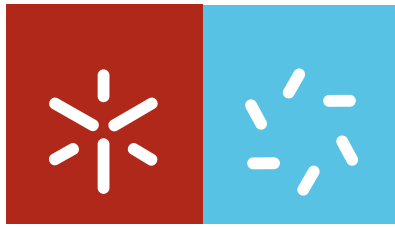




Universidade do Minho
Escola de Ciências

José Maria Gouveia Martins

Thresholds for epidemiological outbreaks



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Tese de Doutoramento em Ciências
Área de Conhecimento em Matemática

Trabalho efectuado sob orientação do
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Título da tese: **Thresholds for epidemiological outbreaks**

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Doutoramento em Ciências, Área de conhecimento Matemática

Novembro de 2009

É AUTORIZADA A REPRODUÇÃO INTEGRAL DESTA TESE
APENAS PARA EFEITOS DE INVESTIGAÇÃO, MEDIANTE DECLARAÇÃO
ESCRITA DO INTERESSADO, QUE A TAL SE COMPROMETE;

Universidade do Minho, 09 de Novembro de 2009

Assinatura:

Acknowledgments

This work would not be like this without the support of my supervisors. Their ideas, their knowledge and their encouragement were essential for the development of this work. Hence, my first acknowledgments go to my supervisors: Professor Alberto Pinto, a brilliant mathematician with a huge amount of new ideas in his head, and Professor Nico Stollenwerk that with his deep knowledge of epidemiological models showed me the beauty of the applications of mathematics.

I also acknowledge the financial support from FCT - *Fundação para a Ciência e a Tecnologia* given by the PhD grant with reference SFRH/BD/37433/2007.

For the conditions offered to this project and the warm host I thank the University of Minho, Mathematics Department of School of Sciences. For all the care in the coordination of my professional work I thank the Mathematics Department of the School of Technology and Management of Polytechnic Institute of Leiria.

A very special thanks goes out to my family. Their encouragement and constant concern were an additional incentive. Especially to my parents, Joaquim and Irene, to whom I owe everything I have and I am, but also to my brother Joaquim and remaining family, I thank from the bottom of my heart.

For all my friends that somehow contributed with comments, discussions or encouragement I express here my gratitude and the certainty that I will never forget them.

My last acknowledgment goes to the main source of my inspiration: Catarina. Thanks for everything.

Abstract

The characterization of the critical thresholds in epidemic models is probably the most important feature of the mathematical epidemiology research due to the drastic change of the disease spread on the critical threshold. Hence, the study of the critical thresholds and the epidemic behaviour near these thresholds, especially in the SIS and the SIRI epidemiological models, is present among all the chapters of this thesis.

In chapter 2, we introduce the stochastic SIS model and study the dynamical evolution of the mean value, the variance and the higher moments of the infected individuals. To establish the dynamical equations for all the moments we develop recursive formulas and we observe that the dynamic of the m first moments of infecteds depend on the $m + 1$ moment. Using the moment closure method we close the dynamical equations for the m first moments of infecteds and we developed for every m a recursive formula to compute the equilibria manifold of these equations.

In chapter 3, we consider equilibria manifold obtained from the dynamical equations for the m first moments of infecteds on the SIS model and we study when the stable equilibria can be a good approximation of the quasi-stationary mean value of infecteds. We discover that the steady states

give a good approximation of the quasi-stationary states of the SIS model not only for large populations of individuals but also for small ones and not only for large infection rate values but also for infection rate values close to its critical values.

In chapter 4, we consider the spatial stochastic SIS model formulated with creation and annihilation operators. We study the perturbative series expansion of the gap between the dominant and subdominant eigenvalues of the evolution operator of the model and we compute explicitly the first terms of the series expansion of the gap.

In chapter 5, we present the reinfection epidemic SIRS model and study the dynamical equations for the state variables. We compute the phase transition diagram in the mean field approximation and observe the so called reinfection threshold. Moreover, we compute the phase transition lines analytically in pair approximation improving the mean field results.

Resumo

A caracterização de limiares críticos em modelos epidemiológicos é provavelmente o aspecto mais importante da investigação matemática em epidemiologia, devido à mudança drástica da propagação epidémica no limiar crítico. Assim, o estudo dos limiares críticos e do comportamento epidémico junto destes limiares críticos, especialmente no modelo SIS e no modelo SIRI, está presente em todos os capítulos desta tese.

No capítulo 2, introduzimos o modelo estocástico SIS e estudamos a evolução dinâmica do valor médio, da variância e dos momentos de ordem mais elevada da quantidade de indivíduos infectados. Para estabelecer as equações dinâmicas para os momentos de todas as ordens desenvolvemos fórmulas recursivas e observamos que a dinâmica dos m primeiros momentos depende do momento de ordem $m + 1$. Utilizando o método “moment closure” fechamos as equações dinâmicas para os m primeiros momentos da quantidade de indivíduos infectados e desenvolvemos para cada m uma fórmula recursiva que permite obter os equilíbrios resultantes da dinâmica dos momentos.

No capítulo 3, consideramos os equilíbrios obtidos a partir das equações de variação dos m primeiros momentos da quantidade de indivíduos

infectados, no modelo SIS, e estudamos quando é que os equilíbrios estáveis constituem boas aproximações do valor médio quase-estacionário desta quantidade. Descobrimos que estes equilíbrios fornecem uma boa aproximação dos estados quase-estacionários do modelo SIS, não só para populações de grande dimensão mas também de pequena dimensão e não só para valores elevados da taxa de infecção mas também para valores da taxa de infecção próximos do valor crítico.

No capítulo 4, consideramos o modelo estocástico SIS com estrutura espacial, formulado a partir dos operadores de criação e de aniquilação. Estudamos a expansão em série da diferença entre o valor próprio dominante e subdominante do operador evolução deste modelo e calculamos explicitamente os primeiros termos desta expansão.

No capítulo 5, apresentamos o modelo epidemiológico de reinfeção SIRI e estudamos as equações dinâmicas para as variáveis de estado. Calculamos o diagrama de transição de fase para a aproximação de campo médio e observamos o chamado limiar crítico de reinfeção. Além disso, calculamos as linhas de transição de fase analiticamente para a aproximação par, melhorando os resultados obtidos na aproximação de campo médio.

Contents

Acknowledgments	iii
Abstract	v
Resumo	vii
1 Introduction	19
2 Moment closure in the SIS model	29
2.1 The stochastic SIS model	29
2.2 The m moment closure SIS ODEs	31
2.2.1 The mean field approximation	38
2.2.2 The Gaussian approximation	41
2.2.3 The moment closure of third order	45
2.3 The threshold evolution	49
3 Quasi-stationarity in the SIS model	55
3.1 Quasi-stationary distribution	55
3.2 Quasi-stationary approximations	62
3.3 Approximating the quasi-stationary states	63
4 The SIS model with creation and annihilation operators	67

4.1	The spatial stochastic SIS model	67
4.1.1	The creation and annihilation operators	68
4.1.2	The σ representation	72
4.2	Series expansion	78
4.3	Explicit calculation of series expansion	86
4.3.1	Critical values	89
5	The phase transition lines in the SIRI model	91
5.1	The SIRI epidemic model	91
5.1.1	The ODEs for the moments	94
5.2	Mean field approximation	107
5.2.1	The reinfection threshold	110
5.3	Critical points and phase transition lines in pair approxima- tion	113
5.3.1	Pair approximation	115
5.3.2	Stationary states of the SIRI model	118
5.3.3	The $\tilde{\beta} = \beta$ limit or SIS limit	119
5.3.4	The $\alpha = \mathbf{0}$ limit	121
5.3.5	The $\tilde{\beta} = \mathbf{0}$ limit or SIR limit	124
5.3.6	Simulations of the pair approximation ODEs	125
5.4	Analytic expression of the phase transition line	128

List of Figures

2.1	<i>Stationary values of $\langle I \rangle$ in dependence of β, for $\alpha = 1$ and $N = 100$, in the mean field approximation.</i>	40
2.2	<i>a) Stationary values of $\langle I \rangle$ in terms of β for $\alpha = 1$ and $N = 100$. b) Real versus the imaginary part of $\langle I \rangle^*$ presented in a).</i>	42
2.3	<i>a) Simulation of the system Eq. (2.25) with the initial condition $X(0) = [1 \ 1]^T$, for the particular case of $\alpha = 1$ and $N = 100$ with $\beta = 1.002$. b) The same simulation of a) but now for $\beta = 1.005$.</i>	44
2.4	<i>The real stationary equilibria of system Eq. (2.31) as function of β. The usual parameters $\alpha = 1$ and $N = 100$ were used.</i>	47

-
- 2.5 *The stationary mean value of infecteds for the m moment closure ODEs, presented Eq. (2.20), for different values of β . In a), we consider the dynamic of the first five moments of infecteds $m = 5$ and therefore the system has 5 equations. In b), we consider $m = 11$. The thick lines correspond to the stable equilibria and the others to the unstable. The parameters $\alpha = 1$ and $N = 100$ were used. 49*
- 3.1 a) *We compare the quasi stationary mean value of infecteds $\langle I \rangle_{QS}$ with the approximated value $\langle I \rangle_{QS,Apx}$, for different infection rates β . b) Distance $|\langle I \rangle_{QS} - \langle I \rangle_{QS,Apx}|$. Parameters $N = 100$ and $\alpha = 1$ 63*
- 3.2 *Distance $|\langle I \rangle_{m,\beta}^* - \langle I \rangle_{QS,\beta}|$ between the first moment of infecteds obtained by the successive m moment closure ODEs $\langle I \rangle_{m,\beta}^*$ and the quasi-stationary mean value $\langle I \rangle_{QS}$. In a), we consider the quasi-stationary mean value obtained from the distribution presented in Eqs. (3.5) to (3.8) and in b), the approximated distribution presented in Eq. (3.20). The population size used is $N = 100$ 64*

- 5.1 a) *The conventional picture of the reinfection threshold, in semi-logarithmic plot [14]. We just use the parameter α instead of the death out of all classes and birth into susceptibles. The value for $\sigma = 1/4$ will also be used in Fig. 5.1 b), and $\varepsilon = 0.00001$ to demonstrate a clear threshold behaviour around $\rho = 1/\sigma$. b) The solution $i_2^* = -\frac{r}{2} + \sqrt{\frac{r^2}{4} - q}$, full line is plotted against the curves $-r$ and its modulus $|r|$. While i_2^* changes from negative to positive at $\rho = 1$, the curves for $-r$ and $|r|$ change at $\rho = 1/\sigma$ for vanishing or small ε . This qualitative change at $\rho = 1/\sigma$ is the reinfection threshold. Parameters are $\sigma = 1/4 = 0.25$ and $\varepsilon = 0.01$ 109*
- 5.2 a) *The stationary value of the number of infected individuals with both parameters ρ and ε shows for high ε values just a threshold behaviour at $\rho = 1$, and for vanishing ε the threshold for $\rho = 1/\sigma$. Here in the graphic plot $\rho = 1/\sigma = 4$, where beforehand σ was fixed to be $\sigma = 1/4$. b) When we look at larger values of ε , here up to $\varepsilon = 0.2$, we also find back the first threshold at $\rho = 1$. The continuous change from behaviour dominated by the first threshold $\rho = 1$ for $\varepsilon = 0.2$ to the behaviour only determined by the behaviour around the second threshold $\rho = 1/\sigma$ for $\varepsilon = 0$ can be seen here. 111*

5.3	<i>Phase diagram for the mean field model. For consistency with the previously investigated two-dimensional case, we set $Q = 4$ neighbours. The mean field phase diagram is however in good agreement with spatial simulations above the upper critical dimension [5].</i>	113
5.4	<i>The mean field solution of the SIS limiting case (isolated dashed line), the pair approximation solution (dotted line) for $\langle I \rangle^*(\beta)$ and the convergence of the time dependent solution of the SIRI pair dynamics. The critical value for the pair contact process is given as well as $\beta_c = 0.4122$.</i>	121
5.5	<i>The critical point in pair approximation for $\tilde{\beta} = \beta$, the SIS limiting case.</i>	122
5.6	<i>The phase transition line for $\alpha = 0$ obtained in pair approximation.</i>	123
5.7	<i>The critical point for $\tilde{\beta} = 0$ (the SIR-limit) obtained in pair approximation.</i>	125
5.8	<i>a) The $I(t_{max})$ obtained integrating the system Eqs. (5.43) to (5.47) numerically up to time t_{max} with changing $\tilde{\beta}$ for $\beta = \gamma/(Q - 1)$, the SIS critical point value. b) The logarithm of $I(t)$ versus $\ln(t)$ for various $\tilde{\beta}$ values.</i>	126
5.9	<i>a) $I(t_{max})$ for $\beta = \gamma/(Q - 2)$, the SIR critical point value in the limit $\alpha = 0$. b) $\ln(I(t))$ versus $\ln(t)$ for various $\tilde{\beta}$ values.</i>	126
5.10	<i>a) $I(t_{max})$ for $\beta = \gamma/(Q - 1.5)$, i.e. between the SIS critical point and the SIR critical point. b) $\ln(I(t))$ versus $\ln(t)$ for various $\tilde{\beta}$ values.</i>	127

-
- 5.11 *Comparison for the phase transition line between no-growth and ring-growth determined numerically for small but finite $\alpha = 0.05$, straight line, and the analytic solution in the limit when α tends to zero, dotted line. 128*
- 5.12 *The phase transition line between no-growth and annular growth determined from the analytic solution in the limiting case when α tends to zero which is explicitly given in Eq. (5.98). The horizontal transition line of the SIRI limiting case when $\alpha = 0$ and the phase transition points of SIS and SIR limiting cases are also presented as calculated in [43]. The SIS and SIR limiting cases are given by dashed lines. (Parameters $Q = 4$ appropriate for spatial two dimensional systems and $\gamma = 1$ were used.) 137*

List of Tables

2.1	The critical values of β , for $N = 100$ and $\alpha = 1$, considering the dynamic of the nine first moments.	50
2.2	The critical values of β , their distances and the ratio between the distances, for $N = 100$ and $\alpha = 1$, considering the dynamic of an odd number of moments m	53
3.1	Values of the cumulants $\langle\langle I^n \rangle\rangle_{QS,\beta}$, $n = 1, 2, 3$, of the quasi-stationary distribution of infecteds for different population sizes $N = 10, 100$ and 1000 , taking $\beta = 5$ and $\alpha = 1$. In the third, fourth and fifth columns we present the distances $d_m = \langle\langle I^n \rangle\rangle_{QS,\beta} - \langle\langle I^n \rangle\rangle_{m,\beta}^* $ between these cumulants and the corresponding cumulants $\langle\langle I^n \rangle\rangle_{m,\beta}^*$ obtained from the $m = 3, 5$ and 15 moment closure ODEs.	65
4.1	The coefficients c_n of the expansion of the gap Γ	89
4.2	Critical parameter λ_c and the critical exponent $v_{ }$, obtained from the Padé approximants.	90

Chapter 1

Introduction

Registries of epidemic outbreaks exist almost from the beginning of the recorded history. Already in the Book of Exodus, from the Christian Old Testament, Moses describes the plagues in Egypt. But many other biblical descriptions of epidemic outbreaks can be found. The understanding of a disease spread has tremendous implications upon the health and wealth of a community. For example, the Black Death throughout Europe and much of Asia in the 14th century, the invasions of cholera in India in the 19th century and the influenza epidemic of 1918/19 in United States, that causes the death of millions of people, clearly justifies the importance of the mathematical epidemiology. More recently, the Ebola virus, the SARS, the avian flu and the current H1N1 flu demand the continuous development of this research field.

Maybe, the first author working in the mathematical modeling of infectious diseases was Daniel Bernoulli in 1766. But many other physicians gave significant contributions to the mathematical modeling theory, such as

Malthus, Verhulst, Hamer, Ross, Soper, etc.. A great triumph of mathematical epidemiology was achieved by W.O. Kermack and A.G. McKendrick in 1927. They divided the population into three different compartments - the susceptibles, the infected and the removed individuals - and formulated the deterministic SIR model. Under the very simple assumptions of the model they observe a threshold phenomenon. If the average number of new infections caused by a single infective individual, called the *basic reproduction number*, is less than 1 the epidemic tends to disappear while if it exceeds 1 the epidemic increases (see [3, 25]). The characterization of the thresholds in epidemic models is important due to the drastic change of the disease spread above and below the threshold (see [44]). For a detailed description of the threshold concept see [29]. In this thesis the analyses of the thresholds for epidemiological outbreaks is a constant concern.

With the evolution of the mathematical epidemiology the stochastic models become more and more important. These are Markov processes with discrete state space. The stochastic version of a model is more realistic for populations with small size N and the deterministic models can be derived as approximations of the stochastic ones by letting the population size N approach infinity. For small populations the spatial structure in epidemic models is also vital since only the interactions with the nearest neighbours are more important to take into account (see [12]). Using the various sources of information, nowadays, the universe of the epidemic models is vast (see [2, 3]). In this work, we focus our study in two epidemiological models: the SIS (Susceptible-Infected-Susceptible) and the SIRI (Susceptible-Infected-Recovered-Infected) model. The SIS model

describes the spread of a disease through a population of individuals that can be susceptibles, infecteds and again susceptibles to the infection. We use the SIS model for endemic infections that do not confer immunity. The SIRS model is a reinfection model that confers partial immunization and is used to describe an infection through a population of individuals that can be susceptibles, infected, recovered and again infected. The work presented in this thesis were developed considering the following assumptions valid for every epidemiological models analysed:

- The disease is transmitted by contact between an infected individual and a susceptible one;
- There is no latent period for the disease, hence it is transmitted instantaneously upon contact;
- All susceptible individuals are equally susceptible and all infected are equally infectious;
- The population under consideration is fixed in size.

Below, we present a more detailed description of the study made in each chapter of this thesis.

Moment closure in the SIS model

The stochastic SIS model is a well known epidemiological model (see [3]) introduced by Weiss and Dishon [48] and a special case of more complex models, like the reinfection SIRS model (see [43, 26]). The letters S and I correspond to the susceptible and infected individuals, respectively, and

the usual designation SIS indicates the successive states of an individual. This simple mathematical model has been extensively used in many other applications, including sociology, chemistry, ecology, etc.. It can also be interpreted, in a different context, as the stochastic logistic model with applications to the study of populations dynamics (see [34]). But it is in the epidemiological context that this model achieved a huge importance and the mathematical theory is most developed. In the SIS model, individuals do not acquire immunity after the infection and return directly to the susceptible class. Hence, this model is used for endemic infections that do not confer immunity. The stochastic SIS model can also be interpreted as a birth-and-death process with a finite state space, correspondent to the number of infected individuals $I(t) \in \{0, 1, 2, \dots, N\}$ at time t and susceptibles $S(t) = N - I(t)$. In an epidemiological context, many authors worked on the SIS model considering only the dynamical evolution of the mean value of the infected individuals or, at most, the variance.

In chapter 2, we present the stochastic version of the SIS epidemic model and we derive recursively the dynamic equations for all the moments, using the moment closure method. We develop a recursive formula to compute the equilibria manifold of the m moment closure ODEs and we analyse the evolution of the SIS threshold with the moment closure method (see also [28]).

Quasi-stationarity in the SIS model

The concept of the quasi-stationarity for continuous Markov chains was introduced by Darroch and Seneta [6]. This distribution is supported in the set of the transient states and it is a useful approximation of the states distribution before the equilibrium being attained. In an epidemic setting the quasi-stationary distribution was first studied by Kryscio and Lefevre (see [23]) and more recently by Nåsell among other authors (see [10, 30, 31, 32, 33]). In epidemic models the importance of the quasi-stationary distribution is concerned with the description of the long-time behaviour of the model and the time to extinction of the epidemics. The absorbing classes correspond to the absence of infection and the equilibrium can be interpreted as extinction of the infection. For the stochastic SIS model, we know that the state $I(t) = 0$ is the only one absorbing and all the other are transient and therefore the stationary distribution is degenerated with probability one at this state. However, the time to reach the equilibrium $I(t) = 0$ can be so long that the stationary distribution is non informative. Hence, our interest goes to compute the quasi-stationary mean value of infecteds $\langle I \rangle_{QS}$. The quasi-stationary distribution of the stochastic SIS model is the stationary distribution of the stochastic process conditioned to the non-extinction of the infected individuals (see [23, 30, 28]). Since the quasi-stationary distribution of the stochastic SIS model does not have explicit form, it is useful to approximate the model in order to obtain explicit approximations of the quasi-stationary distribution. Two possible approximations were studied by Kryscio and Lefevre [23] and by Nåsell [30, 31].

These approximations of the stationary distributions can be determined explicitly and give good approximations of the quasi-stationary distribution of the SIS model when the infection rate β is distinctly smaller or greater than the recovery rate α and the population size N is relatively large (see [31]). A different approach using dynamical systems methods is presented by Nåsell [35]. Nåsell uses the stable equilibria of the 1 to 3 moment closure ODEs to obtain approximations of the quasi-stationary mean value of infecteds for high values of the population size N .

In chapter 3, we observe that the stable equilibria of the m moment closure ODEs can also be used to give a good approximation of the quasi-stationary mean value of infecteds for relatively small populations size N and also for relatively small infection rates β by taking m large enough (see also [28]).

The SIS model with creation and annihilation operators

The simple spatial stochastic SIS epidemic model, also known as the contact process, has a continuous phase transition from the absorbing state devoid of infected individuals to a nonequilibrium state of infectivity. The phase transition point of the SIS model was recently characterized in pair approximation as particular case of the reinfection SIRI model (see [43, 26]), and improves the rough qualitative behaviour in mean field approximation. In the phase transition the dominant eigenvalue of the evolution operator

for the SIS model becomes degenerate, that occurs when the gap between the dominant and the subdominant eigenvalues vanishes. To study the gap value, series expansions in terms of the creation rate have been used (see [8, 21, 7]). This requires the formulation of the epidemic models in terms of creation and annihilation operators (see [11, 16, 17, 37, 45]) starting from the master equation (see [47, 19]). The critical values follows from the series expansion, based on a perturbation ansatz and using a Padé analysis (see [21, 7]).

In chapter 4, we consider the spatial stochastic SIS epidemic model formulated via creation and annihilation operators. For the SIS model in one dimensional lattices, we deduce the perturbative series expansion of the gap between the dominant and subdominant eigenvalues of the evolution operator. The first terms of the series expansion of the gap are computed explicitly. Here, we do not assume the translation invariance of the lattice in contrast to the study made by de Oliveira [7] (see also [27]).

The phase transition lines in the SIRS model

Models for reinfection processes in epidemiology have been recently attracted interest, especially for a first description of multi-strain epidemics (see [14, 15]). In the physics literature models for partial immunization have also found wide interest (see [18, 5]), under somehow different aspects though. Transitions between no-growth, compact growth and annular growth have been observed in both cases (see [18]). Hence, the study of the phase transition lines for the basic epidemic model for reinfection

and partial immunization SIRI - susceptible, infected, recovered and again infected - becomes a difficult but also an important task. Two limiting cases of the SIRI model, depending upon the model parameters, are the SIS and the SIR model. The SIS limiting case corresponds to consider equal primary and secondary infection rates and the SIR limiting case corresponds to vanish the reinfection rate. The transition between annular and compact growth has been found for mean field like models under the name of reinfection threshold by Gomes, White and Medley [14]. In their stationary states analysis they found a first threshold between a disease free state and a non-trivial state with strictly positive endemic equilibrium. Besides this first threshold they found a second threshold characterized by the ratio between first and secondary infection rate. This second threshold they call the “reinfection threshold”. However, this notion of the reinfection threshold has been under debate. Breban and Blower in 2005 simply claim that “The reinfection threshold does not exist” [4]. An immediate reply by Gomes, White and Medley [15] on the importance of the reinfection threshold emphasizes the epidemiological implications of vaccine efforts being successful below the threshold but not above.

In chapter 5, we describe the reinfection SIRI model in its stochastic description. Deriving dynamic equations for the expectation values of total number of susceptibles, infected and recovered we obtain expressions of pairs, then writing dynamic equations for these we obtain triplets, etc.. We start to calculate the mean field approximation of this stochastic spatial epidemiological SIRI model for the dynamics of the mean total numbers of susceptibles, infected and recovered, and we compute the stationary states

of the model. In the limit of vanishing the transition from recovered to susceptibles we obtain a sharp threshold behaviour characterized by the parameter values of the reinfection threshold of Gomes, White and Medley, concluding that the reinfection threshold does exist (see also [46]). We also consider the pair approximation to obtain a closed system of dynamic equations for means and pairs. In this approximation we compute the critical parameters improving the mean field results, in which the limiting cases of SIS and SIR model have the same critical values for the transition from no-growth to a nontrivial stationary state. In the case of the SIS model that is the transition from no-growth to compact growth of an area of infection and in the case of the SIR model it is the transition from no-growth to annular growth, a ring of infecteds leaving recovered behind. In pair approximation these critical points have different values, as previously calculated for the SIS system (see [24]) and the SIR system (see [22]). For the SIRS model in pair approximation, the ODEs for means and pairs are analyzed further to obtain the stationary states and the critical lines. We compute analytically the phase transition lines between no-growth and compact growth, between annular growth and compact growth and between no-growth and annular growth, and compare the especially tricky phase transition line between no-growth and annular growth with simulations. We present a detailed proof of the explicit formula of this last phase transition line, that could only be calculated via a scaling argument (see also [43, 26]).

Chapter 2

Moment closure in the SIS model

In this chapter we introduce one of the simplest stochastic epidemic models: the SIS model. Here, we derive recursively the dynamic equations for all the moments of the infecteds, using the moment closure method, and we derive recursively the stationary states of the state variables.

2.1 The stochastic SIS model

We consider the stochastic SIS (Susceptible-Infected-Susceptible) model that describes the evolution of an infectious disease in a population of N individuals. Each individual can be either infected or susceptible. Denoting the global quantity of susceptible individuals by $S(t)$ and the infected quantity by $I(t)$, at time t , we obtain that $S(t) + I(t) = N$. The stochastic SIS model is a birth-and-death process with a finite state space, correspondent

to the number of infected individuals $I(t) \in \{0, 1, 2, \dots, N\}$ at time t . The birth rate β is the probability, per unit of time, of one infected individual contact with a susceptible one and transmit the disease. The death rate α is the probability, per unit of time, of one infected individual recover and become susceptible again. In an epidemiological context, the rate β is known as the infection rate and α as the recovery rate. Thus, in the SIS model the spreading of the epidemic can be illustrated by



Let $p(I, t)$ denotes the probability of having I infecteds at time t . The time evolution of the probability $p(I, t)$ is given by the master equation of the SIS model

$$\begin{aligned} \frac{d}{dt} p(I, t) &= \beta \frac{N - (I - 1)}{N} (I - 1) p(I - 1, t) \\ &+ \alpha (I + 1) p(I + 1, t) \\ &- \left(\beta \frac{N - I}{N} I + \alpha I \right) p(I, t) \quad , \end{aligned} \tag{2.1}$$

with $I \in \{0, 1, \dots, N\}$. The master equation is a gain-loss equation for the probability of each state, also known as the differential form of the Chapman-Kolmogorov equation, described for general Markov processes in [1] and especially applied to chemical reactions in [47].

2.2 The m moment closure SIS ODEs

We will derive the dynamics of the m first moments of infecteds $\langle I \rangle$, $\langle I^2 \rangle$, ..., $\langle I^m \rangle$, for the m moment closure ODEs, using the moment closure method and we will compute the stable equilibria manifold.

Let $\langle I^n \rangle$ denote the n^{th} moment of the state variable I that is given by

$$\langle I^n \rangle(t) = \sum_{I=0}^N I^n p(I, t) \quad . \quad (2.2)$$

The dynamic ordinary differential equation (ODE) of any moment of infecteds $\langle I^n \rangle$ is stated below in Theorem 2.2.1.

Theorem 2.2.1 *The ODE of the n^{th} moment of infecteds, derived from the master equation, is given by*

$$\frac{d}{dt} \langle I^n \rangle = f_n (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^n \rangle) - \frac{\beta}{N} n \langle I^{n+1} \rangle \quad , \quad (2.3)$$

where

$$\begin{aligned} f_n (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^n \rangle) &= \sum_{j=1}^n \binom{n}{j} (\beta + (-1)^j \alpha) \langle I^{n+1-j} \rangle \\ &\quad - \frac{\beta}{N} \sum_{j=2}^n \binom{n}{j} \langle I^{n+2-j} \rangle \quad . \end{aligned} \quad (2.4)$$

Proof. Using the master equation presented in Eq. (2.1), we compute

the dynamics for the moments of infecteds $\langle I^n \rangle = \sum_{I=0}^N I^n p(I, t)$ by

$$\begin{aligned} \frac{d}{dt} \langle I^n \rangle &= \sum_{I=0}^N \left[\beta I^n \frac{N - (I - 1)}{N} (I - 1) p(I - 1, t) \right. \\ &\quad \left. + \alpha I^n (I + 1) p(I + 1, t) \right. \\ &\quad \left. - \left(\beta \frac{N - I}{N} I^{n+1} + \alpha I^{n+1} \right) p(I, t) \right] . \end{aligned} \quad (2.5)$$

We observe that

$$\begin{aligned} \sum_{I=0}^N \beta I^n \frac{N - (I - 1)}{N} (I - 1) p(I - 1, t) &= \sum_{\tilde{I}=-1}^{N-1} \beta (\tilde{I} + 1)^n \frac{N - \tilde{I}}{N} \tilde{I} p(\tilde{I}, t) \\ &= \sum_{I=0}^N \beta (I + 1)^n \frac{N - I}{N} I p(I, t) . \end{aligned}$$

Assuming that $p(I = N + 1, t) = 0$ in a population of size N , we obtain

$$\begin{aligned} \sum_{I=0}^N \alpha I^n (I + 1) p(I + 1, t) &= \sum_{\tilde{I}=1}^{N+1} \alpha (\tilde{I} - 1)^n \tilde{I} p(\tilde{I}, t) \\ &= \sum_{I=0}^N \alpha (I - 1)^n I p(I, t) . \end{aligned}$$

Therefore, from Eq. (2.5), it follows that

$$\begin{aligned} \frac{d}{dt} \langle I^n \rangle &= \sum_{I=0}^N \left[\beta (I + 1)^n \frac{N - I}{N} I + \alpha (I - 1)^n I - \beta \frac{N - I}{N} I^{n+1} \right. \\ &\quad \left. - \alpha I^{n+1} \right] \cdot p(I, t) . \end{aligned} \quad (2.6)$$

Using that $(a + b)^n = \sum_{j=0}^n \binom{n}{j} a^{n-j} b^j$, we obtain

$$\begin{aligned} \frac{d}{dt} \langle I^n \rangle = \sum_{I=0}^N \left[\beta \sum_{j=0}^n \binom{n}{j} I^{n-j} \frac{N-I}{N} I + \alpha \sum_{j=0}^n \binom{n}{j} I^{n-j} (-1)^j I \right. \\ \left. - \beta \frac{N-I}{N} I^{n+1} - \alpha I^{n+1} \right] \cdot p(I, t) \end{aligned} \quad (2.7)$$

that can be rewritten as follows

$$\begin{aligned} \frac{d}{dt} \langle I^n \rangle &= \sum_{I=0}^N \left[\beta I^n \frac{N-I}{N} I + \beta \sum_{j=1}^n \binom{n}{j} I^{n-j} \frac{N-I}{N} I + \alpha I^n I \right. \\ &\quad \left. + \alpha \sum_{j=1}^n \binom{n}{j} I^{n-j} (-1)^j I - \beta \frac{N-I}{N} I^{n+1} - \alpha I^{n+1} \right] \cdot p(I, t) \\ &= \sum_{I=0}^N \left[\beta \sum_{j=1}^n \binom{n}{j} I^{n+1-j} \frac{N-I}{N} + \alpha \sum_{j=1}^n (-1)^j \binom{n}{j} I^{n+1-j} \right] \\ &\quad \cdot p(I, t) \quad . \quad (2.8) \end{aligned}$$

In the mean value notation, we have

$$\begin{aligned} \frac{d}{dt} \langle I^n \rangle &= \frac{\beta}{N} \sum_{j=1}^n \binom{n}{j} \langle I^{n+1-j} (N-I) \rangle + \alpha \sum_{j=1}^n (-1)^j \binom{n}{j} \langle I^{n+1-j} \rangle \\ &= \sum_{j=1}^n \binom{n}{j} (\beta + (-1)^j \alpha) \langle I^{n+1-j} \rangle - \frac{\beta}{N} \sum_{j=1}^n \binom{n}{j} \langle I^{n+2-j} \rangle \end{aligned} \quad (2.9)$$

and Eq. (2.9) can be easily written like presented in Theorem 2.2.1. ■

We observe that the dynamic of n^{th} moment $\langle I^n \rangle$ depends on the $\langle I^{n+1} \rangle$ moment and therefore the ODE system of the m first moments of infecteds are not closed. However, for analysis purposes we have to close the ODE

system applying the so called moment closure technique and approximate the higher-order moments by a nonlinear function of lower-order moments. The moment closure technique was introduced by Whittle [49] and consists in assuming that the distribution of the state variables are approximately normal. Hence, all cumulants beyond the second are approximately zero. Other moment closure methods was study e.g. in [35, 41].

Let $p : \mathbb{R} \rightarrow \mathbb{C}$ denotes the characteristic function of the state variable I

$$p(k) = \langle e^{ikI} \rangle = \sum_{I=0}^N e^{ikI} p(I, t) \quad , \quad (2.10)$$

and k_n the n^{th} cumulant of I defined implicitly by

$$\ln p(k) = \sum_{n=1}^{\infty} k_n \frac{(ik)^n}{n!} \quad . \quad (2.11)$$

We denote the n^{th} cumulant of I by $k_n = \langle\langle I^n \rangle\rangle$. There is a relation between cumulants and moments [36, 42] given by

$$\langle\langle I^{n+1} \rangle\rangle = \langle I^{n+1} \rangle - \sum_{j=1}^n \binom{n}{j} \langle I^j \rangle \langle\langle I^{n+1-j} \rangle\rangle, \quad n \geq 1 \quad , \quad (2.12)$$

where the first cumulant is equal to the mean value of the infecteds $\langle\langle I \rangle\rangle = \langle I \rangle$. To apply the moment closure technique, we will use the following Lemma that gives the moment closure function.

Lemma 2.2.1 *Assuming that $\langle\langle I^{m+1} \rangle\rangle = 0$, there is a polynomial function $g_m(\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^{m-1} \rangle)$ such that*

$$\langle I^{m+1} \rangle = g_m(\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^{m-1} \rangle) + (m+1)\langle I \rangle \langle I^m \rangle \quad . \quad (2.13)$$

Proof. We know that if I is a random variable with the n first moments $\langle I^k \rangle$, $k \in \{0, 1, \dots, n\}$, then it has cumulants of the same order that can be computed by the recursive formula given in Eq. (2.12) as shown in [36, 42]. Hence, assuming that $\langle\langle I^{m+1} \rangle\rangle = 0$ we obtain that

$$\begin{aligned} \langle I^{m+1} \rangle &= \sum_{j=1}^m \binom{m}{j} \langle I^j \rangle \langle\langle I^{m+1-j} \rangle\rangle \\ &= m\langle I \rangle \langle\langle I^m \rangle\rangle + \sum_{j=2}^{m-1} \binom{m}{j} \langle I^j \rangle \langle\langle I^{m+1-j} \rangle\rangle + \langle I^m \rangle \langle\langle I \rangle\rangle \quad (2.14) \end{aligned}$$

Applying the recursive formula given in Eq. (2.12) to compute the cumulant $\langle\langle I^m \rangle\rangle$, it follows that

$$\begin{aligned} \langle I^{m+1} \rangle &= m\langle I \rangle \left(\langle I^m \rangle - \sum_{j=1}^{m-1} \binom{m-1}{j} \langle I^j \rangle \langle\langle I^{m-j} \rangle\rangle \right) \\ &\quad + \sum_{j=2}^{m-1} \binom{m}{j} \langle I^j \rangle \langle\langle I^{m+1-j} \rangle\rangle + \langle I^m \rangle \langle\langle I \rangle\rangle \quad . \quad (2.15) \end{aligned}$$

We observe that only the first and the last terms of the previous expression depends of the m^{th} moment. Hence, Eq. (2.15) can be reorganized in order to join the terms with this moment and we obtain

$$\begin{aligned} \langle I^{m+1} \rangle &= -m \langle I \rangle \sum_{j=1}^{m-1} \binom{m-1}{j} \langle I^j \rangle \langle \langle I^{m-j} \rangle \rangle + \sum_{j=2}^{m-1} \binom{m}{j} \langle I^j \rangle \langle \langle I^{m+1-j} \rangle \rangle \\ &\quad + m \langle I \rangle \langle I^m \rangle + \langle I^m \rangle \langle \langle I \rangle \rangle . \end{aligned} \quad (2.16)$$

Defining the function g_m by

$$\begin{aligned} g_m (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^{m-1} \rangle) &= -m \langle I \rangle \sum_{j=1}^{m-1} \binom{m-1}{j} \langle I^j \rangle \langle \langle I^{m-j} \rangle \rangle \\ &\quad + \sum_{j=2}^{m-1} \binom{m}{j} \langle I^j \rangle \langle \langle I^{m+1-j} \rangle \rangle , \end{aligned} \quad (2.17)$$

we obtain for the moment $\langle I^{m+1} \rangle$ the equality

$$\langle I^{m+1} \rangle = g_m (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^{m-1} \rangle) + (m+1) \langle I \rangle \langle I^m \rangle , \quad (2.18)$$

as presented in Lemma 2.2.1. ■

The m^{th} moment closure approximation consists in assuming that $\langle \langle I^{m+1} \rangle \rangle = 0$ and therefore to replace the moment $\langle I^{m+1} \rangle$ in Eq. (2.3) by the expression given in Eq. (2.13). Hence, the m moment closure ODEs for the m first moments of infecteds $\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^m \rangle$, after applying the m^{th} moment closure approximation, is as follows: for $n = 1, \dots, m-1$, the ODEs of $\langle I^n \rangle$ are as presented in Eq. (2.3) of Theorem 2.2.1; the ODE of

$\langle I^m \rangle$ is given by

$$\begin{aligned} \frac{d}{dt} \langle I^m \rangle &= f_m (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^m \rangle) \\ &\quad - \frac{\beta}{N} m [g_m (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^{m-1} \rangle) + (m+1) \langle I \rangle \langle I^m \rangle] \end{aligned} \quad (2.19)$$

where f_m and g_m are as presented in Theorem 2.2.1 and Lemma 2.2.1, respectively. For the m moment closure ODE system, we observe that the stationary value of infected individuals $\langle I \rangle_{m,\beta}^*$ is a zero of a $(m+1)^{th}$ order polynomial function. We consider the dynamics of the m first moments of infecteds under the appropriated moment closure approximation,

$$\begin{aligned} \frac{d}{dt} \langle I \rangle &= (\beta - \alpha) \langle I \rangle - \frac{\beta \langle I^2 \rangle}{N} \\ \frac{d}{dt} \langle I^2 \rangle &= (\beta + \alpha) \langle I \rangle + 2(\beta - \alpha) \langle I^2 \rangle - \frac{\beta}{N} \langle I^2 \rangle - 2 \frac{\beta}{N} \langle I^3 \rangle \\ &\dots \\ \frac{d}{dt} \langle I^m \rangle &= f_m (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^m \rangle) \\ &\quad - \frac{\beta}{N} n [g_m (\langle I \rangle, \langle I^2 \rangle, \dots, \langle I^{m-1} \rangle) + (m+1) \langle I \rangle \langle I^m \rangle] \end{aligned} \quad (2.20)$$

To solve this system in stationarity for any dimension m we have the following recursive process:

Step 1: Solve the first equation in the second moment

$$\frac{d}{dt} \langle I \rangle = 0 \Leftrightarrow \langle I^2 \rangle^* = \left(1 - \frac{\alpha}{\beta}\right) N \langle I \rangle^*$$

and substitute the result in the following equations;

Step 2: Solve the second equation in the third moment

$$\frac{d}{dt}\langle I^2 \rangle = 0 \Leftrightarrow \langle I^3 \rangle^* = \left(\frac{\alpha}{\beta} + \left(1 - \frac{\alpha}{\beta}\right)^2 N \right) N \langle I \rangle^*$$

and substitute the result in the following equations;

...

Step m – 1: Solve the $(m - 1)^{th}$ equation in the m^{th} moment

$$\frac{d}{dt}\langle I^{m-1} \rangle = 0 \Leftrightarrow \langle I^m \rangle^* = \langle I^m \rangle^* (\langle I \rangle^*)$$

and substitute the result in the last equation.

In the end, we obtain one polynomial expression in the first moment of infecteds

$$\langle I \rangle^* (c_m \langle I \rangle^{*m} + \dots + c_1 \langle I \rangle^* + c_0) = 0 \quad , \quad (2.21)$$

that is numerically solved for fixed values of α , β and N . Furthermore, all the higher moments $\langle I^n \rangle^*$, $n \geq 2$, at equilibria are determined by the first moment of infecteds $\langle I \rangle^*$.

2.2.1 The mean field approximation

The simplest approximation, and therefore the poorest of all is the mean field approximation. We use this approximation in order to close the dynamic of the first moment, the mean value of infecteds $\langle I \rangle$, which is given

by Theorem 2.2.1 as

$$\frac{d}{dt}\langle I \rangle = (\beta - \alpha)\langle I \rangle - \frac{\beta}{N}\langle I^2 \rangle \quad .$$

From Lemma 2.2.1 and putting $m = 1$, we obtain the approximation

$$\langle I^2 \rangle = \langle I \rangle^2 \quad , \quad (2.22)$$

that is the same as assuming the variance of the infected individuals equal to zero $Var(I) = \langle I^2 \rangle - \langle I \rangle^2 = 0$. Hence, in the mean field approximation, the dynamic of $\langle I \rangle$ becomes

$$\begin{aligned} \frac{d}{dt}\langle I \rangle &= (\beta - \alpha)\langle I \rangle - \frac{\beta}{N}\langle I \rangle^2 \\ &= \langle I \rangle \left((\beta - \alpha) - \frac{\beta}{N}\langle I \rangle \right) . \end{aligned}$$

For the stationary states we obtain the trivial state $\langle I \rangle^* = 0$ and the state $\langle I \rangle^* = N(1 - \alpha/\beta)$. In Fig. 2.1 we present the stationary value of infected individuals for different values of the infection rate β . We consider a population of $N = 100$ individuals and $\alpha = 1$.

To characterize the threshold region of an epidemic model, that separates the persistence of an epidemics from its extinction, we define the critical infection rate β_c as follows.

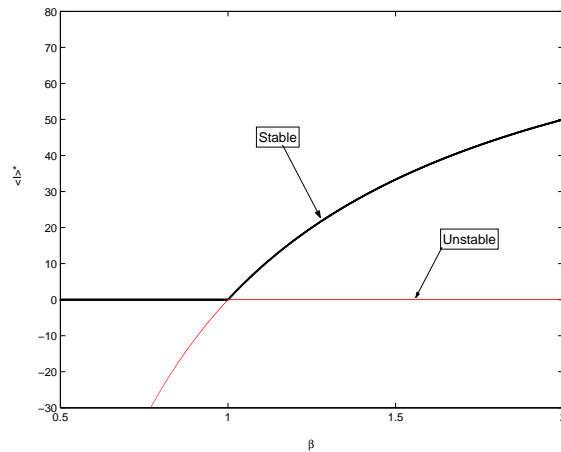


Figure 2.1: *Stationary values of $\langle I \rangle$ in dependence of β , for $\alpha = 1$ and $N = 100$, in the mean field approximation.*

Definition 2.2.1 *Let $\langle I \rangle^*(\beta)$ be a non-zero stable equilibria for the mean value of the infected individuals. We define the critical value of the infection rate β as the smallest value β_c such that*

$$\lim_{\beta \rightarrow \beta_c^+} \langle I \rangle^*(\beta) = 0 .$$

With a stability analysis [20, 40], we observe for the SIS model in the mean field approximation that $\langle I \rangle^* = 0$ is stable if $\beta < \alpha$ and unstable otherwise. For the other stationary value we observe the opposite. Hence, the critical value of the infection rate β in the mean field approximation is given by

$$\beta_c = \alpha . \quad (2.23)$$

2.2.2 The Gaussian approximation

The Gaussian approximation is used to close the dynamic of the two first moments of infecteds, $\langle I \rangle$ and $\langle I^2 \rangle$, which is given in Theorem 2.2.1 by

$$\begin{aligned} \frac{d}{dt}\langle I \rangle &= (\beta - \alpha)\langle I \rangle - \frac{\beta\langle I^2 \rangle}{N} \\ \frac{d}{dt}\langle I^2 \rangle &= 2(\beta - \alpha)\langle I^2 \rangle + (\beta + \alpha)\langle I \rangle - 2\frac{\beta}{N}\langle I^3 \rangle - \frac{\beta}{N}\langle I^2 \rangle \end{aligned} \quad (2.24)$$

This approximation consists in vanishing the third cumulant, which is zero for the normal distribution, or by Lemma 2.2.1 in approximating $\langle I^3 \rangle$ by

$$\langle I^3 \rangle = 3\langle I^2 \rangle\langle I \rangle - 2\langle I \rangle^3 \quad ,$$

leading to the ODE system given by

$$\begin{aligned} \frac{d}{dt}\langle I \rangle &= (\beta - \alpha)\langle I \rangle - \frac{\beta\langle I^2 \rangle}{N} \\ \frac{d}{dt}\langle I^2 \rangle &= 2(\beta - \alpha)\langle I^2 \rangle + (\beta + \alpha)\langle I \rangle - 2\frac{\beta}{N}(3\langle I^2 \rangle\langle I \rangle - 2\langle I \rangle^3) - \frac{\beta}{N}\langle I^2 \rangle \end{aligned} \quad (2.25)$$

To compute the stationary states we use the previous recursive process and obtain $\langle I^2 \rangle^* = N(1 - \alpha/\beta)\langle I \rangle^*$ for the second moment of infecteds and for the first moment we obtain the following three stationary values

$$\langle I \rangle_1^* = 0 \quad \text{and} \quad \langle I \rangle_{2,3}^* = \frac{3}{4}N\left(1 - \frac{\alpha}{\beta}\right) \pm \frac{1}{4}N\sqrt{\left(1 - \frac{\alpha}{\beta}\right)^2 - \frac{8\alpha}{N\beta}} \quad (2.26)$$

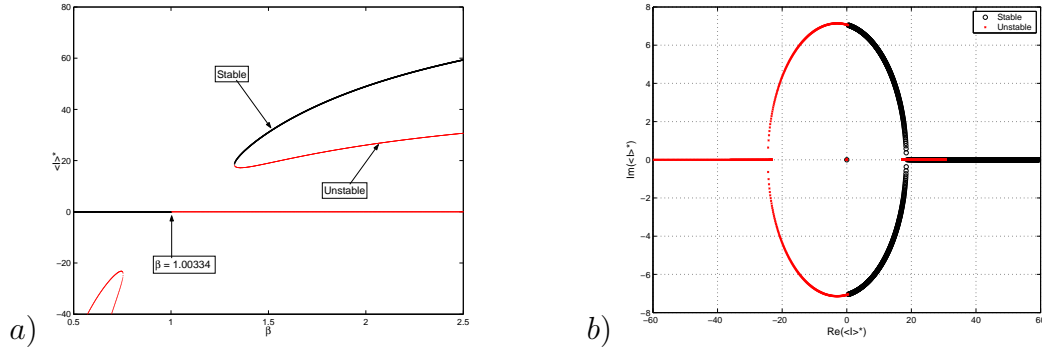


Figure 2.2: a) Stationary values of $\langle I \rangle$ in terms of β for $\alpha = 1$ and $N = 100$. b) Real versus the imaginary part of $\langle I \rangle^*$ presented in a).

The graphic of the stationary values of infecteds, as function of β , is presented in Fig. 2.2 a). We observe the trivial disease free state $\langle I \rangle^* = 0$ and two non-zero states. These two stationary states touch themselves, while still negatives, and becomes complex. After this, they touch themselves again and become real. This behaviour is illustrated in Fig. 2.2 b). Both graphics where made for the particular case of $\alpha = 1$, $N = 100$ and varying the infection rate β between 0.5 and 2.5.

Since the non-zero stationary values of the infecteds $\langle I \rangle_{2,3}^*$ do not cross the stationary value $\langle I \rangle^* = 0$, for finite populations, we can not vanish the non-zero equilibria to compute the critical value of β . To find this value we will study the stability of the stationary state $\langle I \rangle^* = 0$. The critical value of β will be the one that makes $\langle I \rangle^* = 0$ cross from stable to unstable. To apply the Hartman-Grobman theorem (see [40]) and linearize the system Eq. (2.25) we denot by X the state variables and by f the non-linear function that corresponds to system Eq. (2.25), $\dot{X} = f(X)$. The jacobian

matrix of f in the equilibrium $X^* = 0$ is given by

$$D_f(0) = \begin{bmatrix} \beta - \alpha & -\frac{\beta}{N} \\ \beta + \alpha & 2(\beta - \alpha) - \frac{\beta}{N} \end{bmatrix} \quad (2.27)$$

and the eigenvalues are

$$\lambda_{1,2} = \frac{3}{2}(\beta - \alpha) - \frac{\beta}{2N} \pm \frac{1}{2N} \sqrt{(\beta - \alpha)^2 N^2 - \beta^2(6N - 1) - 2\beta\alpha N}, \quad (2.28)$$

with the real part given by

$$Re(\lambda_{1,2}) = \frac{3}{2}(\beta - \alpha) - \frac{\beta}{2N}. \quad (2.29)$$

The expression in Eq. (2.29) vanishes for $\beta = \alpha/(1 - \frac{1}{3N})$ and the equilibrium $X^* = 0$ is a sink if $\beta < \alpha/(1 - \frac{1}{3N})$ and a source if $\beta > \alpha/(1 - \frac{1}{3N})$. This implies that the critical value of β , for the SIS model in the Gaussian approximation, is given by

$$\beta_c = \frac{\alpha}{1 - \frac{1}{3N}}. \quad (2.30)$$

Making a similar analysis for the other equilibria we conclude that the two non-zero equilibria are unstable for $\beta < \beta_c$ and become stable when β crosses its critical value, even though they are complex. But when they touch themselves and become real, one equilibrium is stable and the other one is unstable, like Fig. 2.2 a) suggests.

The Andronov-Hopf bifurcation

From the previous computations we may suspect that a Andronov-Hopf bifurcation (see [20, 40]) occurs for the dynamical system presented in Eq. (2.25) when β crosses its critical value. Indeed, simulations of the system show that the flow is a periodic orbit near the equilibrium $X^* = 0$, which is attracting if $\beta < \beta_c$ and repellent if $\beta > \beta_c$, as illustrated in Fig. 2.3. To prove that the Andronov-Hopf bifurcation occurs at $\beta_c = \frac{\alpha}{1 - \frac{1}{3N}}$ let us

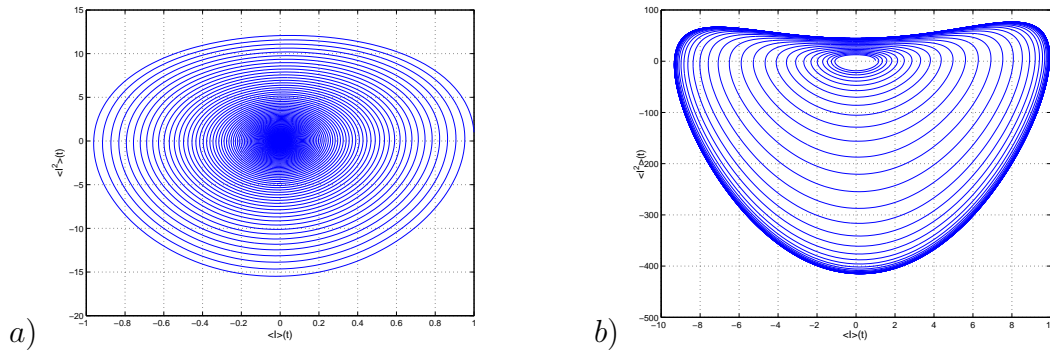


Figure 2.3: *a)* Simulation of the system Eq. (2.25) with the initial condition $X(0) = [1 \ 1]^T$, for the particular case of $\alpha = 1$ and $N = 100$ with $\beta = 1.002$. *b)* The same simulation of *a)* but now for $\beta = 1.005$.

consider the one parameter function $f_\beta(X)$ as before. The condition that $X^* = 0$ is a fixed point of system Eq. (2.25) was already verified. Let us consider now that the eigenvalues of $D_f(0)$ are of the form $\Re(\beta) \pm i\Im(\beta)$, in a neighborhood of β_c , where $\Re(\beta)$ and $\Im(\beta)$ are defined in Eq. (2.28). It is obvious that $\Re(\beta_c) = 0$ and the inequalities $\Im(\beta_c) \neq 0$ and $\Re'(\beta_c) \neq 0$ also hold because

$$\Im\left(\frac{\alpha}{1 - \frac{1}{3N}}\right) = \frac{\alpha\sqrt{2(9N - 2)}}{3N - 1} \quad \text{and} \quad \Re'(\beta) = \frac{3}{2} - \frac{1}{2N} \quad .$$

Hence, the eigenvalues cross the imaginary axis at β_c and therefore we conclude that the ODE system presented in Eq. (2.25) have a supercritical Andronov-Hopf bifurcation at $\beta_c = \alpha/(1 - \frac{1}{3N})$.

Although, the SIS model in the Gaussian approximation can not be totally accepted because does not keep the “biological space” invariant. We observe that the flow of the differential equations considered can be negative or even increase to infinity, which is biologically unacceptable.

2.2.3 The moment closure of third order

The dynamic of the three first moments of infecteds is given by

$$\begin{aligned} \frac{d}{dt}\langle I \rangle &= (\beta - \alpha)\langle I \rangle - \frac{\beta\langle I^2 \rangle}{N} \\ \frac{d}{dt}\langle I^2 \rangle &= 2(\beta - \alpha)\langle I^2 \rangle + (\beta + \alpha)\langle I \rangle - 2\frac{\beta}{N}\langle I^3 \rangle - \frac{\beta}{N}\langle I^2 \rangle \\ \frac{d}{dt}\langle I^3 \rangle &= 3(\beta - \alpha)\langle I^3 \rangle + 3(\beta + \alpha)\langle I^2 \rangle + (\beta - \alpha)\langle I \rangle - \frac{\beta}{N}(3\langle I^4 \rangle + 3\langle I^3 \rangle + \langle I^2 \rangle) \end{aligned} \tag{2.31}$$

as presented in Theorem 2.2.1. To close this system of differential equations we use the moment closure technique and the Lemma 2.2.1 to substitute the $\langle I^4 \rangle$ moment in the last equation by

$$\langle I^4 \rangle = 4\langle I^3 \rangle\langle I \rangle - 12\langle I^2 \rangle\langle I \rangle^2 + 6\langle I \rangle^4 + 3\langle I^2 \rangle^2. \tag{2.32}$$

To obtain the critical value of the infection rate β we compute the stationary values of the infecteds $\langle I \rangle^*$ and then, we discover when the “biological” value crosses the zero state, in order to exist some infected individuals in stationarity. After replace the fourth moment by the expression presented in Eq. (2.32) in the third equation of system Eq. (2.31), we close the ODE system. Using the previous recursive process to compute the stationary states, we obtain for the second moment $\langle I^2 \rangle^* = N(1 - \alpha/\beta)\langle I \rangle^*$, which is exactly the same that we had obtained in the Gaussian approximation. This result does not surprise since the dynamic of the first moment remains unchanged. Only the dynamic of the second moment is now influenced by the third moment, which was not considered before. The last equation, that depends only of the the stationary state $\langle I \rangle^*$, is given by

$$\frac{2\langle I \rangle^* (A_3 \langle I \rangle^{*3} + A_2 \langle I \rangle^{*2} + A_1 \langle I \rangle^* + A_0)}{\beta N (\beta (N - 4\langle I \rangle^* - 1) - \alpha N)} = 0, \quad (2.33)$$

where the coefficients A_i , $i = 0, 1, 2, 3$, are defined by

$$\begin{aligned} A_0 &= N [\beta^3 N^2 - \beta^2 \alpha (3N(N-1) + 1) + 3\beta \alpha^2 N(N-1) - \alpha^3 N^2] \quad , \\ A_1 &= N\beta [-7\alpha^2 N - 7\beta^2 N + 14\beta \alpha N - 4\beta \alpha] \quad , \\ A_2 &= 12\beta^2 N [\beta - \alpha] \quad , \\ A_3 &= -6\beta^3 \quad . \end{aligned}$$

From Eq. (2.33) we obtain the trivial stationary state $\langle I \rangle^* = 0$ and three other. The real stationary values are plotted in Fig. 2.4 for $\alpha = 1$ and $N = 100$. In the threshold region only one of the free non-zero solutions is

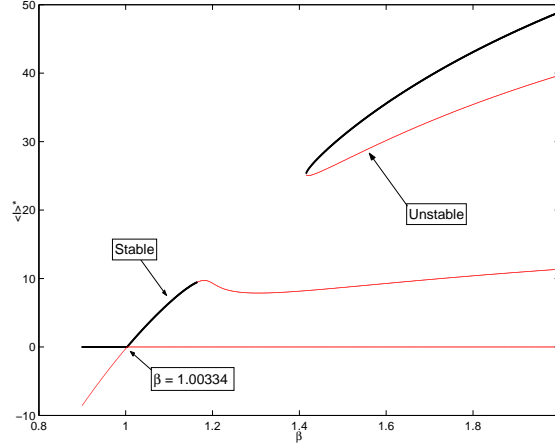


Figure 2.4: *The real stationary equilibria of system Eq. (2.31) as function of β . The usual parameters $\alpha = 1$ and $N = 100$ were used.*

acceptable, since the others are complex for some values of the parameters. This solution vanishes when the coefficient A_0 of Eq. (2.33) also vanishes. Again, this occurs at three different values of β but only one should be considered because the others are complex. The real one is the critical value of β and to obtain its analytic expression we need to apply the Cardano's method. Let c_0 , c_1 and c_2 be the coefficients of β in the equation $A_0 = 0$ after we reduce this polynomial to a monic one,

$$c_0 = -\alpha^3 \quad , \quad c_1 = \frac{3\alpha^2(N-1)}{N} \quad \text{and} \quad c_2 = -\frac{\alpha(3N(N-1)+1)}{N^2} .$$

Let p and q be the transformations of the coefficients given by

$$p = c_1 - \frac{c_2^2}{3} \quad \text{and} \quad q = \frac{2}{27}c_2^3 - \frac{1}{3}c_2c_1 + c_0 .$$

Defining the variable

$$u = \sqrt[3]{-\frac{q}{2} + \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}},$$

we have for β critical the analytic expression $\beta_c = u - p/(3u) - c_2/3$. This expression can be reorganized leading to

$$\beta_c = U - \frac{\alpha^2 W}{9U} + \alpha \left(1 - \frac{1}{N} + \frac{1}{3N^2} \right), \quad (2.34)$$

with U and W defined by the expressions

$$U = \frac{\sqrt[3]{4}}{6} \alpha \sqrt[3]{S + \sqrt{S^2 + 4W^3}} \quad (2.35)$$

$$W = \frac{9N^3 - 15N^2 + 6N - 1}{N^4} \quad (2.36)$$

where

$$S = \frac{108N^4 - 135N^3 + 72N^2 - 18N + 2}{N^6}. \quad (2.37)$$

Hence, we conclude that, in the limit when N tends to infinity, we have $U \rightarrow 0$ and $\frac{W}{U} \rightarrow 0$. Therefore, the critical value of β tends to α when N tends to infinity, in agreement with the critical values of the mean field approximation.

2.3 The threshold evolution

For higher approximations, that result from considering more moments and the respective dynamics, the analytic expressions for the stationary states and for the critical parameters become more complicated to obtain. Therefore, the method of vanishing the stationary states to compute the critical value of the infection rate β is not very helpful. The alternative is to study the stability of the trivial disease free state $\langle I \rangle^* = 0$.

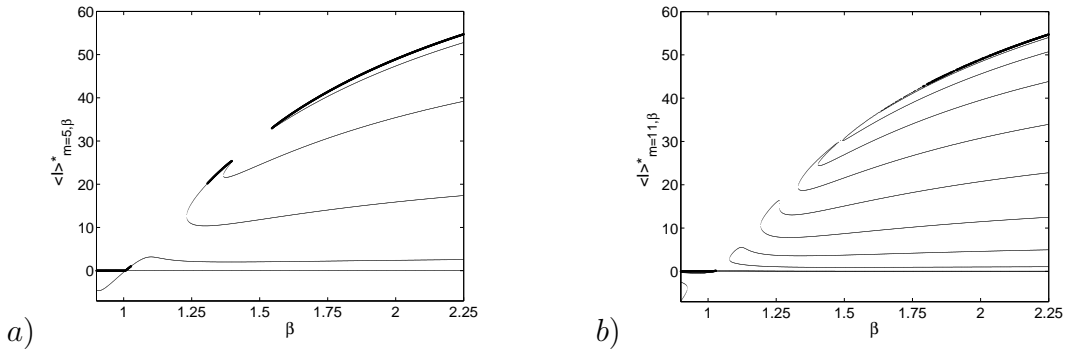


Figure 2.5: *The stationary mean value of infecteds for the m moment closure ODEs, presented Eq. (2.20), for different values of β . In a), we consider the dynamic of the first five moments of infecteds $m = 5$ and therefore the system has 5 equations. In b), we consider $m = 11$. The thick lines correspond to the stable equilibria and the others to the unstable. The parameters $\alpha = 1$ and $N = 100$ were used.*

In Fig. 2.5, we present the real zeros of the polynomial function obtained when are considered the dynamic of 5 and 11 moments, i.e., the $\langle I \rangle_{m, \beta}^*$ for the $m = 5$ and 11 moment closure approximations and different infection rate values β . The values used for the parameters α and N are $\alpha = 1$ and $N = 100$. There are multiple equilibria and we present in thick lines the stable equilibria and in thin lines the unstable ones. Let $[\beta_m; +\infty)$ be the

m	$\beta_c(m)$
1	1
2	1.0033444816
3	1.0033432360
4	1.0066901984
5	1.0067056257
6	1.0101498308
7	1.0100873020
8	1.0136470206
9	1.0134883984

Table 2.1: The critical values of β , for $N = 100$ and $\alpha = 1$, considering the dynamic of the nine first moments.

interval of the infection rate β for which there is a stable equilibria for m moment closure ODEs. We observe that the value β_m tends to $+\infty$ when m tends to $+\infty$. Furthermore, letting the critical value of the infection rate $\beta_c(m)$ be the smallest value of β such that the equilibrium $\langle I \rangle^* = 0$ turns into an unstable equilibrium, for the m moments closed ODEs, we also observe that $\beta_c(m)$ tends to $+\infty$ when m tends to $+\infty$.

To obtain the different values of the critical infection rate $\beta_c(m)$, we consider the dynamics of the m first moments of infecteds under the appropriated moment closure approximation presented in system Eq. (2.20). From the previous knowledge it is obvious that the trivial disease free state $\langle I \rangle^* = \langle I^2 \rangle^* = \dots = \langle I^m \rangle^* = 0$ arises for any moment closure approximation. With a careful analysis it is possible to conclude that the jacobian matrix of system Eq. (2.20), at this trivial zero stationary value, has a

characteristic aspect given by

$$J = \begin{bmatrix} \beta - \alpha & -\frac{\beta}{N} & 0 & 0 & 0 \\ \beta + \alpha & 2(\beta - \alpha) - \frac{\beta}{N} & -2\frac{\beta}{N} & 0 & 0 \\ \beta - \alpha & 3(\beta + \alpha) - \frac{\beta}{N} & 3(\beta - \alpha) - 3\frac{\beta}{N} & -3\frac{\beta}{N} & 0 \\ \beta + \alpha & 4(\beta - \alpha) - \frac{\beta}{N} & 6(\beta + \alpha) - 4\frac{\beta}{N} & 4(\beta - \alpha) - 6\frac{\beta}{N} & -4\frac{\beta}{N} \\ & & & & \ddots \end{bmatrix}$$

where each entry of this matrix is defined by

$$J_{ij} = \begin{cases} \beta + (-1)^i \alpha & , \quad j = 1 \\ \binom{i}{j-1} (\beta - (-1)^{i+j} \alpha) - \binom{i}{j-2} \frac{\beta}{N} & , \quad 1 < j \leq i \\ -i \frac{\beta}{N} & , \quad j = i + 1 \\ 0 & , \quad j > i + 1 \end{cases} .$$

We would like to obtain a triangular matrix but the element above the main diagonal is completely natural, since the dynamic of the n^{th} moment depends on the $(n + 1)^{th}$ moment. The critical value of β is now computed very easily. Fixing the value of N and the parameters α and β , any mathematical program compute the eigenvalues of the jacobian matrix J . The critical value of β will be the one that makes the highest real part of all eigenvalues cross from negative values to positive ones, which is the point where the stationary value zero becomes unstable. Therefore, for any dimension m we can make an iterative program that computes the critical β ,

for a fixed α and N . For lower dimensions ($m = 1$, $m = 2$ and $m = 3$) we already characterize the critical parameters. Applying this technique for higher dimensions the critical values of β , for $N = 100$ and $\alpha = 1$, are given in table 2.1.

Now, it is very interesting to observe the behavior of the distance between the different critical values of β . When we consider an even number of moments, m , the ratio between the distances of the critical values of β does not seem to be very regular. We have, for example,

$$\frac{\beta_c(6) - \beta_c(4)}{\beta_c(4) - \beta_c(2)} \approx 1,0340 \quad \text{and} \quad \frac{\beta_c(8) - \beta_c(6)}{\beta_c(6) - \beta_c(4)} \approx 1,0108, \quad (2.38)$$

where $\beta_c(m)$ represents the critical value of β for the m moment closure approximation. On the other hand, when we consider only odd values of m , we observe that the ratio of these distances are approximately constant

$$\frac{\beta_c(5) - \beta_c(3)}{\beta_c(3) - \beta_c(1)} = \frac{\beta_c(7) - \beta_c(5)}{\beta_c(5) - \beta_c(3)} = \dots \approx 1.0057 \quad . \quad (2.39)$$

Indeed this ratio is not constant. Considering more significant digits we obtain a ratio increasing with the number of the moments considered, like is shown in table 2.2.

Since the constant 1.0057 is higher than one, we conclude that the critical value of β tends to infinity when we increase the value of m . This means that, for a fixed value of β , there will be an approximation that have the critical β higher than the fixed value of β . Therefore, if we consider a sufficient number of moments m , we will have $\beta < \beta_c$ and the infected

m	$\beta_c(m)$	$\Delta\beta_m = \beta_c(m) - \beta_c(m-1)$	$R_m = \frac{\Delta\beta_m}{\Delta\beta_{m-1}}$
1	1,000000000		
3	1,0033432360	0,0033432360	
5	1,0067056257	0,0033623897	1,0057291036
7	1,0100873020	0,0033816763	1,0057359555
9	1,0134883984	0,0034010964	1,0057427550
11	1,0169090494	0,0034206510	1,0057495011
13	1,0203493902	0,0034403408	1,0057561469
15	1,0238095573	0,0034601671	1,0057628945
17	1,0272896873	0,0034801300	1,0057693456
19	1,0307899184	0,0035002311	1,0057759624
21	1,0343103897	0,0035204713	1,0057825414

Table 2.2: The critical values of β , their distances and the ratio between the distances, for $N = 100$ and $\alpha = 1$, considering the dynamic of an odd number of moments m .

individuals tends to disappear. This result agrees with the stationary distribution of the SIS model which states that we do not have any infected individual in stationarity.

Chapter 3

Quasi-stationarity in the SIS model

In this chapter we study the quasi-stationary distributions for epidemic models. For the stochastic SIS model, we discover that the steady states in the moment closure give a good approximation of the quasi-stationary states not only for large populations of individuals but also for small ones and not only for large infection rate values but also for infection rate values close to its critical values.

3.1 Quasi-stationary distribution

For the stochastic SIS model, we know that $I(t) = 0$ is the only absorbing state and is attained for a finite time. Hence, the stationary distribution of

the stochastic SIS model is degenerated with probability one at the origin

$$p(I^* = k) = \begin{cases} 1, & \text{if } k = 0 \\ 0, & \text{if } k \neq 0 \end{cases} .$$

However, the time to reach the equilibrium $I(t) = 0$ can be so long that the stationary distribution is non informative. Hence, our interest goes to the quasi-stationary distribution. The quasi-stationary distribution is the stationary distribution of the stochastic process conditioned to the non-extinction of the infected individuals

$$\{I(t) = i | I(t) > 0\} , \quad i = 1, 2, \dots, N ,$$

and therefore supported on the set of the transient states. Denoting by $\tilde{q}_i(t)$ the probability of having i infecteds in the conditioned process, at time t , and by $p_i(t)$ the same probability in the non-conditioned process, we obtain

$$\tilde{q}_i(t) = p(I(t) = i | I(t) > 0) = \frac{p_i(t)}{1 - p_0(t)}, \quad i = 1, 2, \dots, N . \quad (3.1)$$

The quasi-stationary distribution is the solution of the equation

$$\frac{d}{dt} \tilde{q}_i(t) = 0 \quad .$$

Denoting by $q_i(t)$ these solution probabilities, we observe that

$$\frac{\dot{p}_i(t)}{1 - p_0(t)} + \frac{p_i(t)\dot{p}_0(t)}{(1 - p_0(t))^2} = 0 \quad . \quad (3.2)$$

Observing that $\dot{p}_0(t) = \alpha p_1(t)$ and applying the master equation of the SIS model (see Eq. (2.1)) we obtain in the $q_i(t)$ probabilities that

$$\beta \frac{N - (i - 1)}{N} (i - 1) q_{i-1}(t) + \alpha (i + 1) q_{i+1}(t) - \left(\beta \frac{N - i}{N} i + \alpha i \right) q_i(t) + q_i(t) \alpha q_1(t) = 0, \quad (3.3)$$

or, like shown in [30],

$$\lambda_{i-1} q_{i-1}(t) - k_i q_i(t) + \mu_{i+1} q_{i+1}(t) = -\alpha q_1(t) q_i(t), \quad (3.4)$$

where

$$\lambda_i = \beta \frac{N - i}{N} i, \quad \mu_i = \alpha i \quad \text{and} \quad k_i = \lambda_i + \mu_i.$$

We observe that the system Eq. (3.4) can not be solved explicitly. In [30], it is shown that q_i satisfies the relation

$$q_i = \gamma(i) \alpha(i) R_0^{i-1} q_1, \quad i = 1, 2, \dots, N, \quad (3.5)$$

where $R_0 = \beta/\alpha$,

$$\gamma(i) = \frac{1}{i} \sum_{k=1}^i \frac{1 - \sum_{l=1}^{k-1} q_l}{\alpha(k) R_0^{k-1}}, \quad (3.6)$$

$$\alpha(i) = \frac{N!}{(N - i)! N^i}, \quad (3.7)$$

and

$$q_1 = \frac{1}{\sum_{i=1}^N \gamma(i)\alpha(i)R_0^{i-1}} . \quad (3.8)$$

Eqs. (3.5) to (3.8) do not define explicitly the quasi-stationary distribution. However, we can use iterative methods to approach the q_i values (see [32]). One possible method starts with an initial guess for q_1 and uses Eq. (3.5) to determine the other q_i . Then q_1 can be actualized using Eq. (3.8). This process should be repeated until successive iterations are close enough.

The quasi-stationary distribution can also be computed using eigenvectors. In the following theorem, we present one method to compute numerically the quasi-stationary distribution of the SIS model.

Theorem 3.1.1 *Let $p(t) = (p_0(t), p_1(t), \dots, p_N(t))$ be the vector with the probabilities $p_i(t)$ of having i infecteds at time t . Let A be the real matrix such that*

$$\dot{p}(t) = Ap(t) , \quad (3.9)$$

and let A_q be the A matrix with the first row and the first column removed. Then 0 is the highest eigenvalue of the A matrix. Moreover, A_q has N real distinct negative eigenvalues

$$-\lambda_1 > -\lambda_2 > \dots > -\lambda_N ,$$

and the quasi-stationary distribution of the stochastic SIS model is given by the dominant normalized eigenvector $\vec{v}_{-\lambda_1}$ of the A_q matrix.

Proof. We observe that the SIS master equation, presented in Eq. (2.1), represents a system of linear equations given by

$$\dot{p}(t) = Ap(t) \quad (3.10)$$

where $p(t) = (p_0(t), p_1(t), \dots, p_N(t))$ is the probability vector and A is the matrix given by

$$A = \begin{pmatrix} 0 & \alpha & 0 & 0 & \dots & 0 \\ 0 & -\alpha - \beta(N-1)/N & 2\alpha & 0 & \dots & 0 \\ 0 & \beta(N-1)/N & -2\alpha - 2\beta(N-2)/N & 3\alpha & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & -\alpha N \end{pmatrix}.$$

It is obvious that 0 is an eigenvalue of A and the vector $\vec{v}_0 = (1, 0, \dots, 0)$ is the correspondent eigenvector. Since the stationary distribution of the infected individuals has probability one at the $I(t) = 0$ state all the other eigenvalues should be negative. Assuming that A have $N + 1$ distinct real eigenvalues $0, -\lambda_1, \dots, -\lambda_N$ (for a detailed proof see [38]) then there exists an invertible matrix Q (see [20]), whose columns are the eigenvectors of A , such that

$$Q^{-1}AQ = \text{diag}\{0, -\lambda_1, \dots, -\lambda_N\} = D,$$

and new coordinates $y(t) = Q^{-1}p(t)$ such that

$$\dot{y}(t) = Dy(t) . \quad (3.11)$$

Since D is diagonal and therefore Eq. (3.11) is a system of differential equations of the form

$$\dot{y}_i(t) = -\lambda_i y_i(t) , \quad (3.12)$$

we know that each solution is uniquely determined by

$$y_i(t) = u_i \exp(-\lambda_i t) , \quad (3.13)$$

for the initial condition $u_i = y_i(0)$. Hence, the solution of system Eq. (3.10) is given by

$$p(t) = Qy(t) , \quad (3.14)$$

or, equivalently, by

$$\begin{pmatrix} p_0(t) \\ p_1(t) \\ p_2(t) \\ \vdots \\ p_N(t) \end{pmatrix} = \begin{pmatrix} 1 & v_{01} & v_{02} & & v_{0N} \\ 0 & v_{11} & v_{12} & & v_{1N} \\ 0 & v_{21} & v_{22} & & v_{2N} \\ & & & \ddots & \\ 0 & v_{N1} & v_{N2} & & v_{NN} \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \exp(-\lambda_1 t) \\ u_2 \exp(-\lambda_2 t) \\ \vdots \\ u_N \exp(-\lambda_N t) \end{pmatrix} ,$$

where $\vec{v}_0 = (1, 0, \dots, 0)$, $\vec{v}_1 = (v_{01}, v_{11}, \dots, v_{N1})$, $\vec{v}_2 = (v_{02}, v_{12}, \dots, v_{N2})$, etc.,

form a coordinate system of eigenvectors of A . Hence, each solution $p_i(t)$ of system Eq. (3.10) is given by

$$p_i(t) = v_{i0}u_0 + v_{i1}u_1 \exp(-\lambda_1 t) + v_{i2}u_2 \exp(-\lambda_2 t) + \dots + v_{iN}u_N \exp(-\lambda_N t) \quad (3.15)$$

We recall that the probability of having i infecteds in the SIS model conditioned to the non-extinction is given by $\tilde{q}_i(t)$ in Eq. (3.1) by

$$\begin{aligned} \tilde{q}_i(t) &= \frac{p_i(t)}{1 - p_0(t)} \\ &= \frac{p_i(t)}{\sum_{i=1}^N p_i(t)}, \quad i = 1, 2, \dots, N. \end{aligned} \quad (3.16)$$

Applying the explicit expression of $p_i(t)$ presented in Eq. (3.15), we obtain

$$\tilde{q}_i(t) = \frac{v_{i1}u_1 \exp(-\lambda_1 t) + O(\exp(-\lambda_2 t))}{(v_{11} + v_{21} + \dots + v_{N1})u_1 \exp(-\lambda_1 t) + O(\exp(-\lambda_2 t))}. \quad (3.17)$$

Taking the limit of Eq. (3.17) when t tends to infinity, we obtain the quasi-stationary probabilities q_i . Since $-\lambda_2 < -\lambda_1$ we have that

$$q_i = \frac{v_{i1}}{v_{11} + v_{21} + \dots + v_{N1}}. \quad (3.18)$$

Hence, we conclude that the quasi-stationary probability q_i corresponds to the i^{th} coordinate of \vec{v}_1

$$q_i = \frac{v_{i1}}{\|\vec{v}_1\|}, \quad i = 1, 2, \dots, N, \quad (3.19)$$

which is the the dominant normalized eigenvector of the A_q matrix. ■

3.2 Quasi-stationary approximations

Since the quasi-stationary distribution of the stochastic SIS model does not have an explicit form, it is useful to approximate the model in order to obtain explicit approximations of the quasi-stationary distribution. Two possible approximations were studied by Kryscio and Lefevre [23] and by Nåsell [30, 31]. One is given by the stationary distribution of the SIS model with one permanently infected individual and the other is obtained from the SIS model with the state $\langle I \rangle(t) = 0$ removed, i.e., the recovery rate is zero when there exists only one infected individual while all the others transition rates stay unchanged. The stationary distribution of this last process can be determined explicitly and gives a good approximation of the quasi-stationary distribution of the SIS model, when β is distinctly greater than α and $N \rightarrow +\infty$ (see [31]). For this process the stationary distribution of the infected individuals is given by

$$p_j = \frac{N!}{j(N-j)!N^j} \left(\frac{\beta}{\alpha}\right)^{j-1} p^{(0)}, \quad j = 1, 2, \dots, N, \quad (3.20)$$

where $p_j = P(I^* = j)$ and $p^{(0)}$ is defined by

$$p^{(0)} = \frac{1}{\sum_{j=1}^N \frac{N!}{j(N-j)!N^j} \left(\frac{\beta}{\alpha}\right)^{j-1}}. \quad (3.21)$$

In Fig. 3.1, we compare the mean value of infecteds that arises from the quasi-stationary distribution $\langle I \rangle_{QS}$ with the mean value $\langle I \rangle_{QS, Apx}$ of the approximated distribution presented in Eq. (3.20). The quasi-stationary mean

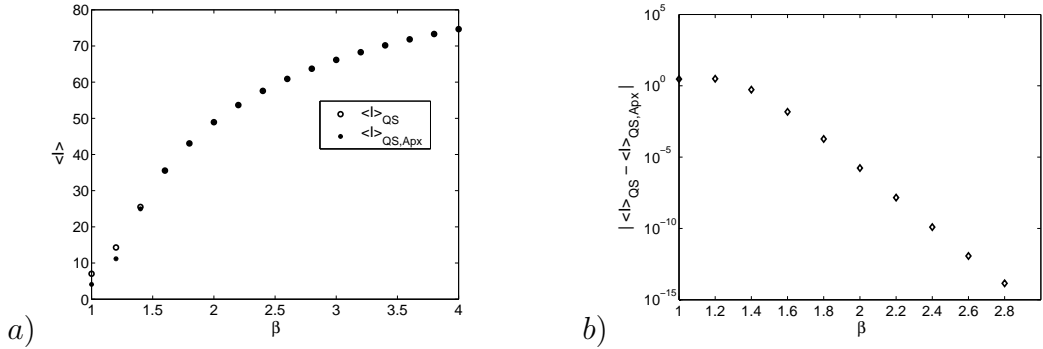


Figure 3.1: a) We compare the quasi stationary mean value of infecteds $\langle I \rangle_{QS}$ with the approximated value $\langle I \rangle_{QS,App}$, for different infection rates β . b) Distance $|\langle I \rangle_{QS} - \langle I \rangle_{QS,App}|$. Parameters $N = 100$ and $\alpha = 1$.

value was computed iteratively from Eqs. (3.5) to (3.8) with a precision of 15 digits. The parameters used are $N = 100$ and $\alpha = 1$.

3.3 Approximating the quasi-stationary states

In [35], Nåsell indicates that the stable equilibria of the 1 to 3 moment closure ODEs can be used to give a good approximation of the quasi-stationary mean value of infecteds $\langle I \rangle_{QS,\beta}$ for high values of the population size N . Here, we study how this approximation can improve using higher moment closure ODEs. In Fig. 3.2, we present the distance $|\langle I \rangle_{m,\beta}^* - \langle I \rangle_{QS,\beta}|$ between the first moment of infecteds obtained by the successive m moment closure ODEs $\langle I \rangle_{m,\beta}^*$ and the quasi-stationary mean value of infecteds $\langle I \rangle_{QS,\beta}$ for the distribution presented in Eq. (3.20). In Fig. 3.2 a), we consider a relatively small infection rate $\beta = 1.6$, above the critical mean field threshold $\beta_c = 1$, taking $\alpha = 1$ and $N = 100$. We observe that the distance $|\langle I \rangle_{m,\beta=1.6}^* - \langle I \rangle_{QS,\beta=1.6}|$ decreases with m while the equilibria $\langle I \rangle_{m,\beta=1.6}^*$ are

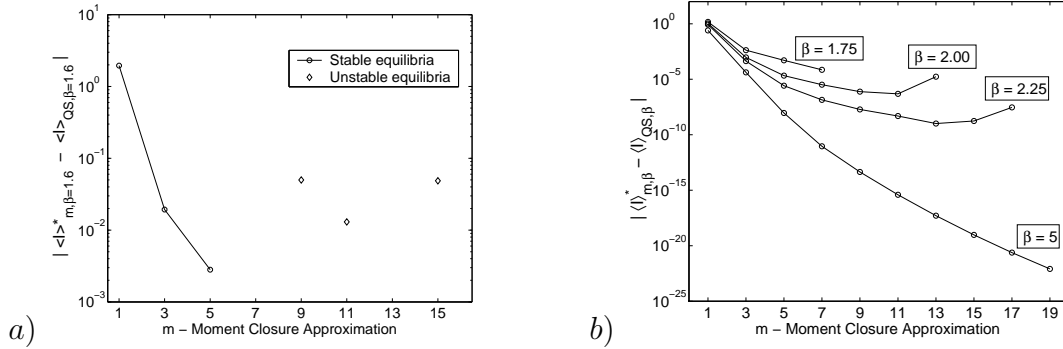


Figure 3.2: Distance $|\langle I \rangle_{m,\beta}^* - \langle I \rangle_{QS,\beta}|$ between the first moment of infecteds obtained by the successive m moment closure ODEs $\langle I \rangle_{m,\beta}^*$ and the quasi-stationary mean value $\langle I \rangle_{QS}$. In a), we consider the quasi-stationary mean value obtained from the distribution presented in Eqs. (3.5) to (3.8) and in b), the approximated distribution presented in Eq. (3.20). The population size used is $N = 100$.

stable (up to $m = 5$). In Fig. 3.2 b), we consider other infection rate values and we observe that the distance $|\langle I \rangle_{m,\beta}^* - \langle I \rangle_{QS,\beta}|$ decreases with m up to a certain m^{th} moment closure approximation that can even occur before the break down of the stable equilibria for the value of the infection rate β under consideration. In Table 3.1, we show the values of the cumulants $\langle \langle I^n \rangle \rangle_{QS,\beta}$, for $n = 1, 2, 3$, obtained by the quasi-stationary distribution of infecteds and the distances $d_m = |\langle \langle I^n \rangle \rangle_{QS,\beta} - \langle \langle I^n \rangle \rangle_{m,\beta}^*|$ between these cumulants and the corresponding cumulants obtained from the m moment closure ODEs, taking $\beta = 5$, $\alpha = 1$ and considering different populations size $N = 10, 100$ and 1000 and different orders $m = 3, 5$ and 15 of the moment closure ODEs. We note that for $N = 10$ and $m = 15$, the stable equilibria break down and the distance d_{15} is not well defined. In table 1 of [35] a similar study is done for the case $m = 3$. Here, we show that the computations of the quasi-stationary cumulants improves when we consider

N	$\langle\langle I^n \rangle\rangle_{QS}$	d_3	d_5	d_{15}
10	$\langle\langle I \rangle\rangle = 7.677$	4.7×10^{-3}	1.3×10^{-2}	
	$\langle\langle I^2 \rangle\rangle = 2.455$	5.2×10^{-2}	7.6×10^{-2}	
	$\langle\langle I^3 \rangle\rangle = -2.790$	4.4×10^{-1}	4.5×10^{-1}	
100	$\langle\langle I \rangle\rangle = 79.745$	4.2×10^{-5}	9.2×10^{-9}	9.4×10^{-20}
	$\langle\langle I^2 \rangle\rangle = 20.322$	3.4×10^{-3}	7.3×10^{-7}	7.5×10^{-18}
	$\langle\langle I^3 \rangle\rangle = -20.493$	2.7×10^{-1}	5.8×10^{-5}	5.9×10^{-16}
1000	$\langle\langle I \rangle\rangle = 799.750$	3.9×10^{-7}	6.4×10^{-13}	2.1×10^{-35}
	$\langle\langle I^2 \rangle\rangle = 200.313$	3.2×10^{-4}	5.1×10^{-10}	1.7×10^{-32}
	$\langle\langle I^3 \rangle\rangle = -200.471$	2.5×10^{-1}	4.1×10^{-7}	1.4×10^{-29}

Table 3.1: Values of the cumulants $\langle\langle I^n \rangle\rangle_{QS,\beta}$, $n = 1, 2, 3$, of the quasi-stationary distribution of infecteds for different population sizes $N = 10, 100$ and 1000 , taking $\beta = 5$ and $\alpha = 1$. In the third, fourth and fifth columns we present the distances $d_m = |\langle\langle I^n \rangle\rangle_{QS,\beta} - \langle\langle I^n \rangle\rangle_{m,\beta}^*|$ between these cumulants and the corresponding cumulants $\langle\langle I^n \rangle\rangle_{m,\beta}^*$ obtained from the $m = 3, 5$ and 15 moment closure ODEs.

a higher m moment closure approximation instead of $m = 3$.

Chapter 4

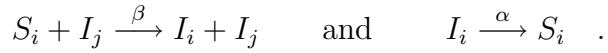
The SIS model with creation and annihilation operators

In this chapter we will formulate the spatial stochastic SIS model using the creation and annihilation operators. We consider the series expansion of the gap between the dominant and subdominant eigenvalues of the evolution operator and we compute explicitly the first terms of this series expansion for the 1 dimensional SIS model.

4.1 The spatial stochastic SIS model

The spatial stochastic SIS (Susceptible-Infected-Susceptible) model is one of the best known epidemic models and one of the simplest. It describes the evolution of an infectious disease through a population of N individuals, which can be either infected or susceptible. This epidemic model is also known as the contact process because it describes an interacting-particle sys-

tem on a regular lattice, where the particles are annihilated spontaneously and created catalytically. We consider that a particle is annihilated with rate α , usually $\alpha = 1$, and created with a rate β times the fraction of the nearest neighbours occupied sites. In an epidemic context, we can illustrate this behaviour by the following scheme



We use the state variables

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (4.1)$$

to represent the site i whenever is empty or occupied, or when the individual i is susceptible or infected. The configuration of the lattice can be represented by

$$|\eta\rangle = |\eta_1 \eta_2 \dots \eta_N\rangle = |\eta_1\rangle \otimes |\eta_2\rangle \otimes \dots \otimes |\eta_N\rangle \quad , \quad (4.2)$$

where \otimes represents the usual tensor product, $|\eta_i\rangle = |0\rangle$ or $|\eta_i\rangle = |1\rangle$ represents the state of each site i and N denotes the total number of the sites.

4.1.1 The creation and annihilation operators

To describe the SIS epidemic model using the creation and annihilation operators, we define the following operators to act on each site of the lattice.

Definition 4.1.1 *The creation operator, c_i^+ , and the annihilation operator,*

c_i , are given by

$$c_i^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad c_i = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} . \quad (4.3)$$

It is obvious that these local operators applied to the state variables give

$$c_i^+ |0\rangle = |1\rangle \quad \text{and} \quad c_i |1\rangle = |0\rangle . \quad (4.4)$$

Let $J_{i,j} \in \{0, 1\}$ be the elements of the $N \times N$ adjacency matrix J , symmetric and with zero diagonal elements, that describes the neighbouring structure of the individuals: if $J_{i,j} = 1$ then the individual i is a neighbour of j and if $J_{i,j} = 0$ then the individual i is not a neighbour of j . We consider that the individuals live on a regular lattice, where each corner has the same number Q of edges. Following [13], we observe that the time evolution of the probability $p(\eta, t) = p(\eta_1, \dots, \eta_N, t)$ is given by the master equation

$$\begin{aligned} \frac{d}{dt} p(\eta, t) = & \sum_{i=1}^N w_{\eta_i, 1-\eta_i} p(\eta_1, \dots, 1 - \eta_i, \dots, \eta_N, t) \\ & - \sum_{i=1}^N w_{1-\eta_i, \eta_i} p(\eta_1, \dots, \eta_i, \dots, \eta_N, t) \quad , \quad (4.5) \end{aligned}$$

for $\eta_i \in \{0, 1\}$ and with the transition rates

$$w_{\eta_i, 1-\eta_i} = \beta \left(\sum_{j=1}^N J_{ij} \eta_j \right) \eta_i + \alpha (1 - \eta_i)$$

$$w_{1-\eta_i, \eta_i} = \beta \left(\sum_{j=1}^N J_{ij} \eta_j \right) (1 - \eta_i) + \alpha \eta_i \quad .$$

We use the term master equation as specified in [47], especially in application to chemical reactions. For spatial systems our approach corresponds to the master equation as used by Glauber [13] for an Ising spin dynamics. There the spin variable at each lattice site σ_i can take values -1 or +1, whereas our state variables, e.g. I_i can take 0 or 1. Whereas Glauber fixed the transition rates to obtain the desired stationary states to give the original Ising model, we fix the transition rates due to the infection dynamics (in the way chemical reactions are described [47]). But the structure of our master equation has the same formal form as the one used in the spatial set-up by Glauber [13].

Now we will use the vector representation given by

$$\begin{aligned} |\psi(t)\rangle &= \sum_{\eta_1=0}^1 \sum_{\eta_2=0}^1 \dots \sum_{\eta_N=0}^1 p(\eta_1, \dots, \eta_N, t) (c_1^+)^{\eta_1} \dots (c_N^+)^{\eta_N} |O\rangle \\ &= \sum_{\eta} p(\eta, t) \prod_{i=1}^N (c_i^+)^{\eta_i} |O\rangle \quad , \end{aligned} \quad (4.6)$$

where $|O\rangle$ represents the vacuum state and $|\eta\rangle$ represents the configuration of the lattice. Hence, the time evolution of the state vector $|\psi(t)\rangle$ is given by

$$\frac{d}{dt} |\psi(t)\rangle = L |\psi(t)\rangle \quad , \quad (4.7)$$

where the evolution operator L can be written in terms of the creation and annihilation operators, after some calculations from the master equation, as

$$\begin{aligned} L &= \alpha \sum_{i=1}^N (\mathbb{1}_i - c_i^\dagger) c_i + \beta Q \sum_{i=1}^N (\mathbb{1}_i - c_i) \left(\frac{1}{Q} \sum_{j=1}^N J_{ij} c_j^\dagger c_j \right) c_i^\dagger \\ &= \alpha W_0 + \lambda V \quad , \end{aligned} \tag{4.8}$$

with $\lambda = \beta Q$, $\mathbb{1}_i$ being the identity matrix at site i and zero elsewhere, and W_0 and V abbreviating the single site respectively multi-site operator expressions. Changing the time scale to $\tau = t/\alpha$, the new rates become $\alpha = 1$ and $\lambda = \beta Q/\alpha$ and the evolution operator L is given by

$$L = W_0 + \lambda V \quad . \tag{4.9}$$

From now on we will consider only 1 dimensional lattices. Hence, each individual has $Q = 2$ neighbours.

In the following definition we present some local operators that will be used in future computations.

Definition 4.1.2 *Let $\mathbf{1}$ be the two-dimensional identity matrix and let \hat{B} , \hat{Q} and \hat{n} be the local operators given by*

$$\hat{B} = (\mathbf{1} - c^+)c \quad , \quad (4.10)$$

$$\hat{Q} = \frac{1}{2}(\mathbf{1} - c)c^+ \quad , \quad (4.11)$$

$$\hat{n} = c^+c \quad . \quad (4.12)$$

The operator \hat{n} is called the number operator. In the following Lemma, we observe the result of applying these operators to the state variables.

Lemma 4.1.1 *The local operators presented in Definition 4.1.2 applied to the state variables $|0\rangle$ and $|1\rangle$ give:*

$$\hat{B}|0\rangle = 0 \quad \text{and} \quad \hat{B}|1\rangle = |0\rangle - |1\rangle \quad , \quad (4.13)$$

$$\hat{Q}|0\rangle = \frac{1}{2}(|1\rangle - |0\rangle) \quad \text{and} \quad \hat{Q}|1\rangle = 0 \quad , \quad (4.14)$$

$$\hat{n}|0\rangle = 0 \quad \text{and} \quad \hat{n}|1\rangle = |1\rangle \quad . \quad (4.15)$$

The proof of this Lemma is trivial and it will not be presented here.

4.1.2 The σ representation

We start to observe that the operator \hat{B} has eigenvalues 0 and -1 associated to the right eigenvectors $|0\rangle$ and $|1\rangle - |0\rangle$. So, it is convenient to change the

coordinated system to these right eigenvectors that we define by

$$|\tilde{0}\rangle = |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad |\tilde{1}\rangle = |1\rangle - |0\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix} . \quad (4.16)$$

The left eigenvectors of \hat{B} are $\langle\tilde{0}| = \langle 0| + \langle 1|$ and $\langle\tilde{1}| = \langle 1|$, associated with the eigenvalues 0 and -1 respectively.

Lemma 4.1.2 *The local operators presented in Definition 4.1.2 applied to the state variables $|\tilde{0}\rangle$ and $|\tilde{1}\rangle$ give*

$$\hat{B} |\tilde{0}\rangle = 0 \quad \text{and} \quad \hat{B} |\tilde{1}\rangle = -|\tilde{1}\rangle , \quad (4.17)$$

$$\hat{Q} |\tilde{0}\rangle = \frac{1}{2} |\tilde{1}\rangle \quad \text{and} \quad \hat{Q} |\tilde{1}\rangle = -\frac{1}{2} |\tilde{1}\rangle , \quad (4.18)$$

$$\hat{n} |\tilde{0}\rangle = 0 \quad \text{and} \quad \hat{n} |\tilde{1}\rangle = |\tilde{1}\rangle + |\tilde{0}\rangle . \quad (4.19)$$

Once again the proof of this Lemma is trivial.

Let the state of two sites of the lattice be denoted by e.g.

$$|\tilde{0}\tilde{0}\rangle = |\tilde{0}\rangle \otimes |\tilde{0}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} . \quad (4.20)$$

Similarly, we define the two sites states $|\tilde{0}\tilde{1}\rangle$, $|\tilde{1}\tilde{0}\rangle$ and $|\tilde{1}\tilde{1}\rangle$. The operators that act on these two sites are given by, e.g., $B_1 + B_2$, where

$$B_1 = \hat{B} \otimes \mathbf{1} = \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (4.21)$$

acts on the first site and

$$B_2 = \mathbf{1} \otimes \hat{B} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad (4.22)$$

acts on the second site. Therefore, $B_1 + B_2$ acts, e.g., on the pair $|\tilde{0}\tilde{1}\rangle$ giving

$$(B_1 + B_2)|\tilde{0}\tilde{1}\rangle = \begin{pmatrix} -2 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} = -|\tilde{0}\tilde{1}\rangle \quad (4.23)$$

This result can also be justified using the properties of the tensor product

$$\begin{aligned}
(B_1 + B_2) |\tilde{0}\tilde{1}\rangle &= B_1 |\tilde{0}\tilde{1}\rangle + B_2 |\tilde{0}\tilde{1}\rangle \\
&= (\hat{B} \otimes \mathbf{1}) (|\tilde{0}\rangle \otimes |\tilde{1}\rangle) + (\mathbf{1} \otimes \hat{B}) (|\tilde{0}\rangle \otimes |\tilde{1}\rangle) \\
&= (\hat{B} |\tilde{0}\rangle) \otimes (\mathbf{1} |\tilde{1}\rangle) + (\mathbf{1} |\tilde{0}\rangle) \otimes (\hat{B} |\tilde{1}\rangle) \quad (4.24) \\
&= 0 \otimes |\tilde{1}\rangle + |\tilde{0}\rangle \otimes (-|\tilde{1}\rangle) \\
&= 0 - (|\tilde{0}\rangle \otimes |\tilde{1}\rangle) \\
&= -|\tilde{0}\tilde{1}\rangle \quad .
\end{aligned}$$

In the same way we obtain that

$$(B_1 + B_2) |\tilde{0}\tilde{0}\rangle = 0 \quad , \quad (4.25)$$

$$(B_1 + B_2) |\tilde{1}\tilde{0}\rangle = -|\tilde{1}\tilde{0}\rangle \quad , \quad (4.26)$$

$$(B_1 + B_2) |\tilde{1}\tilde{1}\rangle = -2|\tilde{1}\tilde{1}\rangle \quad . \quad (4.27)$$

This representation can be generalized for all the sites in the lattice by

$$|\sigma\rangle = |\sigma_1 \sigma_2 \dots \sigma_N\rangle \quad , \quad \sigma_i \in \{\tilde{0}, \tilde{1}\} \quad , \quad (4.28)$$

which we call the σ representation. To act on the $|\sigma\rangle$ vector we define the operator

$$W_0 = \sum_{i=1}^N B_i \quad , \quad (4.29)$$

where

$$\begin{aligned} B_i &= \mathbf{1} \otimes \dots \otimes \mathbf{1} \otimes \hat{B} \otimes \mathbf{1} \otimes \dots \otimes \mathbf{1} \\ &= \mathbf{1}^{\otimes(i-1)} \otimes \hat{B} \otimes \mathbf{1}^{\otimes(N-i)} \quad , \end{aligned} \quad (4.30)$$

with \hat{B} being the operator defined in Eq. (4.10), Def. 4.1.2. Hence, generalizing the calculations presented in Eq. (4.24), we have that

$$\begin{aligned} W_0 |\sigma\rangle &= \sum_{i=1}^N B_i |\sigma_1 \sigma_2 \dots \sigma_N\rangle \\ &= - \sum_{i=1}^N \sigma_i |\sigma_1 \sigma_2 \dots \sigma_N\rangle \quad . \end{aligned} \quad (4.31)$$

Therefore, the operator $W_0 = \sum_{i=1}^N B_i$ has eigenvalues given by

$$\Lambda(\sigma) = - \sum_{i=1}^N \sigma_i \quad . \quad (4.32)$$

To operate in the two sites states we define the operators

$$Q_1 = \hat{Q} \otimes \mathbf{1}, \quad Q_2 = \mathbf{1} \otimes \hat{Q}, \quad n_1 = \hat{n} \otimes \mathbf{1} \quad \text{and} \quad n_2 = \mathbf{1} \otimes \hat{n} \quad .(4.33)$$

where \hat{Q} and \hat{n} are the operators defined in Eqs. (4.11) and (4.12) of Definition 4.1.2.

Theorem 4.1.1 *With the operators presented in Eq. (4.33) the following rules are satisfied*

$$(Q_1 n_2 + n_1 Q_2) |\tilde{0}\tilde{0}\rangle = 0 \quad , \quad (4.34)$$

$$(Q_1 n_2 + n_1 Q_2) |\tilde{0}\tilde{1}\rangle = \frac{1}{2} |\tilde{1}\tilde{0}\rangle + \frac{1}{2} |\tilde{1}\tilde{1}\rangle \quad , \quad (4.35)$$

$$(Q_1 n_2 + n_1 Q_2) |\tilde{1}\tilde{0}\rangle = \frac{1}{2} |\tilde{0}\tilde{1}\rangle + \frac{1}{2} |\tilde{1}\tilde{1}\rangle \quad , \quad (4.36)$$

$$(Q_1 n_2 + n_1 Q_2) |\tilde{1}\tilde{1}\rangle = -\frac{1}{2} |\tilde{0}\tilde{1}\rangle - \frac{1}{2} |\tilde{1}\tilde{0}\rangle - |\tilde{1}\tilde{1}\rangle \quad . \quad (4.37)$$

Proof. Due to the similarity of the calculations, here we prove only the second rule of the theorem. We start to observe that

$$\begin{aligned} Q_1 n_2 &= (\hat{Q} \otimes \mathbf{1}) (\mathbf{1} \otimes \hat{n}) \\ &= (\hat{Q}\mathbf{1}) \otimes (\mathbf{1}\hat{n}) \\ &= \hat{Q} \otimes \hat{n} \quad , \end{aligned} \quad (4.38)$$

and, in the same way, we have $n_1 Q_2 = \hat{n} \otimes \hat{Q}$. Hence, applying the Lemma 4.1.2, we obtain that

$$\begin{aligned} Q_1 n_2 |\tilde{0}\tilde{1}\rangle &= (\hat{Q} \otimes \hat{n}) (|\tilde{0}\rangle \otimes |\tilde{1}\rangle) \\ &= (\hat{Q} |\tilde{0}\rangle) \otimes (\hat{n} |\tilde{1}\rangle) \\ &= \frac{1}{2} |\tilde{1}\rangle \otimes (|\tilde{1}\rangle + |\tilde{0}\rangle) \\ &= \frac{1}{2} |\tilde{1}\tilde{1}\rangle + \frac{1}{2} |\tilde{1}\tilde{0}\rangle \quad , \end{aligned} \quad (4.39)$$

and

$$\begin{aligned}
n_1 Q_2 |\tilde{0}\tilde{1}\rangle &= (\hat{n} \otimes \hat{Q}) (|\tilde{0}\rangle \otimes |\tilde{1}\rangle) \\
&= (\hat{n} |\tilde{0}\rangle) \otimes (\hat{Q} |\tilde{1}\rangle) \\
&= 0 \otimes \left(-\frac{1}{2} |\tilde{1}\rangle\right) \\
&= 0 \quad .
\end{aligned} \tag{4.40}$$

Therefore, summing Eqs. (4.39) and (4.40) it follows immediately that $(Q_1 n_2 + n_1 Q_2) |\tilde{0}\tilde{1}\rangle = \frac{1}{2} |\tilde{1}\tilde{0}\rangle + \frac{1}{2} |\tilde{1}\tilde{1}\rangle$. ■

4.2 Series expansion

We observe that the annihilation and creation operators that appear in the evolution operator L presented in Eq. (4.9) are given (see [16, 45]) by the expressions

$$W_0 = \sum_{i=1}^N B_i \quad , \tag{4.41}$$

and

$$V = \sum_{i=1}^N Q_i (n_{i-1} + n_{i+1}) \quad , \tag{4.42}$$

where the V operator can be reorganized and written in the form

$$V = \sum_{i=1}^N (Q_i n_{i+1} + n_i Q_{i+1}) \quad . \tag{4.43}$$

From Eq. (4.31) we observe that

$$\begin{aligned} \sum_{i=1}^N B_i |O\rangle &= \sum_{i=1}^N B_i |\tilde{0} \dots \tilde{0}\rangle \\ &= - \sum_{i=1}^N 0 |\tilde{0} \dots \tilde{0}\rangle = 0 \quad , \end{aligned} \quad (4.44)$$

and from Eq. (4.34) we also observe that

$$\sum_{i=1}^N (Q_i n_{i+1} + n_i Q_{i+1}) |O\rangle = 0 \quad . \quad (4.45)$$

Therefore, we conclude that $|O\rangle = |\tilde{0} \dots \tilde{0}\rangle$ is an eigenvector of L for the zero eigenvalue

$$L |O\rangle = \sum_{i=1}^N B_i |O\rangle + \lambda \sum_{i=1}^N (Q_i n_{i+1} + n_i Q_{i+1}) |O\rangle \quad (4.46)$$

$$= 0 + \lambda 0 = 0 \quad . \quad (4.47)$$

From Eq. (4.31) we also observe that the subdominant eigenvalue of W_0 is -1 and the correspondent eigenvector is $|\psi_0\rangle = |.\tilde{1}.\rangle$, where the two dots means that all sites at the right and the left of $\tilde{1}$ are $\tilde{0}$,

$$\begin{aligned} W_0 |\psi_0\rangle &= \sum_{i=1}^N B_i |.\tilde{1}\rangle \\ &= - |.\tilde{1}\rangle \\ &= - |\psi_0\rangle \quad . \end{aligned} \quad (4.48)$$

Now, we are interested in determining the subdominant eigenvalue of the evolution operator L . Let $|\psi\rangle$ denote this subdominant eigenvector and A the correspondent eigenvalue

$$L|\psi\rangle = A|\psi\rangle \quad . \quad (4.49)$$

Hence, the gap between the dominant eigenvalue and the subdominant eigenvalue of L is given by

$$\Gamma = 0 - A = -A \quad . \quad (4.50)$$

We assume that $|\psi\rangle$ and A can be expanded in powers of λ

$$|\psi\rangle = |\psi_0\rangle + \lambda|\psi_1\rangle + \lambda^2|\psi_2\rangle + \dots = \sum_{n=0}^{\infty} \lambda^n |\psi_n\rangle \quad , \quad (4.51)$$

$$A = A_0 + \lambda A_1 + \lambda^2 A_2 + \dots = \sum_{n=0}^{\infty} A_n \lambda^n \quad , \quad (4.52)$$

where $|\psi_0\rangle = |\tilde{1}\rangle$ and $A_0 = -1$. Therefore, the expansion of the gap between the dominant and the subdominant eigenvalues Γ is given by

$$\Gamma = 1 - \lambda A_1 - \lambda^2 A_2 - \dots \quad . \quad (4.53)$$

We choose the vectors $|\psi_n\rangle$ to be orthogonal to the vector $|\psi_0\rangle$

$$\langle \psi_0 | \psi_n \rangle = 0 \quad , \quad \forall n = 1, 2, \dots \quad . \quad (4.54)$$

We show how to obtain A_n and $|\psi_n\rangle$ in the following computations. Inserting the expanded expressions of $|\psi\rangle$ and A in Eq. (4.49) we obtain

$$\begin{aligned}
(W_0 + \lambda V) \sum_{n=0}^{\infty} \lambda^n |\psi_n\rangle &= \left(\sum_{m=0}^{\infty} A_m \lambda^m \right) \left(\sum_{n=0}^{\infty} \lambda^n |\psi_n\rangle \right) \\
\Leftrightarrow \sum_{n=0}^{\infty} W_0 |\psi_n\rangle \lambda^n + \sum_{n=0}^{\infty} V |\psi_n\rangle \lambda^{n+1} &= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A_m |\psi_n\rangle \lambda^{m+n} \\
\Leftrightarrow \sum_{n=0}^{\infty} W_0 |\psi_n\rangle \lambda^n + \sum_{n=1}^{\infty} V |\psi_{n-1}\rangle \lambda^n &= \sum_{n=0}^{\infty} \sum_{m=0}^n A_m |\psi_{n-m}\rangle \lambda^n \\
\Leftrightarrow W_0 |\psi_0\rangle + \sum_{n=1}^{\infty} (W_0 |\psi_n\rangle + V |\psi_{n-1}\rangle) \lambda^n &= \\
&= A_0 |\psi_0\rangle + \sum_{n=1}^{\infty} \sum_{m=0}^n A_m |\psi_{n-m}\rangle \lambda^n . \quad (4.55)
\end{aligned}$$

Comparing the coefficients of the same powers of λ in both sides of Eq. (4.55) we verify that

$$W_0 |\psi_0\rangle = A_0 |\psi_0\rangle \quad , \quad (4.56)$$

in the case of $n = 0$ and for other values

$$W_0 |\psi_n\rangle + V |\psi_{n-1}\rangle = \sum_{m=0}^n A_m |\psi_{n-m}\rangle \quad . \quad (4.57)$$

Multiplying by $\langle \psi_0 |$ and using the orthogonality $\langle \psi_0 | \psi_n \rangle, \forall n \neq 0$, we obtain

$$\begin{aligned}
 \langle \psi_0 | W_0 | \psi_n \rangle + \langle \psi_0 | V | \psi_{n-1} \rangle &= \sum_{m=0}^n A_m \langle \psi_0 | \psi_{n-m} \rangle \\
 \Leftrightarrow A_0 \langle \psi_0 | \psi_n \rangle + \langle \psi_0 | V | \psi_{n-1} \rangle &= \sum_{m=0}^n A_m \delta_{0, n-m} \\
 \Leftrightarrow A_0 0 + \langle \psi_0 | V | \psi_{n-1} \rangle &= A_n \quad . \quad (4.58)
 \end{aligned}$$

Hence, the coefficients A_n of the expansion of the subdominant eigenvalue of L can be computed recursively by the formula

$$A_n = \langle \psi_0 | V | \psi_{n-1} \rangle, \quad \forall n \geq 1, \quad \text{and} \quad A_0 = -1 \quad . \quad (4.59)$$

Now, we have to determine the vectors $|\psi_n\rangle$. Since W_0 has eigenvalues given by $\Lambda(\sigma) = -\sum_{i=1}^N \sigma_i$ (see Eqs. (4.31) and (4.32)) this operator can be written by the expression

$$\begin{aligned}
 W_0 &= \sum_{\substack{\sigma_1=\bar{0} \\ \sigma_1+\dots+\sigma_N \neq 0}}^1 \dots \sum_{\sigma_N=\bar{0}}^1 |\sigma_1 \dots \sigma_N\rangle \Lambda(\sigma_1 \dots \sigma_N) \langle \sigma_1 \dots \sigma_N| \\
 &= \sum_{\sigma} '|\sigma\rangle \Lambda(\sigma) \langle \sigma| \quad . \quad (4.60)
 \end{aligned}$$

Let R be the operator given by

$$\begin{aligned}
 R &= \sum_{\substack{\sigma_1=\tilde{0} \\ \sigma_1+\dots+\sigma_N \notin \{0,-1\}}}^1 \dots \sum_{\sigma_N=\tilde{0}}^1 |\sigma_1 \dots \sigma_N\rangle \frac{1}{\Lambda(\sigma_1 \dots \sigma_N) - A_0} \langle \sigma_1 \dots \sigma_N| \\
 &= \sum_{\sigma} "|\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} \langle \sigma| \quad . \quad (4.61)
 \end{aligned}$$

From Eq. (4.57) we observe that

$$\begin{aligned}
 W_0 |\psi_n\rangle + V |\psi_{n-1}\rangle &= A_0 |\psi_n\rangle + \sum_{m=1}^n A_m |\psi_{n-m}\rangle \\
 \Leftrightarrow (W_0 - A_0) |\psi_n\rangle &= -V |\psi_{n-1}\rangle + \sum_{m=1}^n A_m |\psi_{n-m}\rangle \quad , \quad (4.62)
 \end{aligned}$$

and applying R we obtain

$$R(W_0 - A_0) |\psi_n\rangle = -RV |\psi_{n-1}\rangle + \sum_{m=1}^n A_m R |\psi_{n-m}\rangle \quad . \quad (4.63)$$

But

$$\begin{aligned}
R(W_0 - A_0) &= \sum_{\sigma} "|\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} \langle\sigma| (W_0 - A_0) \\
&= \sum_{\sigma} "|\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} (\langle\sigma| W_0 - \langle\sigma| A_0) \\
&= \sum_{\sigma} "|\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} (\Lambda(\sigma) \langle\sigma| - A_0 \langle\sigma|) \\
&= \sum_{\sigma} "|\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} (\Lambda(\sigma) - A_0) \langle\sigma| \\
&= \sum_{\sigma} "|\sigma\rangle \langle\sigma| \quad , \tag{4.64}
\end{aligned}$$

and joining to this sum the terms for the cases $\sigma_1 + \dots + \sigma_N = 0$ and $\sigma_1 + \dots + \sigma_N = -1$ we complete the eigenbasis $\sum_{\sigma} |\sigma\rangle \langle\sigma| = \mathbf{1}$. Hence,

$$R(W_0 - A_0) = \sum_{\sigma} |\sigma\rangle \langle\sigma| - |O\rangle \langle O| - |\psi_0\rangle \langle\psi_0| \quad , \tag{4.65}$$

and therefore,

$$\begin{aligned}
R(W_0 - A_0) |\psi_n\rangle &= \mathbf{1} |\psi_n\rangle - |O\rangle \langle O|\psi_n\rangle - |\psi_0\rangle \langle\psi_0|\psi_n\rangle \\
&= |\psi_n\rangle \quad . \tag{4.66}
\end{aligned}$$

Hence, from Eq. (4.63) we obtain for the calculation of the state $|\psi_n\rangle$ the difference equation

$$\begin{aligned} |\psi_n\rangle &= -RV|\psi_{n-1}\rangle + \sum_{m=1}^n A_m R|\psi_{n-m}\rangle \\ &= -RV|\psi_{n-1}\rangle + \sum_{m=1}^{n-1} A_m R|\psi_{n-m}\rangle \quad . \end{aligned} \quad (4.67)$$

In conclusion, we observe that the expansion of the gap Γ

$$\Gamma = 1 - \lambda A_1 - \lambda^2 A_2 - \dots \quad (4.68)$$

is given by the recursive process

$$A_n = \langle \psi_0 | V | \psi_{n-1} \rangle, \quad \forall n \geq 1 \quad , \quad (4.69)$$

with the vectors

$$|\psi_0\rangle = |.\tilde{1}.\rangle \quad , \quad (4.70)$$

$$|\psi_1\rangle = -RV|\psi_0\rangle \quad , \quad (4.71)$$

$$|\psi_n\rangle = -RV|\psi_{n-1}\rangle + \sum_{m=1}^{n-1} A_m R|\psi_{n-m}\rangle, \quad \forall n \geq 2 \quad . \quad (4.72)$$

4.3 Explicit calculation of series expansion

We will now compute explicitly some coefficients of the expansion of the gap between the dominant and the subdominant eigenvector of the evolution operator for the SIS model. Here, we do not consider the translation invariance of the lattice, in contrast to de Oliveira [7]. For the initial state

$$|\psi_0\rangle = |\tilde{0}\tilde{1}\tilde{0}\rangle \quad (4.73)$$

and unperturbed eigenvalue $A_0 = -1$ we obtain

$$A_1 = \langle \psi_0 | V | \psi_0 \rangle = 0 \quad . \quad (4.74)$$

This value results from

$$\begin{aligned} V|\psi_0\rangle &= \left((Q_1 n_2 + n_1 Q_2) + (Q_2 n_3 + n_2 Q_3) + (Q_3 n_1 + n_3 Q_1) \right) |\tilde{0}\tilde{1}\tilde{0}\rangle \\ &= \frac{1}{2} \left(|\tilde{1}\tilde{0}\tilde{0}\rangle + |\tilde{1}\tilde{1}\tilde{0}\rangle + |\tilde{0}\tilde{0}\tilde{1}\rangle + |\tilde{0}\tilde{1}\tilde{1}\rangle \right) \end{aligned} \quad (4.75)$$

and therefore

$$A_1 = \langle \tilde{0}\tilde{1}\tilde{0} | V | \psi_0 \rangle = 0 \quad (4.76)$$

since $\langle \tilde{0}\tilde{1}\tilde{0} | \tilde{1}\tilde{1}\tilde{0} \rangle = 0$ etc. due to the orthonormality of the states. The state vector of first order in the series expansion is given by

$$\begin{aligned} |\psi_1\rangle &= -RV|\psi_0\rangle \\ &= - \sum_{\Lambda(\sigma) \notin \{0, -1\}} |\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} \langle \sigma | \cdot V | \psi_0 \rangle \quad . \end{aligned} \quad (4.77)$$

Since

$$\sum_{\Lambda(\sigma) \notin \{0, -1\}} |\sigma\rangle \frac{1}{\Lambda(\sigma) - A_0} \langle \sigma| = |\tilde{1}\tilde{1}\tilde{0}\rangle \frac{1}{-2+1} \langle \tilde{1}\tilde{1}\tilde{0}| + |\tilde{1}\tilde{0}\tilde{1}\rangle \frac{1}{-2+1} \langle \tilde{1}\tilde{0}\tilde{1}| \\ + |\tilde{0}\tilde{1}\tilde{1}\rangle \frac{1}{-2+1} \langle \tilde{0}\tilde{1}\tilde{1}| + |\tilde{1}\tilde{1}\tilde{1}\rangle \frac{1}{-3+1} \langle \tilde{1}\tilde{1}\tilde{1}| \quad ,$$

we find from Eq. (4.77)

$$|\psi_1\rangle = -\frac{1}{2} \left(\frac{1}{-2+1} |\tilde{1}\tilde{1}\tilde{0}\rangle + \frac{1}{-2+1} |\tilde{0}\tilde{1}\tilde{1}\rangle \right) \\ = \frac{1}{2} (|\tilde{1}\tilde{1}\tilde{0}\rangle + |\tilde{0}\tilde{1}\tilde{1}\rangle) \quad . \quad (4.78)$$

For the next terms in the expansion we have to start with system size $N = 5$, hence starting with state

$$|\psi_0\rangle = |\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\rangle \quad (4.79)$$

then because of $(\hat{Q}_i \hat{n}_{i+1} + \hat{n}_i \hat{Q}_{i+1})|\tilde{0}\tilde{0}\rangle = 0$ we obtain as before

$$A_1 = 0 \quad , \quad |\psi_1\rangle = \frac{1}{2} \left(|\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle + |\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\rangle \right) \quad (4.80)$$

and computing $V|\psi_1\rangle$ as in Eq. (4.75) we obtain now

$$A_2 = \langle \psi_0 | V | \psi_1 \rangle = -\frac{1}{2} \quad . \quad (4.81)$$

The second state $|\psi_2\rangle$ of the series expansion

$$|\psi_2\rangle = -RV|\psi_1\rangle + A_1 R|\psi_0\rangle \quad (4.82)$$

gives, with $A_1 = 0$, explicitly

$$\begin{aligned}
 |\psi_2\rangle &= \frac{1}{4}|\tilde{1}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{1}{8}|\tilde{1}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle - \frac{1}{2}|\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{1}{2}|\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\rangle \\
 &\quad + \frac{1}{4}|\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\rangle - \frac{1}{2}|\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\rangle + \frac{1}{4}|\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{1}\rangle + \frac{1}{8}|\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{1}\rangle \quad (4.83)
 \end{aligned}$$

and the third coefficient gives

$$A_3 = \langle \psi_0 | V | \psi_2 \rangle = \frac{1}{2} \quad . \quad (4.84)$$

With the previous coefficients A_i and the vectors $|\psi_i\rangle$, we obtain for

$$|\psi_3\rangle = -RV|\psi_2\rangle + A_2R|\psi_1\rangle \quad (4.85)$$

the explicit expression given by

$$\begin{aligned}
 |\psi_3\rangle &= \frac{1}{4}|\tilde{1}\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle + \frac{1}{16}|\tilde{1}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle + \frac{15}{16}|\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle - \frac{1}{8}|\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle \\
 &\quad + \frac{1}{16}|\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\tilde{0}\rangle + \frac{3}{8}|\tilde{0}\tilde{1}\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{1}{8}|\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{1}{32}|\tilde{1}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle \\
 &\quad + \frac{1}{48}|\tilde{1}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle - \frac{3}{8}|\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\tilde{0}\rangle + \frac{5}{32}|\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{1}{16}|\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle \\
 &\quad - \frac{3}{4}|\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\rangle - \frac{1}{4}|\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{15}{16}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{0}\rangle + \frac{3}{8}|\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\tilde{1}\tilde{0}\rangle \\
 &\quad + \frac{5}{32}|\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\rangle + \frac{1}{8}|\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\rangle + \frac{1}{16}|\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\rangle - \frac{3}{8}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{0}\rangle \\
 &\quad - \frac{1}{8}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{0}\rangle + \frac{1}{16}|\tilde{0}\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\rangle + \frac{1}{8}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{0}\tilde{1}\rangle + \frac{1}{16}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{0}\tilde{1}\tilde{1}\rangle \\
 &\quad + \frac{1}{32}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{0}\tilde{1}\rangle + \frac{1}{48}|\tilde{0}\tilde{0}\tilde{0}\tilde{1}\tilde{1}\tilde{1}\tilde{1}\rangle \quad .
 \end{aligned}$$

Then for the A_4 coefficient we obtain

$$A_4 = \langle \psi_0 | V | \psi_3 \rangle = -\frac{15}{16} \quad (4.86)$$

which can serve as a test value for numeric programs. Continue with similar computations in an elementary computer for the other coefficients A_n of the expansion of the gap Γ , we obtain the values presented in Table 4.1.

n	$c_n = -A_n$
0	1
1	0
2	0.5
3	-0.5
4	0.9375
5	-1.8125
6	3.94010416666667
7	-8.79687500000000
8	20.45668764467593
9	-48.49340518904322

Table 4.1: The coefficients c_n of the expansion of the gap Γ .

4.3.1 Critical values

In the critical point the dominant eigenvalue becomes degenerate and the gap has a singular behaviour given by

$$\Gamma \sim (\lambda - \lambda_c)^{v_{||}} \quad , \quad (4.87)$$

and taking the logarithm derivative we have

$$\frac{d}{d\lambda} \ln \Gamma \sim \frac{v_{\parallel}}{(\lambda - \lambda_c)} \quad . \quad (4.88)$$

Hence, to obtain the critical values of λ we compute the poles of the Padé approximant of the logarithm derivative. The results are shown in the Table 4.2 for some approximations. After discover the critical parameters λ_c , we compute the Padé approximant of the left hand side of

$$(\lambda - \lambda_c) \frac{d}{d\lambda} \ln \Gamma \sim v_{\parallel} \quad , \quad (4.89)$$

to evaluate at $\lambda = \lambda_c$ giving the critical exponent v_{\parallel} . The results obtained for the previous critical parameters λ_c are also presented in Table 4.2.

Approximant	λ_c	v_{\parallel}
[2, 2]	-2.135557	-2.209077
[3, 3]	0.672395	-0.007224
[4, 4]	0.644608	-0.006032

Table 4.2: Critical parameter λ_c and the critical exponent v_{\parallel} , obtained from the Padé approximants.

These are the critical values obtained using the first coefficients of the expansion of the gap Γ . We observe that the computation of the c_n coefficient involves a square matrix of size 2^{2n+1} . Hence, to obtain the c_9 coefficient we already use matrices of size 2^{19} . To accurate the critical values we should continue with this process and compute more coefficients c_n in more sophisticated computers, with a higher memory capacity.

Chapter 5

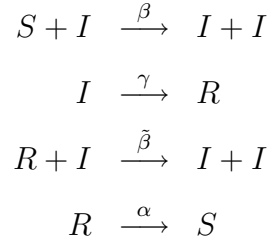
The phase transition lines in the SIRI model

In this chapter we will consider the spatial stochastic SIRI epidemic model, that includes reinfection and partial immunization. The dynamical equations for the moments will be investigated and the phase transition lines calculated analytically in the mean field and pair approximation.

5.1 The SIRI epidemic model

To describe reinfection in a simple epidemic model, we investigate an extension on classical SIS or SIR models extending to the SIRI model (see [43]). We consider the following transitions between host classes for N individuals

being either susceptible S , infected I by a disease or recovered R



resulting in the master equation (see [47]) for variables S_i, I_i and $R_i \in \{0, 1\}$, $i = 1, 2, \dots, N$, for N individuals, with constraint $S_i + I_i + R_i = 1$.

The first infection $S + I \xrightarrow{\beta} I + I$ occurs with infection rate β , whereas after recovery with rate γ the respective host becomes resistant up to a possible reinfection $R + I \xrightarrow{\tilde{\beta}} I + I$ with reinfection rate $\tilde{\beta}$. Hence the recovered are only partially immunized. For further analysis of possible stationary states we include a transition from recovered to susceptibles α , which might be simply due to demographic effects (or very slow waning immunity for some diseases). We will later consider the limit of vanishing or very small α . In case of demography that would be in the order of inverse 70 years, whereas for the basic epidemic processes like first infection β we would expect inverse a few weeks. We consider that the N individuals live on a regular lattice, where each corner has the same number Q of edges.

Let $p(S_1, I_1, R_1, S_2, I_2, R_2, \dots, R_N, t)$ be the probability of the state $S_1, I_1, R_1, S_2, I_2, R_2, \dots, R_N$ occur at time t . Let $J_{i,j} \in \{0, 1\}$ be the elements of the $N \times N$ adjacency matrix J that describes the neighbouring structure of the N individuals. Following Glauber [13], the master equation for the SIRI model gives the time evolution of the probability

$p(S_1, I_1, R_1, S_2, I_2, R_2, \dots, R_N, t)$ with respect to the underlying regular grid describing the spatial interactions of the model:

$$\begin{aligned}
\frac{d}{dt} p(S_1, I_1, R_1, S_2, I_2, R_2, \dots, R_N, t) &= \sum_{i=1}^N \beta \left(\sum_{j=1}^N J_{ij} I_j \right) (1 - S_i) p(S_1, I_1, R_1, \dots, 1 - S_i, 1 - I_i, R_i, \dots, R_N, t) \\
&+ \sum_{i=1}^N \gamma (1 - I_i) p(S_1, I_1, R_1, \dots, S_i, 1 - I_i, 1 - R_i, \dots, R_N, t) \\
&+ \sum_{i=1}^N \tilde{\beta} \left(\sum_{j=1}^N J_{ij} I_j \right) (1 - R_i) p(S_1, I_1, R_1, \dots, S_i, 1 - I_i, 1 - R_i, \dots, R_N, t) \\
&+ \sum_{i=1}^N \alpha (1 - R_i) p(S_1, I_1, R_1, \dots, 1 - S_i, I_i, 1 - R_i, \dots, R_N, t) \\
&- \sum_{i=1}^N \left[\beta \left(\sum_{j=1}^N J_{ij} I_j \right) S_i + \gamma I_i + \tilde{\beta} \left(\sum_{j=1}^N J_{ij} I_j \right) R_i + \alpha R_i \right] \\
&\quad \cdot p(\dots S_i, I_i, R_i \dots) \quad .
\end{aligned} \tag{5.1}$$

The expectation value of the total number of infected hosts $\langle I \rangle$ at a given time t is

$$\begin{aligned}
\langle I \rangle(t) &= \sum_{SIR} \left(\sum_{i=1}^N I_i \right) p(S_1, I_1, R_1, S_2, \dots, R_N, t) \\
&= \sum_{i=1}^N \sum_{SIR} I_i p(S_1, I_1, R_1, S_2, \dots, R_N, t) \\
&= \sum_{i=1}^N \langle I_i \rangle(t) \quad .
\end{aligned} \tag{5.2}$$

where \sum_{SIR} denotes the sum $\sum_{S_1=0}^1 \sum_{I_1=0}^1 \sum_{R_1=0}^1 \sum_{S_2=0}^1 \cdots \sum_{R_N=0}^1$, and $p(S_1, I_1, R_1, S_2, \dots, R_N, t)$ is the probability of the state $S_1, I_1, R_1, S_2, \dots, R_N$ occurs at time t given by the master equation for the SIRI model.

Similarly to the first moment, the second moment $\langle SI \rangle$ of the expectation value of two individuals neighbours in which one is susceptible and one is infected is the pair given by

$$\begin{aligned} \langle SI \rangle(t) &= \sum_{SIR} \left(\sum_{i=1}^N \sum_{j=1}^N J_{ij} S_i I_j \right) p(S_1, I_1, R_1, \dots, R_N, t) \\ &= \sum_{i=1}^N \sum_{j=1}^N J_{ij} \langle S_i I_j \rangle(t) \quad . \end{aligned} \quad (5.3)$$

The other first and second moments are defined similarly. These are dynamic variables, e.g. $\langle I \rangle(t)$, and the stationary values will be denoted by $\langle I \rangle^*$, $\langle R \rangle^*$ etc.

5.1.1 The ODEs for the moments

We are going to determine the dynamic equations for the first moments $\langle S \rangle$, $\langle I \rangle$ and $\langle R \rangle$ (see Eq. (5.12)), and for the second moments $\langle SS \rangle$, $\langle II \rangle$, $\langle RR \rangle$, $\langle SI \rangle$, $\langle SR \rangle$ and $\langle IR \rangle$ (see Eq. (5.20)) using the master equation of the spatial stochastic SIRI model presented in Eq. (5.1).

In the next theorem we present the ODE for the first moment of infecteds $\langle I \rangle$ and for the other moments the ODEs are computed similarly.

Theorem 5.1.1 *The ODE for the mean values of infected individuals $\langle I \rangle$, derived from the master equation of SIRI model, is given by*

$$\frac{d}{dt}\langle I \rangle = \beta \langle SI \rangle - \gamma \langle I \rangle + \tilde{\beta} \langle RI \rangle \quad ,$$

where $\langle SI \rangle$ is defined in Eq. (5.3) and $\langle RI \rangle$ is the pair given by

$$\langle RI \rangle(t) = \sum_{SIR} \left(\sum_{i=1}^N \sum_{j=1}^N J_{ij} R_i I_j \right) p(S_1, I_1, R_1, \dots, R_N, t) \quad .$$

Proof. The expectation value of the marginal quantity I_i is defined by

$$\begin{aligned} \langle I_i \rangle(t) &= \sum_{S_1=0}^1 \sum_{I_1=0}^1 \sum_{R_1=0}^1 \sum_{S_2=0}^1 \dots \sum_{R_N=0}^1 I_i p(S_1, I_1, R_1, S_2, \dots, R_N, t) \\ &= \sum_{SIR} I_i p(S_1, I_1, R_1, S_2, \dots, R_N, t) \quad , \end{aligned}$$

where \sum_{SIR} denotes the sum $\sum_{S_1=0}^1 \sum_{I_1=0}^1 \sum_{R_1=0}^1 \sum_{S_2=0}^1 \dots \sum_{R_N=0}^1$, and its dynamics is given by

$$\begin{aligned} \frac{d}{dt}\langle I_i \rangle &= \sum_{SIR} I_i \frac{d}{dt} p(S_1, I_1, R_1, S_2, \dots, R_N) \\ &= A + B + C + D + E \quad , \end{aligned} \tag{5.4}$$

with

$$A = \sum_{SIR} I_i \sum_{k=1}^N \beta \left(\sum_{j=1}^N J_{kj} I_j \right) (1 - S_k) p(\dots, 1 - S_k, 1 - I_k, R_k \dots) \tag{5.5}$$

$$\begin{aligned}
B &= \sum_{SIR} I_i \sum_{k=1}^N \gamma (1 - I_k) p(\dots, S_k, 1 - I_k, 1 - R_k \dots) \\
C &= \sum_{SIR} I_i \sum_{k=1}^N \tilde{\beta} \left(\sum_{j=1}^N J_{kj} I_j \right) (1 - R_k) p(\dots, S_k, 1 - I_k, 1 - R_k \dots) \\
D &= \sum_{SIR} I_i \sum_{k=1}^N \alpha (1 - R_k) p(\dots, 1 - S_k, I_k, 1 - R_k \dots) \\
E &= - \sum_{SIR} I_i \sum_{k=1}^N \left[\beta \left(\sum_{j=1}^N J_{kj} I_j \right) S_k + \gamma I_k + \tilde{\beta} \left(\sum_{j=1}^N J_{kj} I_j \right) R_k + \alpha R_k \right] \\
&\quad \cdot p(\dots, S_k, I_k, R_k, \dots) \quad .
\end{aligned}$$

Making a change of variables we observe, for any expression f , that

$$\begin{aligned}
&\sum_{I_k=0}^1 \sum_{R_k=0}^1 f(S_k, I_k, R_k) p(S_1, \dots, S_k, 1 - I_k, 1 - R_k, \dots, R_N) \\
&= \sum_{I_k=0}^1 \sum_{R_k=0}^1 f(S_k, 1 - I_k, 1 - R_k) p(S_1, \dots, S_k, I_k, R_k, \dots, R_N) \quad . (5.6)
\end{aligned}$$

Hence, we have $A = A_1 + A_2$, where

$$\begin{aligned}
A_1 &= \sum_{SIR} I_i \sum_{k=1 \wedge k \neq i}^N \beta \left(\sum_{j=1}^N J_{kj} I_j \right) S_k p(\dots, S_k, I_k, R_k \dots) \\
A_2 &= \sum_{SIR} (1 - I_i) \beta \left(\sum_{j=1}^N J_{ij} I_j \right) S_i p(\dots, S_i, I_i, R_i \dots) \quad .
\end{aligned}$$

Similarly, we have $B = B_1 + B_2$, where

$$\begin{aligned} B_1 &= \sum_{SIR} I_i \sum_{k=1 \wedge k \neq i}^N \gamma I_k p(\dots, S_k, I_k, R_k \dots) \\ B_2 &= \sum_{SIR} (1 - I_i) \gamma I_i p(\dots, S_i, I_i, R_i \dots), \end{aligned}$$

we have $C = C_1 + C_2$, where

$$\begin{aligned} C_1 &= \sum_{SIR} I_i \sum_{k=1 \wedge k \neq i}^N \tilde{\beta} \left(\sum_{j=1}^N J_{kj} I_j \right) R_k p(\dots, S_k, I_k, R_k \dots) \\ C_2 &= \sum_{SIR} (1 - I_i) \tilde{\beta} \left(\sum_{j=1}^N J_{ij} I_j \right) R_i p(\dots, S_i, I_i, R_i \dots), \end{aligned}$$

we have $D = D_1 + D_2$, where

$$\begin{aligned} D_1 &= \sum_{SIR} I_i \sum_{k=1 \wedge k \neq i}^N \alpha R_k p(\dots, S_k, I_k, R_k \dots) \\ D_2 &= \sum_{SIR} I_i \alpha R_i p(\dots, S_i, I_i, R_i \dots), \end{aligned}$$

and we have $E = E_1 + E_2$, where

$$\begin{aligned} E_1 &= - \sum_{SIR} I_i \sum_{k=1 \wedge k \neq i}^N \left[\beta \left(\sum_{j=1}^N J_{kj} I_j \right) S_k + \gamma I_k + \tilde{\beta} \left(\sum_{j=1}^N J_{kj} I_j \right) R_k + \alpha R_k \right] \\ &\quad \cdot p(\dots, S_k, I_k, R_k, \dots) \\ E_2 &= - \sum_{SIR} I_i \left[\beta \left(\sum_{j=1}^N J_{ij} I_j \right) S_i + \gamma I_i + \tilde{\beta} \left(\sum_{j=1}^N J_{ij} I_j \right) R_i + \alpha R_i \right] \\ &\quad \cdot p(\dots, S_i, I_i, R_i, \dots) . \end{aligned}$$

We note that $A_1 + B_1 + C_1 + D_1 + E_1 = 0$. Observing that $I_i \cdot (1 - I_i) = 0$, we obtain that $B_2 = 0$. Since one individual can not stay in more than one state, we obtain that $I_i \cdot R_i = 0$ and $I_i \cdot S_i = 0$. Therefore, $D_2 = 0$ and

$$\begin{aligned}
 E_2 &= -\gamma \sum_{SIR} I_i^2 p(\dots, S_i, I_i, R_i, \dots) \\
 &= -\gamma \sum_{SIR} I_i p(\dots, S_i, I_i, R_i, \dots) \\
 &= -\gamma \langle I_i \rangle \quad .
 \end{aligned} \tag{5.7}$$

Hence, Eq. (5.4) becomes

$$\frac{d}{dt} \langle I_i \rangle = A_2 + C_2 + E_2 \quad . \tag{5.8}$$

Observing that $(1 - I_i) \cdot S_i = S_i - I_i \cdot S_i = S_i$, we get

$$\begin{aligned}
 A_2 &= \beta \sum_{SIR} \sum_{j=1}^N J_{ij} I_j S_i p(\dots, S_i, I_i, R_i, \dots) \\
 &= \beta \sum_{j=1}^N J_{ij} \langle I_j S_i \rangle \quad .
 \end{aligned} \tag{5.9}$$

Since $(1 - I_i) \cdot R_i = R_i - I_i \cdot R_i = R_i$, we obtain that

$$\begin{aligned}
 C_2 &= \tilde{\beta} \sum_{SIR} \sum_{j=1}^N J_{ij} I_j R_i p(\dots, S_i, I_i, R_i, \dots) \\
 &= \tilde{\beta} \sum_{j=1}^N J_{ij} \langle I_j R_i \rangle \quad .
 \end{aligned} \tag{5.10}$$

Applying the formulas in Eqs. (5.7), (5.9) and (5.10) into Eq. (5.8), we

obtain the dynamics of $\langle I_i \rangle$

$$\frac{d}{dt}\langle I_i \rangle = \beta \sum_{j=1}^N J_{ij} \langle I_j S_i \rangle + \tilde{\beta} \sum_{j=1}^N J_{ij} \langle I_j R_i \rangle - \gamma \langle I_i \rangle \quad . \quad (5.11)$$

The expectation value of the total number of infected hosts at a given time is defined in Eq. (5.2). Hence, by Eq. (5.11) follows that

$$\begin{aligned} \frac{d}{dt}\langle I \rangle &= \sum_{i=1}^N \frac{d}{dt} \langle I_i \rangle \\ &= \beta \sum_{i=1}^N \sum_{j=1}^N J_{ij} \langle I_j S_i \rangle + \tilde{\beta} \sum_{i=1}^N \sum_{j=1}^N J_{ij} \langle I_j R_i \rangle - \gamma \sum_{i=1}^N \langle I_i \rangle \\ &= \beta \langle SI \rangle + \tilde{\beta} \langle RI \rangle - \gamma \langle I \rangle \quad , \end{aligned}$$

where $\langle RI \rangle$ is defined by

$$\langle RI \rangle(t) = \sum_{SIR} \left(\sum_{i=1}^N \sum_{j=1}^N J_{ij} R_i I_j \right) p(S_1, I_1, R_1, \dots, R_N, t) \quad .$$

and $\langle SI \rangle$ is defined in Eq. (5.3). ■

Doing a similar reasoning for the mean total number of susceptible and recovered hosts we obtain the following ODE system for the first moments $\langle S \rangle$, $\langle I \rangle$ and $\langle R \rangle$

$$\begin{aligned} \frac{d}{dt}\langle S \rangle &= \alpha \langle R \rangle - \beta \langle SI \rangle \\ \frac{d}{dt}\langle I \rangle &= \beta \langle SI \rangle - \gamma \langle I \rangle + \tilde{\beta} \langle RI \rangle \\ \frac{d}{dt}\langle R \rangle &= \gamma \langle I \rangle - \alpha \langle R \rangle - \tilde{\beta} \langle RI \rangle \end{aligned} \quad (5.12)$$

involving pairs of susceptibles and infected or pairs of infected and recovered. Now, either we have to continue to calculate the ODEs for the pairs, which will involve even higher clusters, or we can try to approximate the higher moments by lower ones. The simplest scheme is the mean field approximation, leading to a closed system of ODEs for the total number of infected, recovered and susceptibles only. For the present system the mean field approximation will be analysed in section 5.2. In this thesis we also go one step beyond by considering the dynamics of the pairs and approximating the triples into pairs (see section 5.3). We will compute now the ODEs for the second moments. We present the details for dynamic of the pair $\langle SI \rangle$ defined in Eq. (5.3) and the ODEs for the order moments follow similarly.

Theorem 5.1.2 *The ODE for the second moment $\langle SI \rangle$ derived from the master equation of the spatial stochastic SIRI model is given by*

$$\frac{d}{dt}\langle SI \rangle = \beta \langle SSI \rangle + \tilde{\beta} \langle SRI \rangle + \alpha \langle RI \rangle - \beta \langle ISI \rangle - \gamma \langle SI \rangle \quad ,$$

where appear the triples, e.g.

$$\begin{aligned} \langle SRI \rangle(t) &= \sum_{SIR} \left(\sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{jk} S_i R_j I_k \right) p(S_1, I_1, R_1, \dots, R_N, t) \\ &= \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{jk} \langle S_i R_j I_k \rangle \end{aligned}$$

and $\langle I_i S_j I_k \rangle$ is the local expectation value.

Proof. The local expectation value $\langle S_i I_j \rangle(t)$ is defined by

$$\langle S_i I_j \rangle(t) = \sum_{SIR} S_i I_j p(S_1, I_1, R_1, S_2, \dots, R_N, t) \quad ,$$

where \sum_{SIR} denotes the sum $\sum_{S_1=0}^1 \sum_{I_1=0}^1 \sum_{R_1=0}^1 \sum_{S_2=0}^1 \cdots \sum_{R_N=0}^1$, and its dynamics is given by

$$\begin{aligned} \frac{d}{dt} \langle S_i I_j \rangle &= \sum_{SIR} S_i I_j \frac{d}{dt} p(S_1, I_1, R_1, S_2, \dots, R_N) \\ &= A + B + C + D + E \quad , \end{aligned} \quad (5.13)$$

with

$$\begin{aligned} A &= \sum_{SIR} S_i I_j \sum_{l=1}^N \beta \left(\sum_{k=1}^N J_{lk} I_k \right) (1 - S_l) p(\dots, 1 - S_l, 1 - I_l, R_l, \dots) \\ B &= \sum_{SIR} S_i I_j \sum_{l=1}^N \gamma (1 - I_l) p(\dots, S_l, 1 - I_l, 1 - R_l, \dots) \\ C &= \sum_{SIR} S_i I_j \sum_{l=1}^N \tilde{\beta} \left(\sum_{k=1}^N J_{lk} I_k \right) (1 - R_l) p(\dots, S_l, 1 - I_l, 1 - R_l, \dots) \\ D &= \sum_{SIR} S_i I_j \sum_{l=1}^N \alpha (1 - R_l) p(\dots, 1 - S_l, I_l, 1 - R_l, \dots) \\ E &= - \sum_{SIR} S_i I_j \sum_{l=1}^N \left[\beta \left(\sum_{k=1}^N J_{lk} I_k \right) S_l + \gamma I_l + \tilde{\beta} \left(\sum_{k=1}^N J_{lk} I_k \right) R_l + \alpha R_l \right] \\ &\quad \cdot p(\dots, S_l, I_l, R_l, \dots) \quad . \end{aligned}$$

Hence, making a change of variables like in Eq. (5.6) we have $A = A_1 +$

$A_2 + A_3$, where

$$\begin{aligned}
 A_1 &= \sum_{SIR} S_i I_j \sum_{l=1 \wedge l \neq i \wedge l \neq j}^N \beta \left(\sum_{k=1}^N J_{lk} I_k \right) S_l p(\dots, S_l, I_l, R_l, \dots) \quad , \\
 A_2 &= \sum_{SIR} (1 - S_i) I_j \beta \left(\sum_{k=1}^N J_{ik} I_k \right) S_i p(\dots, S_i, I_i, R_i, \dots) \quad , \\
 A_3 &= \sum_{SIR} S_i (1 - I_j) \beta \left(\sum_{k=1}^N J_{jk} I_k \right) S_j p(\dots, S_j, I_j, R_j, \dots) \quad .
 \end{aligned}$$

Similarly, we have $B = B_1 + B_2 + B_3$, where

$$\begin{aligned}
 B_1 &= \sum_{SIR} S_i I_j \sum_{l=1 \wedge l \neq i \wedge l \neq j}^N \gamma I_l p(\dots, S_l, I_l, R_l, \dots) \quad , \\
 B_2 &= \sum_{SIR} S_i I_j \gamma I_i p(\dots, S_i, I_i, R_i, \dots) \quad , \\
 B_3 &= \sum_{SIR} S_i (1 - I_j) \gamma I_j p(\dots, S_j, I_j, R_j, \dots) \quad ,
 \end{aligned}$$

we have $C = C_1 + C_2 + C_3$, where

$$\begin{aligned}
 C_1 &= \sum_{SIR} S_i I_j \sum_{l=1 \wedge l \neq i \wedge l \neq j}^N \tilde{\beta} \left(\sum_{k=1}^N J_{lk} I_k \right) R_l p(\dots, S_l, I_l, R_l, \dots) \quad , \\
 C_2 &= \sum_{SIR} S_i I_j \tilde{\beta} \left(\sum_{k=1}^N J_{ik} I_k \right) R_i p(\dots, S_i, I_i, R_i, \dots) \quad , \\
 C_3 &= \sum_{SIR} S_i (1 - I_j) \tilde{\beta} \left(\sum_{k=1}^N J_{jk} I_k \right) R_j p(\dots, S_j, I_j, R_j, \dots) \quad ,
 \end{aligned}$$

we have $D = D_1 + D_2 + D_3$, where

$$\begin{aligned} D_1 &= \sum_{SIR} S_i I_j \sum_{l=1 \wedge l \neq i \wedge l \neq j}^N \alpha R_l p(\dots, S_l, I_l, R_l, \dots) \quad , \\ D_2 &= \sum_{SIR} (1 - S_i) I_j \alpha R_i p(\dots, S_i, I_i, R_i, \dots) \quad , \\ D_3 &= \sum_{SIR} S_i I_j \alpha R_j p(\dots, S_j, I_j, R_j, \dots) \quad , \end{aligned}$$

and we have $E = E_1 + E_2 + E_3$, where

$$\begin{aligned} E_1 &= - \sum_{SIR} S_i I_j \sum_{l=1 \wedge l \neq i \wedge l \neq j}^N \left[\beta \left(\sum_{k=1}^N J_{lk} I_k \right) S_l + \gamma I_l + \tilde{\beta} \left(\sum_{k=1}^N J_{lk} I_k \right) R_l + \alpha R_l \right] \\ &\quad \cdot p(\dots, S_l, I_l, R_l, \dots) \quad , \\ E_2 &= - \sum_{SIR} S_i I_j \left[\beta \left(\sum_{k=1}^N J_{ik} I_k \right) S_i + \gamma I_i + \tilde{\beta} \left(\sum_{k=1}^N J_{ik} I_k \right) R_i + \alpha R_i \right] \\ &\quad \cdot p(\dots, S_i, I_i, R_i, \dots) \quad , \\ E_3 &= - \sum_{SIR} S_i I_j \left[\beta \left(\sum_{k=1}^N J_{jk} I_k \right) S_j + \gamma I_j + \tilde{\beta} \left(\sum_{k=1}^N J_{jk} I_k \right) R_j + \alpha R_j \right] \\ &\quad \cdot p(\dots, S_j, I_j, R_j, \dots) \quad . \end{aligned}$$

We start to note that $A_1 + B_1 + C_1 + D_1 + E_1 = 0$. Observing that the state variables are in the set $\{0; 1\}$ and therefore e.g. $(1 - S_i) \cdot S_i = 0$, we have that $A_2 = 0$ and $B_3 = 0$. We also observe that e.g. $S_i \cdot I_i = 0$, because one individual can not stay in more than one state. Hence, $B_2 = 0$, $C_2 = 0$,

$D_3 = 0$,

$$\begin{aligned}
E_2 &= - \sum_{SIR} S_i^2 I_j \beta \left(\sum_{k=1}^N J_{ik} I_k \right) \cdot p(\dots, S_i, I_i, R_i, \dots) \\
&= -\beta \sum_{k=1}^N J_{ik} \sum_{SIR} S_i I_j I_k \cdot p(\dots, S_i, I_i, R_i, \dots) \\
&= -\beta \sum_{k=1}^N J_{ik} \langle S_i I_j I_k \rangle \quad , \tag{5.14}
\end{aligned}$$

and

$$\begin{aligned}
E_3 &= - \sum_{SIR} S_i I_j^2 \gamma \cdot p(\dots, S_j, I_j, R_j, \dots) \\
&= -\gamma \sum_{SIR} S_i I_j \cdot p(\dots, S_j, I_j, R_j, \dots) \\
&= -\gamma \langle S_i I_j \rangle \quad . \tag{5.15}
\end{aligned}$$

Therefore, Eq. (5.13) reduces to

$$\frac{d}{dt} \langle S_i I_j \rangle = A_3 + C_3 + D_2 + E_2 + E_3 \quad . \tag{5.16}$$

Observing that $S_i (1 - I_j) S_j = S_i S_j - S_i I_j S_j = S_i S_j$, we obtain that

$$\begin{aligned}
A_3 &= \beta \sum_{SIR} S_i S_j \left(\sum_{k=1}^N J_{jk} I_k \right) p(\dots, S_j, I_j, R_j, \dots) \\
&= \beta \sum_{k=1}^N J_{jk} \sum_{SIR} S_i S_j I_k p(\dots, S_j, I_j, R_j, \dots) \\
&= \beta \sum_{k=1}^N J_{jk} \langle S_i S_j I_k \rangle \quad . \tag{5.17}
\end{aligned}$$

Similarly, since $S_i(1 - I_j)R_j = S_iR_j$, we have

$$\begin{aligned}
 C_3 &= \sum_{SIR} S_i R_j \tilde{\beta} \left(\sum_{k=1}^N J_{jk} I_k \right) p(\dots, S_j, I_j, R_j, \dots) \\
 &= \tilde{\beta} \sum_{k=1}^N J_{jk} \sum_{SIR} S_i R_j I_k p(\dots, S_j, I_j, R_j, \dots) \\
 &= \tilde{\beta} \sum_{k=1}^N J_{jk} \langle S_i R_j I_k \rangle \quad , \tag{5.18}
 \end{aligned}$$

and with the relation $(1 - S_i)I_j R_i = R_i I_j$, we also have

$$\begin{aligned}
 D_2 &= \sum_{SIR} R_i I_j p(\dots, S_i, I_i, R_i, \dots) \\
 &= \alpha \langle R_i I_j \rangle \quad . \tag{5.19}
 \end{aligned}$$

Applying Eqs. (5.14), (5.15), (5.17), (5.18) and (5.19) in the dynamics of $\langle S_i I_j \rangle$ given in Eq. (5.16), we obtain that

$$\begin{aligned}
 \frac{d}{dt} \langle S_i I_j \rangle &= \beta \sum_{k=1}^N J_{jk} \langle S_i S_j I_k \rangle + \tilde{\beta} \sum_{k=1}^N J_{jk} \langle S_i R_j I_k \rangle + \alpha \langle R_i I_j \rangle \\
 &\quad - \beta \sum_{k=1}^N J_{ik} \langle S_i I_j I_k \rangle - \gamma \langle S_i I_j \rangle \quad .
 \end{aligned}$$

Hence, by Eq.(5.3) we obtain for the dynamics of the pair $\langle SI \rangle$ the ODE

$$\begin{aligned}
\frac{d}{dt}\langle SI \rangle &= \sum_{i=1}^N \sum_{j=1}^N J_{ij} \frac{d}{dt}\langle S_i I_j \rangle \\
&= \beta \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{jk} \langle S_i S_j I_k \rangle + \tilde{\beta} \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{jk} \langle S_i R_j I_k \rangle \\
&\quad + \alpha \sum_{i=1}^N \sum_{j=1}^N J_{ij} \langle R_i I_j \rangle - \beta \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{ik} \langle S_i I_j I_k \rangle \\
&\quad - \gamma \sum_{i=1}^N \sum_{j=1}^N J_{ij} \langle S_i I_j \rangle \\
&= \beta \langle SSI \rangle + \tilde{\beta} \langle SRI \rangle + \alpha \langle RI \rangle - \beta \langle ISI \rangle - \gamma \langle SI \rangle \quad ,
\end{aligned}$$

where $\langle SRI \rangle$ is the triple defined by

$$\begin{aligned}
\langle SRI \rangle(t) &= \sum_{SIR} \left(\sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{jk} S_i R_j I_k \right) p(S_1, I_1, R_1, \dots, R_N, t) \\
&= \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N J_{ij} J_{jk} \langle S_i R_j I_k \rangle
\end{aligned}$$

and the other triples are defined similarly. ■

Doing similar computations for the others pairs, we obtain for the dynamics of the second moments $\langle SS \rangle$, $\langle II \rangle$, $\langle RR \rangle$, $\langle SI \rangle$, $\langle SR \rangle$ and $\langle IR \rangle$ the following ODE system:

$$\begin{aligned}
\frac{d}{dt}\langle SS \rangle &= 2\alpha\langle RS \rangle - 2\beta\langle SSI \rangle \\
\frac{d}{dt}\langle II \rangle &= 2\beta\langle ISI \rangle - 2\gamma\langle II \rangle + 2\tilde{\beta}\langle IRI \rangle \\
\frac{d}{dt}\langle RR \rangle &= 2\gamma\langle IR \rangle - 2\tilde{\beta}\langle RRI \rangle - 2\alpha\langle RR \rangle \\
\frac{d}{dt}\langle SI \rangle &= \beta\langle SSI \rangle + \tilde{\beta}\langle SRI \rangle - \gamma\langle SI \rangle - \beta\langle ISI \rangle + \alpha\langle RI \rangle \\
\frac{d}{dt}\langle RS \rangle &= \gamma\langle SI \rangle - \beta\langle RSI \rangle - \tilde{\beta}\langle SRI \rangle + \alpha\langle RR \rangle - \alpha\langle RS \rangle \\
\frac{d}{dt}\langle RI \rangle &= \gamma\langle II \rangle + \beta\langle RSI \rangle + \tilde{\beta}\langle RRI \rangle - \gamma\langle IR \rangle - \tilde{\beta}\langle IRI \rangle - \alpha\langle RI \rangle
\end{aligned} \tag{5.20}$$

5.2 Mean field approximation

In mean field approximation, the interaction term which gives the exact number of inhabited neighbors is replaced by the average number of infected individuals in the full system, acting like a mean field on the actually considered site. Hence we set

$$\begin{aligned}
\sum_{j=1}^N J_{ij} I_j &\approx \sum_{j=1}^N J_{ij} \frac{\langle I \rangle}{N} \\
&= \frac{Q}{N} \langle I \rangle
\end{aligned} \tag{5.21}$$

where the last line of Eq. (5.21) only holds for regular lattices where Q is the number of neighbours of each individual i . For the pair e.g. $\langle SI \rangle$ we

obtain the mean field approximation given by

$$\begin{aligned}
\langle SI \rangle &= \left\langle \sum_{i=1}^N \sum_{j=1}^N J_{ij} S_i I_j \right\rangle \\
&= \left\langle \sum_{i=1}^N S_i \sum_{j=1}^N J_{ij} I_j \right\rangle \\
&\approx \left\langle \sum_{i=1}^N S_i \frac{Q}{N} \langle I \rangle \right\rangle \\
&= \frac{Q}{N} \left\langle \sum_{i=1}^N S_i \right\rangle \langle I \rangle \\
&= \frac{Q}{N} \langle S \rangle \langle I \rangle
\end{aligned} \tag{5.22}$$

and similar approximations for the other pairs.

For the SIRI model, the mean field approximation gives

$$\begin{aligned}
\frac{d}{dt} \langle S \rangle &= \alpha \langle R \rangle - \beta \frac{Q}{N} \langle S \rangle \langle I \rangle \\
\frac{d}{dt} \langle I \rangle &= \beta \frac{Q}{N} \langle S \rangle \langle I \rangle - \gamma \langle I \rangle + \tilde{\beta} \frac{Q}{N} \langle R \rangle \langle I \rangle \\
\frac{d}{dt} \langle R \rangle &= \gamma \langle I \rangle - \alpha \langle R \rangle - \tilde{\beta} \frac{Q}{N} \langle R \rangle \langle I \rangle .
\end{aligned} \tag{5.23}$$

This ODE system can be studied in simplified coordinates, time changed to $\tau = t/\gamma$ and consequently

$$\rho = \beta Q/\gamma , \quad \varepsilon = \alpha/\gamma \tag{5.24}$$

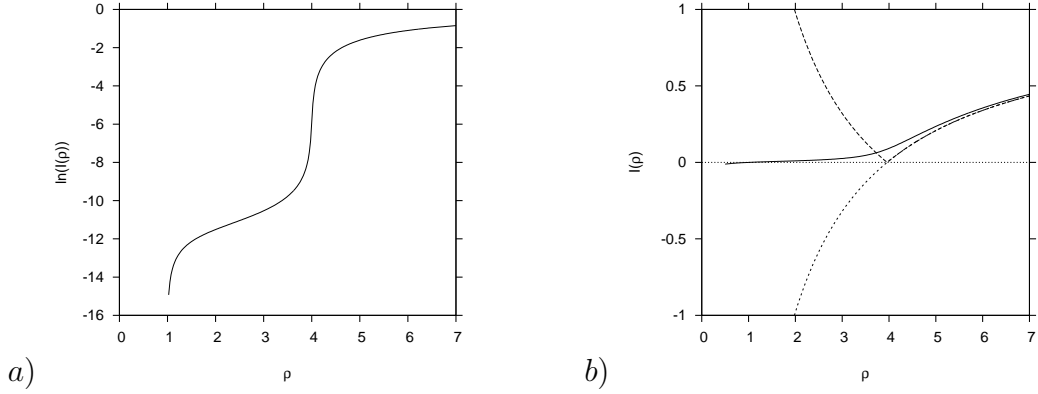


Figure 5.1: a) The conventional picture of the reinfection threshold, in semi-logarithmic plot [14]. We just use the parameter α instead of the death out of all classes and birth into susceptibles. The value for $\sigma = 1/4$ will also be used in Fig. 5.1 b), and $\varepsilon = 0.00001$ to demonstrate a clear threshold behaviour around $\rho = 1/\sigma$. b) The solution $i_2^* = -\frac{r}{2} + \sqrt{\frac{r^2}{4} - q}$, full line is plotted against the curves $-r$ and its modulus $|r|$. While i_2^* changes from negative to positive at $\rho = 1$, the curves for $-r$ and $|r|$ change at $\rho = 1/\sigma$ for vanishing or small ε . This qualitative change at $\rho = 1/\sigma$ is the reinfection threshold. Parameters are $\sigma = 1/4 = 0.25$ and $\varepsilon = 0.01$.

and the ratio of infectivities given by

$$\sigma = \tilde{\beta}/\beta \quad . \quad (5.25)$$

Further, we consider densities of susceptibles, infected, and recovered, hence $s = \langle S \rangle/N$, $i = \langle I \rangle/N$. Then with $\langle R \rangle/N = 1 - s - i$ we obtain the two-dimensional ODE system

$$\frac{d}{d\tau} s = \varepsilon(1 - s - i) - \rho s i \quad (5.26)$$

$$\frac{d}{d\tau} i = \rho i (s + \sigma(1 - s - i)) - i$$

to compare with the formulation in [14]. The stationary solution is either $i_1^* = 0$ or

$$i_2^* = -\frac{r}{2} + \sqrt{\frac{r^2}{4} - q} \quad (5.27)$$

with

$$r = \frac{1}{\rho\sigma} (1 - \rho\sigma + \varepsilon) \quad \text{and} \quad q = \frac{\varepsilon}{\rho^2\sigma} (1 - \rho) \quad . \quad (5.28)$$

In original coordinates this gives $\langle I \rangle_1^* = 0$ and $(\langle I \rangle_2^*/N)^2 + r \cdot (\langle I \rangle_2^*/N) + q = 0$ with

$$r = \left(\frac{\gamma + \alpha}{\tilde{\beta}Q} - 1 \right) \quad , \quad q = \frac{\alpha}{\tilde{\beta}Q} \left(\frac{\gamma}{\beta Q} - 1 \right) \quad . \quad (5.29)$$

At $\rho = 1$ the solutions i_1^* and i_2^* meet each other, i.e. $i_2^* = 0$, coinciding with $q = 0$. And at $\varepsilon = 0$ we obtain another change of regime with $r = 0$, which is slightly more subtle in the first inspection. This second threshold behaviour, known as the reinfection threshold will be analysed in the next section.

5.2.1 The reinfection threshold

The whole concept of the reinfection threshold was questioned in [4] as a comment to [14]. They in turn justified the concept of the reinfection threshold by looking at the behaviour of the basic mean field model under vaccination, showing that the first threshold can be shifted towards larger ρ values by the introduction of vaccination, but cannot be shifted beyond the second threshold by any means of vaccination [15]. Here, we demonstrate that in the SIRI model the reinfection threshold appears in the limit of α decreasing to zero as a sharp threshold. So we conclude that the reinfection

threshold does exist in the sense that any other threshold in physical phase transitions exists or any bifurcation behaviour in mean field models exist. From the studies of spatial stochastic epidemics with partial immunization [18, 5] we even know that the mean field threshold behaviour is qualitatively describing also the threshold behaviour of spatial models, namely the transition between annular growth and compact growth.

In the following, we just analyse the mean field behaviour of the SIRI model and investigate the limiting behaviour of vanishing α , the transition from recovered to susceptible, finding a sharp transition at $1/\sigma$, the reinfection threshold. In Fig. 5.1 b) the solution $i_2^* = -\frac{r}{2} + \sqrt{\frac{r^2}{4} - q}$, full line, is

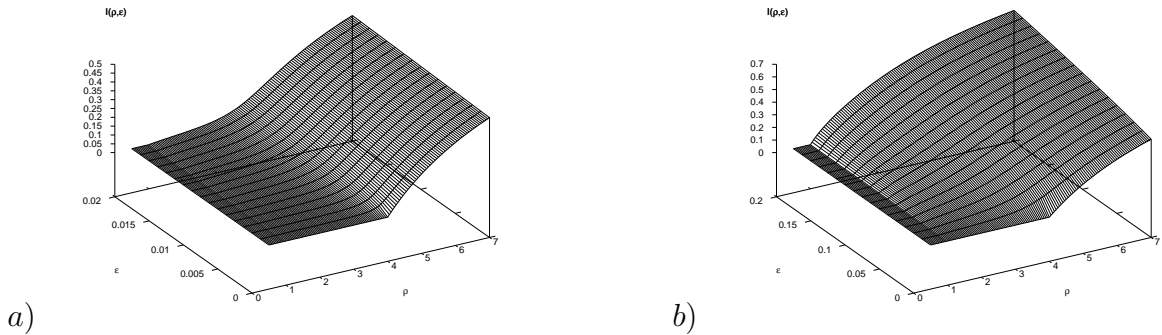


Figure 5.2: a) The stationary value of the number of infected individuals with both parameters ρ and ε shows for high ε values just a threshold behaviour at $\rho = 1$, and for vanishing ε the threshold for $\rho = 1/\sigma$. Here in the graphic plot $\rho = 1/\sigma = 4$, where beforehand σ was fixed to be $\sigma = 1/4$. b) When we look at larger values of ε , here up to $\varepsilon = 0.2$, we also find back the first threshold at $\rho = 1$. The continuous change from behaviour dominated by the first threshold $\rho = 1$ for $\varepsilon = 0.2$ to the behaviour only determined by the behaviour around the second threshold $\rho = 1/\sigma$ for $\varepsilon = 0$ can be seen here.

plotted against the curves $-r$ and its modulus $|r|$. While i_2^* changes from negative to positive at $\rho = 1$, the curves for $-r$ and $|r|$ change at $\rho = 1/\sigma$ for

vanishing or small ε . This qualitative change at $\rho = 1/\sigma$ is the reinfection threshold as predicted by [14].

When plotting the stationary state solution as function of both independent parameters ρ and ε (see Fig. 5.2), the threshold behaviour for vanishing $\varepsilon = 0$ is clearly visible, whereas for finite ε the curves for $I^*(\rho)$ are smoothed out around the reinfection threshold. It is interesting to see that for large values of e.g. $\varepsilon = 0.2$ the behaviour of I^* is completely dominated by the simple threshold behaviour around $\rho = 1$, the reinfection threshold not visible even qualitatively (see Fig. 5.2 b)). In contrast, for vanishing $\varepsilon = 0$ there is only the qualitative behaviour left from the behaviour around the second threshold at $\rho = 1/\sigma$. The change between these two extremes is quite continuous, as can be seen in Fig. 5.2 b). However, close to the reinfection threshold $\rho = 1/\sigma$, the solutions for I^* for small ε are a smoothed out version of that threshold, as better seen in Fig. 5.2 a).

Finally, we look at the phase diagram in the original coordinates, β and $\tilde{\beta}$, as opposed to the changed variables ρ and ε , remembering the definitions for these, Eq. (5.24). The phase diagram for the mean field model for the two-dimensional case, $Q = 4$ neighbours is shown in Fig. 5.3. The threshold at $\rho = 1$ gives the critical value for β with $\beta = \gamma/Q$, the vertical line. The threshold for $\rho = 1/\sigma$ gives the critical value for $\tilde{\beta}$ with $\tilde{\beta} = \gamma/Q$, the horizontal line. This phase diagram can be compared well with the phase diagrams of higher dimensional spatial stochastic simulation where the mean field behaviour is approached in about six dimensions [5].

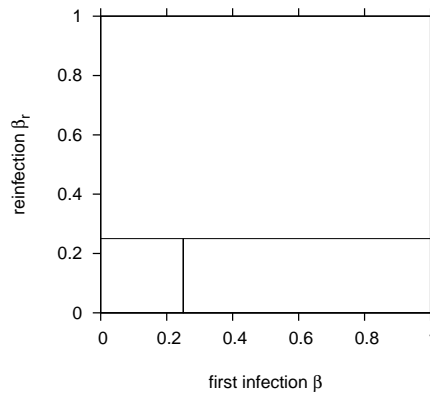


Figure 5.3: *Phase diagram for the mean field model. For consistency with the previously investigated two-dimensional case, we set $Q = 4$ neighbours. The mean field phase diagram is however in good agreement with spatial simulations above the upper critical dimension [5].*

5.3 Critical points and phase transition lines in pair approximation

Now, we will consider the dynamic of the second moments and compute the critical points and the phase transition lines of the SIRI model in the pair approximation. We start to use the balance equations to reduce the number of the equations in the ODEs for the first moments (see Eq. (5.12)) and second moments (see Eq. (5.20)) to the five equations presented in Eq. (5.43) to Eq. (5.47). The balance equations are also used in section 5.3.1 to find a closed form of the ODEs for the moments.

From $S_i + I_i + R_i = 1$ it follows immediately that for the means

$$\langle S \rangle + \langle I \rangle + \langle R \rangle = N \tag{5.30}$$

holds, and from this that

$$\frac{d}{dt}N = 0 = \frac{d}{dt}\langle S \rangle + \frac{d}{dt}\langle I \rangle + \frac{d}{dt}\langle R \rangle \quad (5.31)$$

also holds. A check of the results of the dynamics Eq. (5.12) is to insert the three equations into Eq. (5.31) and verify the sum to be equal to zero. In this case it can be confirmed by eye immediately. For the pair dynamics in all variables S , I and R , however, the check of the balance is not so obvious. The balance equation is now, again for regular lattices,

$$\langle SS \rangle + \langle II \rangle + \langle RR \rangle + 2\langle SI \rangle + 2\langle SR \rangle + 2\langle IR \rangle = N \cdot Q \quad (5.32)$$

which can be obtained by explicitly expressing all terms including variable S in terms of the independent variables I and R , hence

$$\langle SR \rangle + \langle IR \rangle + \langle RR \rangle = Q\langle R \rangle \quad (5.33)$$

etc. The pair balance dynamics is now

$$\frac{d}{dt}(N \cdot Q) = 0 = \frac{d}{dt}\langle SS \rangle + \frac{d}{dt}\langle II \rangle + \frac{d}{dt}\langle RR \rangle + 2\frac{d}{dt}\langle SI \rangle + 2\frac{d}{dt}\langle SR \rangle + 2\frac{d}{dt}\langle IR \rangle \quad (5.34)$$

which is exactly fulfilled by the ODE system for the pair dynamics given in Eq. (5.20). From these balance equations we can reduce the ODE system for total expectation values and for pair expectation values to five independent variables $\langle I \rangle$, $\langle R \rangle$, $\langle SI \rangle$, $\langle RI \rangle$ and $\langle SR \rangle$.

5.3.1 Pair approximation

To obtain approximate expressions for the triples appearing in the equation system Eq. (5.20) in terms of pairs we will do some assumptions in the model. For a detailed discussion of the pair approximation in general, see [24, 22, 39]. We will study the pair approximation for the triples $\langle RSI \rangle$ and $\langle IRI \rangle$. The approximations for the other triples follow similarly.

We consider only the true triples $\widetilde{\langle IRI \rangle}$, where the last site of e.g. infected is not identical with the first, hence with the definition

$$\widetilde{\langle IRI \rangle} = \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1, k \neq i}^N J_{ij} J_{jk} \langle I_i R_j I_k \rangle \quad (5.35)$$

we have

$$\langle IRI \rangle = \widetilde{\langle IRI \rangle} + \langle RI \rangle \quad (5.36)$$

when the local variable at site k , here I_k , is of the same type as the one in i , here I_i and simply

$$\langle RSI \rangle = \widetilde{\langle RSI \rangle} \quad (5.37)$$

when the local variable at site k , now I_k , is different from the one in i , now R_i . For triples, which are by nature just pairs, i.e., with $i = k$, we have locally $\langle I_i R_j I_k \rangle = \langle I_i^2 R_j \rangle = \langle I_i R_j \rangle$, since $I_i \in \{0, 1\}$, so they should be counted as pairs, i.e., given by Eq. (5.36), whereas in Eq. (5.37) for $i = k$ we have $\langle R_i S_j I_k \rangle = \langle R_i S_j I_i \rangle = 0$, since $R_i, I_i \in \{0, 1\}$ and $S_i + I_i + R_i = 1$. The difference between $\widetilde{\langle IRI \rangle}$ and $\langle IRI \rangle$ does first appear in the triples, since in the pairs the diagonal of the adjacency matrix is zero, avoiding the eventual double counting of singlets.

Then we consider all the possible combinations, where sums over the adjacency matrix only come to play $\sum_{j=1}^N J_{ij} = Q_i$. These indicate the number of neighbours to a lattice site i , and from now on we will only consider regular lattices (later the square lattice with periodic boundary conditions). Hence we can assume that all Q_i are equal, i.e., $Q = Q_i$ for each individual i .

The pair approximation yields

$$\langle RSI \rangle = \widetilde{\langle RSI \rangle} \approx \frac{Q-1}{Q} \cdot \frac{\langle RS \rangle \cdot \langle SI \rangle}{\langle S \rangle} \quad (5.38)$$

obtained from an analog for the Bayesian formula for conditional probabilities applied to the local expectation values

$$\langle R_i S_j I_k \rangle \approx \frac{\langle R_i S_j \rangle \cdot \langle S_j I_k \rangle}{\langle S_j \rangle} \quad (5.39)$$

and a spatial homogeneity argument, namely

$$\langle S_j I_k \rangle \approx \langle S_i I_j \rangle \approx \frac{\langle SI \rangle}{NQ} \quad (5.40)$$

and

$$\langle S_j \rangle \approx \frac{\langle S \rangle}{N} \quad (5.41)$$

For the triple $\langle IRI \rangle$ the pair approximation is given by

$$\langle IRI \rangle = \widetilde{\langle IRI \rangle} + \langle RI \rangle \approx \frac{Q-1}{Q} \cdot \frac{\langle RI \rangle^2}{\langle R \rangle} + \langle RI \rangle \quad (5.42)$$

With expressions like the one in Eq. (5.38) and Eq. (5.42) and using

the balance equations we obtain the closed equation system for the first moments $\langle S \rangle$, $\langle I \rangle$ and $\langle R \rangle$ (see Eq. (5.2)), and for the second moments $\langle SS \rangle$, $\langle II \rangle$, $\langle RR \rangle$, $\langle SI \rangle$, $\langle SR \rangle$ and $\langle IR \rangle$ (see Eq. (5.3)):

$$\frac{d}{dt}\langle I \rangle = \beta \langle SI \rangle - \gamma \langle I \rangle + \tilde{\beta} \langle RI \rangle \quad (5.43)$$

$$\frac{d}{dt}\langle R \rangle = \gamma \langle I \rangle - \alpha \langle R \rangle - \tilde{\beta} \langle RI \rangle \quad (5.44)$$

$$\begin{aligned} \frac{d}{dt}\langle SI \rangle &= \alpha \langle RI \rangle - (\gamma + \beta) \langle SI \rangle + \beta(Q - 1) \langle SI \rangle \\ &\quad - \beta \frac{Q - 1}{Q} \frac{(2\langle SI \rangle + \langle SR \rangle) \cdot \langle SI \rangle}{N - \langle I \rangle - \langle R \rangle} \\ &\quad + \tilde{\beta} \frac{Q - 1}{Q} \frac{\langle SR \rangle \langle RI \rangle}{\langle R \rangle} \end{aligned} \quad (5.45)$$

$$\begin{aligned} \frac{d}{dt}\langle RI \rangle &= \gamma (Q \langle I \rangle - \langle SI \rangle) - (\alpha + 2\gamma + \tilde{\beta}) \langle RI \rangle \\ &\quad + \beta \frac{Q - 1}{Q} \frac{\langle SR \rangle \langle SI \rangle}{N - \langle I \rangle - \langle R \rangle} \\ &\quad + \tilde{\beta} \frac{Q - 1}{Q} \frac{(Q \langle R \rangle - \langle SR \rangle - 2\langle RI \rangle) \cdot \langle RI \rangle}{\langle R \rangle} \end{aligned} \quad (5.46)$$

$$\begin{aligned} \frac{d}{dt}\langle SR \rangle &= \gamma \langle SI \rangle + \alpha (Q \langle R \rangle - 2\langle SR \rangle - \langle RI \rangle) \\ &\quad - \beta \frac{Q - 1}{Q} \frac{\langle SR \rangle \langle SI \rangle}{N - \langle I \rangle - \langle R \rangle} \\ &\quad - \tilde{\beta} \frac{Q - 1}{Q} \frac{\langle RI \rangle \langle SR \rangle}{\langle R \rangle} \end{aligned} \quad (5.47)$$

We investigate the stationary states of the closed system Eq. given by Eqs. (5.43) to (5.47) in order to obtain the phase transition lines which have

been described in stochastic simulations of simpler time discrete models [18].

5.3.2 Stationary states of the SIRI model

The full SIRI system in pair approximation cannot be solved analytically in stationarity. After some simplifications, expressing $\langle RI \rangle^*$, $\langle SI \rangle^*$ and $\langle SR \rangle^*$ as functions of the the variables $\langle I \rangle^*$ and $\langle R \rangle^*$ only, we are left with two implicit equations for the remaining variables $\langle I \rangle^*$ and $\langle R \rangle^*$. Explicitly, we obtain the following equations:

From the ODE system Eq. (5.44), second equation, in stationarity, giving $0 = \frac{d}{dt} \langle R \rangle^* = \gamma \langle I \rangle^* - \alpha \langle R \rangle^* - \tilde{\beta} \langle RI \rangle^*$ we obtain directly $\langle RI \rangle^*$ as function of $\langle I \rangle^*$ and $\langle R \rangle^*$, hence

$$\langle RI \rangle^* = \frac{\gamma}{\tilde{\beta}} \langle I \rangle^* - \frac{\alpha}{\tilde{\beta}} \langle R \rangle^* \quad . \quad (5.48)$$

From $0 = \frac{d}{dt} \langle I \rangle^* = \beta \langle SI \rangle^* - \gamma \langle I \rangle^* + \tilde{\beta} \langle RI \rangle^*$ we obtain using Eq. (5.48)

$$\langle SI \rangle^* = \frac{\alpha}{\beta} \langle R \rangle^* \quad . \quad (5.49)$$

Further from $0 = \frac{d}{dt} \langle SR \rangle^*$ we obtain

$$\langle SR \rangle^* = \frac{\alpha Q \langle R \rangle^* - \alpha \langle RI \rangle^* + \gamma \langle SI \rangle^*}{2\alpha + \frac{Q-1}{Q} \left(\beta \frac{\langle SI \rangle^*}{N - \langle I \rangle^* - \langle R \rangle^*} + \tilde{\beta} \frac{\langle RI \rangle^*}{\langle R \rangle^*} \right)} \quad (5.50)$$

which is explicitly also expressable as function of $\langle I \rangle^*$ and $\langle R \rangle^*$ only.

But from

$$0 = \frac{d}{dt} \langle RI \rangle^* = f(\langle I \rangle^*, \langle R \rangle^*) \quad (5.51)$$

and

$$0 = \frac{d}{dt} \langle SI \rangle^* = g(\langle I \rangle^*, \langle R \rangle^*) \quad (5.52)$$

we only get implicit equations for the variables $\langle I \rangle^*$ and $\langle R \rangle^*$. We will first consider some special cases where the above system can be solved analytically very easily, namely the limiting case for reinfection rate equal to first infection rate (the SIS limit of the SIRS model), then vanishing reinfection rate (the SIR limit of the SIRS model), and finally the limit of vanishing transition from recovered to susceptible α . In these cases we can give the stationary values $\langle I \rangle^*$ etc. as well as the critical parameters respectively critical line. For the general case, Eq. (5.48) to (5.52), we finally can calculate in the limit near criticality via a scaling argument the critical line. No general solution for the total number of infected etc. in stationarity can be given.

5.3.3 The $\tilde{\beta} = \beta$ limit or SIS limit

The ODE Eq. system given by Eqs. (5.43) to (5.47) can be treated analytically to obtain the stationary solution $\langle I \rangle^*$ as a function of the parameters in various situations, e.g. for $\tilde{\beta} = \beta$. This is the limit in which the SIRS system behaves in stationarity like an SIS system. When $\tilde{\beta} = \beta$, there is no difference any more between recovered and the susceptibles, hence we can add the recovered individuals to the susceptibles and treat the SIRS model as an SIS model with infection rate β and recovery rate γ . Now, we only need to consider the dynamics of $\langle I \rangle$ and $\langle SI \rangle$ which is given, under pair

approximation, by the following equations

$$\begin{aligned}\frac{d}{dt}\langle I \rangle &= \beta \langle SI \rangle - \gamma \langle I \rangle \\ \frac{d}{dt}\langle SI \rangle &= \gamma Q \langle I \rangle + (\beta(Q-2) - 2\gamma) \langle SI \rangle - 2\beta \frac{Q-1}{Q} \frac{\langle SI \rangle^2}{N - \langle I \rangle} .\end{aligned}$$

From this we can calculate the stationary value of infected, giving either the trivial disease free state $\langle I \rangle_1^* = 0$ or the endemic state

$$\langle I \rangle_2^* = N \frac{Q(Q-1)\beta - Q\gamma}{Q(Q-1)\beta - \gamma} \quad (5.53)$$

and then for the SIS limit the critical value for β is given by

$$\beta_c = \frac{\gamma}{Q-1} \quad (5.54)$$

as was calculated previously in the literature (see [24]) for the SIS epidemics. In Fig. 5.4, we compare the mean field solution (isolated dashed line) with the pair approximation (dotted line) for $\langle I \rangle^*(\beta)$ and the convergence of the time dependent solution of the SIRI pair dynamics (straight lines for various stopping times t_{max} approximating the dotted line). Further the critical value for the pair contact process is given as well, as obtained from extended spatial stochastic simulation reported in the literature (see [9]) as $\beta_c = 0.4122$. The pair approximation solution approaches the simulation value better than the mean field solution. We use the parameters $Q = 4$, appropriate for spatial two dimensional systems, $\gamma = 1$ throughout the figures. Here also $N = 100$. In Fig. 5.5, we present the critical point in pair

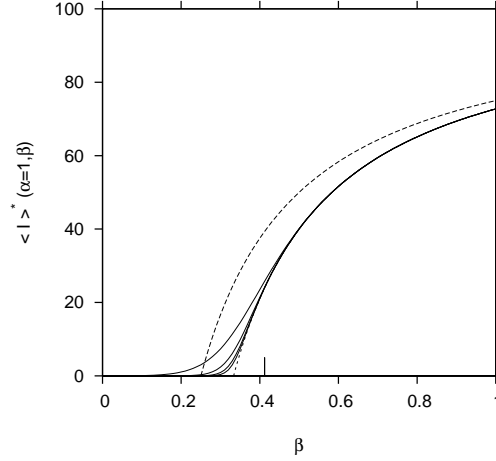


Figure 5.4: The mean field solution of the SIS limiting case (isolated dashed line), the pair approximation solution (dotted line) for $\langle I \rangle^*(\beta)$ and the convergence of the time dependent solution of the SIRI pair dynamics. The critical value for the pair contact process is given as well as $\beta_c = 0.4122$.

approximation along the line where $\tilde{\beta} = \beta$, the SIS limiting case, in the β - $\tilde{\beta}$ phase diagram. (In the figures we set $\tilde{\beta} \equiv \beta_s$, s for secondary infection.)

5.3.4 The $\alpha = 0$ limit

Considering the stationary state equations Eq. (5.48) to Eq. (5.52) in section 5.3.2 in the special case of $\alpha = 0$ we obtain

$$\langle RI \rangle^* = \frac{\gamma}{\tilde{\beta}} \langle I \rangle^* \quad (5.55)$$

and

$$\langle SI \rangle^* = 0 \quad , \quad \langle SR \rangle^* = 0 \quad (5.56)$$

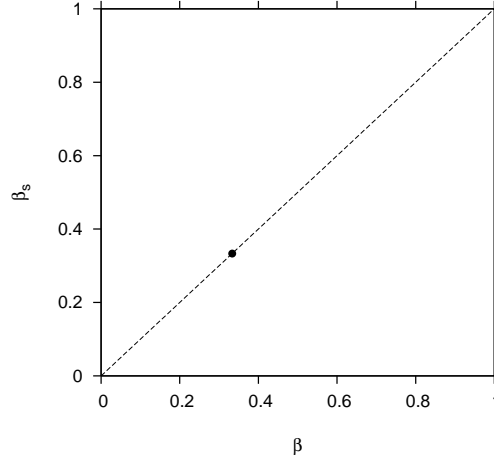


Figure 5.5: *The critical point in pair approximation for $\tilde{\beta} = \beta$, the SIS limiting case.*

so that also $\langle S \rangle^* = 0$. Hence $\langle R \rangle^* = N - \langle I \rangle^*$. Eq. (5.52) in the limit $\alpha = 0$ becomes identical $0 = 0$, and the remaining Eq. (5.51) becomes

$$\gamma Q \langle I \rangle^* - (2\gamma + \tilde{\beta}) \langle RI \rangle^* + \tilde{\beta} \frac{Q-1}{Q} \frac{(Q \langle R \rangle^* - 2 \langle RI \rangle^*) \cdot \langle RI \rangle^*}{\langle R \rangle^*} = 0 \quad (5.57)$$

and inserting the above equations, Eq. (5.55) and (5.56), gives

$$\gamma Q \langle I \rangle^* - (2\gamma + \tilde{\beta}) \frac{\gamma}{\tilde{\beta}} \langle I \rangle^* + \gamma \frac{Q-1}{Q} \frac{(QN - Q \langle I \rangle^* - 2 \frac{\gamma}{\tilde{\beta}} \langle I \rangle^*) \cdot \langle I \rangle^*}{N - \langle I \rangle^*} = 0 \quad (5.58)$$

an equation which is independent of β . It has as one stationary state $\langle I \rangle_1^* =$

0. The remaining equation

$$\gamma Q - (2\gamma + \tilde{\beta}) \frac{\gamma}{\tilde{\beta}} + \gamma \frac{Q-1}{Q} \frac{(QN - Q \langle I \rangle^* - 2 \frac{\gamma}{\tilde{\beta}} \langle I \rangle^*)}{N - \langle I \rangle^*} = 0 \quad (5.59)$$

gives the solution for $\langle I \rangle_2^*$. It is explicitly after some calculation

$$\langle I \rangle_2^* = N \frac{Q(Q-1)\tilde{\beta} - Q\gamma}{Q(Q-1)\tilde{\beta} - \gamma} \quad (5.60)$$

which is the solution of the SIS pair approximation dynamics in stationarity Eq. (5.53). From Eq. (5.59) directly (or from Eq. (5.60)) the critical value $\tilde{\beta}_c$ for the parameter $\tilde{\beta}$ can be calculated considering the condition that $\langle I \rangle_2^* \rightarrow \langle I \rangle_1^* = 0$, hence setting $\langle I \rangle_2^* = 0$. The result is

$$\tilde{\beta}_c = \frac{\gamma}{Q-1} \quad (5.61)$$

independently of the parameter β . This solution Eq. (5.61) gives a straight

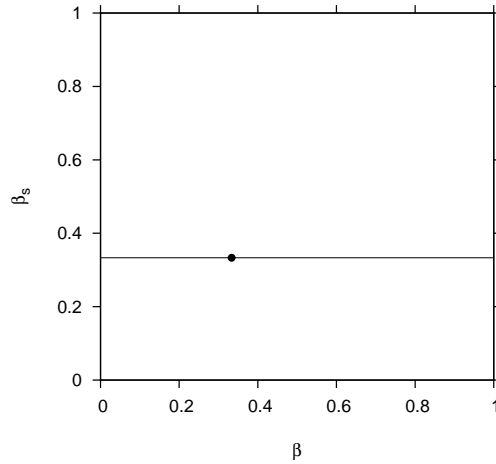


Figure 5.6: *The phase transition line for $\alpha = 0$ obtained in pair approximation.*

horizontal line in the parameter phase diagram for β and $\tilde{\beta}$, as shown in Fig. 5.6.

5.3.5 The $\tilde{\beta} = 0$ limit or SIR limit

In analogy to subsection 5.3.4 we can calculate from the system Eq. given by Eqs. (5.43) to (5.47) the stationary state solution for the limit $\tilde{\beta} = 0$. The stationary state $\langle I \rangle_1^* = 0$ can be found and the other stationary state follows from an equation of the form

$$a_2 (\langle I \rangle_2^*)^2 + a_1 \langle I \rangle_2^* + a_0 = 0 \quad (5.62)$$

with the coefficients

$$\begin{aligned} a_2 &= \beta Q^2 (Q - 1) (\alpha^3 + 2\alpha^2\gamma + 2\alpha\gamma^2 + \gamma^3) - Q\gamma (\alpha^3 + \gamma^3) \\ &\quad - (\alpha + \gamma) (2\alpha\gamma Q + \beta Q (\alpha + \gamma) + \alpha\gamma) \gamma \\ a_1 &= -\alpha\beta Q^2 N [2\alpha^2(Q - 1) + 3\gamma(Q\alpha - \gamma) + 2\gamma(Q\gamma - 2\alpha)] \\ &\quad + \alpha\gamma Q N [Q(\alpha^2 + \alpha\gamma + \gamma^2) + \beta(\alpha + \gamma) + (\alpha^2 + 3\alpha\gamma + \gamma^2)] \\ a_0 &= \alpha^2 Q^2 N^2 (\alpha\beta (Q - 1) + \beta\gamma (Q - 2) - \gamma(\alpha + \gamma)) \quad . \end{aligned}$$

Setting $\langle I \rangle_2^* = 0$ (which is the same as $a_0 = 0$), like shown in subsection 5.3.4, gives the explicit solution for the critical value β_c as

$$\beta_c = \frac{\gamma + \alpha}{Q - 2 + (Q - 1)\frac{\alpha}{\gamma}} \quad (5.63)$$

and in the limit of $\alpha = 0$

$$\beta_c = \frac{\gamma}{Q - 2} \quad (5.64)$$

in agreement with previously reported results (see [22]). The solution of the

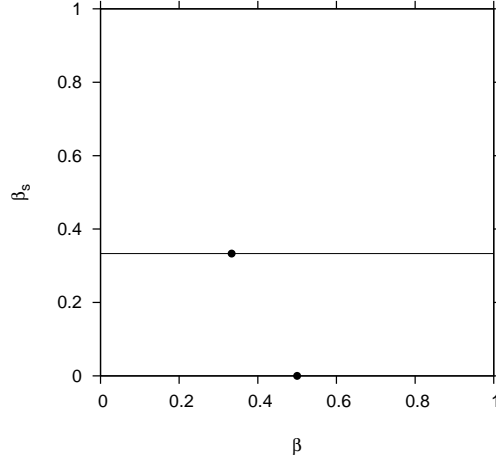


Figure 5.7: *The critical point for $\tilde{\beta} = 0$ (the SIR-limit) obtained in pair approximation.*

critical value $\beta_c = \frac{\gamma}{Q-2}$ is shown in the phase diagram for β and $\tilde{\beta}$ in Fig. 5.7 in addition to the previously calculated results Fig. 5.5 and Fig. 5.6.

5.3.6 Simulations of the pair approximation ODEs

We simulate the ODE system Eq. given by Eqs. (5.43) to (5.47) for fixed $\gamma = 1$ and small $\alpha = 0.05$, varying the infection rates β and $\tilde{\beta}$. In Fig. 5.8 a), we integrate the system Eqs. (5.43) to (5.47) numerically up to time t_{max} to obtain $I(t_{max})$. We change $\tilde{\beta}$ and fix $\beta = \gamma/(Q - 1)$, the SIS critical point value. In Fig. 5.8 b), we plot the logarithm of $I(t)$, $\ln(I(t))$, versus $\ln(t)$ for various $\tilde{\beta}$ values. A clear distinction is visible for the subcritical (going towards minus infinity) versus the supercritical values (going to finite values at t_{max}). In Fig. 5.9 a), we present the $I(t_{max})$ obtained integrating the system Eqs. (5.43) to (5.47) numerically up to time t_{max} , as in Fig. 5.8 a), but fixing now $\beta = \gamma/(Q - 2)$, the SIR critical point value

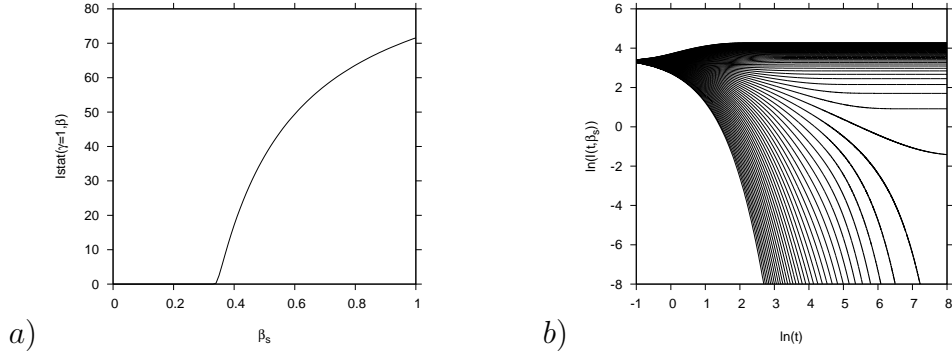


Figure 5.8: a) The $I(t_{max})$ obtained integrating the system Eqs. (5.43) to (5.47) numerically up to time t_{max} with changing $\tilde{\beta}$ for $\beta = \gamma/(Q - 1)$, the SIS critical point value. b) The logarithm of $I(t)$ versus $\ln(t)$ for various $\tilde{\beta}$ values.

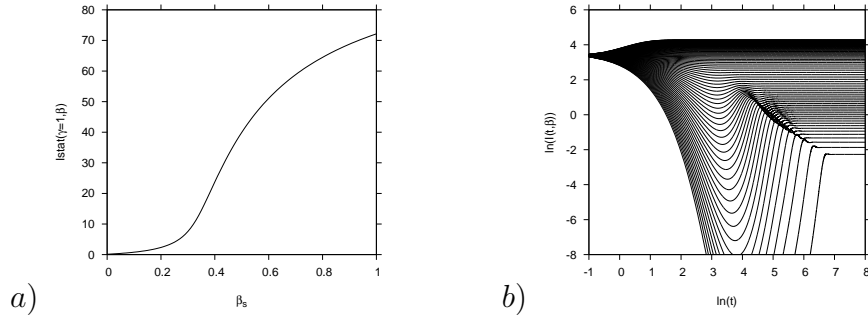


Figure 5.9: a) $I(t_{max})$ for $\beta = \gamma/(Q - 2)$, the SIR critical point value in the limit $\alpha = 0$. b) $\ln(I(t))$ versus $\ln(t)$ for various $\tilde{\beta}$ values.

in the limit $\alpha = 0$. However the simulations are done for small but finite $\alpha = 0.05$. In Fig. 5.9 b), we plot the logarithm of $I(t)$, $\ln(I(t))$, versus $\ln(t)$ for various $\tilde{\beta}$ values. For all $\tilde{\beta}$ values the curves go to finite values, none towards minus infinity, hence all $\tilde{\beta}$ values are supercritical. The result of integrating the system Eqs. (5.43) to (5.47) for a fixed β between the values for the SIS critical point value $\beta = \gamma/(Q - 1)$ and the SIR critical point value $\beta = \gamma/(Q - 2)$ is presented in Fig. 5.10 a). In Fig. 5.10 b), we

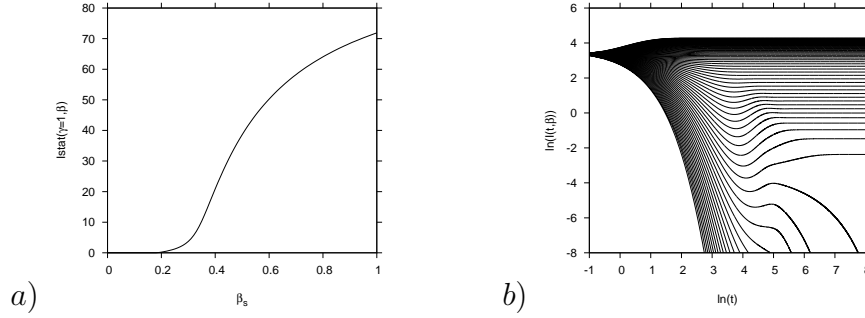


Figure 5.10: a) $I(t_{max})$ for $\beta = \gamma/(Q - 1.5)$, i.e. between the SIS critical point and the SIR critical point. b) $\ln(I(t))$ versus $\ln(t)$ for various $\tilde{\beta}$ values.

plot the logarithm of $I(t)$ versus $\ln(t)$ for various $\tilde{\beta}$ values. Sub-critical and super-critical values for $\tilde{\beta}$ can be distinguished finally, but initially some of the supercritical curves go to very low numbers, which for smaller t_{max} could be mistaken as sub-critical.

From the simulations analogously to Figs. 5.8 to 5.10 we can determine the critical line for a small but finite α value between the no-growth and the annular growth region in pair approximation. We can determine for small values of α from the numeric solutions of the SIRI pair dynamics directly the critical values. The result is shown in Fig. 5.11 as a line between the SIS limiting critical point and the SIR limiting critical point. The SIRI pair dynamics, Eqs. (5.43) to (5.47), is varied between $\beta = \gamma/(Q - 1)$ and $\beta = \gamma/(Q - 2)$, then the critical value for $\tilde{\beta}$ is determined for each value of β . The simulations for Fig. 5.11 have $\alpha = 0.05$ as small α value. We also compare this finite $\alpha = 0.05$ case with the analytic solution in the limit when α tends to zero (see Corollary 5.4.1), finding only small differences. So the numerical procedure shown above gives a rather good impression of

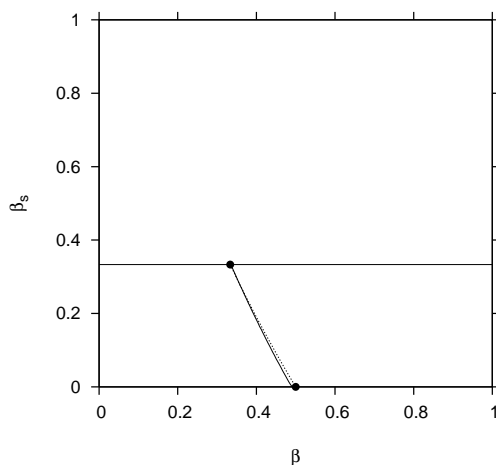


Figure 5.11: Comparison for the phase transition line between no-growth and ring-growth determined numerically for small but finite $\alpha = 0.05$, straight line, and the analytic solution in the limit when α tends to zero, dotted line.

the phase diagram in the limiting but numerically difficult to access case of vanishing α as expected. This is a good sign for future studies of purely stochastic simulations, which close to criticality are expected to be rather time consuming.

5.4 Analytic expression of the phase transition line

Let

$$E = \alpha + \gamma Q + \tilde{\beta} \quad , \quad (5.65)$$

$$F = D + \sqrt{D^2 + 4\alpha(Q-1)E} \quad , \quad (5.66)$$

where

$$D = \gamma Q - \tilde{\beta}(Q-1) - \alpha(Q-2) \quad . \quad (5.67)$$

We observe for the transition line between no-growth and annular growth that the stationary value $\langle I \rangle^*$ tends to zero and the stationary value $\langle R \rangle^*$ also tends to zero but their ratio stays finite. Hence, we conclude the following lemma:

Lemma 5.4.1 *The scaling limit of $\langle R \rangle^* / \langle I \rangle^*$ when $\langle I \rangle^*$ tends to zero is given by*

$$\lim_{\langle I \rangle^* \rightarrow 0} \frac{\langle R \rangle^*}{\langle I \rangle^*} = \frac{\gamma F}{2\alpha E} \quad . \quad (5.68)$$

Proof. We consider the equilibrium manifold of ODE system given by Eq. (5.43) to Eq. (5.47). We use equations (5.43), (5.44) and (5.47) to compute $\langle SI \rangle^*$, $\langle RI \rangle^*$ and $\langle SR \rangle^*$ and we replace their values in equation (5.45) and (5.46) giving the following two implicit equations:

$$\begin{aligned} & Q\langle I \rangle^* - \frac{\tilde{\beta} + 2\gamma}{\tilde{\beta}} \left(\langle I \rangle^* - \frac{\alpha}{\gamma} \langle R \rangle^* \right) + \left((Q-1) \langle I \rangle^* + \frac{\alpha}{\gamma} \langle R \rangle^* \right) \\ & \cdot \left(1 - 2 \frac{N - \langle I \rangle^* - \langle R \rangle^* - \frac{\alpha}{\beta Q} \langle R \rangle^*}{\frac{Q}{Q-1} (N - \langle I \rangle^* - \langle R \rangle^*) + \langle R \rangle^*} - \frac{2}{\tilde{\beta} Q} \frac{\gamma \langle I \rangle^* - \alpha \langle R \rangle^*}{\langle R \rangle^*} \right) = 0 \end{aligned} \quad (5.69)$$

and

$$\begin{aligned}
& Q\langle I \rangle^* - \frac{\alpha(\beta + 2\gamma)}{\beta\gamma}\langle R \rangle^* - \frac{\tilde{\beta} + 2\gamma}{\tilde{\beta}} \left(\langle I \rangle^* - \frac{\alpha}{\gamma}\langle R \rangle^* \right) \\
& + \frac{\alpha}{\gamma}(Q - 1)\langle R \rangle^* \left(1 - \frac{2\alpha\langle R \rangle^*}{\beta Q(N - \langle I \rangle^* - \langle R \rangle^*)} \right) \\
& + (Q - 1) \left(\langle I \rangle^* - \frac{\alpha}{\gamma}\langle R \rangle^* \right) \left(1 - \frac{2(\gamma\langle I \rangle^* - \alpha\langle R \rangle^*)}{\tilde{\beta}Q\langle R \rangle^*} \right) = 0 \quad .
\end{aligned} \tag{5.70}$$

We start proving that if $\langle I \rangle^*$ tends to zero then $\langle R \rangle^*$ also converges to zero.

We observe that the function in Eq. (5.69) is continuous at $\langle I \rangle^* = 0$ and its value is

$$\frac{\tilde{\beta} + 2\gamma}{\tilde{\beta}} \frac{\alpha}{\gamma} \langle R \rangle^* + \frac{\alpha}{\gamma} \langle R \rangle^* \left(1 - 2 \frac{N - \langle R \rangle^* - \frac{\alpha}{\beta Q} \langle R \rangle^*}{\frac{Q}{Q-1}(N - \langle R \rangle^*) + \langle R \rangle^*} + \frac{2\alpha}{\tilde{\beta}Q} \right) = 0 \tag{5.71}$$

Hence, we obtain that $\langle R \rangle^* = 0$ or

$$\langle R \rangle^* = - \frac{\beta Q (\tilde{\beta} + \gamma Q + \alpha)}{\beta \tilde{\beta} Q (Q - 2) + \tilde{\beta} \alpha (Q - 1) - \beta (\gamma Q + \alpha)} \quad . \tag{5.72}$$

But the value presented in Eq. (5.72) is not a solution of Eq. (5.70) for $\langle I \rangle^* = 0$. Hence, the stationary state $\langle R \rangle^*$ converges to zero when $\langle I \rangle^*$ tends to zero. Let

$$\begin{aligned}
N_{1,2} &= -\alpha \tilde{\beta} \gamma Q \quad , \\
N_{0,3} &= \tilde{\beta} \alpha (-\gamma Q + \alpha(Q-1)) \quad , \\
N_{0,2} &= \alpha \tilde{\beta} \gamma N Q \quad ,
\end{aligned} \tag{5.73}$$

and

$$\begin{aligned}
D_{3,0} &= \gamma^2(Q-1) \quad , \\
D_{2,1} &= -\tilde{\beta} \gamma Q(Q-1) - 2\alpha \gamma (Q-1) + 2\gamma^2(Q-1) \quad , \\
D_{1,2} &= \alpha^2(Q-1) - \tilde{\beta} \gamma Q(Q-1) - 3\alpha \gamma Q + 2\alpha \gamma + \gamma^2 Q \quad , \\
D_{0,3} &= \alpha^2(Q-1) - \alpha \gamma Q \quad , \\
D_{2,0} &= -\gamma^2 N(Q-1) \quad , \\
D_{1,1} &= N \gamma (2\alpha(Q-1) + \tilde{\beta} Q(Q-1) - \gamma Q) \quad , \\
D_{0,2} &= N \alpha (\gamma Q - \alpha(Q-1)) \quad .
\end{aligned} \tag{5.74}$$

Solving Eq. (5.70) in order to isolate the parameter β , we obtain that

$$\beta(\tilde{\beta}) = \frac{N_\beta(\langle I \rangle^*, \langle R \rangle^*, \tilde{\beta})}{D_\beta(\langle I \rangle^*, \langle R \rangle^*, \tilde{\beta})} \quad , \tag{5.75}$$

where N_β is given by

$$N_\beta(\langle I \rangle^*, \langle R \rangle^*, \tilde{\beta}) = N_{1,2} \langle I \rangle^* \langle R \rangle^{*2} + N_{0,3} \langle R \rangle^{*3} + N_{0,2} \langle R \rangle^{*2} \quad , \tag{5.76}$$

and D_β is given by

$$D_\beta(\langle I \rangle^*, \langle R \rangle^*, \tilde{\beta}) = D_{3,0} \langle I \rangle^{*3} + D_{2,1} \langle I \rangle^{*2} \langle R \rangle^* + D_{1,2} \langle I \rangle^* \langle R \rangle^{*2} \quad (5.77) \\ + D_{0,3} \langle R \rangle^{*3} + D_{2,0} \langle I \rangle^{*2} + D_{1,1} \langle I \rangle^* \langle R \rangle^* + D_{0,2} \langle R \rangle^{*2} .$$

Substituting in Eq. (5.69) the expression for β given in Eq. (5.75), we obtain

$$\frac{N(\langle I \rangle^*, \langle R \rangle^*; \tilde{\beta})}{D(\langle I \rangle^*, \langle R \rangle^*; \tilde{\beta})} = 0 \quad , \quad (5.78)$$

where the denominator is given by

$$D(\langle I \rangle^*, \langle R \rangle^*; \tilde{\beta}) = \tilde{\beta} Q \langle R \rangle^* (\gamma Q N - \langle R \rangle^* (\gamma Q - \alpha(Q - 1)) - \gamma Q \langle I \rangle^*) \\ \cdot (\langle R \rangle^* - Q(N - \langle I \rangle^*)) \quad , \quad (5.79)$$

and the numerator is given by

$$N(\langle I \rangle^*, \langle R \rangle^*; \tilde{\beta}) = C_{4,0} \langle I \rangle^{*4} + C_{3,1} \langle I \rangle^{*3} \langle R \rangle^* + C_{2,2} \langle I \rangle^{*2} \langle R \rangle^{*2} \\ + C_{1,3} \langle I \rangle^* \langle R \rangle^{*3} + C_{0,4} \langle R \rangle^{*4} + C_{3,0} \langle I \rangle^{*3} \quad (5.80) \\ + C_{2,1} \langle I \rangle^{*2} \langle R \rangle^* + C_{1,2} \langle I \rangle^* \langle R \rangle^{*2} + C_{0,3} \langle R \rangle^{*3} \\ + C \langle I \rangle^{*2} + B \langle I \rangle^* \langle R \rangle^* + A \langle R \rangle^{*2} \quad ,$$

with

$$A = -2\alpha N^2 Q^2 (\alpha + \gamma Q + \tilde{\beta}) \quad , \quad (5.81)$$

$$B = 2\gamma N^2 Q^2 (\gamma Q - \tilde{\beta}(Q - 1) - \alpha(Q - 2)) \quad , \quad (5.82)$$

$$C = 2\gamma^2 N^2 Q^2 (Q - 1) \quad . \quad (5.83)$$

The other coefficients $C_{i,j}$ of the numerator are not presented here, because we will not use them in the future computations. We are going to find the limit of the ratio $\langle R \rangle^* / \langle I \rangle^*$, when $\langle I \rangle^*$ tends to zero, such that

$$N(\langle I \rangle^*, \langle R \rangle^*; \tilde{\beta}) = 0 \quad (5.84)$$

is satisfied. Dividing Eq. (5.84) by $\langle I \rangle^{*2}$ and furthermore defining the ratio of recovered over infected $\langle V \rangle^* = \langle R \rangle^* / \langle I \rangle^*$, we obtain that

$$\begin{aligned} & C_{4,0} \langle I \rangle^{*2} + C_{3,1} \langle I \rangle^* \langle R \rangle^* + C_{2,2} \langle R \rangle^{*2} + C_{1,3} \langle V \rangle^* \langle R \rangle^{*2} + C_{0,4} \langle V \rangle^{*2} \langle R \rangle^{*2} \\ & + C_{3,0} \langle I \rangle^* + C_{2,1} \langle R \rangle^* + C_{1,2} \langle V \rangle^* \langle R \rangle^* + C_{0,3} \langle V \rangle^{*2} \langle R \rangle^* \\ & + C + B \langle V \rangle^* + A \langle V \rangle^{*2} = 0 \quad . \end{aligned} \quad (5.85)$$

When $\langle I \rangle^*$ tends to zero we already proved that $\langle R \rangle^*$ converges to zero. Hence, from Eq. (5.85), we obtain

$$A \langle V \rangle^{*2} + B \langle V \rangle^* + C = 0 \quad , \quad (5.86)$$

in the limiting case when $\langle I \rangle^*$ tends to 0. Therefore, there are two solutions $\langle V \rangle_{1,2}^*$ for $\langle V \rangle^*$ given by

$$\langle V \rangle_{1,2}^* = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} \quad . \quad (5.87)$$

Since $C = 2\gamma^2 N^2 Q^2 (Q - 1) > 0$ and $A = -2\alpha N^2 Q^2 (\alpha + \gamma Q + \tilde{\beta}) < 0$, we conclude that $-4AC > 0$ and so $B^2 - 4AC > B^2$. Hence, Eq. (5.86) has a

unique positive solution

$$\langle V \rangle^* = \frac{-B - \sqrt{B^2 - 4AC}}{2A} . \quad (5.88)$$

Inserting into Eq. (5.88) the expressions of A , B and C presented in Eqs. (5.81) to (5.83), we obtain Eq. (5.68). ■

Now we will use the value of the ratio $\langle R \rangle^* / \langle I \rangle^*$ at criticality to obtain the analytic expression of the phase transition line.

Let

$$G(\tilde{\beta}) = \gamma \tilde{\beta} Q \cdot F^2 , \quad (5.89)$$

and

$$\begin{aligned} H(\tilde{\beta}) &= 2 \left(2\alpha(Q-1) + \tilde{\beta}Q(Q-1) - \gamma Q \right) \cdot E \cdot F \\ &+ (\gamma Q - \alpha(Q-1)) \cdot F^2 \\ &- 4\alpha(Q-1) \cdot E^2 , \end{aligned} \quad (5.90)$$

where E and F are defined in Eq. (5.65) and Eq. (5.66) respectively.

Theorem 5.4.1 *Let $\alpha > 0$. The phase transition line $\beta(\tilde{\beta}) = \beta_c(\tilde{\beta}, \alpha, \gamma, Q, N)$ between no-growth and annular growth for the spatial epidemic SIRS model in pair approximation is given by*

$$\beta(\tilde{\beta}) = \frac{G(\tilde{\beta})}{H(\tilde{\beta})} , \quad (5.91)$$

with $0 \leq \tilde{\beta} \leq \gamma/(Q-1)$.

Proof. We observe that Eq. (5.75) can be rewritten in terms of $\langle I \rangle^*$, $\langle R \rangle^*$ and $\langle V \rangle^* = \langle R \rangle^* / \langle I \rangle^*$ as follows:

$$\beta(\tilde{\beta}) = \frac{L_1 \langle R \rangle^* + N_{0,2} \langle V \rangle^{*2}}{D_{3,0} \langle I \rangle^* + L_2 \langle R \rangle^* + D_{2,0} + D_{1,1} \langle V \rangle^* + D_{0,2} \langle V \rangle^{*2}} \quad , \quad (5.92)$$

where

$$L_1 = N_{1,2} \langle V \rangle^* + N_{0,3} \langle V \rangle^{*2} \quad , \quad (5.93)$$

$$L_2 = D_{2,1} + D_{1,2} \langle V \rangle^* + D_{0,3} \langle V \rangle^{*2} \quad , \quad (5.94)$$

and the coefficients $N_{i,j}$ and $D_{i,j}$ are presented in Eqs. (5.73) and (5.74) respectively. The phase transition curve follows from Eq. (5.92) by letting $\langle I \rangle^*$ tends to zero. Under this limit, Eq. (5.92) reduces to

$$\beta(\tilde{\beta}) = \frac{N_{0,2} \langle V \rangle^{*2}}{D_{2,0} + D_{1,1} \langle V \rangle^* + D_{0,2} \langle V \rangle^{*2}} \quad . \quad (5.95)$$

Hence, the numerator of Eq. (5.95) is given by

$$\begin{aligned} N_{0,2} \langle V \rangle^{*2} &= \alpha \tilde{\beta} \gamma N Q \frac{\gamma^2 F^2}{4 \alpha^2 E^2} \\ &= \tilde{\beta} \gamma^3 N Q \frac{F^2}{4 \alpha E^2} \quad , \end{aligned} \quad (5.96)$$

and the denominator is given by

$$\begin{aligned}
& -\gamma^2 N(Q-1) + N\gamma(2\alpha(Q-1) + \tilde{\beta}Q(Q-1) - \gamma Q) \frac{\gamma F}{2\alpha E} \\
& \quad + N\alpha(\gamma Q - \alpha(Q-1)) \frac{\gamma^2 F^2}{4\alpha^2 E^2} \\
= & \gamma^2 N \left(-(Q-1) + (2\alpha(Q-1) + \tilde{\beta}Q(Q-1) - \gamma Q) \frac{F}{2\alpha E} \right. \\
& \quad \left. + (\gamma Q - \alpha(Q-1)) \frac{F^2}{4\alpha E^2} \right) \quad (5.97)
\end{aligned}$$

Dividing Eq. (5.96) by Eq. (5.97), we obtain the explicit formula for the phase transition curve of the SIRI model, that can be written as given in Eq. (5.91). ■

This completes the expression for the critical curve $\beta(\tilde{\beta})$ for the general α and γ case. When α tend to 0, we obtain the following expression for $\beta(\tilde{\beta})$:

Corollary 5.4.1 *In the limit when α tends to zero the phase transition line between no-growth and annular growth $\beta(\tilde{\beta})$ for the spatial epidemic SIRI model is given by*

$$\lim_{\alpha \rightarrow 0} \beta(\tilde{\beta}) = \frac{\gamma^2 Q - \gamma \tilde{\beta}(Q-1)}{\gamma Q(Q-2) + \tilde{\beta}(Q-1)} \quad . \quad (5.98)$$

In Fig. 5.12, we show the horizontal transition line corresponding in the left hand side to transition from no-growth to compact growth and in the right hand side to transition from annular growth to compact growth (see [43]) and the obliquel line is the phase transition between no-growth and

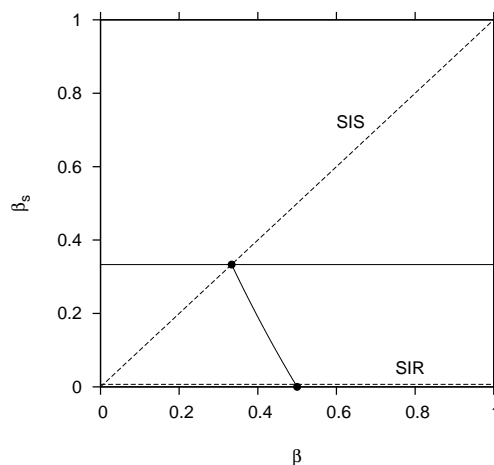


Figure 5.12: *The phase transition line between no-growth and annular growth determined from the analytic solution in the limiting case when α tends to zero which is explicitly given in Eq. (5.98). The horizontal transition line of the SIRS limiting case when $\alpha = 0$ and the phase transition points of SIS and SIR limiting cases are also presented as calculated in [43]. The SIS and SIR limiting cases are given by dashed lines. (Parameters $Q = 4$ appropriate for spatial two dimensional systems and $\gamma = 1$ were used.)*

annular growth as determined in corollary 5.4.1. The intersection of these two lines is the phase transition for the SIS model and the intersection of the oblique line with the horizontal axis is the phase transition line for the SIR model.

Summary

In this thesis we characterize the critical thresholds and the phase transition lines for different epidemiological models, namely the SIS and the SIRS model. The stochastic SIS model was first introduced in chapter 2, where we studied recursively the moment closure ODE's for the infected individuals. We developed for every number of the moments m a recursive formula to compute the equilibria manifold of the m moment closure ODE's. Nåsell used the stable equilibria of the 1 to 3 moment closure ODE's to obtain approximations of the quasi-stationary mean value of infecteds for high values of the population size N . In chapter 3, we concluded that the stable equilibria of the m moment closure ODE's can also be used to give a good approximation of the quasi-stationary mean value of infecteds for relatively small populations size N and also for relatively small infection rates β by taking m large enough. In chapter 4 we considered the spatial stochastic SIS model with creation and annihilation operators. We studied the series expansion of the gap between the dominant and subdominant eigenvalues of the evolution operator for the SIS model in 1 dimension and we computed explicitly the first terms of this series expansion. The spatial reinfection SIRS model was considered in chapter 5, where we determined

the phase transition diagram in the mean field approximation and in the pair approximation. In the mean field approximation we observe that this epidemiological model exhibits a first critical threshold between a disease free state and a non-trivial endemic state and a second threshold known as the reinfection threshold. We also have computed the analytic expression of the phase transition lines for the spatial SIRI model using the pair approximation. We have introduced a scaling argument that allowed us to determine analytically an explicit formula for the phase transition line between no-growth and annular growth. This scaling argument consisted in computing the ratio $\langle R \rangle^* / \langle I \rangle^*$ of the average of the recovered individuals $\langle R \rangle^*$ against the infected individuals $\langle I \rangle^*$.

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