

# Mathematical Physics and the Microscopic Origin of Macroscopic Behavior

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## Abstract

“Mathematical physics is the discipline of people who try to reach a deep understanding of physical phenomena by following the rigorous style and method of mathematics.” This is a quote from Freeman Dyson which captures the spirit of the discipline.

My own area of mathematical physics is statistical mechanics which is concerned with the microscopic origin of macroscopic behavior. I will discuss the mathematical framework which statistical mechanics provides for explaining how the laws governing the microscopic constituents of matter, the atoms, determine the behavior of macroscopic systems involving very many atoms.

- ① Statistical Mechanics: An Overview
  - ① Hierarchical nature of the world
  - ② Simple microscopic laws, complex macroscopic cooperative behavior: phase transitions
- ② Equilibrium states: a beautiful theory
  - ① Gibbs ensembles
  - ② Phase diagrams
- ③ Nonequilibrium states
  - ① Approach to Equilibrium
  - ② Dynamical phase transitions
  - ③ Hydrodynamic equations

Nature has a hierarchical structure, with time, length and energy scales ranging from the sub-microscopic to the supergalactic. Surprisingly, it is possible, and in many cases essential, to discuss these levels independently — quarks are irrelevant for understanding protein folding and atoms are a distraction when studying ocean currents. Nevertheless, it is a central lesson of science, as developed in the past five hundred years, that there are no new fundamental laws, only new phenomena, as one goes up the hierarchy. Explanations are therefore always to be looked for in the smaller scales.

In some cases this is fairly straightforward — at least on the conceptual level — stars form galaxies because of the gravitational attraction between them, protons and electrons form atoms because of the electrical attractions between them (in the framework of quantum mechanics). In other cases — such as molecules forming human brains with the property of consciousness and ability to formulate “explanations” —our understanding is still quite minimal at present.

Going beyond the conceptual, the quantitative study of the microscopic origin of macroscopic behavior is the subject of statistical mechanics. Fortunately, many striking features of macroscopic systems can be obtained from simplified microscopic models.

We therefore often take as our lowest level starting point Feynman's description of atoms as "little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another." This crude classical picture (a refined version of that held by some ancient greek philosophers) gives predictions which are, in many cases, not only qualitatively correct but also quantitatively accurate.

Using this starting point statistical mechanics combines physical insight with beautiful mathematics to connect the macroscopic to the microscopic.

## Microscopic: Equilibrium Gibbs Ensembles

To compute the equilibrium properties of a macroscopic system of  $N$  particles,  $N \gg 1$ , in a domain  $\Lambda \subset \mathbb{R}^d$ , statistical mechanics uses probability distributions (ensembles) over different microscopic states  $X = (\mathbf{r}_1, \mathbf{p}_1, \dots, \mathbf{r}_N, \mathbf{p}_N)$ ,  $\mathbf{r}_i \in \Lambda$ ,  $\mathbf{p}_i \in \mathbb{R}^d$ . Given the system's Hamiltonian

$$H(X) = \sum \mathbf{p}_i^2 / 2m + \sum v(r_{ij})$$

in “equilibrium” at temperature  $T$ , the probability of being in a phase space region  $dX$  is given by the canonical ensemble

$$\mu(dX) = Z^{-1} e^{-\beta H(X)} dX, \quad \beta = (kT)^{-1},$$
$$Z = \frac{1}{N!} (2\pi m / \hbar \beta)^{dN/2} \int_{\Lambda} \dots \int e^{-\beta \sum v(r_{ij})} d\mathbf{r}_1 \dots d\mathbf{r}_N.$$

$Z$  is a normalization factor taking into account the symmetry and the appropriate units coming from the classical limits of quantum mechanics.

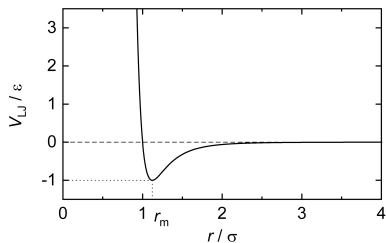


Figure 1: Lennard-Jones potential.

Connection between microscopic and macroscopic becomes precise in the thermodynamic limit,  $N \rightarrow \infty$ ,  $|\Lambda| \rightarrow \infty$ ,  $N/|\Lambda| \rightarrow \rho$ ,  $|\Lambda| =$  volume of  $\Lambda$ ,

$$f(\rho, T) = -kT \lim\{[\log Z(\beta, N, \Lambda)]/|\Lambda|\}.$$

$f(\rho, T)$  is the thermodynamic free energy per unit volume from which one can compute many properties of equilibrium systems.

Theorem: (van Hove, Ruelle, Fischer, ...) This limit exists and  $f(\rho, T)$  is convex in  $\rho$ , etc. under some general assumptions on  $v(r)$  e.g.  $v(r) \geq C/r^{d+\varepsilon}$  for  $r < R$  and  $|v(r)| \leq K/r^{d+\varepsilon}$  for  $r > R$ .

For neutral systems with Coulomb interactions, which decay as  $1/r$  the result (for quantum systems) was proven by Lebowitz and Lieb in 1968.

It is sometimes simpler to consider the consider the “equivalent” grand canonical ensemble where instead of fixing  $N$  we consider different possible  $N$ 's in  $\Lambda$  with probabilities

$$W(N, \Lambda, T; \lambda) = e^{\lambda\beta N} Z(\beta, N, \Lambda) / \sum_{N=0}^{\infty} e^{+\beta\lambda N} Z(\beta, N, \Lambda),$$

where  $\lambda$  is the chemical potential, and

$$p(\lambda, T) = kT \lim_{|\Lambda| \rightarrow \infty} \left\{ \frac{1}{|\Lambda|} \log \sum e^{-\beta\lambda N} Z(\beta, N, \Lambda) \right\},$$

is the pressure of the system.

## 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 parameters at which two pure phases can coexist. At the triple point, the system can coexist in any of three pure phases.

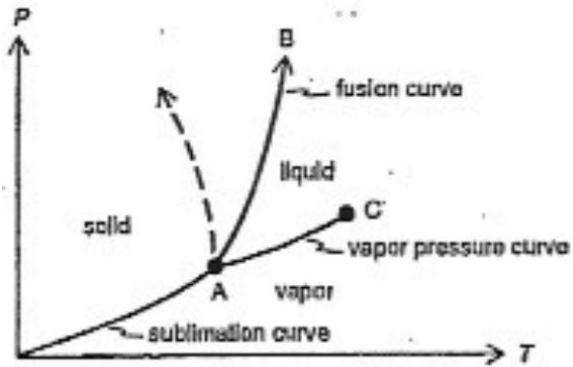


Figure 2: Coexistence curves for a typical pure PVT system: point A is the triple point and point C is the critical point. The dashed line is an example of a fusion curve with negative slope.

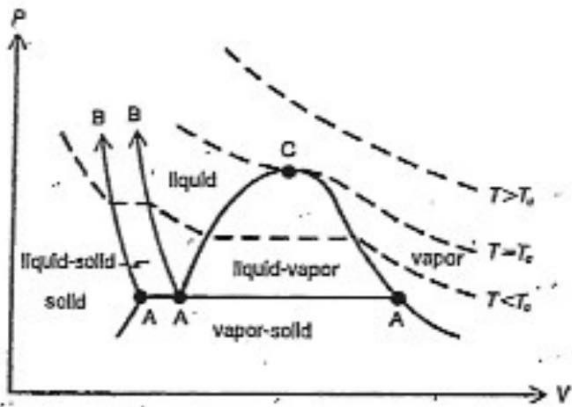


Figure 3: A plot of the coexistence regions for a typical PVT system; all the phase transitions are first order; the dashed lines represent isotherms.

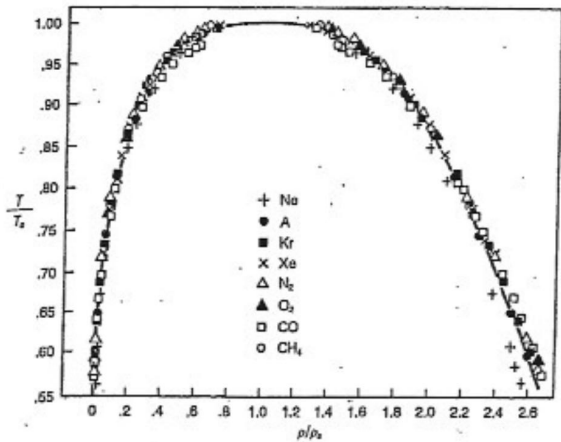


Figure 4: Experimental vapor-liquid coexistence curve for a variety of substances: the plot is of reduced temperature versus reduced density. Here  $\rho - \rho_c \sim (1 - T/T_c)^{0.326}$ .

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. On the other hand, when one moves between two points in the thermodynamic parameter space along a path which does not intersect any coexistence line the properties of the system change smoothly.

How do we connect these discontinuities in the macroscopic properties with the behavior of the microscopic entities, which do not change in such a transition? An argon atom in the vapor is the same as in the liquid.

This is an example of “emergent” collective phenomena.

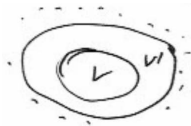
## Emergent Phenomena

In general, a macroscopic system with a given Hamiltonian 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.

One gets these different phases by considering the infinite volume limit with different “boundary conditions”. The coexisting phases all have the same pressure and free energy.

Formal mathematics of infinite volume Gibbs measures: boundary conditions Dobrushin-Lanford-Ruelle eqs.

This is essentially a Markov type characterization



**Figure 5:** A visualization of a Markov type characterization with  $(V \cup V')^c = V''$ .

$\text{Prob}(X_V | X_{V'}, X_{V''}) = Z^{-1}(X_{V'}) \exp[-\Phi(X_V \cup X_{V'}) - \Phi(X_{V'})]$ , for potential  $\Phi$ , approximately independent of  $X_{V''}$  when  $V'$  is 'sufficiently large'. Phase transitions correspond to non uniqueness of solutions to the DLR equations for defining an infinite volume measure.

# Lattice Systems

How can we prove the existence of phase transitions for a system with a given Hamiltonian?

This is generally a very difficult and mostly open problem. We can do better if we simplify the model system further by considering instead of continuous position of the particles,  $\mathbf{r} \in \mathbb{R}^d$ , we consider instead the lattice  $\mathbb{Z}^d$  and set  $\eta(\mathbf{x}) = 1$  if site  $\mathbf{x} \in \mathbb{Z}^d$  is occupied by a particle and  $\eta(\mathbf{x}) = 0$  if site  $\mathbf{x}$  is empty. One can think of dividing up  $\Lambda \in \mathbb{R}^d$  into small cells each of which is either occupied or empty forgetting about momentum.

Setting  $\sigma(\mathbf{x}) = 2\eta(\mathbf{x}) - 1 = \pm 1$  one gets an Ising spin system. This can represent a crystal in which the atoms have spins which can point “up or down”.

The best understood system exhibiting a phase transition is the Ising model with ferromagnetic pair interaction

$$U(\sigma) = - \sum J(i-j)\sigma(i)\sigma(j) - h \sum \sigma(i),$$
$$J(i-j) \geq 0, \quad i \in \mathbb{Z}^d.$$

The phase diagram of the system in the  $T - h$  plane is

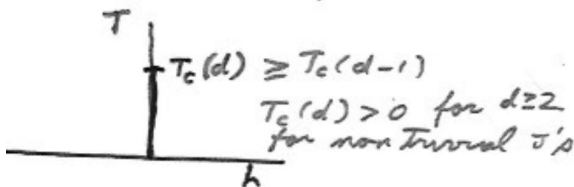


Figure 6: Ferromagnetic pair interaction system phase transition.



**Figure 7:** Ferromagnetic pair interaction system phase transition hysteresis curve. The vertical axis is the magnetization,  $\langle \sigma_0 \rangle$ .

The free energy and all correction functions are analytic functions of  $T$  and  $h$  (in fact of the  $J$ 's) whenever  $h \neq 0$  and for  $h = 0$  at high temperature (in fact) for  $T > T_c$  the critical temperature for spontaneous magnetization.

Our detailed knowledge about this system is based: (i) on the Lee-Yang theorem about the location of zeros of the partition function in the complex  $z = e^{i\beta h}$  plane: they all lie on the circle  $|z| = 1$ , (ii) on various inequalities, GKS, FKG, . . . .

In 1944 Onsager solved exactly the nearest neighbor Ising model in two dimensions with energy  $H(\sigma) = U$ ,

$$\beta U = -K_1 \sum_{x \in \mathbb{Z}^2} \sigma(x)\sigma(x + e_1) - K_2 \sum_{x \in \mathbb{Z}^2} \sigma(x)\sigma(x + e_2) - h \sum_{x \in \mathbb{Z}^2} \sigma(x),$$
$$x \in \mathbb{Z}^2, \quad \sigma(x) = \pm 1.$$

He found a critical temperature  $\sinh K_x^c \sinh K_y^c = 1$ ,  $h = 0$ .

In some recent work with David Ruelle we have been able to extend these results to Ising systems with multi-spin interactions. As an example consider the square lattice with four spin interactions on alternate squares all pairs all four spins on the alternate squares.



Figure 8: Multi-spin system interactions.

$$U = -J_2 \sum_{i,j} \sigma(i)\sigma(j) - J_4 \sum_{i,j} \sigma(i)\sigma(j)\sigma(k)\sigma(l)$$

For this system with  $J_4 \geq 0$  the only phase transitions can occur at  $h = 0$ . In fact, for  $J_2 > 0$  a phase transition will occur at low temperature while for  $J_2 \leq 0$  there is no phase transition at any temperature. The proof is based on Ruelle's extension of the Lee-Yang circle theorem for multi-spin interactions at low temperatures and on the GKS inequalities. For  $J_4 > 0$  the Lee-Yang theorem does not hold at higher temperature but one then shows that the zeros stay away from the positive  $z$ -axis, i.e.  $z \geq 0$ .

There are no results of that type 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 symmetric mixture of species 1 and 2

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

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

# Open Problem

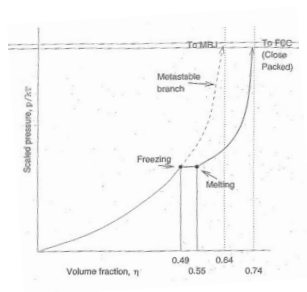


Figure 9: Phase diagram of one component hard sphere system with diameter  $d$  in 3 dimensions (no proof).

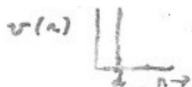


Figure 10: Phase diagram of hard spheres (balls) of volume 1.

## Time evolution of isolated macroscopic systems

Using a macroscopic description in terms of hydrodynamic density profiles of locally conserved quantities,  $\xi_X(\mathbf{x}) = (n(\mathbf{x}), \mathbf{u}(\mathbf{x}), e(\mathbf{x}))$ ,  $\mathbf{x} \in V$ . 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 longer time and space scales, than the microscopic dynamics

On these scales one can expect (hope) that the description of their evolution will be given 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.

To actually carry out this scaling rigorously is unfortunately beyond our mathematical abilities. To make progress we have to resort to stochastic dynamics. These are, with few exceptions, the only dynamics for which we are currently able to derive such macroscopic equations. These dynamics (probably) mimic many aspects of the chaotic deterministic classical Hamiltonian dynamics (and also that of quantum systems).

Before going on to describe such a derivation of macroscopic equations I will give a general overview of stochastic dynamics for lattice systems, which are simpler to analyze than continuum systems. Along the way I will discuss some models the dynamics and stationary states of which are of independent interest.

## 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:

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

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.

## Stochastic models not satisfying detailed balance

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

### Basic Voter Model

A voter at site  $x \in \mathbb{Z}^d$  with two options, represented by  $\sigma(x) = \pm 1$ , 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  $\mathbb{Z}^d$ ?

The latter depends strongly on  $d$ .

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  $\lambda$ . 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  $\lambda$  is varied.

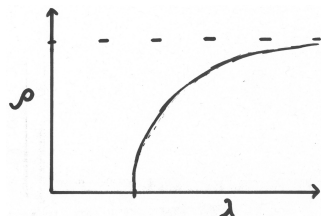
Stationary states ?

$\rho$  = 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 probabilistic cellular automaton

A very interesting nonequilibrium model which exhibits a phase transition, without having any absorbing states, is the Toom model due to Andre Toom.

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  $\sigma_{ij}$  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  $0 \leq p + q \leq 1$ .

## Stochastic Dynamics: Simple Exclusion Process

In  $d = 1$ , with nearest neighbor jumps

$$\tau = \{\tau_i\}, \quad \tau_i = \{0, 1\}, \quad i \in \mathbb{Z}.$$

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 site on which the attempt to jump is empty, otherwise nothing happens. All stationary translation invariant measures on  $\mathbb{Z}$  are (superpositions) of Bernoulli or product measures with density  $r \in [0, 1]$ ,  $\text{prob}\{\tau_i = 1\} = r$ .

Also true for  $\mathbb{Z}^d$ ,  $d > 1$ , and more general jumps.

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

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

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

## Hydrodynamical Scaling of SEP

$i \rightarrow x/\epsilon$ ,  $s = t/\epsilon^\alpha$ ,  $x$  and  $t$  are macroscopic space and time scales, while  $i \in \mathbb{Z}$  and  $s$  is the microscopic time variable.

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

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

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.

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

For  $q < 1$  ASEP: set  $\alpha = 1$ , then

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

Burger's Equation.

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

$$\frac{\partial \rho}{\partial t} + \frac{1}{2} \frac{\partial}{\partial x} \left[ D(\rho) \frac{\partial \rho}{\partial x} \right] = 0, \quad D = 1, \quad \text{for SSEP.}$$

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

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