

Collective Phenomena in Multi Particle Systems

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1. Statistical Mechanics: An Overview
2. Phase Transitions
3. Derivation of Macroscopic Equations

The modern search for a quantitative microscopic theory of macroscopic phenomena dates to the middle of the nineteenth century. At that time the experiments of Joule and others made it clear that phenomena like boiling and freezing, heat conduction, diffusion, etc., have their origins in the dynamics of the atoms and molecules which are the constituents of matter.

It was also soon recognized that the large disparity in the spatial and temporal scales between the world of atoms and the world of macroscopic experience not only necessitated a statistical theory but also assured, in analogy to the law of large numbers in probability theory, that such a theory will give predictions precise enough to have the force of “law”, as in Fourier’s law or in the second law of thermodynamics

Thus was born the subject of statistical mechanics, whose aim is to explain how the cooperative behavior of many individual entities can give rise to new phenomena having no counterpart in the properties or dynamics of the separate entities. The nature of these entities can vary widely: in the traditional studies they are atoms in a fluid, spins in a magnet, electrons in a metal, etc. In more recent applications they can also be birds in a flock, people in a soccer stadium or at a demonstration. The emergent phenomena can be the boiling/freezing of water, people clapping rhythmically at a performance, etc.

The twentieth century saw the development of the subject into a physically very successful and mathematically very beautiful theory of statistical mechanics of systems in thermal equilibrium.

The development of a comparable theory for the more complex world of nonequilibrium phenomena, including in particular those occurring in biological systems, remains a challenge for physicists, mathematicians, biologists, etc.

Microstates: classical

Every bit of macroscopic matter is composed of an enormous number of quasi-autonomous units, e.g. atoms in a simple fluid. If one treats these atoms as classical particles moving according to non-relativistic Hamiltonian equations then the complete microscopic (or micro) state of an isolated classical system of N particles is specified at any time t by a point $X(t)$ in its phase space Γ ,

$$X = (\mathbf{r}_1, \mathbf{v}_1, \dots, \mathbf{r}_N, \mathbf{v}_N), \quad \mathbf{r}_i \in \mathbf{V} \subset \mathbb{R}^d, \quad \mathbf{v}_i \in \mathbb{R}^d,$$

with $X(t)$, $t \in \mathbb{R}$, given by the Hamiltonian evolution.

A typical (isolated, non-relativistic) Hamiltonian for a simple fluid, say Argon, has the form (using units in which the mass of a particle is 1)

$$H(X) = \frac{1}{2} \sum \mathbf{v}_i^2 + \frac{1}{2} \sum_{i \neq j} \phi(|\mathbf{r}_{ij}|), \quad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j,$$

with appropriate boundary conditions on ∂V . The equations of motion

$$\dot{\mathbf{r}}_i(t) = \mathbf{v}_i(t), \quad \dot{\mathbf{v}}_i(t) = - \sum_{j \neq i} \frac{\partial}{\partial \mathbf{r}_i} \phi(\mathbf{r}_{ij}),$$

give an evolution

$$X(t) = T_{t-t_0} X(t_0), \quad t, t_0 \in \mathbb{R}.$$

The evolution preserves Liouville volume, $d\Gamma = \prod d\mathbf{r}_i d\mathbf{v}_i$. and also conserves energy

$$H(X_t) = E, \text{ constant}$$

so the evolution takes place on an energy surface Γ_E .

Since the real world is quantum mechanical, such a classical description is clearly “not realistic”. That it works so well in many cases is (to me at least) very surprising. I will use it as a model of reality for this presentation.

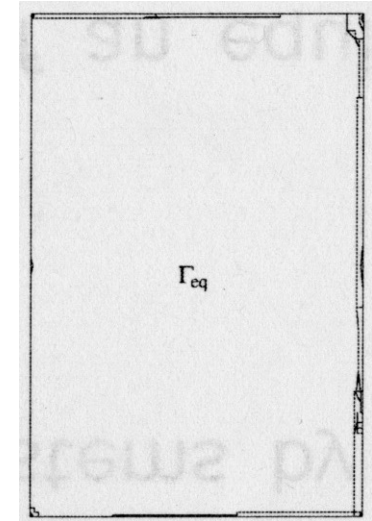
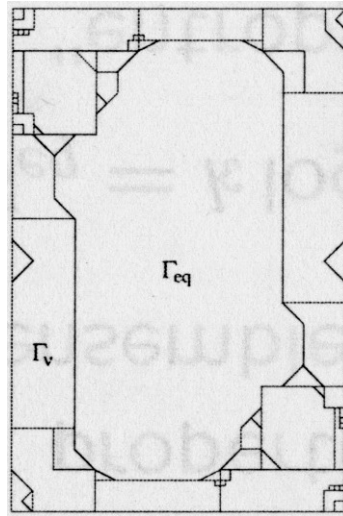
Macrostates

To describe the macroscopic state of a system of N atoms in a box V , say $N \gtrsim 10^{20}$, we make use of a much cruder description than that provided by the microstate X . We shall denote by M such a macroscopic description of a macrostate, and by $M(X)$ the macrostate corresponding to the microstate X . As an example, we may divide V into K cells, where K is large but still $K \ll N$, and specify the number of particles, the total momentum, and the amount of energy in each cell, with some tolerance.

Clearly, there are many microstates, in fact a continuum which correspond to the same macrostate, M . Let Γ_M be the region in the phase space Γ consisting of all microstates X corresponding to a given macrostate M , and denote by $|\Gamma_M|$ its (Liouville) volume.

The equilibrium macrostate M_{eq} of an isolated system with energy E is defined as that state for which $|\Gamma_{M_{eq}}| \sim |\Gamma_E|$, the “volume” of the whole “energy shell.” When M specifies a non-equilibrium state, $|\Gamma_M|$ is much smaller. Thus, if a dilute gas contains N atoms in a volume V , then the ratio of $|\Gamma_{M_{eq}}|$ for the macrostate M_{eq} in which there are $\left(\frac{1}{2} \pm 10^{-10}\right) N$ particles in the left half of the box to $|\Gamma_M|$, where M is a macrostate in which all the particles are in the left half, is of order 2^N . For any macroscopic value of N , this is far larger than the ratio of the volume of the known universe to the volume of one proton.

Pictorially



The second picture is slightly more faithful. Neither shows the topology or differences in relative sizes of the different Γ_M 's.

The fact that $|\Gamma_{M_{eq}}| \sim |\Gamma_E|$ explains why typical properties of equilibrium systems, i.e. those true for almost all $X \in \Gamma_{eq}$, are also typical for all $X \in \Gamma_E$ and can thus be obtained from the “microcanonical ensemble”, which gives a uniform measure on Γ_E . It also explains why isolated systems started in a nonequilibrium macro-state M_0 typically evolve into macrostates M_t such that $|\Gamma_{M_t}|$ is increasing and end up in $\Gamma_{M_{eq}}$, where they typically stay for very, very long times.

Equating the entropy of a macroscopic system in the state M with $\log |\Gamma_M|$, Boltzmann gave a natural (and correct) explanation of the origin of the second law of thermodynamics: “the entropy of an isolated macroscopic system (almost) never decreases.”

How this Boltzmann entropy is related (or unrelated) to other entropies, like the Gibbs-Shannon entropy of measures, the Kolmogorov-Sinai entropy of dynamical systems, the topological entropy, etc. is a very interesting subject, which I shall not go into here. I would like to note however that large entropy (of a macrostate), i.e. the large number of microstates corresponding to the macrostate, is not necessarily the same as what one would normally call large disorder. Thus at small energy (or temperature) the maximal entropy state of most systems is that of a crystal, which one would normally think of as being ordered.

Clustering in Gravitational Systems at all Energies

R. Penrose: Inflationary Cosmology

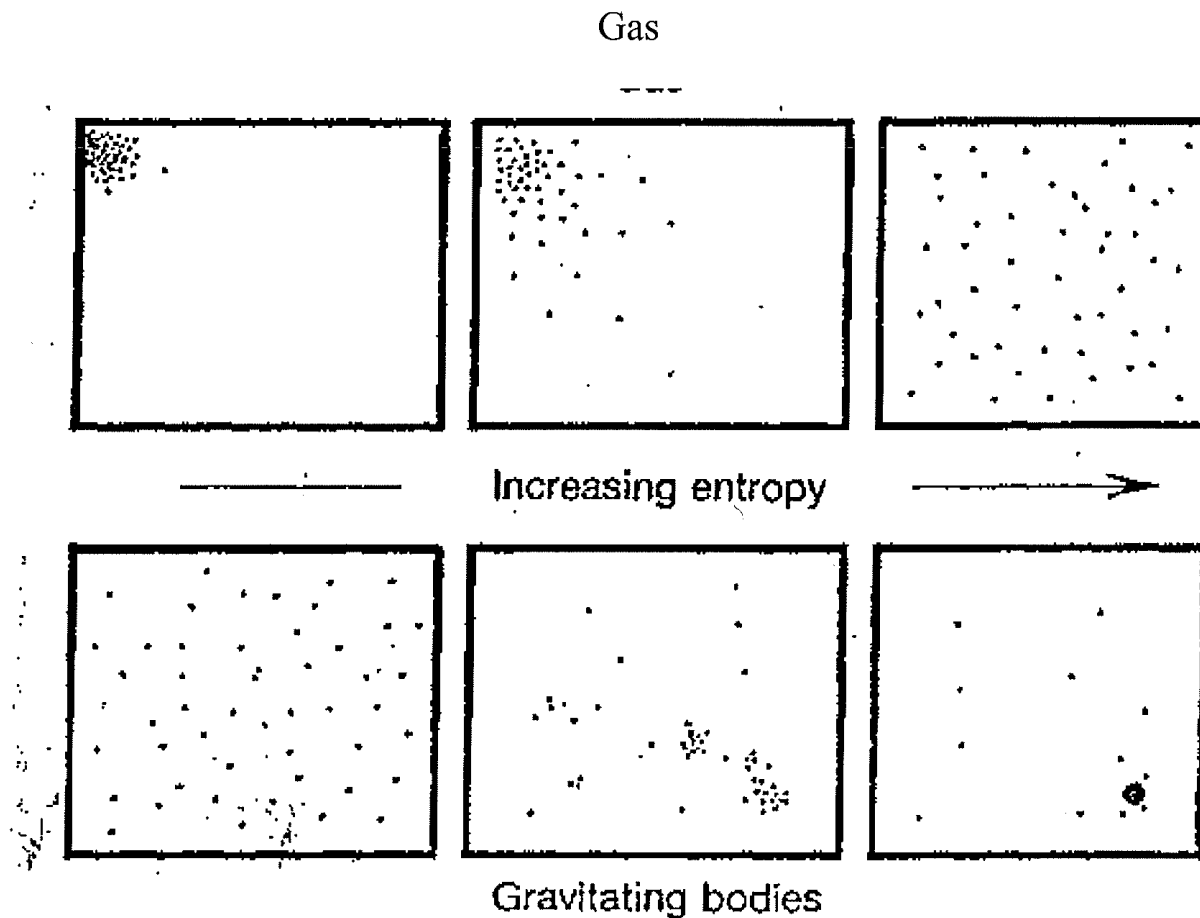
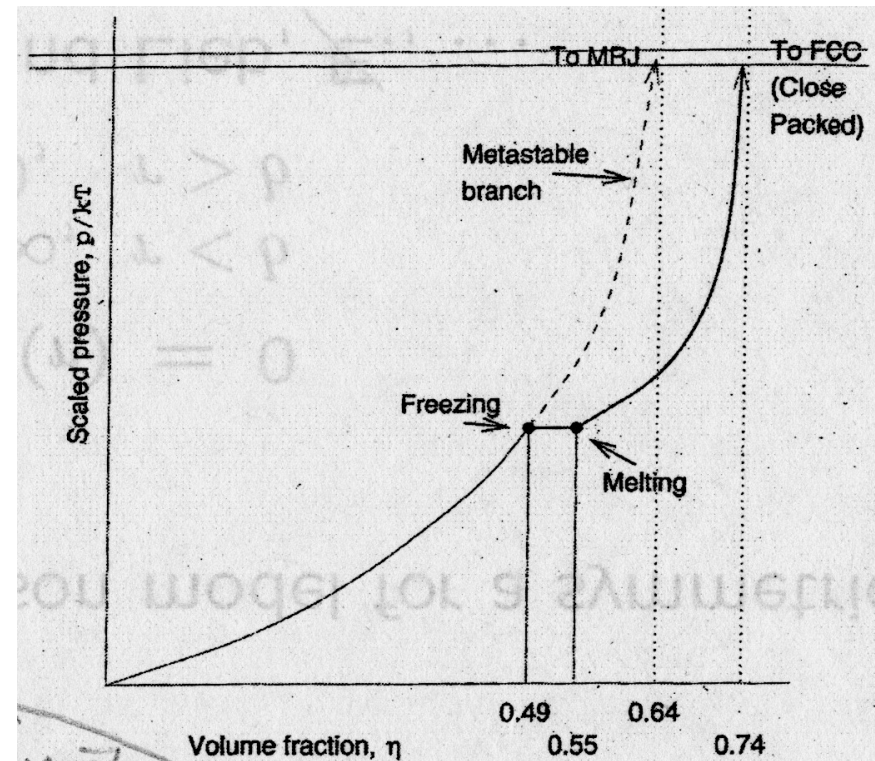
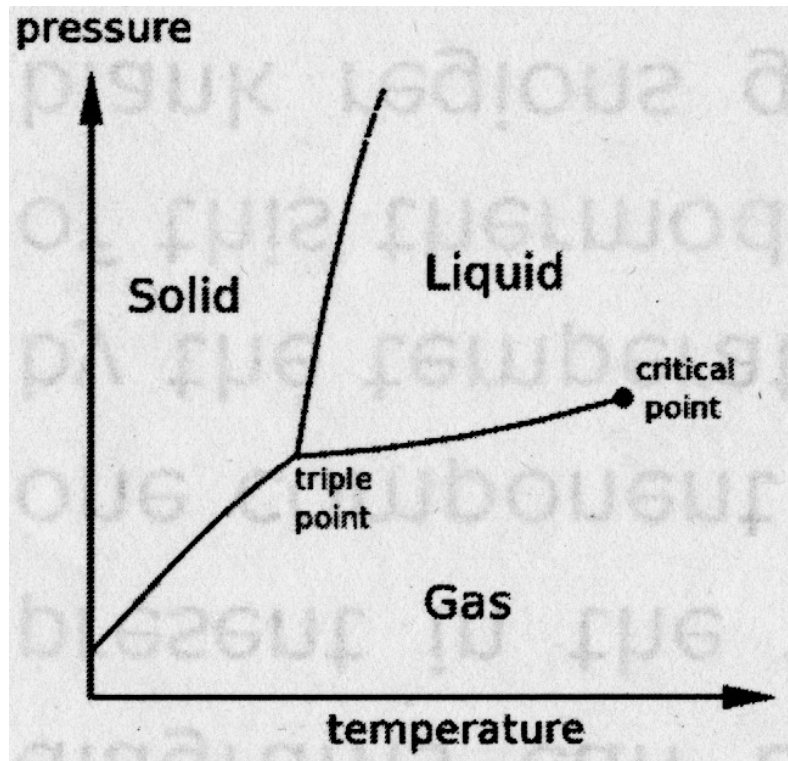


FIGURE 6. With a gas in a box, the maximum entropy state (thermal equilibrium) has the gas distributed uniformly; however, with a system of gravitating bodies, entropy can be increased from the uniform state by gravitational clumping to a black hole finally.

Phase Transitions in Equilibrium Systems

Information about the equilibrium phases of a homogeneous macroscopic system is conveniently encoded in its phase diagram. Phase diagrams can be very complicated, but their essence is already present in the familiar, simplified two dimensional diagram for a one component system like water or argon. This has axes marked by the temperature T and pressure p , and gives the decomposition of this thermodynamic parameter space into different regions: the blank regions generally correspond to parameter values in which there is a unique pure phase — gas, liquid, or solid — while the lines between these regions represent values of the parameters at which two pure phases can coexist. At the triple point, the system can coexist in any of three pure phases.



(1) System with attractive interactions. (2) Hard sphere system, 3D.

The phase transition for hard spheres from a disordered fluid to an fcc crystal is based entirely on simulations. If correct it is driven entirely by entropy maximization.

The mathematically precise formulation of what is meant by coexistence of phases is a beautiful part of statistical mechanics. It is based on the observation that “boundary conditions” may influence the bulk state of a macroscopic system even when the volume V goes to infinity.

In general, a macroscopic system is said to *undergo* or *be at* a first-order phase transition when the temperature and pressure (or more generally, the temperature and chemical potentials) do not uniquely specify its homogeneous equilibrium state: the different boundary conditions will give rise to different pure phases. The different properties of the pure phases coexisting at such a transition manifest themselves as discontinuities in certain observables, e.g. a discontinuity in the density as a function of temperature at the boiling point.

To make this precise we need to take the “thermodynamic limit”

$$N \rightarrow \infty, \quad V \rightarrow \infty, \quad \frac{N}{|V|} \rightarrow \rho, \quad E \rightarrow \infty, \quad \frac{E}{|V|} \rightarrow e.$$

Real systems of course contain only a finite number of particles but physically this limit is a good idealization for systems containing 10^{20} particles (or even much smaller ones used in computer simulations).

31. SOME REMINISCENCES ABOUT EINSTEIN'S VISITS TO LEIDEN

George E. Uhlenbeck

Harry Woolf (ed.), *Some Strangeness in the Proportion:*

I started to study in the beginning of 1927 the paper of Einstein in which he claims that an ideal gas like helium would show a condensation phenomena as a consequence of the Bose statistics.¹ This seemed very paradoxical, and to my surprise I came to the conclusion that Einstein was wrong! In my opinion his error was to replace the partition function over the discrete energy levels of the particles by an integral that was not allowed near the condensation point. The exact formula did not show any kind of singularity, so that, for instance, the equation of state would be quite smooth. I was of course quite excited, especially because Ehrenfest was convinced that I was right when I told him my reasoning. I know that he lectured about it at a few places and also that he wrote a letter to Einstein in which at the end he quoted some phrases of Schiller, I think, which I do not quite remember except that the sense was: If the masters fail, then the young people must do the work! I hope that Martin Klein can dig up the letter.²

In retrospect I think one should say that, although I was technically right, Einstein had somehow intuitively understood that a phase transition like the Bose condensation can occur only for large systems and is a kind of limit property. This should justify the replacement of sums by integrals. Of course Einstein did not prove this! In fact I know from a later conversation with him, in the thirties, that he agreed with my criticism. The insight that only in the so-called bulk or thermodynamic limit the partition function of a system can show singularities like phase transitions became clear and generally accepted in the late thirties. My late student Boris Kahn played an important role in this clarification process.

3. Martin Klein has found the letter of Ehrenfest. It is in the form of a manuscript to the *Z. f. Physik* and it is very witty, although difficult to read. I have tried to translate the beginning to give some idea of the style. The title is:

Does the Bose-Einstein Statistics Lead for Ideal Gases to
a Condensation in the Degenerate State?

G. E. Uhlenbeck and P. Ehrenfest (Leiden)

Motto: When kings are building, then the sewer cleaners
have work to do.

Summary: No!

In this way it goes on. There is also an answer by Einstein, who appreciated the jokes, but who was at this point not yet convinced.

How do we prove the existence of phase transitions?

There are no mathematically rigorous results showing a phase transition for continuum systems with “realistic effective interactions” such as Lennard-Jones pair potentials, but computer simulations on such systems give results in (semi) quantitative agreement with experiments.

An exception is the Widom–Rowlinson model for a symmetric mixture of species 1 and 2:

$$\begin{aligned}\phi_{11}(r) &= \phi_{22}(r) = 0 \\ \phi_{12}(r) &= \begin{cases} \infty, & r < b \\ 0, & r > b \end{cases}\end{aligned}$$

and its generalizations: Ruelle, L. and Lieb, etc.

One can also prove (L-Penrose, L-Presutti-Mazel) gas-liquid phase transitions for models in which the interaction potential extends over distances which are very large compared to the inter-particle spacing, but this becomes technical so I will not discuss it here.

Nonequilibrium systems

I will now go on to time dependent phenomena. Refining the description given in terms of macrostates (slide 8) we are led in suitable cases to a macroscopic description in terms of hydrodynamic density profiles, $\xi_X(\mathbf{x}) = (n(\mathbf{x}), \mathbf{u}(\mathbf{x}), e(\mathbf{x}))$, $\mathbf{x} \in V$. The time evolution of such profiles $\xi(\mathbf{x}, t) = \xi_{X(t)}(\mathbf{x})$, while coming from the dynamics of the microstates $X(t)$, takes place on much coarser time and space scales.

This permits the description of their evolution by autonomous equations, such as the Navier-Stokes and diffusion equation. The derivation (and solution) of such equations is one of the main subjects of classical non-equilibrium statistical mechanics. The basic approach is to use a rescaling of space-time to go from the microscopic dynamics to the macroscopic ones. I will describe this later when I discuss stochastic dynamics. These are the only dynamics for which we are currently able to derive such macroscopic equations.

Stochastic dynamics for lattice systems

Let $x \in \Lambda \subset \mathbb{Z}^d$, $\underline{\eta} = \{\eta(x)\}$, $\underline{\sigma} = \{\sigma(x)\}$,

$\eta(x) = \{1, 0\}$, occupied/empty,

$\sigma(x) = 1 - 2\eta(x) = \pm 1$, up/down spin

Glauber: $\sigma(x) \rightarrow -\sigma(x)$, with rate $c(x; \underline{\sigma})$

i.e, $\underline{\sigma} \rightarrow \underline{\sigma}^x$, $\underline{\sigma}^x(y) = \begin{cases} \sigma(y) & , y \neq x \\ -\sigma(y) & , y = x \end{cases}$

same as $\eta(x) \rightarrow 1 - \eta(x)$.

Kawasaki: spin exchange or hopping is given by:

$$\begin{aligned} \eta(x), \eta(y) &\rightarrow \eta(y), \eta(x), & \underline{\eta} &\rightarrow \underline{\eta}^{x,y} \\ \sigma(x), \sigma(y) &\rightarrow \sigma(y), \sigma(x), & \underline{\sigma} &\rightarrow \underline{\sigma}^{x,y} \end{aligned}$$

with rate $c(x, y; \underline{\eta})$ or $c(x, y; \underline{\sigma})$. We can think of this as a particle “hopping” to an empty site or spin exchanges.

Master Equation

Stochastic dynamics give transition rates $K(\underline{\sigma}, \underline{\sigma}')$ for $\underline{\sigma}' \rightarrow \underline{\sigma}$. This leads to an evolution equation for the probability $\mu(\underline{\sigma}, t)$,

$$\begin{aligned}\frac{\partial \mu(\underline{\sigma}, t)}{\partial t} &= \sum_{\underline{\sigma}'} [K(\underline{\sigma}, \underline{\sigma}') \mu(\underline{\sigma}', t) - K(\underline{\sigma}', \underline{\sigma}) \mu(\underline{\sigma}, t)] \\ &= \mathcal{L} \mu\end{aligned}$$

for Glauber

$$\mathcal{L}_G \mu = - \sum_x c(x; \underline{\sigma}) \mu(\underline{\sigma}) + \sum_x c(x; \underline{\sigma}^x) \mu(\underline{\sigma}^x)$$

for Kawasaki

$$\mathcal{L}_K \mu = - \sum_{x,y} c(x, y; \underline{\sigma}) \mu(\underline{\sigma}) + \sum_{x,y} c(x, y; \underline{\sigma}^{x,y}) \mu(\underline{\sigma}^{x,y})$$

Stationary state, $\tilde{\mu}$

$$\frac{\partial \tilde{\mu}}{\partial t} = 0 = \mathcal{L} \tilde{\mu}$$

Detailed balance of dynamics wrt $\tilde{\mu}$ iff :

$$K(\underline{\sigma}, \underline{\sigma}') \tilde{\mu}(\underline{\sigma}') = K(\underline{\sigma}', \underline{\sigma}) \tilde{\mu}(\underline{\sigma}).$$

Historically the Glauber and Kawasaki rates were chosen to satisfy detailed balance wrt some Gibbs measure $\tilde{\mu}$, which describes the equilibrium state of the system:

$$\tilde{\mu} = \mu_{\text{eq}} = \exp[-\beta U(\underline{\sigma})].$$

Detailed balance then means,

$$\frac{c(x; \underline{\sigma})}{c(x; \underline{\sigma}^x)} = \exp\{-\beta[U(\underline{\sigma}^x) - U(\underline{\sigma})]\},$$

$$\frac{c(x, y; \underline{\sigma})}{c(x, y; \underline{\sigma}^{x,y})} = \exp\{-\beta[U(\underline{\sigma}^{x,y}) - U(\underline{\sigma})]\}.$$

Clearly, there are infinitely many rates satisfying detailed balance for the same $\tilde{\mu}$. If one is only interested in the properties of the stationary equilibrium state, which are obtained as time averages over the evolution, one uses whichever rate is more convenient to implement.

Dynamic (Nonequilibrium) Models

In non-equilibrium situations the stochastic model is what describes the phenomena to be studied. The transition rates will then not generally satisfy detailed balance wrt the stationary state. Some examples of that are:

Basic Voter Model

A voter at site $x \in \mathbb{Z}^d$ with two options, $\sigma(x) = \pm 1$, randomly chooses a neighbor and adopts the neighbors politics at a rate

$$c_v(x; \underline{\sigma}) = 1 - \sigma(x) \frac{1}{2d} \sum_{y: |y-x|=1} \sigma(y)$$

What are the stationary states:

For finite domain $\Lambda \subset \mathbb{Z}^d$? For all of $\mathbb{Z}^d$?

There are very many variations on this model.

Contact Process (epidemics)

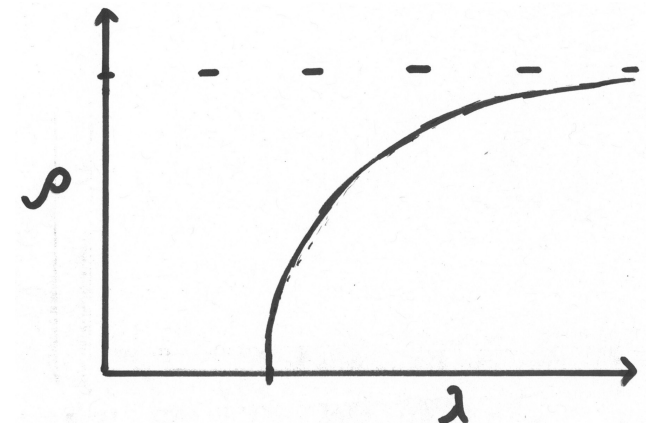
(SIS) Susceptible Infected Susceptible

An infected site ($\sigma(x) = 1$) gets cured at rate 1 and while infected it infects its neighbors at rate λ . This is a bit like the voter model with the probability that someone in the wrong party (infected) spontaneously sees the light. It has however only one (rather than two) absorbing states and a second order phase transition as λ is varied.

Stationary states ?

ρ = fraction of sites (probability of a given site being) infected. There is a phase transition at $\lambda_c = \lambda_c(d)$

Generalizations: SIRS, long range infection, etc.



Toom Model

A very interesting nonequilibrium model which exhibits a phase transition is the Toom model due to Andre Toom who developed it in 1980 while working at one of the USSR academy institutes.

The system consists of Ising spins located on the two-dimensional integer lattice, $\mathbb{Z}^2$, $\sigma_{ij} = \pm 1$. In this model the time evolution is done at discrete times, $t = 1, 2, \dots$. At each time step, all spins σ_{ij} are updated according to the rule

$$\sigma_{ij}(t+1) = \begin{cases} \text{sign}[\sigma_{i,j+1}(t) + \sigma_{i+1,j}(t) + \sigma_{ij}(t)] & \text{with prob. } 1 - p - q, \\ +1 & \text{with prob. } p, \\ -1 & \text{with prob. } q, \end{cases}$$

with $0 \leq p + q \leq 1$.

Such systems are generally referred to as probabilistic cellular automata but were called in the soviet literature Stavskaya systems.

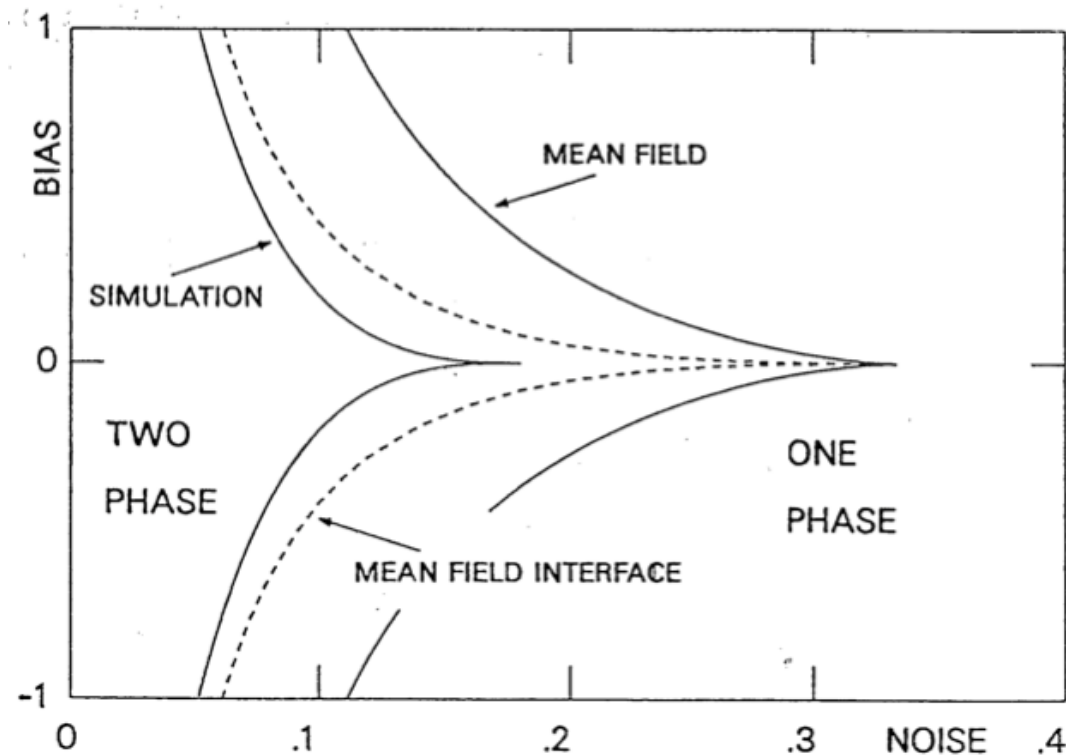
The parameters $p + q$ and $(p - q)/(p + q)$ are called *noise* and *bias*, respectively. For $p = q = 0$, the evolution is deterministic: each updated spin becomes equal to the majority of itself, its northern, and its eastern neighbor. Toom proved that for p and q sufficiently small (low noise), but otherwise unrestricted, there exist (at least) two stationary states, in which the spins are predominantly $+1$ or -1 , respectively. The proof uses the “eroder” property which comes from the spatial asymmetry of the process.

Eroder: Consider a lattice filled with $+$ spins enclosing a finite region of diameter R containing $-$ spins. In the absence of noise, this region will disappear in time R for the Toom Model

+	+	+	+
+	-	-	+
+	-	-	+
+	+	+	+

The existence of two phases at low noise levels is surely true but is not proven for the case when you take majority of self and the four nearest neighbors, and add a small noise $p = q$, “corresponding” to low temperature and zero magnetic field. The above picture would not change under this deterministic evolution.

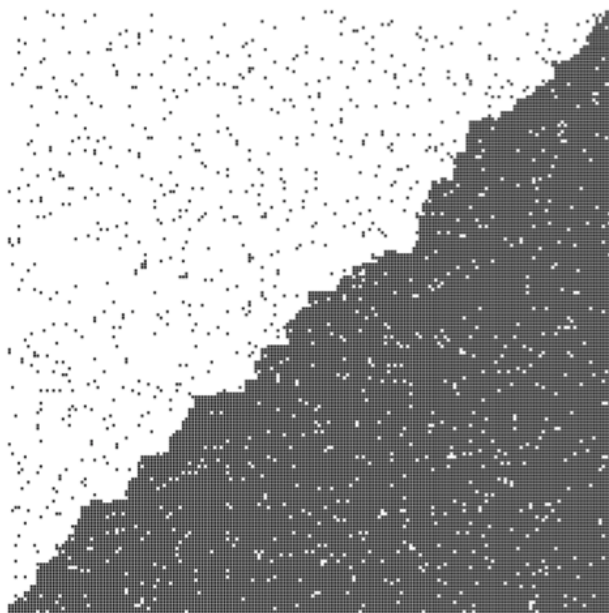
Phase Diagram of the Toom Model



Notice that the existence of two phases holds for small noise and all biases. This includes the case where the bias is 1 or -1, i.e. in the case when one of the states, all plus ones or all minus ones, is a trapping state. In that case, the transition is clearly first order.

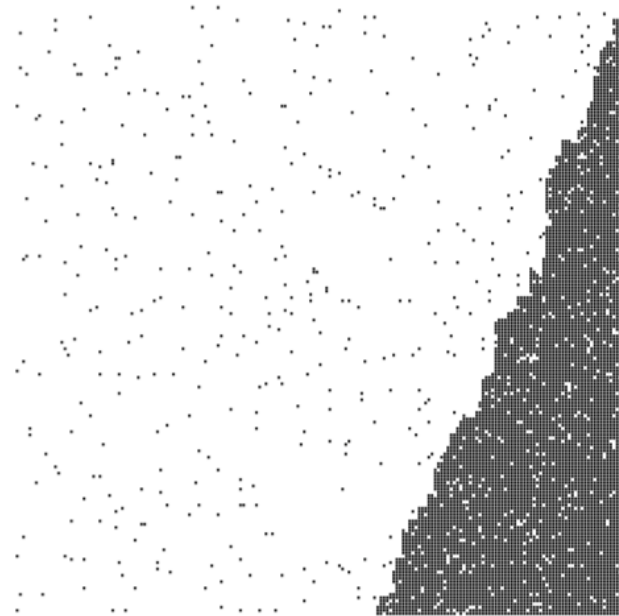
Derrida-L-Speer-Spohn Model

One can introduce a non-equilibrium interface between two low-noise phases by considering the system in the third quadrant only and imposing the following boundary conditions: $\sigma_{i0} = +1$ and $\sigma_{0i} = -1$ for all $i < 0$ and all t . That is, the spins are all fixed as $+1$ along the negative x -axis and -1 along the negative y -axis. The interface is anchored at the origin.



unbiased, $p = q = 0.02$

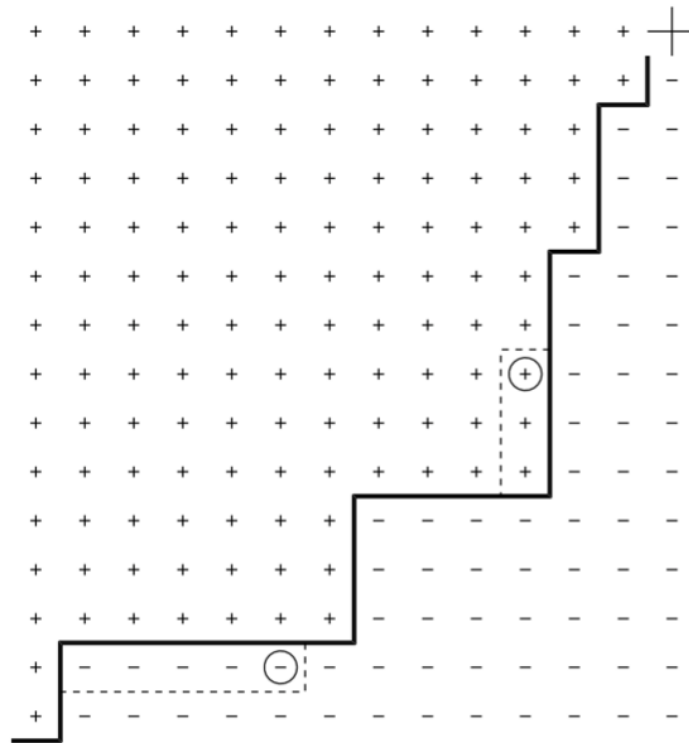
FIGURE 1a



biased, $p = 0.032$, $q = 0.008$

FIGURE 1b

At the zero-noise level ($p = q = 0$), the interface forms a staircase with all spins equal to $+1$ above the staircase and -1 below the staircase. All such staircases are stationary and can be represented as a sequence of spins $\{S_n : n \geq 1\}$ with $S_n = \pm 1$ where $+1$ represents a vertical edge and -1 a horizontal edge in the staircase.

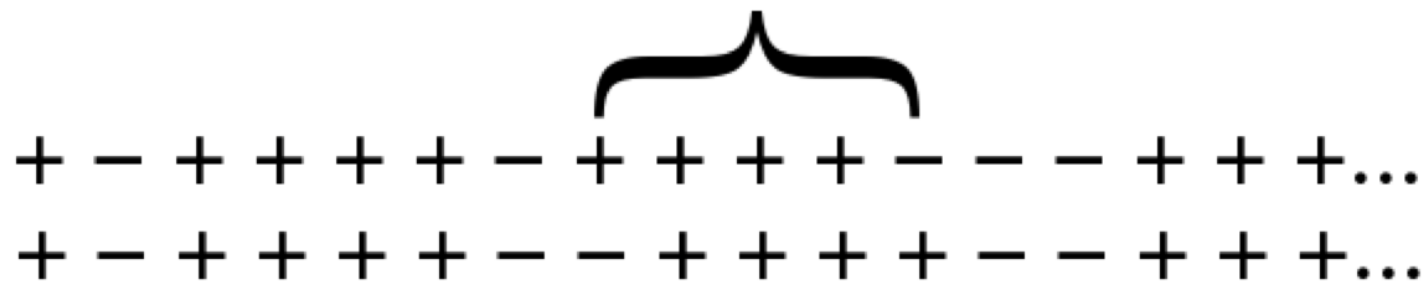


$$\underline{S} = (+ - + + + - + + + + + - - - - \dots)$$

Under the effect of noise there will be spin flips. When the noise is very weak flips away from the interface will have a very short life-time whereas flips adjacent to the interface will typically change the staircase rapidly to another staircase. The change of the interface is described by exchanging the spin S_n , which corresponds to the edge adjacent to the spin σ_{ij} flipped by noise, with the first spin following S_n which has a different value from S_n .

Spin Exchange Model on $\mathbb{Z}^+$ (joint work with Derrida, Speer and Spohn)

Under suitable scaling of noise and time, the time evolution of the interface can be represented by a continuous time Markov process on $\mathbb{Z}^+$ where a $+1$ (respectively, -1) is exchanged with the first -1 (respectively, $+1$) to its right at rate λ_+ (respectively, λ_-), with $\lambda_+/\lambda_- = q/p$, in the limit $q + p \rightarrow 0$.



The properties of the interface, such as average position and fluctuations, are then directly related to the stationary state of this spin exchange model.

Let me begin by noting a very interesting property of this system, inherited from the interface model.

Start with any initial state on $\mathbb{Z}^+$ in which there is a non-vanishing density of both $+$'s and $-$'s. Then consider the dynamics in the interval $[1, L]$ with the additional rule that if one picks a site j in the last block then one simply changes S_j to $-S_j$. A little thought then shows that

$$\mu_L(S_1, \dots, S_L) \equiv \mu(S_1, \dots, S_L)$$

where $\mu(S_{j_1}, \dots, S_{j_k})$ is simply the projection of the measure $\mu(\underline{S})$ on $\mathbb{Z}^+$, onto the spins at sites $\{j_i\}$. This reflects the fact that in the Toom model all the influences come from the North-East.

Consequently we can compute the projected measure exactly for “any” fixed L . In particular we have done this for the stationary measure μ_L , the focus of our attention from now on, for $L \leq 16$.

Thus, for the unbiased case, $\lambda_+ = \lambda_- = 1$,

$$\mu_1(+) = \mu_1(-) = \frac{1}{2},$$

$$\mu_2(+, +) = \mu_2(-, -) = \frac{1}{6}, \quad \mu_2(+, -) = \mu_2(-, +) = \frac{1}{3}.$$

One can also readily show that

$$\mu_k(\text{all } +) = \mu_k(\text{all } -) = \frac{1}{(k+1)!}$$

The quantity of primary interest is the variance of the magnetization which corresponds to the fluctuations in the position of the interface

$$V_L = \langle M_L^2 \rangle - \langle M_L \rangle^2 \quad \text{for} \quad M_L = \sum_{j=1}^L S_j.$$

It is clear from considerations of symmetry that for the unbiased model we are considering $\langle S_j \rangle = 0$, and thus $\langle M_L \rangle = 0$.

My first question is: How does V_L depend on L ? (A purse of \$200 for solution).

To give you a hint:

L	$\langle M_L^2 \rangle$ simulation	R_L	$\langle M_L^2 \rangle_{CV}$	$\sqrt{3L/2}$
2	4/3	3.00	1.33	1.73
4	1.920 ...	2.95	1.92	2.45
8	2.733 ...	3.00	2.76	3.46
16	3.890 ...	3.02	4.02	4.90
32	5.576 ± 0.002	3.03	5.88	6.92
64	8.02 ± 0.02	3.04	8.60	9.80
128	11.58 ± 0.03	3.05	12.53	13.86
256	16.76 ± 0.03	3.04	18.16	19.60
512	24.22 ± 0.04	3.04	26.19	27.71
1024	35.01 ± 0.03	3.05	37.60	39.19
2048	50.54 ± 0.09	3.03	53.78	55.43
4096	73.1 ± 0.1	3.04	76.69	78.38
8192	105.3 ± 0.2	3.05	109.1	110.9
16384	151.7 ± 0.4	3.02	155.0	156.8
65536	313 ± 1		311.7	313.5
131072	449 ± 1		441.6	443.4
262144	644 ± 4		625.3	627.7
524288	924 ± 3			886.1

$R_L = \langle M_L^4 \rangle / \langle M_L^2 \rangle^2$ obtained from simulation.

This is of course very different from the “standard” central limit theorem case where $V_L \sim bL$. In fact if one considers the same dynamics on the full $\mathbb{Z}$ then there is for any $m \in [-1, 1]$ a (presumably unique) translation invariant state which is Bernoulli with $\langle S_j \rangle = m$. On the circle all configurations with specified number of $+$ ’s have equal weight.

Please note also that the quantity $R_L = \langle M_L^4 \rangle / \langle M_L^2 \rangle^2$ is quite close to its Gaussian value of 3. The other two columns in the table give the results of the “collective variable approximation” or CVA which is asymptotic to a Gaussian with $V_L \sim \sqrt{3L/2}$. (I will come back to this later.)

The CVA is quite a good approximation which slightly underestimates V_L for large L . A better fit to the simulations is obtained by setting

$$V_L \sim c \sqrt{L} \log^\beta \left(\frac{L}{L_0} \right), \quad \beta \sim \frac{1}{4}.$$

The use of a logarithmic correction is suggested from studying the interface via a (modified) KPZ type equation

Speaking mathematically I do not know (despite various attempts over the years) of even a bound which would say that $V_L < cL$ for any c . The same is true also in the opposite direction: we do not have a proof that $V_L \rightarrow \infty$ as $L \rightarrow \infty$.

The CVA and the PDE

We note that the only moves which change the magnetization M_L are spin flips in the last block which ends with spin S_L . Let K_L be the number of sites in that block, i.e.

$S_j = S_{j+1} = \dots = S_L = -S_{j-1}$, with $j = L - K_L + 1$. Then the generator for any function $\phi(M_L)$

$$\begin{aligned}\mathcal{L}_L \phi(M_L) &= K_L(\underline{S}) [\phi(M_L - 2S_L) - \phi(M_L)] \\ &= K_L(\underline{S}) [\phi(M_{L-1} - S_L) - \phi(M_{L-1} + S_L)] \\ &= K_L(\underline{S}) S_L [\phi(M_{L-1} - 1) - \phi(M_{L-1} + 1)] \\ &= K_L(\underline{S}) S_L \Psi(M_{L-1}).\end{aligned}$$

In the stationary state $\langle K_L(\underline{S}) S_L \Psi(M_{L-1}) \rangle = 0$, for all Ψ .

The collective variable approximation which, as noted before, gives quite good results, is based on the following ansatz:

$$\langle S_{l+1} | K_l = k, M_l = m \rangle = \langle S_{l+1} | M_l = m \rangle.$$

When this is combined with various exact relations, valid in the stationary state, it leads to a recursive formula for $W_l(m)$, the probability that $M_l = m$.

For large values of l , assuming that $W_l(m)$ is slowly varying, one can write a scaling relation

$$W_l(m) \sim w(\varepsilon^4 l, \varepsilon m) \xrightarrow{\varepsilon \rightarrow 0} w(t, x),$$

with $w(t, x)$ satisfying the nonlinear fourth order equation

$$\frac{\partial}{\partial t} w(t, x) = -\frac{3}{8} \frac{\partial^2}{\partial x^2} \left[w \frac{\partial^2}{\partial x^2} (\log w) \right]$$

(DLSS)

The equation has a (relevant) solution

$$w_G(t, x) = \sqrt{2\pi\gamma(t)} \exp\left(-\frac{x^2}{2\gamma(t)}\right), \quad \gamma(t) = \sqrt{3t/2}.$$

This gives then, in this approximation

$$\langle M_l^2 \rangle_{CV} \sim \sqrt{\frac{3l}{2}},$$

in approximate agreement with the “leading order” numerical simulations.

The PDE for the symmetric case turned out to be of much interest in various other unrelated physical situations, e.g. thin liquid films and of all places in some quantum transport problems. It now goes under the name of DLSS equation. We (Bleher, L, Speer) proved global existence of positive solutions on the circle under some conditions. Others proved more.

The CVA for the biased case leads in the scaling limit with $W_l(m) \sim w(\varepsilon^3 l, \varepsilon(m - \mu l))$ to the equation

$$\frac{\partial}{\partial t} w(t, x) = A \left[\frac{4}{3} \frac{\partial^3}{\partial x^3} w - \frac{\partial}{\partial x} \left(\frac{\left(\frac{\partial}{\partial x} w \right)^2}{w} \right) \right],$$

with A a known constant. This equation yields the result

$$V_L \sim cL^{3/2},$$

“in agreement” with KPZ and simulations.

Microscopic Dynamics to Macroscopic Equations

The formal way of going from a microscopic time evolution to a macroscopic one is via the rescaling of space and time. Let me illustrate this in the simplest example: the so called simple exclusion process (SEP). The dynamics of this model is of the Kawasaki exchange type and thus conserves particle number.

The Simple Exclusion Process

In $d = 1$, the microscopic configuration is specified by η :

$$\underline{\eta} = \{\eta(i)\} \quad \eta(i) = \{0, 1\}, \quad i \in \mathbb{Z}.$$

With nearest neighbor jumps, particles attempt to jump to the neighboring site on right with rate 1 and to the left with rate $q \leq 1$: they succeed if the site on which they attempt to jump is empty, otherwise nothing happens.

For M particles on L sites, with periodic b.c., all $\binom{L}{M}$ configurations have equal weight in the stationary state.

For $q = 1$, SSEP, symmetric SEP, the dynamics satisfies *detailed balance* with respect to the stationary measure.

For $q < 1$, ASEP, asymmetric SEP, the dynamics doesn't satisfy detailed balance with respect to stationary measure.

For both SSEP and ASEP all stationary translation invariant measures on $\mathbb{Z}$ are (superpositions of) Bernoulli or product measures with density $r \in [0, 1]$, $\text{prob}\{\eta(i) = 1\} = r$. Also true for $\mathbb{Z}^d$, $d > 1$, and more general jumps.

Hydrodynamical Scaling of SEP

$i \rightarrow x/\epsilon$, $s = t/\epsilon^\alpha$, x and t are macroscopic space and time scales, while i and s are the microscopic time variables.

Starting with initial configuration (or measure) on a system with L sites, whose density profile converges to $\rho_0(x)$, when $L \rightarrow \infty$,

$$\frac{1}{(b-a)L} \sum_{i=aL}^{bL} \eta(i) \rightarrow \int_a^b \rho_0(x) dx, \quad L = \epsilon^{-1}$$

The density profile $\rho(x, t)$ will then evolve in time according to a deterministic macroscopic equation:

$$\frac{\partial \rho(x, t)}{\partial t} = F(\{\rho\}), \quad \rho(x, 0) = \rho_0(x)$$

i.e.

$$\frac{1}{(b-a)L} \sum_{i=aL}^{bL} \eta(t/\epsilon^\alpha) \rightarrow \int_a^b \rho(x, t) dx.$$

Also true for $\mathbb{Z}^d$.

Euler Scaling, $\alpha = 1$

For $q < 1$ ASEP, $\alpha = 1$

$$\frac{\partial \rho(x, t)}{\partial t} + (1 - q) \frac{\partial}{\partial x} [\rho(1 - \rho)] = 0$$

Burger's Equation.

Diffusive Scaling, $\alpha = 2$

For $q = 1$, SSEP, “nothing” happens “on macroscopic scale” for times of order ϵ^{-1} . If, however, one waits for macroscopic times of order ϵ^{-2} one gets diffusive behavior

$$\frac{\partial \rho}{\partial t} = \frac{1}{2} \frac{\partial}{\partial x} [D(\rho) \frac{\partial \rho}{\partial x}]; \quad D = 1 \quad \text{for} \quad \text{SSEP}$$

For $q = 1 - \lambda\epsilon$, WASEP, and $\alpha = 2$: one gets the viscous Burger's equation

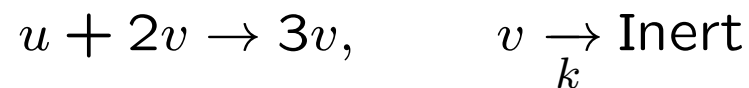
$$\frac{\partial \rho(x, t)}{\partial t} + \lambda \frac{\partial}{\partial x} \rho(1 - \rho) = \frac{\partial^2 \rho}{\partial x^2}$$

Reaction-Diffusion Equation (RDE)

Let me mention now briefly some old and current work on the derivation of RDE from stochastic lattice models with both Glauber (reaction) and Kawasaki (diffusion) dynamics. An example of a RDE involving two species, with densities $u(x, t)$ and $v(x, t)$, is the well known (to some) Gray-Scott model

$$\begin{aligned}\frac{\partial u(x, t)}{\partial t} &= D_u \nabla^2 u - uv^2 + F(1 - u), \\ \frac{\partial v(x, t)}{\partial t} &= D_v \nabla^2 v + uv^2 - (F + k)v, \quad D_u > D_v\end{aligned}$$

where D_u and D_v are diffusion constants and the chemical reactions are



and F is some inflow/outflow rate to/from the system.

These equations which were derived to model an idealized form of some chemical reactions incorporate the “law of mass action”. One imagines that the “chemical tank” in which the reaction takes place is constantly stirred so that there are no correlations between the positions of the reacting molecules.

We model this on a lattice by having a particle hop very rapidly to neighboring empty sites as in a symmetric simple exclusion process (SSEP) and undergoing reactions, being created or annihilated, at rates which depend on its surrounding.

Formally the generator of the evolution (for a single species) in which $\eta(i) = 1, 0$ is given by

$$\mathcal{L} = \varepsilon^{-2} \mathcal{L}_K + \mathcal{L}_G.$$

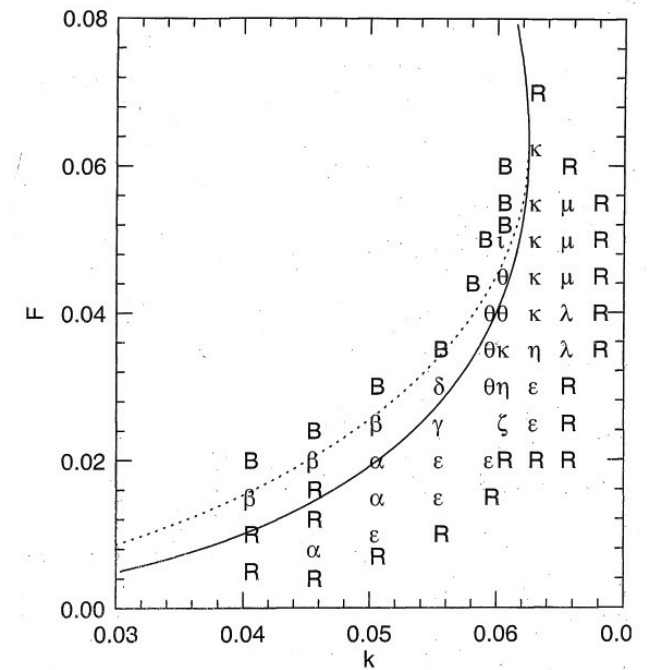
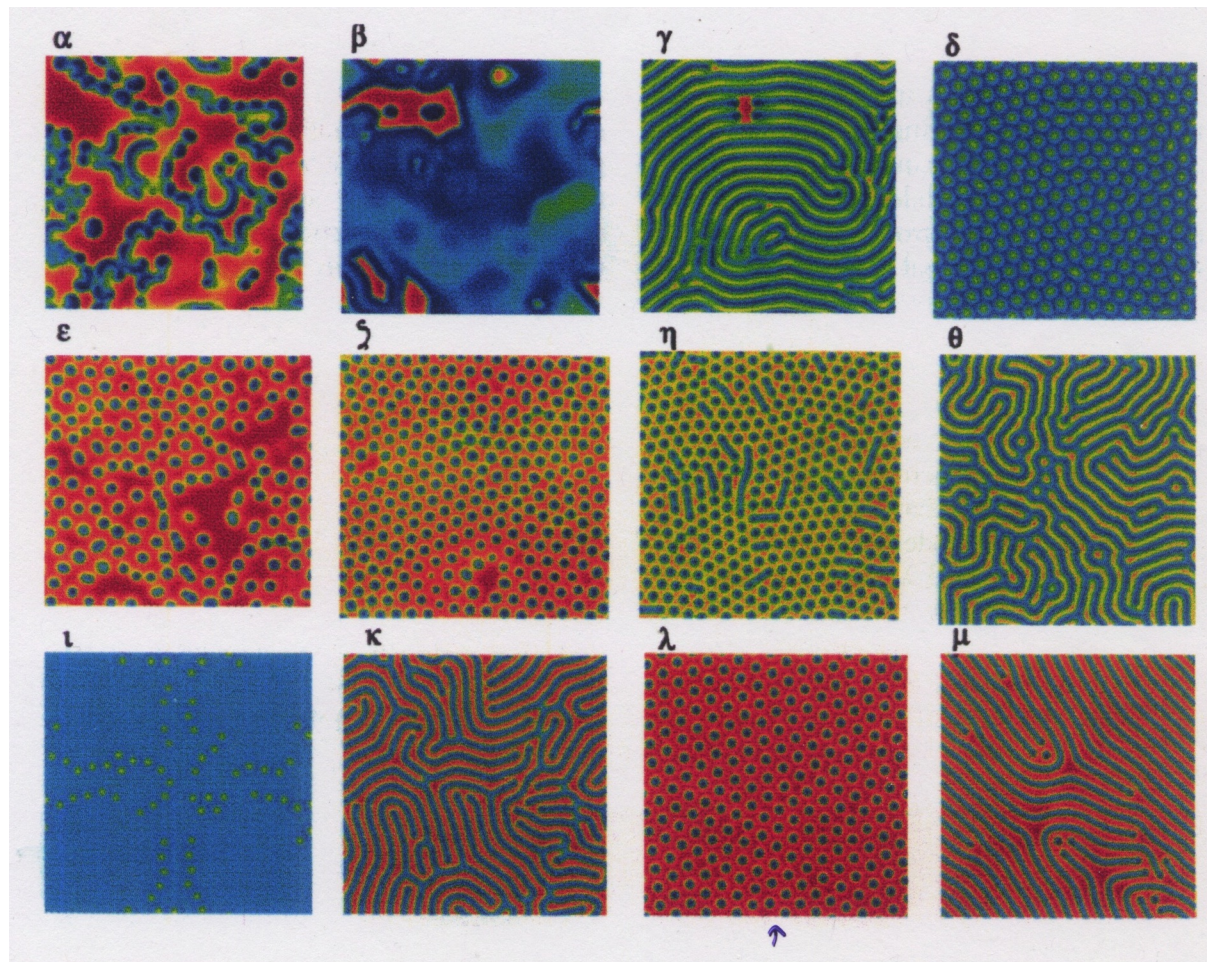
Then scaling space by ε , i.e. making the lattice spacing equal to ε , we rigorously obtain when $\varepsilon \rightarrow 0$, a RDE of the form

$$\frac{\partial \rho(x, t)}{\partial t} = D \nabla^2 \rho(x, t) + \mathcal{P}(\rho(x, t)),$$

where $\mathcal{P}(\rho)$ is a polynomial in ρ .

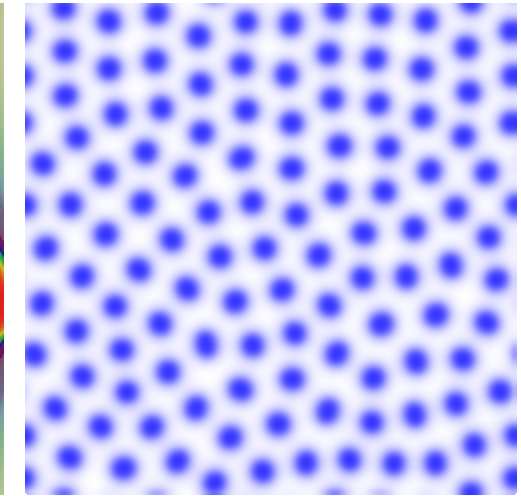
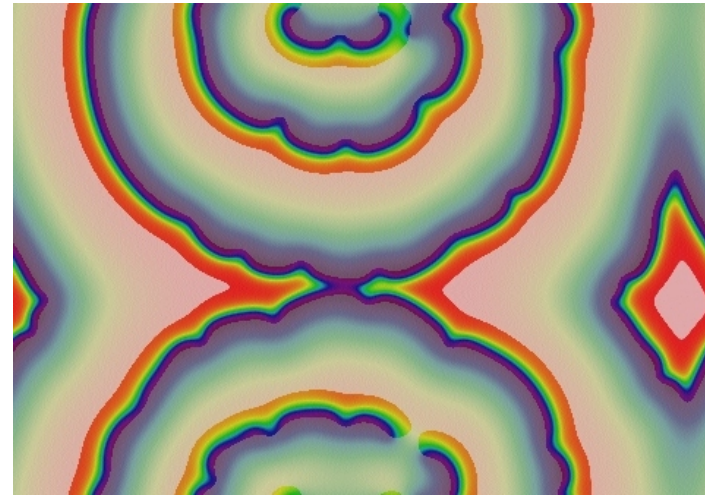
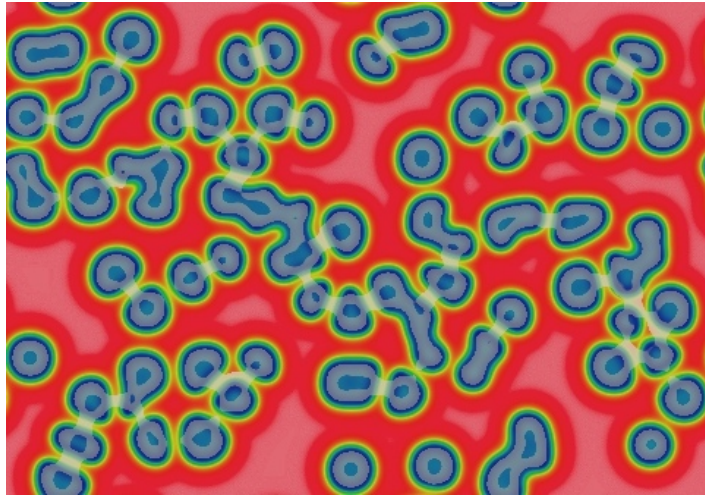
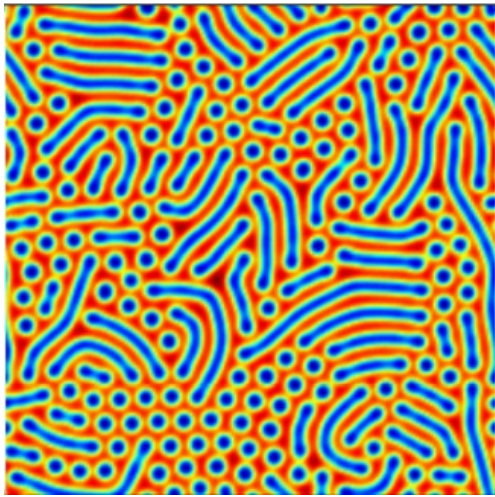
The analysis is similar for modeling multispecies RDE such as the Gray-Scott one. There we permit at most one particle of each species per site.

Full disclosure: we have to twist a bit those equations to get them in our form but this does not seem to change the nature of the solutions, pictures of which I will now show you.



$$D_u = 2 \times 10^{-5}, \quad D_v = 10^{-5}, \quad F \in [.02, .06], \quad k \in [.04, .06].$$

Initial condition $u = 1, v = 0$ except in a small square in the middle where $u = \frac{1}{2}, v = \frac{1}{4}$.



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