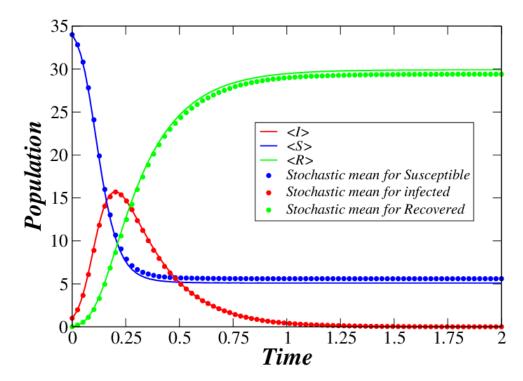


Figure 16: Numeric solution via Fock space approach versus the mean of stochastic simulations, for $N=35, S_0=34, I_0=1, \alpha=1.0$ and $\beta=5.0$.

Bellow, in the figures 16 and 17 we have the comparison between the numeric solutions using the Fock space approach and the mean of 500 experiments realized by Cain software, using the direct method of Gillespie stochastic simulation algorithm, 80 frames and allowed 80 max steps in a single trajectory. Without loss of generality, we can fix $\alpha = 1.0$ for different values of β , so that $\rho = \beta$ and thus is possible to see the difference between the epidemic peak for various values of ρ .

Infected populations as function of time

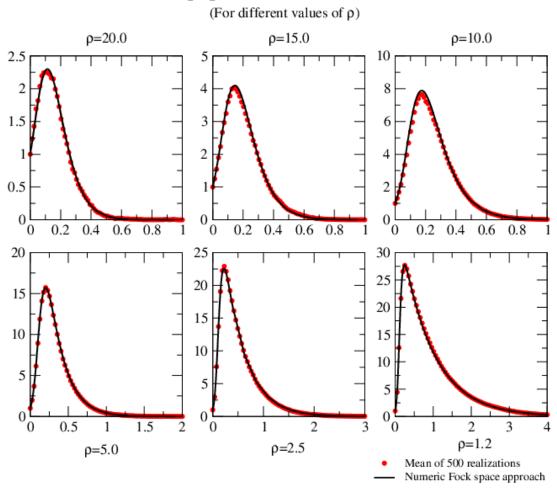


Figure 17: Different epidemic curves in function of time.

It is clear by the figure 17 that the exacts solutions for infectives are good approach to the mean of this realizations, no matter the values of ρ . The variation of this values represents graphically a changing of the power and duration of epidemic. More precisely, the number of infected and total time of epidemic are increasing as the values of ρ decays.

5 DISCUSSION

We introduced quantum mechanical techniques to study an important stochastic epidemic model which serves as gateway to other models in epidemiology that still can benefit from several analytic treatments to make its understanding reasonable. Using an approach equivalent to (SANTOS; GADÊLHA; GAFFNEY, 2015), we made possible a deeper and easier understanding of the stochastic SIR model. Analyzing the problem via Master equations was a way to re-obtain the results found by Kermarck and McKendrick (KERMACK; MCKENDRICK, 1927), without the necessity of using several tools and techniques adopted in (BAILEY et al., 1975), besides having the analytic expressions of the stochastic model, one of the main objectives of this work. Yet, by using the Fock space representation, the calculus of the total size of epidemic now can be obtained from the analytic solution, just as in the definition in Eq.(10), by taking the limits of solutions corresponding to the states whose infected are zero, in analogy with a first exit time problem.

Furthermore, the Fock-space approach implemented on Maple software made possible to express the analytic solution for a small number individuals, besides having an explicit symbolic process to express a recursive formula for the eigenvalues, for $N \geq 3$, and a direct formula for all natural number N, which can be verified in the Appendix.

We also pointed out that the full general expression of the eigenvalues of the Hamiltonian presented in this work can be used as a strategy to get the analytic solution to the stochastic model using Laplace transform, presented in (SANTOS; GADÊLHA; GAFFNEY, 2015) and can be an alternative to the Fock-space method, for computing $\exp(-Ht)$.

One efficient strategy, given that we had control of the solution for small sizes of the system, was to analyze the general form of the eigenvalues as a function of the size of the system. We noticed a recurrence relation between the eigenvalues for a immediately smaller population (N-1) and the current population (N). In fact, the sequence if eigenvalues found for a fixed population of size N contains all the terms of a population size N-1 plus an extra number of eigenvalues. This results imply that the set of eigenvalues of the Hamiltonian for a big sized population carries the mathematical information of the eigenvalues from populations of smaller sizes recursively, as explained in section 4.0.1.

Although we analyzed a classical epidemic model, this alternative approach allow us to compute analytically new results for the SIR model, in particular for the mean time prediction for the duration of an epidemic. This result becomes a powerful tool, since coupled to its biological parameters, and can be easily obtained from the matrix exponential $\exp(-Ht)$, as expressed in the equation 4.0.38, in contrast with the methods usually adopted to study epidemic spread which was unable to give analytic information about the mean time realized by stochastic simulations.

This method is successfully implemented for small system size. However, the method has a computation limitation, since the complexity of the algorithm and the time of computation blows up as the total number of population becomes large. This limitation does not diminish the importance of the work, since in the beginning and in the end of an outbreak we may have small number of individuals, a regime where our approach holds. Yet, we also used numeric linear algebra techniques for a large systems. The comparison between the numerical plot and the mean of stochastic realizations are practically indistinguishable, as seen in the figure 17.

Even being limited the analytic expression to small populations, the method still a interesting way to study the approaches some more complex epidemic models, as arboviruses and veneral disease, as we will discuss in the next section.

5.1 FUTURE PLANS

As we said before, we have a interest in the approach of arboviruses epidemic models, motivated by the actual situation of health public in Brazil. This work open the prospect of using Fock Space representation for different stochastic epidemic models, including models for arboviruses. Comparing to the stochastic SIR model, the dynamics associated with this new model is more complex due to insertion of two new variables with crucial information between human and vector population. Although the implementation is similar to the SIR model, the logical treatment becomes complex even for a small population of humans and vectors. Basically, the first attempt will still be working on simple models with human and vectors using conservation of total population size. The Human population is distributed in susceptible, infected and recovered, or removed, as before, while the vector dynamics will be treated as susceptible and infected, once that the most of disease vectors cannot be recovered. For a more realistic model we can consider the removal of vectors as the number of death vector population. We point out that a more realistic celular automata based dynamics of arboviruses was performed in (MELLO; CASTILHO, 2014; MEDEIROS et al., 2011). The same analysis can be applied to humans, even for the SIR model, this is not the focus here. Performing a simple analysis, we can consider birth and death in the model kept at same rate so that we do not have change in the population size over time. Considering the simplest model (without the birth-and-death process) we have S_H , I_H and R_H the human population and S_V , I_V the vectors satisfying

$$S_H + I_H + R_H = N, (5.1.1)$$

and

$$S_V + I_V = M, (5.1.2)$$

this way, respecting the conservation of total population. The interaction between populations are similar to the SIR model, but we do not have the contagion between human species by direct touch anymore. Once a susceptible human it is needed to interact with an infected vector to get the disease, so the relation is given by:

$$S_H + I_V \to I_H + I_V. \tag{5.1.3}$$

The same happens to vector population. In turn, infected humans interactions may transmit the disease to a susceptible vector:

$$I_H + S_V \to I_H + I_V \tag{5.1.4}$$

We still have the possibility of infected humans become recovered as the time goes by:

$$I_H \to R_H.$$
 (5.1.5)

From now, we can associate rates of recovering and infection, as before, to treat our model in a stochastic approach. As a perspective, we hope to obtain the same qualitative approach using Fock space techniques as the one used in SIR stochastic epidemic models, willing to get the analytic solutions to this class of systems.

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APPENDIX A – MAPLE CODE FOR THE SIR FOCK SPACE

```
> #In this worksheet we will show the buinding of the SIR
   stochastic model in a Fock-Space
> restart;
   with(Physics) : with(LinearAlgebra) : with(Student) :
      # First, you have to be sure that you are using the latest version of Physics Package,
      otherwise some commands may not work properly. In this work, we used the update
      Physics61.3 availabe on http://www.maplesoft.com/products/maple/features/physicsresearch.
      aspx
   Physics:-Version();
          "C:\Program Files\Maple 2015\lib\update.mla", 2015, May 19, 16:0 hours
                                                                                     (1)
> # Setting the main variables to build the quantum operators:
> Setup(op = S,In,R);
                * Partial match of 'op' against keyword 'quantumoperators'
                  * Partial match of 'In' against keyword 'spinorindices'
* Partial or misspelled keyword matches more than one possible keyword. Please select the
    correct one from below and try again.
                      redo, readusersetup, realobjects, redefinesum
                                                                                     (2)
> #Restricting the size of matrices, just for aesthetic reasons:
> interface(rtablesize=150);
                                        10
                                                                                     (3)
> #Cheking the package version:
> version(Physics);
 User Interface: 1045715
            Kernel: 1045715
          Library: 1045715
                                                                                     (4)
                                     1045715
> # Notation S = "susceptible fock space" Sp = Creation Operator
   for the Susceptible, Sm = #Annihilation operator for the
   Susceptible
> # Creating a set of creation operators and ajusting for the
   suitable phase
  N:=1;
   for i from 1 to N do
   Sp[i]:= Creation(S,i,phaseconvention= proc(n) 1 end proc,notation
   = explicit);
   # Same thing for the Annihilation operator
   Sm[i]:=Annihilation(S,i,phaseconvention= proc(n) n end
  proc,notation = explicit);
   end do;
                                    Sp_1 := a^+_{S_1}
Sm_1 := a^-_{S_1}
                                                                                     (5)
```

> # Notation In = "Infected fock space" Inp = Creation Operator for
the Infected, Inm = #Annihilation operator for Infected
> # Creating a set of creation operators and ajusting for the
suitable phase

```
N:=1;
  for i from 1 to N do
  Inp[i]:= Creation(In,i,phaseconvention= proc(n) 1 end proc,
  notation = explicit);
  # Same thing for the Annihilation operator
  Inm[i]:=Annihilation(In,i,phaseconvention= proc(n) n end
  proc,notation = explicit);
  end do;
                                Inp_1 := a^+_{In_1}
                                Inm_1 := a^-_{In_1}
                                                                             (6)
> # Notation R = "Recovered fock space" Rp = Creation Operator for
  the Recovered, Rm = #Annihilation operator for the Recovered
> # Creating a set of creation operators and ajusting for the
  suitable phase
  N := 1;
  for i from 1 to N do
  Rp[i]:= Creation(R,i,phaseconvention= proc(n) 1 end proc,notation
  = explicit);
  # Same thing for the Annihilation operator
  Rm[i]:=Annihilation(R,i,phaseconvention= proc(n) n end
  proc,notation = explicit);
  end do;
                                Rp_1 := a^+_{R_1}
                                Rm_1 := a^-_R
                                                                             (7)
> #Reminding the transitions for the SIR model so we can buind the
     Hamiltonian in therms of the quantum operators.
> #Transictions:
> # First transiction
  \# S + In -> 2In (k1)
  # Seccond transition
  \# In -> R (k2)
  #First Hamiltonian piece, coupled to the constant k1 and defined
  as a procedure depending of this constant:
  H1:=proc(k1) -Expand(k1*(Inp[1]*Inp[1]*Sm[1]*Inm[1]-Sp[1]*Sm[1]*
  Inp[1]*Inm[1])); end proc;
H1 := \mathbf{proc}(k1)
                                                                             (8)
   (-1) * Physics:-Expand(k1 * (Inp[1] * Inp[1] * Sm[1] * Inm[1] - Sp[1] * Sm[1] * Inp[1]
   * Inm[1]))
end proc
> H1(k1);
          -k1 '*' ( '^' ( a^+_{In_1} , 2 ), a^-_{S_1} , a^-_{In_1} ) +k1 '*' ( a^+_{S_1} , a^-_{S_1} , a^+_{In_1} , a^-_{In_1} )
                                                                             (9)
```

```
#The same to the second Hamiltonian piece, dependending of k2,
   H2:=proc(k2) -Expand(k2*(Rp[1]*Inm[1]-Inp[1]*Inm[1])); end proc;
H2 := \mathbf{proc}(k2)
                                                                                                           (10)
    (-1) * Physics:-Expand(k2 * (Rp[1] * Inm[1] - Inp[1] * Inm[1]))
end proc
> H2(k2);
                            -k2 '*' \left(a^{+}_{R_{1}}, a^{-}_{In_{1}}\right) + k2 '*' \left(a^{+}_{In_{1}}, a^{-}_{In_{1}}\right)
                                                                                                           (11)
> #Conecting the pieces:
   H:=proc(k1,k2) H1(k1)+H2(k2); end proc;
                          H := \mathbf{proc}(k1, k2) \ H1(k1) + H2(k2) end proc
                                                                                                           (12)
-k1 \stackrel{\text{`*`}}{(} \stackrel{\text{``}}{(} \stackrel{a^{+}}{a^{-}}_{I_{1}}, 2 \stackrel{\text{}}{)}, a^{-}_{S_{1}}, a^{-}_{I_{1}} \stackrel{\text{}}{)} + k1 \stackrel{\text{`*`}}{(} \stackrel{a^{+}}{s_{1}}, a^{-}_{S_{1}}, a^{+}_{I_{1}}, a^{-}_{I_{1}} \stackrel{\text{}}{)} - k2 \stackrel{\text{`*`}}{(} \stackrel{a^{+}}{s_{1}}, a^{-}_{I_{1}} \stackrel{\text{}}{)} 
                                                                                                           (13)
     + k2 '*' \left(a^{+}_{In_{1}}, a^{-}_{In_{1}}\right)
> #Here, we will express each Hamiltonian's matrix element.
    (Bra(S,si).Bra(In,ii).Bra(R,ri)).(H(k1,k2)).(Ket(R,rj).Ket(In,ij))
    .Ket(S,sj));
    -ij\left(\left(-\delta_{ii,\ ij}\ (k1\ sj+k2)\ \delta_{si,\ sj}+k1\ \delta_{si,\ sj-1}\ sj\ \delta_{ii,\ ij+1}\right)\delta_{ri,\ rj}+k2\ \delta_{si,\ sj}\ \delta_{ii,\ ij-1}\ \delta_{ri,\ rj+1}\right)
                                                                                                           (14)
> #Creating the Basis (Now as a function of S, In, R). Here, we
   suppose some conservations #laws to reduce the dimension of fock
   space. In fact we use that S + In + R = N.
   Baseset:=proc(N) global B; global ket; global bra;global Bdim;
   for si from 0 to N
         do
               for ii from 0 to N
                     do
                          for ri from 0 to N
                                do
                                     if si+ii+ri = N then
                                           B[i]:=(si,ii,ri);
                                           ket[i]:=Ket(S,si).Ket(In,ii).Ket(R,ri);
                                           bra[i]:=Bra(R,ri).Bra(In,ii).Bra(S,si);
                                           print(i,B[i] = ket[i]);
                                           i:=i+1;
                                           end if;
                                     end do;
                          end do:
                end do;
   end proc;
Baseset := \mathbf{proc}(N)
                                                                                                           (15)
```

```
local i, si, ii, ri;
   global B, ket, bra, Bdim;
   i := 1:
   for si from 0 to N do
      for ii from 0 to N do
          for ri from 0 to N do
             if si + ii + ri = N then
                B[i] := si, ii, ri;
                ket[i] := Physics:-Ket(S, si). Physics:-Ket(In, ii). Physics:-Ket(R, ri);
                bra[i] := Physics:-Bra(R, ri). Physics:-Bra(In, ii). Physics:-Bra(S, si);
                print(i, B[i] = ket[i]);
                i := i + 1
             end if
          end do
      end do
   end do
end proc
> #Defining a new procedure to generate the matrix whose basis
  depends of S, In and
> Mat:=proc(N, k1, k2)
  delta:=proc(a,b) piecewise(a=b,1,0); end proc;
  #Creating the Basis (Now as a function of sm, im, rm).
  Baseset:=proc(N)
  global B; global ket; global bra;global Bdim;
  i:=1;
  for si from 0 to N
       do
           for ii from 0 to N
               do
                   for ri from 0 to N
                            if si+ii+ri = N then
                                B[i]:=(si,ii,ri);
                                ket[i]:=Ket(S,si).Ket(In,ii).Ket(R,ri);
                                bra[i]:=Bra(R,ri).Bra(In,ii).Bra(S,si);
                                       i:=i+1;
                                   end if;
                       end do;
                   end do;
            end do;
  Bdim:=i-1;
  end proc;
  Baseset(N):
      for i from 1 to Bdim do
          for j from 1 to Bdim do
```

```
#Replacing the Hamiltonian's matrix element found from the
      equation (14).
                               A[i,j] := -B[j][2]*((-delta(B[i][2], B[j][2])*(k1*B[j][1]+
      k2)*delta(B[i][1], B[j][1])+k1*delta(B[i][1], B[j][1]-1)*B[j][1]*
      delta(B[i][2], B[j][2]+1))*delta(B[i][3], B[j][3])+k2*delta(B[i]
       [1], B[j][1])*delta(B[i][2], B[j][2]-1)*delta(B[i][3], B[j][3]+1)
      );
                               end do;
                 end do;
      Mt := Array(1..Bdim, 1..Bdim, (i,j) \rightarrow A[i,j]);
      end proc;
                                                                                                                                                                                                                                           (16)
Mat := \mathbf{proc}(N, k1, k2)
         local delta, Baseset, i, j, A, Mt;
         delta := proc(a, b) piecewise(a = b, 1, 0) end proc;
         Baseset := \mathbf{proc}(N)
                   local si, ii, ri;
                   global B, ket, bra, Bdim;
                   i := 1;
                   for si from 0 to N do
                             for ii from 0 to N do
                                      for ri from 0 to N do
                                                 if si + ii + ri = N then
                                                          B[i] := si, ii, ri;
                                                          ket[i] := Physics:-Ket(S, si) . Physics:-Ket(In, ii) . Physics:-Ket(R, si)
                                                          bra[i] := Physics:-Bra(R, ri). Physics:-Bra(In, ii). Physics:-Bra(S, ri)
                                                          si);
                                                          i := i + 1
                                                 end if
                                       end do
                             end do
                   end do:
                   Bdim := i - 1
         end proc;
         Baseset(N);
         for i to Bdim do
                   for j to Bdim do
                             A[i,j] := (-1) * B[j][2] * ((-\text{delta}(B[i][2], B[j][2]) * (k1 * B[j][1] + k2)
                             * \det(B[i][1], B[j][1]) + k1 * \det(B[i][1], B[j][1] - 1) * B[j][1] * \det(B[i][1], B[j][1]) + k1 * \det(B[i][1], B[i][1]) + k1 * \det(B[i][1
                             [2], B[j][2] + 1) * delta(B[i][3], B[j][3]) + k2 * delta(B[i][1], B[j][1])
                              * \det(B[i][2], B[j][2] - 1) * \det(B[i][3], B[j][3] + 1)
                   end do
         end do:
         Mt := Array(1 ..Bdim, 1 ..Bdim, (i, j) \rightarrow A[i, j])
```

```
end proc
>
  #Defining the solution to the Hamiltonian from the matrix
  exonential - Mat (in the fock space).
> ExpHt:= proc(N,k1,k2,t)
  MatrixExponential(-Mat(N,k1,k2)*t); end proc;
                                                                                    (17)
ExpHt := \mathbf{proc}(N, k1, k2, t)
   LinearAlgebra:-MatrixExponential((-1)*Mat(N, k1, k2)*t)
end proc
> # Defining a way to give each element (depending of each row and
  column) of the matrix exponential,
  #ExpHt.
> Expi:=proc(R,C,N,k1,k2,t)
  evalf(ExpHt(N, k1, k2, t)[R][C]);
  end proc;
                                                                                    (18)
        Expi := \mathbf{proc}(R, C, N, k1, k2, t) evalf (ExpHt(N, k1, k2, t) \lceil R \rceil \lceil C \rceil) end proc
> #Defining a way to give the column vector from the matrix
  exponential
  Vexp:=proc(N,C,k1,k2,t)
  Mat(N,k1,k2):
  <seq(ExpHt(N,k1,k2,t)[i,C],i=1..Bdim)>: end proc;
                                                                                    (19)
Vexp := \mathbf{proc}(N, C, k1, k2, t)
   Mat(N, k1, k2); \leq seq(ExpHt(N, k1, k2, t) [i, C], i = 1 ..Bdim) >
end proc
> #Taking the vector of susceptible population condition definded
  by the Baseset
  Vs:=proc(k,N)
  Mat(N,k1,k2):
  <seq(B[i][1]**k,i=1..Bdim)>: end proc;
       Vs := \mathbf{proc}(k, N) \ Mat(N, k1, k2); \le seq(B[i][1]^k, i = 1..Bdim) \ge \mathbf{end} \ \mathbf{proc}
                                                                                    (20)
> Vs (1,2)
                                        0
                                        0
                                        0
                                                                                    (21)
                                        1
                                        2
> #The same for Infectives:
  Vin:= proc(k,N)
  Mat(N,k1,k2):
  <seq(B[i][2]**k,i=1..Bdim)>: end proc;
      Vin := \mathbf{proc}(k, N) \ Mat(N, k1, k2); \le seq(B[i][2]^k, i=1...Bdim) \ge \mathbf{end} \ \mathbf{proc}
                                                                                    (22)
> Vin(1, 2);
```

```
0
                                                                                    (23)
> #The same for recovered:
  Vr := proc(k,N)
  Mat(N,k1,k2):
  <seq(B[i][3]**k,i=1..Bdim)>: end proc;
       Vr := \mathbf{proc}(k, N) \ Mat(N, k1, k2); \le seq(B[i][3]^k, i = 1..Bdim) \ge end proc
                                                                                    (24)
> Vr(1, 2);
                                                                                    (25)
> #Finally, getting the k-th moments (in particular, the mean, fot
      k=1) in function of time of each population, given the
      poplation size, N, the initial condition, C (the C-th choice
      of the baseset), and the constants of interaction, k1 and k2.
> Sk:=proc(k,N,C,k1,k2,t) DotProduct(Vs(k,N),Vexp(N,C,k1,k2,t));
  end proc;
Sk := \mathbf{proc}(k, N, C, k1, k2, t)
                                                                                    (26)
   LinearAlgebra:-DotProduct(Vs(k, N), Vexp(N, C, k1, k2, t))
end proc
> Ink:=proc(k,N,C,k1,k2,t) DotProduct(Vin(k,N),Vexp(N,C,k1,k2,t));
  end proc;
Ink := \mathbf{proc}(k, N, C, k1, k2, t)
                                                                                    (27)
   LinearAlgebra:-DotProduct(Vin(k, N), Vexp(N, C, k1, k2, t))
end proc
> Rk:=proc(k,N,C,k1,k2,t) DotProduct(Vr(k,N),Vexp(N,C,k1,k2,t));
  end proc;
Rk := \mathbf{proc}(k, N, C, k1, k2, t)
                                                                                    (28)
   LinearAlgebra:-DotProduct(Vr(k, N), Vexp(N, C, k1, k2, t))
> #Testing the solutions for N=3 and initial condition (S0,I0,R0)=(2,1,0):
> Sk(1,3,9,1,2,t);
                             -\frac{1}{9}e^{-6t} + \frac{8}{9}e^{-3t} + \frac{11}{9}
                                                                                    (29)
  Ink(1, 3, 9, 1, 2, t);
```

$$\frac{1}{6} e^{-6t} - \frac{8}{3} e^{-3t} + \frac{7}{2} e^{-2t}$$
 (30)

> Rk(1, 3, 9, 1, 2, t);

$$-\frac{1}{18} e^{-6t} + \frac{16}{9} e^{-3t} - \frac{7}{2} e^{-2t} + \frac{16}{9}$$
 (31)

> #Displaying the graph for susceptible (with the deviation):

> DispS = proc(N, C, k1, k2, s)plot([Sk(1, N, C, k1, k2, t), Sk

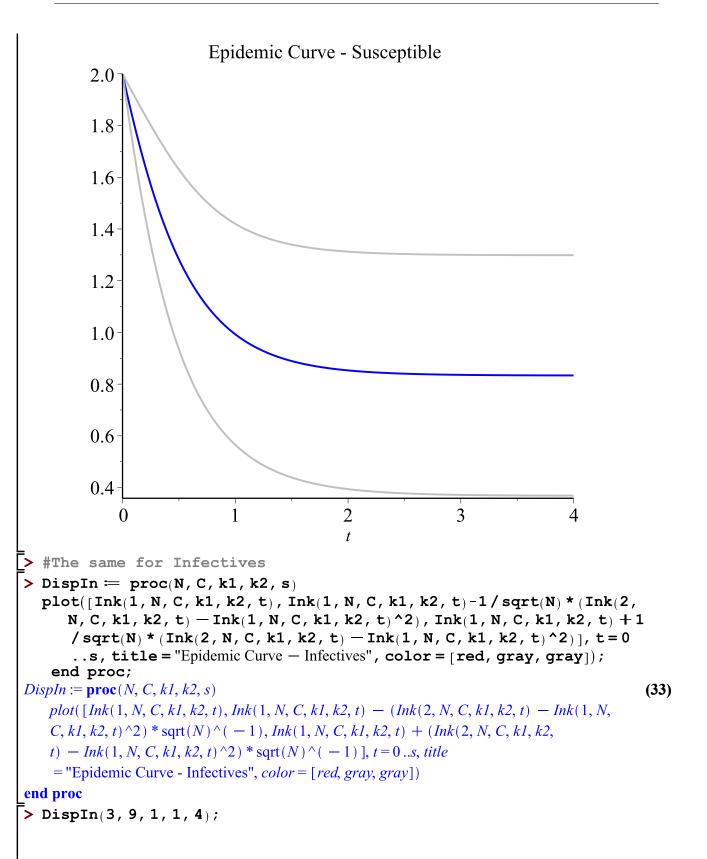
plot([Sk(1, N, C, k1, k2, t), Sk(1, N, C, k1, k2, t)-1/sqrt(N)*(Sk(2, N, C, k1, k2, t)-Sk(1, N, C, k1, k2, t)-1/sqrt(N)*(Sk(2, N, C, k1, k2, t)-2), Sk(1, N, C, k1, k2, t)+1/sqrt(N)*(Sk(2, N, C, k1, k2, t)-Sk(1, N, C, k1, k2, t)-2)], t=0..s, title="Epidemic Curve — Susceptible", color=[blue, gray, gray]); end proc;

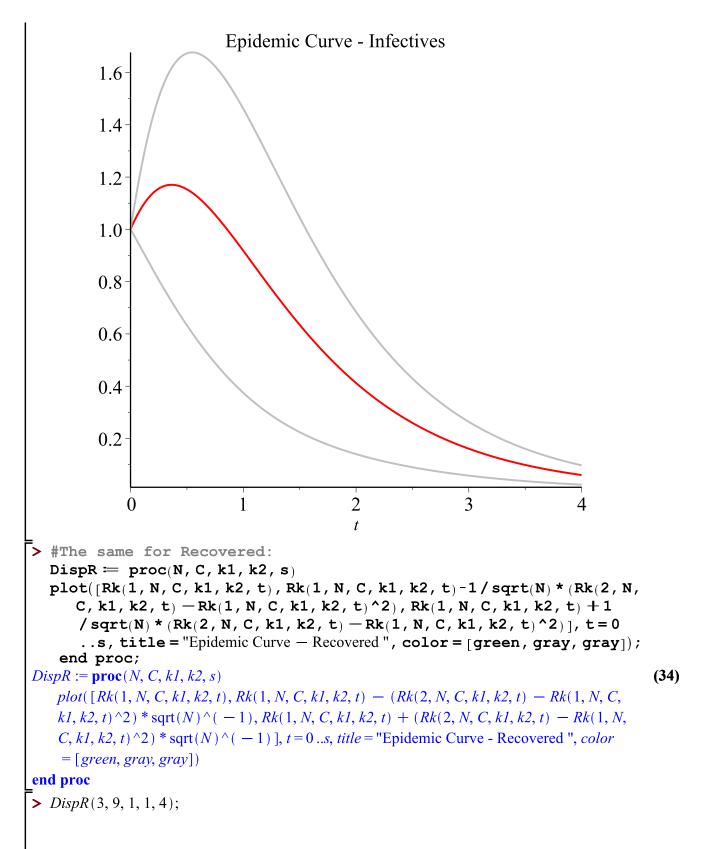
$$DispS := \mathbf{proc}(N, C, k1, k2, s)$$

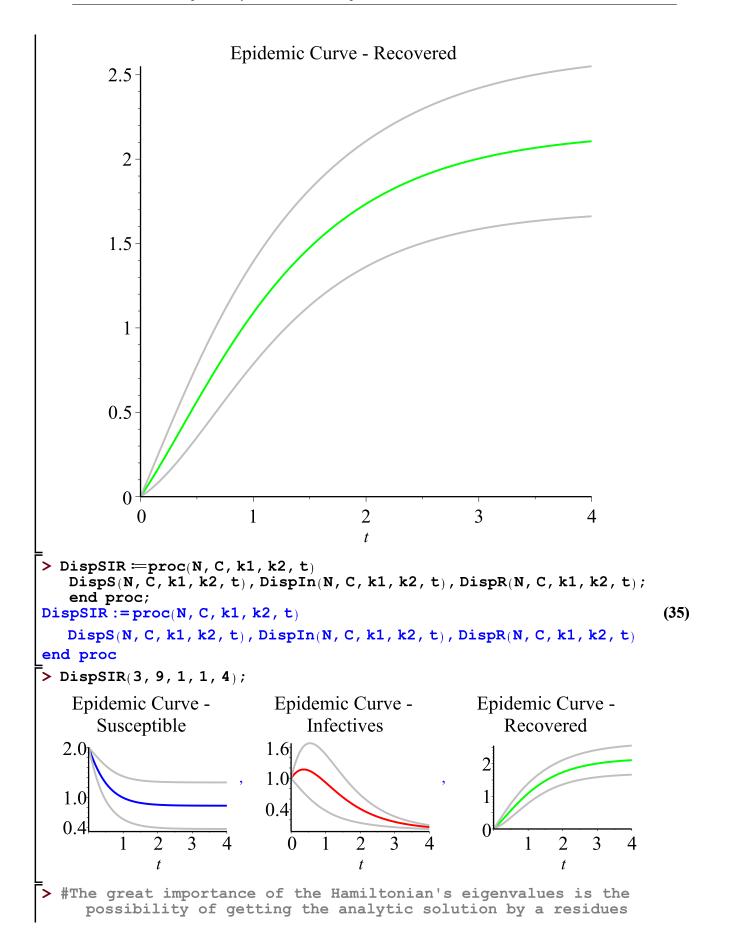
$$plot([Sk(1, N, C, k1, k2, t), Sk(1, N, C, k1, k2, t) - (Sk(2, N, C, k1, k2, t) - Sk(1, N, C, k1, k2, t)^2) * \operatorname{sqrt}(N)^{(-1)}, Sk(1, N, C, k1, k2, t) + (Sk(2, N, C, k1, k2, t) - Sk(1, N, C, k1, k2, t)^2) * \operatorname{sqrt}(N)^{(-1)}, t = 0 ...s, title = "Epidemic Curve - Susceptible ", color = [blue, gray, gray])$$
(32)

end proc

> DispS(3, 9, 1, 1, 4);







formula. To our happiness, this eigenvalues follows a rule depending on the size of population N and it's constants of interactions, k1 and k2. You can check this as follows:

> Eigenvalues(Mat(1, alpha, beta)); $\begin{bmatrix}
0 \\
0 \\
\beta
\end{bmatrix}$ (36)

Eigenvalues(Mat(2, alpha, beta));

 $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 2\beta \\ \beta \\ \alpha + \beta \end{bmatrix}$ (37)

Eigenvalues(Mat(3, alpha, beta));

$$\begin{array}{c|c}
0 \\
0 \\
0 \\
0 \\
\beta \\
2 \beta \\
3 \beta \\
2 \alpha + 2 \beta \\
2 \alpha + \beta \\
\alpha + \beta
\end{array}$$
(38)

Eigenvalues(Mat(4, alpha, beta));

(39)

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 3 \alpha + \beta \\ 4 \alpha + 2 \beta \\ 3 \alpha + 3 \beta \\ 4 \beta \\ 2 \alpha + \beta \\ 2 \alpha + 2 \beta \\ 3 \beta \\ \alpha + \beta \\ 2 \beta \\ \beta \end{bmatrix}$$

Eigenvalues(Mat(5, alpha, beta));

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 4\alpha + \beta \\ 6\alpha + 2\beta \\ 6\alpha + 3\beta \\ 4\alpha + 4\beta \\ 5\beta \\ 3\alpha + \beta \\ 4\alpha + 2\beta \\ 3\alpha + 3\beta \\ 4\beta \\ 2\alpha + \beta \\ 2\alpha + \beta \\ 2\alpha + \beta \\ 2\alpha + \beta \\ 2\beta \\ \beta \end{bmatrix}$$

Eigenvalues(Mat(6, alpha, beta));

(40)

```
0
      0
      0
 5\alpha + \beta
8\alpha + 4\beta
5\alpha + 5\beta
    6 β
4\alpha + \beta
6\alpha + 2\beta
6\alpha + 3\beta
4\alpha + 4\beta
    5 β
3\alpha + \beta
4\alpha + 2\beta
3\alpha + 3\beta
    4 β
2\alpha + \beta
2\alpha + 2\beta
   3 β
  \alpha + \beta
    2 β
      β
```

Eigenvalues(Mat(7, alpha, beta));

(41)

0
0
0
0
0
0
0
0
$6 \alpha + \beta$
$10 \alpha + 2 \beta$
$12 \alpha + 3 \beta$
$12 \alpha + 4 \beta$
$10 \alpha + 5 \beta$
$6\alpha + 6\beta$
7 β
$5 \alpha + \beta$
$8\alpha + 2\beta$
$9\alpha + 3\beta$
$8\alpha + 4\beta$
$5\alpha + 5\beta$
6β
•
$4\alpha + \beta$
$6\alpha + 2\beta$
$6\alpha + 3\beta$
$4\alpha + 4\beta$
5 β
$3 \alpha + \beta$
$4\alpha + 2\beta$
$3\alpha + 3\beta$
4 β
$2\alpha + \beta$

```
(42)
```

> #Due to a long time of computation, an alternative Maple
 worksheet was built to compute this eigenvalues. You can
 compare them to certify the authenticity.

APPENDIX B – MAPLE CODE FOR THE MATRIX EIGENVALUES

```
> #This worksheet has as prurpose display step by step all the computational work necessary
       and mady for us to have an easy way of getting the eigenvalues of the hamiltonian
       's SIR stochastic model without needing to resort the exaustive job made in the Fock
        — space due to extensive computational time of processing.
> #Here, all the comentaries will be in gray text, while de commands will be wrote in black text
       . When the commands are accepted than the text will give as a blue text as output
       . Otherwise, a pink error text informing the issue.
  #The next command will clean all the variables to avoid future errors or glitches.
  restart:
  #Calling the package necessary to find recorrent sequences.
> with(genfunc);
[rgf charseq, rgf encode, rgf expand, rgf findrecur, rgf hybrid, rgf norm, rgf pfrac,
                                                                                                   (1)
    rgf relate, rgf sequence, rgf_simp, rgf_term, termscale]
> #Here we will try to find the nonzero eigenvalues for N=9. At first,
       we observe that we need all the nonzero eingevalues for N = 8, 7,...1. More generally,
       to find the results for N=M we need the rest of the results for N=M-1, M-2,..., 2,
       1. Taking all the eigenvalues on this ordenaded list, we have a recurence sequence
       in commun for all the sizes of population. First, lets find de sequence acoupled
       to the constant alpha. The comand rgf_findrecur will help us
       to find the recurrent sequence depending on the 3 first therms of the sequence.
> #First piece of the list (for N=9)
> rgf \ findrecur(3, [8, 14, 18, 20, 20, 18, 14, 8, 0], a, k);
                         a(k) = 3 \ a(k-1) - 3 \ a(k-2) + a(k-3)
                                                                                                   (2)
> #Second piece of the list (N=8)
> rgf findrecur(3, [7, 12, 15, 16, 15, 12, 7, 0], a, k);
                         a(k) = 3 \ a(k-1) - 3 \ a(k-2) + a(k-3)
                                                                                                   (3)
> #And so on, the other pieces:
> #N=7
> rgf findrecur(3, [6, 10, 12, 12, 10, 6, 0], a, k);
                         a(k) = 3 \ a(k-1) - 3 \ a(k-2) + a(k-3)
                                                                                                   (4)
> #N=6
> rgf_findrecur(3, [5, 8, 9, 8, 5, 0], a, k);
                         a(k) = 3 a(k-1) - 3 a(k-2) + a(k-3)
                                                                                                   (5)
> #N=5
  rgf_findrecur(3, [4, 6, 6, 4, 0], a, k);
> rgf \ findrecur(3, [3, 4, 3, 0], a, k);
  rgf \ findrecur(3, [2, 2, 0], a, k);
  \#N=2
```

```
> rgf_findrecur(3, [0, 0, 1], a, k):
                                        ndrecur) second argument is not a list
  \#N=1: Has just one therm, that is 0.
> #NOTE: All the errors here are justified by the fact of the comand rgf findrecur limitates the
       research for a number of therms greather than 2 times the size of the explicit sequence.
       You can see this at the help page. Even so, for N=6,5,4 the recurrent sequence keeps the
       same of the others. You can check this manually. For N=2,1, we can write them
       explicitally. For N=3, we can find a direct sequence, just like for N>3, and it can be done
       by the comand rsolve, as follows:
> simplify(rsolve(\{a(k) = 3 \cdot a(k-1) - 3 \cdot a(k-2) + a(k-3), a(0) = r-1, a(1) = 2(r-1)\}
        (-2), a(2) = 3(r-3), a(k));
                                     -k^2 + kr - 2k + r - 1
                                                                                                      (6)
> #By the same method, we will find the other sequence acoupled to the constant beta. We will
       name it b. Looking at the resultos of the eigenvalues we have cleary a simpler sequence
       given by the recursive formula b(k)=b(k-1)+1, where b(0)=1. Using the comand rsolve one
       more time we find as follows:
> rsolve(\{b(k) = b(k-1) + 1, b(0) = 1\}, b(k));
                                                                                                      (7)
> #Now, we will define the sequences found as a procidure and get them together to have all the
       nonzero eigenvalues defined from the lists of pieces of this sequences, the new complete
       sequences, a and b, now depends on two index, r and k:
> a := \operatorname{proc}(r, k)
    -k^2 + (r-2)k + r - 1
   end proc;
                    a := \mathbf{proc}(r, k) - k^2 + (r-2) * k + r - 1 end proc
                                                                                                      (8)
  b := \operatorname{proc}(r, k)
   k+1
   end proc;
                                b := \mathbf{proc}(r, k) \ k + 1 \ \mathbf{end} \ \mathbf{proc}
                                                                                                      (9)
> #Here, we will define Ev1, the procedure to express the piece of nonzero eigenvalues, including
       N=1 and 2:
> Ev1 = proc(N, k1, k2)
   local i:
   if N=2 then print(lambda(2, 0) = k1 \cdot a(2, 0) + k2 \cdot b(2, 0)); print(lambda(2, 1) = k1 \cdot a(2, 0))
       1) +k2 \cdot b(2,1); print(lambda(1,0) = k2 \cdot b(2,0)) else
   for i from 0 to N-1 do print (lambda (N, i) = k1 \cdot a(N, i) + k2 \cdot b(N, i));
   end do:
   end if:
   end proc;
Ev1 := \mathbf{proc}(N, k1, k2)
                                                                                                     (10)
    local i;
    if N=2 then
        print(lambda(2, 0) = k1 * a(2, 0) + k2 * b(2, 0));
        print(lambda(2, 1) = k1 * a(2, 1) + k2 * b(2, 1));
        print(lambda(1, 0) = k2 * b(2, 0))
```

```
else
         for i from 0 to N-1 do print(lambda(N, i) = k1 * a(N, i) + k2 * b(N, i)) end do
     end if
end proc
> Ev1(1, k1, k2);
                                                \lambda(1,0) = k2
                                                                                                                   (11)
> Ev1(2, k1, k2);
                                             \lambda(2,0) = k1 + k2
                                               \lambda(2, 1) = 2 k2
                                                \lambda(1,0) = k2
                                                                                                                   (12)
> #Finally, we will define Ev, the procedure that shows all the nonzero eigenvalues by sequences
        of the Ev1 previously defined. This way, we have:
> Ev = \operatorname{proc}(N, k1, k2)
    local i;
   if N=1 then print(lambda(1, 0) = k2);
    seq(Ev1(N-i, k1, k2), i=0..N-2);
    end if;
    end proc;
Ev := \mathbf{proc}(N, k1, k2)
                                                                                                                   (13)
    local i;
     if N=1 then print(lambda(1,0)=k2) else seq(Ev1(N-i,k1,k2), i=0..N-2) end if
end proc
> Ev(1, alpha, beta);
                                                                                                                   (14)
                                                 \lambda(1,0) = \beta
> Ev(2, alpha, beta);
                                              \lambda(2,0) = \alpha + \beta
                                                \lambda(2, 1) = 2 \beta
                                                 \lambda(1,0) = \beta
                                                                                                                   (15)
> Ev(3, alpha, beta);
                                             \lambda(3,0) = 2\alpha + \beta
                                             \lambda(3, 1) = 2 \alpha + 2 \beta
                                                \lambda(3,2) = 3 \beta
                                               \lambda(2,0) = \alpha + \beta
                                                \lambda(2, 1) = 2 \beta
                                                 \lambda(1,0) = \beta
                                                                                                                   (16)
> Ev(4, alpha, beta);
                                             \lambda(4,0) = 3 \alpha + \beta
                                             \lambda(4,1) = 4 \alpha + 2 \beta
                                             \lambda(4,2) = 3 \alpha + 3 \beta
                                                \lambda(4,3) = 4 \beta
```

(17)

(18)

$$\lambda(3,0) = 2 \alpha + \beta$$

$$\lambda(3,1) = 2 \alpha + 2 \beta$$

$$\lambda(3,2) = 3 \beta$$

$$\lambda(2,0) = \alpha + \beta$$

$$\lambda(2,1) = 2 \beta$$

$$\lambda(1,0) = \beta$$

> Ev(5, alpha, beta);

$$\lambda(5,0) = 4 \alpha + \beta$$

$$\lambda(5,1) = 6 \alpha + 2 \beta$$

$$\lambda(5,2) = 6 \alpha + 3 \beta$$

$$\lambda(5,3) = 4 \alpha + 4 \beta$$

$$\lambda(5,4) = 5 \beta$$

$$\lambda(4,0) = 3 \alpha + \beta$$

$$\lambda(4,1) = 4 \alpha + 2 \beta$$

$$\lambda(4,2) = 3 \alpha + 3 \beta$$

$$\lambda(4,3) = 4 \beta$$

$$\lambda(3,0) = 2 \alpha + \beta$$

$$\lambda(3,1) = 2 \alpha + 2 \beta$$

$$\lambda(3,2) = 3 \beta$$

$$\lambda(2,0) = \alpha + \beta$$

$$\lambda(2,1) = 2 \beta$$

$$\lambda(1,0) = \beta$$

> Ev(6, alpha, beta);

$$\lambda(6,0) = 5 \alpha + \beta$$

$$\lambda(6,1) = 8 \alpha + 2 \beta$$

$$\lambda(6,2) = 9 \alpha + 3 \beta$$

$$\lambda(6,3) = 8 \alpha + 4 \beta$$

$$\lambda(6,4) = 5 \alpha + 5 \beta$$

$$\lambda(6,5) = 6 \beta$$

$$\lambda(5,0) = 4 \alpha + \beta$$

$$\lambda(5,1) = 6 \alpha + 2 \beta$$

$$\lambda(5,2) = 6 \alpha + 3 \beta$$

$$\lambda(5,3) = 4 \alpha + 4 \beta$$

$$\lambda(5,4) = 5 \beta$$

$$\lambda(4,0) = 3 \alpha + \beta$$

$$\lambda(4,1) = 4 \alpha + 2 \beta$$

$$\lambda(4, 2) = 3 \alpha + 3 \beta$$

$$\lambda(4, 3) = 4 \beta$$

$$\lambda(3, 0) = 2 \alpha + \beta$$

$$\lambda(3, 1) = 2 \alpha + 2 \beta$$

$$\lambda(3, 2) = 3 \beta$$

$$\lambda(2, 0) = \alpha + \beta$$

$$\lambda(2, 1) = 2 \beta$$

$$\lambda(1, 0) = \beta$$
(19)

> #To have sure about the behavior of this work, just take a look of the eigenvalues found in the Fock-space worksheet.

Next, we have the sample for N=35. We can observe the several dependence of the sequences of lower sizes of population.

> Ev(35, alpha, beta);

$$\lambda(35, 0) = 34 \alpha + \beta$$
 $\lambda(35, 1) = 66 \alpha + 2 \beta$
 $\lambda(35, 2) = 96 \alpha + 3 \beta$
 $\lambda(35, 3) = 124 \alpha + 4 \beta$
 $\lambda(35, 4) = 150 \alpha + 5 \beta$
 $\lambda(35, 5) = 174 \alpha + 6 \beta$
 $\lambda(35, 6) = 196 \alpha + 7 \beta$
 $\lambda(35, 7) = 216 \alpha + 8 \beta$
 $\lambda(35, 8) = 234 \alpha + 9 \beta$
 $\lambda(35, 9) = 250 \alpha + 10 \beta$
 $\lambda(35, 10) = 264 \alpha + 11 \beta$
 $\lambda(35, 11) = 276 \alpha + 12 \beta$
 $\lambda(35, 12) = 286 \alpha + 13 \beta$
 $\lambda(35, 13) = 294 \alpha + 14 \beta$
 $\lambda(35, 14) = 300 \alpha + 15 \beta$
 $\lambda(35, 15) = 304 \alpha + 16 \beta$
 $\lambda(35, 16) = 306 \alpha + 17 \beta$
 $\lambda(35, 17) = 306 \alpha + 18 \beta$
 $\lambda(35, 18) = 304 \alpha + 19 \beta$
 $\lambda(35, 19) = 300 \alpha + 20 \beta$
 $\lambda(35, 20) = 294 \alpha + 21 \beta$
 $\lambda(35, 21) = 286 \alpha + 22 \beta$
 $\lambda(35, 22) = 276 \alpha + 23 \beta$

$$\lambda(35, 23) = 264 \alpha + 24 \beta$$
 $\lambda(35, 24) = 250 \alpha + 25 \beta$
 $\lambda(35, 25) = 234 \alpha + 26 \beta$
 $\lambda(35, 26) = 216 \alpha + 27 \beta$
 $\lambda(35, 27) = 196 \alpha + 28 \beta$
 $\lambda(35, 28) = 174 \alpha + 29 \beta$
 $\lambda(35, 29) = 150 \alpha + 30 \beta$
 $\lambda(35, 30) = 124 \alpha + 31 \beta$
 $\lambda(35, 31) = 96 \alpha + 32 \beta$
 $\lambda(35, 32) = 66 \alpha + 33 \beta$
 $\lambda(35, 33) = 34 \alpha + 34 \beta$
 $\lambda(35, 34) = 35 \beta$
 $\lambda(34, 0) = 33 \alpha + \beta$
 $\lambda(34, 1) = 64 \alpha + 2 \beta$
 $\lambda(34, 3) = 120 \alpha + 4 \beta$
 $\lambda(34, 4) = 145 \alpha + 5 \beta$
 $\lambda(34, 6) = 189 \alpha + 7 \beta$
 $\lambda(34, 7) = 208 \alpha + 8 \beta$
 $\lambda(34, 9) = 240 \alpha + 10 \beta$
 $\lambda(34, 10) = 253 \alpha + 11 \beta$
 $\lambda(34, 11) = 264 \alpha + 12 \beta$
 $\lambda(34, 12) = 273 \alpha + 13 \beta$
 $\lambda(34, 13) = 280 \alpha + 14 \beta$
 $\lambda(34, 14) = 285 \alpha + 16 \beta$
 $\lambda(34, 15) = 288 \alpha + 16 \beta$
 $\lambda(34, 16) = 289 \alpha + 17 \beta$
 $\lambda(34, 17) = 288 \alpha + 18 \beta$
 $\lambda(34, 18) = 285 \alpha + 19 \beta$
 $\lambda(34, 19) = 280 \alpha + 20 \beta$
 $\lambda(34, 20) = 273 \alpha + 21 \beta$
 $\lambda(34, 21) = 264 \alpha + 22 \beta$
 $\lambda(34, 22) = 253 \alpha + 23 \beta$
 $\lambda(34, 23) = 240 \alpha + 24 \beta$

$$\lambda(34, 24) = 225 \alpha + 25 \beta$$
 $\lambda(34, 25) = 208 \alpha + 26 \beta$
 $\lambda(34, 26) = 189 \alpha + 27 \beta$
 $\lambda(34, 27) = 168 \alpha + 28 \beta$
 $\lambda(34, 28) = 145 \alpha + 29 \beta$
 $\lambda(34, 29) = 120 \alpha + 30 \beta$
 $\lambda(34, 30) = 93 \alpha + 31 \beta$
 $\lambda(34, 31) = 64 \alpha + 32 \beta$
 $\lambda(34, 32) = 33 \alpha + 33 \beta$
 $\lambda(34, 33) = 34 \beta$
 $\lambda(33, 0) = 32 \alpha + \beta$
 $\lambda(33, 2) = 90 \alpha + 3 \beta$
 $\lambda(33, 3) = 116 \alpha + 4 \beta$
 $\lambda(33, 4) = 140 \alpha + 5 \beta$
 $\lambda(33, 5) = 162 \alpha + 6 \beta$
 $\lambda(33, 6) = 182 \alpha + 7 \beta$
 $\lambda(33, 7) = 200 \alpha + 8 \beta$
 $\lambda(33, 8) = 216 \alpha + 9 \beta$
 $\lambda(33, 10) = 242 \alpha + 11 \beta$
 $\lambda(33, 11) = 252 \alpha + 12 \beta$
 $\lambda(33, 13) = 266 \alpha + 14 \beta$
 $\lambda(33, 14) = 270 \alpha + 15 \beta$
 $\lambda(33, 15) = 272 \alpha + 16 \beta$
 $\lambda(33, 16) = 272 \alpha + 16 \beta$
 $\lambda(33, 17) = 200 \alpha + 8 \beta$
 $\lambda(33, 18) = 266 \alpha + 14 \beta$
 $\lambda(33, 19) = 260 \alpha + 20 \beta$
 $\lambda(33, 19) = 260 \alpha + 20 \beta$
 $\lambda(33, 20) = 252 \alpha + 21 \beta$
 $\lambda(33, 20) = 252 \alpha + 21 \beta$
 $\lambda(33, 20) = 252 \alpha + 23 \beta$
 $\lambda(33, 22) = 230 \alpha + 23 \beta$
 $\lambda(33, 23) = 216 \alpha + 24 \beta$
 $\lambda(33, 24) = 200 \alpha + 25 \beta$
 $\lambda(33, 25) = 182 \alpha + 26 \beta$

$$\lambda(33, 26) = 162 \alpha + 27 \beta$$
 $\lambda(33, 27) = 140 \alpha + 28 \beta$
 $\lambda(33, 28) = 116 \alpha + 29 \beta$
 $\lambda(33, 29) = 90 \alpha + 30 \beta$
 $\lambda(33, 30) = 62 \alpha + 31 \beta$
 $\lambda(33, 31) = 32 \alpha + 32 \beta$
 $\lambda(33, 32) = 33 \beta$
 $\lambda(32, 0) = 31 \alpha + \beta$
 $\lambda(32, 1) = 60 \alpha + 2 \beta$
 $\lambda(32, 2) = 87 \alpha + 3 \beta$
 $\lambda(32, 3) = 112 \alpha + 4 \beta$
 $\lambda(32, 3) = 112 \alpha + 4 \beta$
 $\lambda(32, 4) = 135 \alpha + 5 \beta$
 $\lambda(32, 6) = 175 \alpha + 7 \beta$
 $\lambda(32, 7) = 192 \alpha + 8 \beta$
 $\lambda(32, 8) = 207 \alpha + 9 \beta$
 $\lambda(32, 10) = 231 \alpha + 11 \beta$
 $\lambda(32, 11) = 240 \alpha + 12 \beta$
 $\lambda(32, 12) = 247 \alpha + 13 \beta$
 $\lambda(32, 13) = 252 \alpha + 14 \beta$
 $\lambda(32, 14) = 255 \alpha + 15 \beta$
 $\lambda(32, 15) = 256 \alpha + 16 \beta$
 $\lambda(32, 16) = 255 \alpha + 17 \beta$
 $\lambda(32, 17) = 252 \alpha + 18 \beta$
 $\lambda(32, 18) = 247 \alpha + 19 \beta$
 $\lambda(32, 19) = 240 \alpha + 20 \beta$
 $\lambda(32, 20) = 231 \alpha + 21 \beta$
 $\lambda(32, 20) = 231 \alpha + 23 \beta$
 $\lambda(32, 20) = 231 \alpha + 23 \beta$
 $\lambda(32, 20) = 231 \alpha + 24 \beta$

$$\lambda(32, 29) = 60 \alpha + 30 \beta$$

$$\lambda(32, 30) = 31 \alpha + 31 \beta$$

$$\lambda(32, 31) = 32 \beta$$

$$\lambda(31, 0) = 30 \alpha + \beta$$

$$\lambda(31, 1) = 58 \alpha + 2 \beta$$

$$\lambda(31, 2) = 84 \alpha + 3 \beta$$

$$\lambda(31, 3) = 108 \alpha + 4 \beta$$

$$\lambda(31, 3) = 108 \alpha + 4 \beta$$

$$\lambda(31, 4) = 130 \alpha + 5 \beta$$

$$\lambda(31, 5) = 150 \alpha + 6 \beta$$

$$\lambda(31, 6) = 168 \alpha + 7 \beta$$

$$\lambda(31, 7) = 184 \alpha + 8 \beta$$

$$\lambda(31, 8) = 198 \alpha + 9 \beta$$

$$\lambda(31, 9) = 210 \alpha + 10 \beta$$

$$\lambda(31, 10) = 220 \alpha + 11 \beta$$

$$\lambda(31, 11) = 228 \alpha + 12 \beta$$

$$\lambda(31, 12) = 234 \alpha + 13 \beta$$

$$\lambda(31, 13) = 238 \alpha + 14 \beta$$

$$\lambda(31, 14) = 240 \alpha + 15 \beta$$

$$\lambda(31, 15) = 240 \alpha + 16 \beta$$

$$\lambda(31, 16) = 238 \alpha + 17 \beta$$

$$\lambda(31, 17) = 234 \alpha + 18 \beta$$

$$\lambda(31, 18) = 228 \alpha + 19 \beta$$

$$\lambda(31, 19) = 220 \alpha + 20 \beta$$

$$\lambda(31, 20) = 210 \alpha + 21 \beta$$

$$\lambda(31, 20) = 210 \alpha + 21 \beta$$

$$\lambda(31, 20) = 210 \alpha + 22 \beta$$

$$\lambda(31, 20) = 184 \alpha + 23 \beta$$

$$\lambda(31, 20) = 184 \alpha + 24 \beta$$

$$\lambda$$

$$\lambda(30, 2) = 81 \alpha + 3 \beta$$
 $\lambda(30, 3) = 104 \alpha + 4 \beta$
 $\lambda(30, 4) = 125 \alpha + 5 \beta$
 $\lambda(30, 5) = 144 \alpha + 6 \beta$
 $\lambda(30, 6) = 161 \alpha + 7 \beta$
 $\lambda(30, 7) = 176 \alpha + 8 \beta$
 $\lambda(30, 8) = 189 \alpha + 9 \beta$
 $\lambda(30, 9) = 200 \alpha + 10 \beta$
 $\lambda(30, 10) = 209 \alpha + 11 \beta$
 $\lambda(30, 11) = 216 \alpha + 12 \beta$
 $\lambda(30, 12) = 221 \alpha + 13 \beta$
 $\lambda(30, 13) = 224 \alpha + 14 \beta$
 $\lambda(30, 14) = 225 \alpha + 15 \beta$
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 $\lambda(24, 4) = 95 \alpha + 5 \beta$
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 $\lambda(23, 6) = 112 \alpha + 7 \beta$
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$$\lambda(7,0) = 6 \alpha + \beta$$

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$$\lambda(4,0) = 3 \alpha + \beta$$

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(20)

APPENDIX C – MAPLE CODE FOR THE MEAN TIME OF EPIDEMIC

```
> #In this worksheet we will use the buinding of the Fock space of
  the SIR stochastic model to introduce the Mean time of epidemic.
> restart;
  with(Physics) : with(LinearAlgebra) : with(Student) :
      # First, you have to be sure that you are using the latest version of Physics Package,
      otherwise some commands may not work properly. In this work, we used the update
      Physics61.3 availabe on http://www.maplesoft.com/products/maple/features/physicsresearch.
      aspx
  Physics:-Version();
         "C:\Program Files\Maple 2015\lib\update.mla", 2015, May 19, 16:0 hours
                                                                                    (1)
> #Creating the Basis (Now as a function of S, In, R). Here, we
  suppose some conservations laws to reduce the dimension of fock
  space. In fact we use that S + In + R = N.
  Baseset:=proc(N) global B; global ket; global bra; global Bdim;
  for si from 0 to N
       do
           for ii from 0 to N
                do
                    for ri from 0 to N
                         do
                             if si+ii+ri = N then
                                  B[i]:=(si,ii,ri);
                                  ket[i]:=Ket(S,si).Ket(In,ii).Ket(R,ri);
                                  bra[i]:=Bra(R,ri).Bra(In,ii).Bra(S,si);
                                  print(i,B[i] = ket[i]);
                                  i:=i+1;
                                  end if;
                             end do;
                    end do;
            end do;
  end proc;
Baseset := \mathbf{proc}(N)
                                                                                    (2)
   local i, si, ii, ri;
   global B, ket, bra, Bdim;
   i := 1:
   for si from 0 to N do
       for ii from 0 to N do
          for ri from 0 to N do
              if si + ii + ri = N then
                 B[i] := si, ii, ri;
                 ket[i] := Physics:-Ket(S, si) . Physics:-Ket(In, ii) . Physics:-Ket(R, ri);
                 bra[i] := Physics:-Bra(R, ri). Physics:-Bra(In, ii). Physics:-Bra(S, si);
                 print(i, B[i] = ket[i]);
```

```
i := i + 1
            end if
         end do
      end do
   end do
end proc
> #Defining a new procedure to generate the matrix whose basis
  depends of S, In and
> Mat:=proc(N,k1,k2)
  delta:=proc(a,b) piecewise(a=b,1,0); end proc;
  #Creating the Basis (Now as a function of sm, im, rm).
  Baseset:=proc(N)
  global B; global ket; global bra;global Bdim;
  i:=1;
  for si from 0 to N
      do
          for ii from 0 to N
               do
                  for ri from 0 to N
                      do
                           if si+ii+ri = N then
                              B[i]:=(si,ii,ri);
                              ket[i]:=Ket(S,si).Ket(In,ii).Ket(R,ri);
                              bra[i]:=Bra(R,ri).Bra(In,ii).Bra(S,si);
                                     i := i+1;
                                  end if;
                      end do;
                  end do;
           end do;
  Bdim:=i-1;
  end proc;
  Baseset(N):
     for i from 1 to Bdim do
          for j from 1 to Bdim do
          A[i,j] := -B[j][2]*((-delta(B[i][2], B[j][2])*(k1*B[j][1]+
  k2) *delta(B[i][1], B[j][1]) +k1 *delta(B[i][1], B[j][1]-1) *B[j][1] *
  delta(B[i][2], B[j][2]+1))*delta(B[i][3], B[j][3])+k2*delta(B[i]
  [1], B[j][1])*delta(B[i][2], B[j][2]-1)*delta(B[i][3], B[j][3]+1)
  );
          end do;
     end do;
  Mt:= Array(1..Bdim, 1..Bdim, (i,j) \rightarrow A[i,j]);
  end proc;
Mat := \mathbf{proc}(N, k1, k2)
                                                                            (3)
   local delta, Baseset, i, j, A, Mt;
   delta := proc(a, b) piecewise(a = b, 1, 0) end proc;
   Baseset := \mathbf{proc}(N)
      local si, ii, ri;
```

```
global B, ket, bra, Bdim;
                     i := 1:
                     for si from 0 to N do
                                for ii from 0 to N do
                                          for ri from 0 to N do
                                                    if si + ii + ri = N then
                                                              B[i] := si, ii, ri;
                                                              ket[i] := Physics:-Ket(S, si) . Physics:-Ket(In, ii) . Physics:-Ket(R, si)
                                                              ri):
                                                              bra[i] := Physics:-Bra(R, ri). Physics:-Bra(In, ii). Physics:-Bra(S, ri)
                                                              i := i + 1
                                                    end if
                                         end do
                                end do
                      end do:
                     Bdim := i - 1
            end proc;
            Baseset(N);
            for i to Bdim do
                     for j to Bdim do
                               A[i,j] := (-1) * B[j][2] * ((-\text{delta}(B[i][2], B[j][2]) * (k1 * B[j][1] + k2))
                                * \det(B[i][1], B[j][1]) + k1 * \det(B[i][1], B[j][1] - 1) * B[j][1] * \det(B[i][1], B[j][1]) + k1 * \det(B[i][1], B[i][1]) + k1 * \det(B[i][1
                                |[2], B[j][2] + 1) * delta(B[i][3], B[j][3]) + k2 * delta(B[i][1], B[j][1])
                                * \det(B[i][2], B[j][2] - 1) * \det(B[i][3], B[j][3] + 1))
                      end do
            end do:
            Mt := Array(1 ..Bdim, 1 ..Bdim, (i, j) \rightarrow A[i, j])
 end proc
        #Defining the solution to the Hamiltonian from the matrix
        exonential - Mat (in the fock space).
 > ExpHt:= proc(N,k1,k2,t)
        MatrixExponential(-Mat(N,k1,k2)*t); end proc;
 ExpHt := \mathbf{proc}(N, k1, k2, t)
                                                                                                                                                                                                                                                      (4)
            LinearAlgebra:-MatrixExponential((-1)*Mat(N, k1, k2)*t)
 end proc
> #defining the moments of the epidemic time
 > TimeMoment = proc(l, N, alpha, beta)
        #calculating the Hamiltonian
         Mat(N, alpha, beta):
          #Initial condition (one infected)
        C := Vector[column](Array([seq(piecewise(j = Bdim - 1, 1, 0), j = 1 ..Bdim)])):
        #Mapping the poisions of zero infectives
```

$$p \coloneqq seq\left(\frac{(N+1)(N+2)}{2} - sum(j, j=2..k), k=1..N+1\right)[i]:$$

#Calculating the vectors carring the states of zero infectives

V := Vector(Array([seq(piecewise(j=p, 1, 0), j=1 ..Bdim)])):

#Calculating the cumulating distribuction function

$$F := sum(V. ExpHt(N, alpha, beta, s).C, i = 1..N + 1)$$
:

#Calculating the probability distribuction function

f := subs(s = t, diff(F, s)):

#Finally, obtaing the moments of epidemic time

$$subs(|alpha| = alpha, |beta| = beta, int(t', f, t = 0...infinity));$$

end proc;

 $TimeMoment := \mathbf{proc}(l, N, alpha, beta)$ (5)

local C, p, V, F, f;

Mat(N, alpha, beta);

C := Vector[column](Array([seq(piecewise(j = Bdim - 1, 1, 0), j = 1 .. Bdim)]));

$$p := seq(1*2^{(-1)}*(N+1)*(N+2) - (sum(j, j=2..k)), k=1..N+1)[i];$$

V := Vector(Array([seq(piecewise(j = p, 1, 0), j = 1 ..Bdim)]));

abs(alpha), abs(beta), s)), C), i = 1..N + 1);

f := subs(s = t, diff(F, s));

 $subs(abs(alpha) = alpha, abs(beta) = beta, int(Typesetting:-delayDotProduct(t^l, f), t = 0$...infinity))

end proc

- > #Testing the results
- > TimeMoment(1, 1, alpha, beta);

$$\frac{1}{\beta}$$
 (6)

> TimeMoment(1, 2, alpha, beta);

$$\frac{1}{2} \frac{3 \alpha + 2 \beta}{\beta (\alpha + \beta)} \tag{7}$$

> TimeMoment(1, 3, alpha, beta);

$$\frac{1}{3} \frac{11 \alpha^3 + 26 \alpha^2 \beta + 15 \alpha \beta^2 + 3 \beta^3}{\beta (2 \alpha^3 + 5 \alpha^2 \beta + 4 \alpha \beta^2 + \beta^3)}$$
(8)

> TimeMoment(1, 4, alpha, beta);

$$\frac{1}{2} \frac{50 \alpha^{6} + 213 \alpha^{5} \beta + 361 \alpha^{4} \beta^{2} + 282 \alpha^{3} \beta^{3} + 111 \alpha^{2} \beta^{4} + 23 \alpha \beta^{5} + 2 \beta^{6}}{\beta \left(12 \alpha^{6} + 52 \alpha^{5} \beta + 91 \alpha^{4} \beta^{2} + 82 \alpha^{3} \beta^{3} + 40 \alpha^{2} \beta^{4} + 10 \alpha \beta^{5} + \beta^{6}\right)}$$
(9)

> TimeMoment(1, 5, alpha, beta);

$$\frac{1}{5} \left(3288 \,\alpha^{10} + 20948 \,\alpha^{9} \,\beta + 58424 \,\alpha^{8} \,\beta^{2} + 93578 \,\alpha^{7} \,\beta^{3} + 92475 \,\alpha^{6} \,\beta^{4} + 58110 \,\alpha^{5} \,\beta^{5} \right)$$
 (10)

$$+23659 \alpha^{4} \beta^{6} +6310 \alpha^{3} \beta^{7} +1085 \alpha^{2} \beta^{8} +110 \alpha \beta^{9} +5 \beta^{10})/(\beta (288 \alpha^{10} +1848 \alpha^{9} \beta^{10}))$$

$$+ 5204 \alpha^{8} \beta^{2} + 8458 \alpha^{7} \beta^{3} + 8777 \alpha^{6} \beta^{4} + 6072 \alpha^{5} \beta^{5} + 2835 \alpha^{4} \beta^{6} + 882 \alpha^{3} \beta^{7}$$

$$+ 175 \alpha^{2} \beta^{8} + 20 \alpha \beta^{9} + \beta^{10}))$$

APPENDIX D - MAPLE CODE FOR THE BASIC REPRODUCTION NUMBER

```
> #In this worksheet we will show the buinding of the SIR
  stochastic Ro from the Fock-Space approach
> restart;
  with(Physics) : with(LinearAlgebra) : with(Student) :
      # First, you have to be sure that you are using the latest version of Physics Package,
      otherwise some commands may not work properly. In this work, we used the update
      Physics61.3 availabe on http://www.maplesoft.com/products/maple/features/physicsresearch.
      aspx
  Physics:-Version();
         "C:\Program Files\Maple 2015\lib\update.mla", 2015, May 19, 16:0 hours
                                                                                     (1)
> #Creating the Basis (Now as a function of S, In, R). Here, we
  suppose some conservations #laws to reduce the dimension of fock
  space. In fact we use that S + In + R = N.
  Baseset:=proc(N) global B; global ket; global bra; global Bdim;
  for si from 0 to N
       do
           for ii from 0 to N
                do
                    for ri from 0 to N
                         do
                             if si+ii+ri = N then
                                  B[i]:=(si,ii,ri);
                                  ket[i]:=Ket(S,si).Ket(In,ii).Ket(R,ri);
                                  bra[i]:=Bra(R,ri).Bra(In,ii).Bra(S,si);
                                  print(i,B[i] = ket[i]);
                                  i:=i+1;
                                  end if;
                             end do;
                    end do;
            end do;
  end proc;
Baseset := \mathbf{proc}(N)
                                                                                     (2)
   local i, si, ii, ri;
   global B, ket, bra, Bdim;
   i := 1:
   for si from 0 to N do
       for ii from 0 to N do
          for ri from 0 to N do
              if si + ii + ri = N then
                 B[i] := si, ii, ri;
                 ket[i] := Physics:-Ket(S, si) . Physics:-Ket(In, ii) . Physics:-Ket(R, ri);
                 bra[i] := Physics:-Bra(R, ri). Physics:-Bra(In, ii). Physics:-Bra(S, si);
                 print(i, B[i] = ket[i]);
```

```
i := i + 1
            end if
         end do
      end do
   end do
end proc
> #Defining a new procedure to generate the matrix whose basis
  depends of S, In and
> Mat:=proc(N,k1,k2)
  delta:=proc(a,b) piecewise(a=b,1,0); end proc;
  #Creating the Basis (Now as a function of sm, im, rm).
  Baseset:=proc(N)
  global B; global ket; global bra;global Bdim;
  i:=1;
  for si from 0 to N
      do
          for ii from 0 to N
              do
                  for ri from 0 to N
                      do
                          if si+ii+ri = N then
                              B[i]:=(si,ii,ri);
                              ket[i]:=Ket(S,si).Ket(In,ii).Ket(R,ri);
                              bra[i]:=Bra(R,ri).Bra(In,ii).Bra(S,si);
                                    i := i+1;
                                 end if;
                      end do;
                 end do;
           end do;
  Bdim:=i-1;
  end proc;
  Baseset(N):
     for i from 1 to Bdim do
          for j from 1 to Bdim do
  #Replacing the Hamiltonian's matrix element found from the
  equation (14).
          A[i,j]:= -B[j][2]*((-delta(B[i][2], B[j][2])*(k1*B[j][1]+
  k2) *delta(B[i][1], B[j][1]) +k1 *delta(B[i][1], B[j][1]-1) *B[j][1] *
  delta(B[i][2], B[j][2]+1))*delta(B[i][3], B[j][3])+k2*delta(B[i]
  [1], B[j][1])*delta(B[i][2], B[j][2]-1)*delta(B[i][3], B[j][3]+1)
  );
          end do;
     end do;
  Mt := Array(1..Bdim, 1..Bdim, (i,j) \rightarrow A[i,j]);
  end proc;
Mat := \mathbf{proc}(N, k1, k2)
                                                                          (3)
   local delta, Baseset, i, j, A, Mt;
   delta := proc(a, b) piecewise(a = b, 1, 0) end proc;
```

```
Baseset := \mathbf{proc}(N)
        local si, ii, ri;
        global B, ket, bra, Bdim;
        i := 1:
        for si from 0 to N do
            for ii from 0 to N do
                for ri from 0 to N do
                    if si + ii + ri = N then
                        B[i] := si, ii, ri;
                        ket[i] := Physics:-Ket(S, si) . Physics:-Ket(In, ii) . Physics:-Ket(R, si)
                        bra[i] := Physics:-Bra(R, ri). Physics:-Bra(In, ii). Physics:-Bra(S, ri)
                        si);
                        i := i + 1
                    end if
                end do
            end do
        end do:
        Bdim := i - 1
    end proc;
    Baseset(N);
    for i to Bdim do
        for j to Bdim do
            A[i,j] := (-1) * B[j][2] * ((-\text{delta}(B[i][2], B[j][2]) * (k1 * B[j][1] + k2)
            * \det(B[i][1], B[j][1]) + k1* \det(B[i][1], B[j][1] - 1)* B[j][1]* \det(B[i][1], B[j][1]
            [2], B[j][2] + 1) * delta(B[i][3], B[j][3]) + k2 * delta(B[i][1], B[j][1])
            * \det(B[i][2], B[j][2] - 1) * \det(B[i][3], B[j][3] + 1))
        end do
    end do;
    Mt := Array(1 ..Bdim, 1 ..Bdim, (i, j) \rightarrow A[i, j])
end proc
   #Defining the solution to the Hamiltonian from the matrix
   exonential - Mat (in the fock space).
> ExpHt:= proc(N,k1,k2,t)
  MatrixExponential(-Mat(N,k1,k2)*t); end proc;
ExpHt := \mathbf{proc}(N, k1, k2, t)
                                                                                                 (4)
    LinearAlgebra:-MatrixExponential((-1)*Mat(N, k1, k2)*t)
end proc
\rightarrow Expi:=proc(R,C,N,k1,k2,t)
   evalf(ExpHt(N,k1,k2,t)[R][C]);
   end proc;
         Expi := \mathbf{proc}(R, C, N, k1, k2, t) evalf (ExpHt(N, k1, k2, t) [R][C]) end \mathbf{proc}
                                                                                                 (5)
```

```
> #Defining a way to give the column vector from the matrix
   exponential
   Vexp:=proc(N,C,k1,k2,t)
   Mat(N,k1,k2):
   <seq(ExpHt(N,k1,k2,t)[i,C],i=1..Bdim)>: end proc;
 Vexp := \mathbf{proc}(N, C, k1, k2, t)
                                                                                           (6)
    Mat(N, k1, k2); \leq seg(ExpHt(N, k1, k2, t) [i, C], i = 1 ..Bdim) >
end proc
> #Taking the vector of susceptible population condition definded
   by the Baseset
   Vs:=proc(k,N)
   Mat(N,k1,k2):
   <seq(B[i][1]**k,i=1..Bdim)>: end proc;
        Vs := \mathbf{proc}(k, N) \ Mat(N, k1, k2); \le seq(B[i][1]^k, i = 1..Bdim) \ge \mathbf{end} \ \mathbf{proc}
                                                                                           (7)
> Vs(1,2)
                                                                                           (8)
> #Defining de susceptible population
> Sk:=proc(k,N,C,k1,k2,t) DotProduct(Vs(k,N),Vexp(N,C,k1,k2,t));
   end proc;
                                                                                           (9)
Sk := \mathbf{proc}(k, N, C, k1, k2, t)
    LinearAlgebra:-DotProduct(Vs(k, N), Vexp(N, C, k1, k2, t))
end proc
> #Defining the R0 from susceptible population and the parameters,
   alpha and beta
> R\theta = proc(N, alpha, beta)
    local M:
   M = \frac{(N+1)\cdot(N+2)}{2} - 1:
   subs(|alpha| = alpha, |beta| = beta, |alpha| \cdot int(exp(-|beta| \cdot s) \cdot Sk(1, N, M, |alpha|, |beta|, s), s
       = 0 ... infinity );
    end proc;
                                                                                          (10)
R\theta := \mathbf{proc}(N, \text{ alpha, beta})
    local M:
    M := 1 * 2^{(-1)} * (N+1) * (N+2) - 1;
    subs(abs(alpha) = alpha, abs(beta) = beta, abs(alpha) * (int(exp((-1) * abs(beta) * s)
     * Sk(1, N, M, abs(alpha), abs(beta), s), s = 0 ...infinity))
```

end proc

> *R0*(1, alpha, beta);

= > *R0*(2, alpha, beta);

$$\frac{2\alpha}{2\beta + \alpha} \tag{12}$$

= > *R0*(3, alpha, beta);

$$\frac{\alpha \left(5 \alpha^{2} + 20 \alpha \beta + 12 \beta^{2}\right)}{2 \alpha^{3} + 9 \alpha^{2} \beta + 13 \alpha \beta^{2} + 6 \beta^{3}}$$
(13)

> *R0*(4, alpha, beta);

$$\frac{6 \alpha \left(34 \alpha^{5} + 232 \alpha^{4} \beta + 628 \alpha^{3} \beta^{2} + 739 \alpha^{2} \beta^{3} + 378 \alpha \beta^{4} + 72 \beta^{5}\right)}{72 \alpha^{6} + 522 \alpha^{5} \beta + 1531 \alpha^{4} \beta^{2} + 2325 \alpha^{3} \beta^{3} + 1928 \alpha^{2} \beta^{4} + 828 \alpha \beta^{5} + 144 \beta^{6}}$$
(14)

$$\begin{array}{l} \hline > R\theta(5, \text{alpha, beta}); \\ & \left(2\alpha\left(1776\alpha^8 + 16244\alpha^7\beta + 63580\alpha^6\beta^2 + 139751\alpha^5\beta^3 + 181371\alpha^4\beta^4 + 138806\alpha^3\beta^5 \right) \\ & + 61076\alpha^2\beta^6 + 14472\alpha\beta^7 + 1440\beta^8)\right) / \left(1152\alpha^9 + 10944\alpha^8\beta + 45016\alpha^7\beta^2 \right) \\ & + 105204\alpha^6\beta^3 + 153902\alpha^5\beta^4 + 146111\alpha^4\beta^5 + 90009\alpha^3\beta^6 + 34696\alpha^2\beta^7 + 7596\alpha\beta^8 \\ & + 720\beta^9) \end{array}$$