



# Stochastic approaches to out-of-equilibrium dynamics

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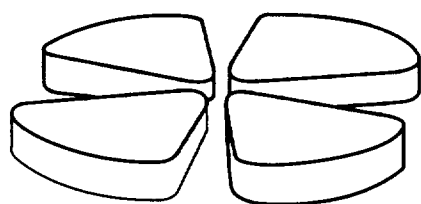
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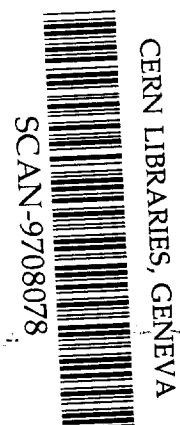


## Stochastic Approaches to Out-of-Equilibrium Dynamics

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*Cours*

# **Stochastic Approaches to Out-of-Equilibrium Dynamics**

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**Abstract:**

In these lectures we summarise several approaches to describe out of equilibrium systems. Using variational principle either for wave functions or for density matrices we derive generalised mean-field approaches as Ehrenfest equations for a set of observables. With the help of projection methods we reinterpret these mean-field approaches in order to justify the stochastic extensions of these theories. In this derivation we emphasise the physical importance of the observables and of the result of the measurement : the observation.

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## I) Introduction

In these lectures we present an overview of several statistical descriptions of out of equilibrium processes. We have restricted our-selves to variationnal approaches and projection methods in order to derive dynamical equations for observations. Because of the lack of time and space we have not discussed nor Heisenberg picture for the dynamics of observable neither methods based on Greens functions. These classical methods can be found in many text books.

In these lectures we have concentrate our efforts to describe results of observations performed at a time  $t$ . This is based on the fact that a physical theory should be a tool to predict results of measurements performed on a wide ensemble of systems always prepared in the same way. This means that we can measure any ensemble of observables "simultaneously", even non commuting observables. The point is that non-commuting observables should be measured at the same time but for different events or ensemble of events.

The goal of the descriptions we will summarised in these lectures is to follow in time the evolution of the observation of few important observables. The main problem we will face is that most of the time the information we are able to control (prepare and measure) is not enough or even is much to small compared with a full description of the system which often require an infinite number of observations. Therefore the disregarded information will strongly influence the dynamics of the pertinent degrees of freedom not only in a deterministic way by making the whole dynamics non linear but also in a stochastic way the unknown observation introducing some random terms in the evolution.

## II) Variationnal evolution of wave functions, coherent states and generalised stochastic mean field approaches

The first method to face the problem of the description of static as well as dynamical properties of a complex system is to try to solve the Schrödinger equation in an approximate way since an exact solution is in general impossible. The first idea one can get is therefore to construct an approximate wave function in order to describe the system. Then in order to obtained either a good approximation for the ground-state or for the dynamical evolution the safer way is to use a variationnal principle. This is the approach we will follow in this first chapter.

### II.1) Coherent states and trial wave functions

In variationnal methods the first step is to define an ensemble of wave functions which will allow us to describe the system. Let me introduce a general parametrised wave function

$$|\psi\rangle = |\psi(\mathbf{Z})\rangle \quad (\text{II.1})$$

where  $\mathbf{Z} \equiv \{Z_i\}$  are an ensemble of real parameters. In principle, these trial wave functions can be whatever we like. In particular they can be some specific functions such as for example gaussian wave packets.

Often, trial wave functions are generalised coherent states

$$|\psi(\mathbf{Z})\rangle = \hat{R}(\mathbf{Z})|\psi(\mathbf{0})\rangle = \exp(i \mathbf{Z} \cdot \hat{\mathbf{A}})|\psi(\mathbf{0})\rangle \quad (\text{II.2})$$

where  $\hat{R}(\mathbf{Z})$  is an element of a Lie group of unitary transformations associated with the Lie algebra constructed using the set generators  $\hat{A} \equiv \{\hat{A}_\ell\}$ . The state  $|\psi(0)\rangle$  is most of the time a simple state of an irreducible representation of the considered group. In such a case one can use group theory tools to solve the variational problem.

In this framework it is often useful to introduce the transformed operators

$$\hat{O}(\mathbf{Z}) = \hat{R}(\mathbf{Z}) \hat{O} \hat{R}^{-1}(\mathbf{Z}) \quad (\text{II.3})$$

because then the average value of any operator  $\hat{O}$  can be obtained as an average value of the operator  $\hat{O}(\mathbf{Z})$  on the state  $|\psi(0)\rangle$

$$\langle \hat{O} \rangle_{\mathbf{Z}} \equiv \langle \psi(\mathbf{Z}) | \hat{O} | \psi(\mathbf{Z}) \rangle = \langle \psi(0) | \hat{O}(\mathbf{Z}) | \psi(0) \rangle$$

On the other hand, it should be noticed that the variable  $\mathbf{Z}$  defining the coherent states are entirely defined by the expectation value of the infinitesimal generators of the group:

$$\langle \hat{A}_\ell \rangle_{\mathbf{Z}} = \langle \psi(\mathbf{Z}) | \hat{A}_\ell | \psi(\mathbf{Z}) \rangle \quad (\text{II.4})$$

Using the relation (II.3) this mean-value can be related to an average value over the initial state  $|\psi(0)\rangle$

$$\langle \hat{A}_\ell \rangle_{\mathbf{Z}} = \langle \psi(0) | \hat{A}_\ell(\mathbf{Z}) | \psi(0) \rangle \quad (\text{II.5})$$

It should be noticed that then any observation  $\langle \hat{O} \rangle_{\mathbf{Z}}$  can thus be seen as a function of the average values  $\langle \hat{A}_\ell \rangle_{\mathbf{Z}}$

$$\langle \hat{O} \rangle_{\mathbf{Z}} = \mathcal{O}(\langle \hat{A}_\ell \rangle_{\mathbf{Z}})$$

In all these cases the problem of finding the static solution reduces to the selection of the best set of  $\mathbf{Z}$  or in an equivalent way in the cases of coherent states to define the best expectation values  $\langle \hat{A}_\ell \rangle_{\mathbf{Z}}$ .

On the other hand, the dynamical problem is the definition of the trajectory  $\mathbf{Z}(t)$  (or  $\langle \hat{A} \rangle(t)$ ). One should then stress that whatever we started with a quantum mechanical problem we end up with a classical problem concerning the trajectory of a point in the parameter space  $\mathbf{Z}$  (or the observation space  $\langle \hat{A} \rangle$ ). Therefore the introduction of a parametrised wave-function  $|\psi(\mathbf{Z})\rangle$  must always be viewed as a classical approach in a very general sense of course. Therefore, we must always ask about the need of a requantification of the whole theory.

## II.2) Variational methods

Let us now study the static and dynamical properties of the considered system. To describe it, we need to define its hamiltonian operator; we will call it  $\hat{H}$ . Then, the parameters  $\mathbf{Z}$  of the wave functions  $|\psi(\mathbf{Z})\rangle$  describing either the ground state (or equilibrium states) or the dynamical evolution of a system can be obtained using variational methods.

### II.2.A) Ground state wave functions

For example if we want to define the ground state of a system we can minimize its energy

$$E(\mathbf{Z}) = \langle \hat{H} \rangle_{\mathbf{Z}} = \langle \psi(\mathbf{Z}) | \hat{H} | \psi(\mathbf{Z}) \rangle \quad (\text{II.6})$$

in the space of the parametrised wave functions discussed above. This minimisation of  $E(\mathbf{Z})$  defines the best parameters  $\mathbf{Z}$  which give the best description of the ground state. Of course in the case of the generalised coherent states this condition can be transformed as a condition on the expectation values  $\langle \hat{A}_i \rangle_{\mathbf{Z}}$  using relation (II.4).

### II.2.B) Variational principle for the dynamics

If we now want to address the problem of the evolution of the system we will rather introduce a variational formulation of the Schrödinger equation

$$i \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle \quad (\text{II.7})$$

using an integral along a given trajectory

$$I[\psi] = \int_{t_0}^{t_1} dt \langle \psi | i \frac{\partial}{\partial t} - \hat{H} | \psi \rangle \quad (\text{II.8})$$

completed with a boundary condition defining the states of the system at  $t=t_0$ . The equivalence between the Schrödinger equation (II.7) and the variational expression (II.8) can be easily demonstrated. Indeed, let me first introduce a continuous or discrete basis of the Hilbert space:  $|i\rangle$ . Then (II.8) reads

$$I[\psi] = \int_0^1 dt \sum_{ij} \psi_i^* \left( i \dot{\psi}_i - \hat{H}_{ij} \psi_j \right) \quad (\text{II.9})$$

Since the coefficients  $\psi_i$  are complex numbers we can either consider the variations of their real and imaginary parts independently or we can rather use  $\psi_i$  and  $\psi_i^*$  as two independent variables. Therefore, the requirement that the action  $I$  is stationary when we add a small variation  $\delta\psi_i^*$  to  $\psi_i^*$  leads to

$$\delta I[\psi] = 0 = \int_0^1 dt \sum_{ij} \delta\psi_i^*(t) \left( i \dot{\psi}_i(t) - \hat{H}_{ij} \psi_j(t) \right) \quad (\text{II.10})$$

If we apply no restriction on the wave functions this relation should hold for any variation  $\delta\psi_i^*$  this implies that

$$0 = i \dot{\psi}_i(t) - \sum_j \hat{H}_{ij} \psi_j(t) \quad (\text{II.11})$$

which is nothing but the Schrödinger equation.

### II.2.C) Dynamical wave functions and mean field approximation



If we introduce the parametrised states  $|\psi(\mathbf{Z})\rangle$  in the action (II.8) we get the following classical like action :

$$I[\mathbf{Z}] = \int_{t_0}^{t_1} dt \mathcal{L}(\mathbf{Z}(t), \dot{\mathbf{Z}}(t)) \equiv \int_{t_0}^{t_1} dt \langle \psi(\mathbf{Z}(t)) | i \frac{\partial}{\partial t} - \hat{H} | \psi(\mathbf{Z}(t)) \rangle \quad (\text{II.12})$$

which can be expressed as an integral of a Lagrange function  $\mathcal{L}(\mathbf{Z}(t), \dot{\mathbf{Z}}(t))$ . Then, the equation of motion for the trajectory  $\mathbf{Z}(t)$  is found as the stationary conditions for the considered action

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{Z}}_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{Z}_i} \quad (\text{II.13})$$

which are equivalent to classical equation of motion for the trajectory  $\mathbf{Z}(t)$ . In the case of coherent states, these dynamical equations can be transformed into equations for the expectation values  $\langle \hat{A}_i \rangle(t)$ . In fact we can directly use an infinitesimal transformation around the stationary solution  $|\psi(\mathbf{Z}(t))\rangle$  using the generators of the considered group

$$|\psi(\mathbf{Z}(t) + \delta \mathbf{Z}(t))\rangle = (1 + i \delta \mathbf{Z}'(t) \cdot \hat{\mathbf{A}}) |\psi(\mathbf{Z}(t))\rangle \quad (\text{II.14})$$

where it should be noticed that in the general case of a non-abelian group (i.e. in the case where at least one commutator of two generators  $\hat{A}_i$  and  $\hat{A}_j$  are non 0) the variations of the parameters  $\delta \mathbf{Z}$  are related to the parameters  $\delta \mathbf{Z}'$  of the infinitesimal transformation (II.14) in a non trivial way.

Introducing the relation (II.14) directly into the action (II.12) we get

$$I[\mathbf{Z} + \delta \mathbf{Z}] = \int_{t_0}^{t_1} dt \left( \langle \psi(\mathbf{Z}) | -i \langle \psi(\mathbf{Z}) | \delta \mathbf{Z}' \cdot \hat{\mathbf{A}} \left( i \frac{\partial}{\partial t} - \hat{H} \right) | \psi(\mathbf{Z}) \rangle + i \delta \mathbf{Z} \cdot \hat{\mathbf{A}} | \psi(\mathbf{Z}) \rangle \right) \quad (\text{II.15})$$

keeping only the lowest order in  $\delta \mathbf{Z}$  the variation of the action can be written as

$$I[\mathbf{Z} + \delta \mathbf{Z}] - I[\mathbf{Z}] = \int_{t_0}^{t_1} dt \left( \langle \psi(\mathbf{Z}) | \delta \mathbf{Z}' \cdot \hat{\mathbf{A}} \left( \frac{\partial}{\partial t} + i \hat{H} \right) \psi(\mathbf{Z}) \rangle + \langle \psi(\mathbf{Z}) | \left( \frac{\partial}{\partial t} - i \hat{H} \right) \delta \mathbf{Z} \cdot \hat{\mathbf{A}} | \psi(\mathbf{Z}) \rangle \right) \quad (\text{II.16})$$

By applying the time derivative either to the right or to the left this leads to

$$\delta I[\mathbf{Z}] = \int_{t_0}^{t_1} dt \delta \mathbf{Z}' \cdot \left( \frac{\partial \langle \psi(\mathbf{Z}) | \hat{\mathbf{A}} | \psi(\mathbf{Z}) \rangle}{\partial t} + \langle \psi(\mathbf{Z}) | i \hat{\mathbf{A}} \hat{H} - i \hat{H} \hat{\mathbf{A}} | \psi(\mathbf{Z}) \rangle \right) \quad (\text{II.17})$$

Therefore, the stationarity condition leads to a generalised Ehrenfest equation

$$\frac{d}{dt} \langle \hat{A}_i \rangle_{\mathbf{Z}} = - \langle \{ \hat{H}, \hat{A}_i \} \rangle_{\mathbf{Z}} \quad (\text{II.18})$$

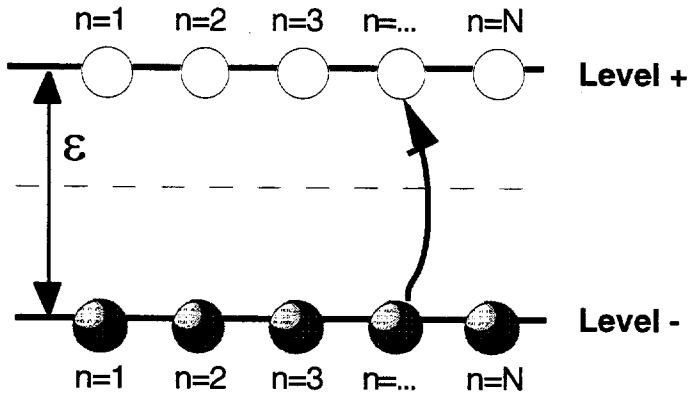
the expectation values being evaluated directly onto the stationary coherent state. In the equation (II.18) the brackets are directly related to the commutators  $\{ . , . \} = [ . , . ] / i$ .

This equation can be understood as a generalised mean-field equation since the expectation value of the commutator present in the right hand side of equation (II.18) can directly be expressed in terms of the mean values  $\langle \hat{A}_i \rangle_{\mathbf{Z}}$  eliminating the  $\mathbf{Z}$  variables using relation (II.4) [Ri81].

From this discussion, it is clear that this type of approximations tries to define the best path in the space of the  $\mathbf{Z}$  variables i.e. as far as the Hilbert space is concerned on the manifold generates by the  $|\psi(\mathbf{Z})\rangle$ . In the complete Hilbert space, the exact solution will follow a different trajectory. The difference between the exact solution and its best approximation  $|\psi(\mathbf{Z})\rangle$  are called correlations.

### II.3) One example: $SU(2)$ dynamics and the Lipkin model

Let me first illustrate this method on a simple model: the Lipkin model. In this model two levels containing  $N$  states labelled by the quantum number  $n$ , can be occupied by  $N$  particles.



**Figure II.1:**  
Schematic representation of the Lipkin model in which two levels with  $N$  available sites can be occupied by  $N$  particles.  $\varepsilon$  is the energy distance between the two levels.

#### II.3.A) The Hamiltonian

The energy difference between the two levels is  $\varepsilon$  but we also introduce a residual interaction between the various particles in such a way that the Hamiltonian reads

$$\hat{H} = \varepsilon \frac{\hat{c}_{+,n}^+ \hat{c}_{+,n} - \hat{c}_{-,n}^+ \hat{c}_{-,n}}{2} + V \left( \frac{\hat{c}_{+,n}^+ \hat{c}_{-,n} + \hat{c}_{-,n}^+ \hat{c}_{+,n}}{2} \right)^2 \quad (\text{II.19})$$

where the  $\hat{c}_{\varepsilon,n}^+$  and  $\hat{c}_{\varepsilon,n}$  create or annihilate a particle on the level  $\varepsilon = \pm$  with the quantum number  $n$ . Looking at the form of the residual interaction we can see that it can only generate jumps from the lower level to the upper one or vis versa without changing the  $n$  quantum number. Therefore, each particle can only occupy two levels  $\pm$  a spin 1/2 which is called pseudo-spin. The algebra

$$\begin{aligned} \hat{k}_n^0 &= \frac{\hat{c}_{+,n}^+ \hat{c}_{+,n} - \hat{c}_{-,n}^+ \hat{c}_{-,n}}{2} \\ \hat{k}_n^+ &= \hat{c}_{+,n}^+ \hat{c}_{-,n} \\ \hat{k}_n^- &= \hat{c}_{-,n}^+ \hat{c}_{+,n} \end{aligned} \quad (\text{II.20})$$

does correspond to the  $SU(2)$  algebra. The Hamiltonian can then be written

$$\hat{H} = \varepsilon \hat{K}^z + V \hat{K}^x{}^2 \quad (\text{II.21})$$

where we have introduced the total pseudo-spin

$$\begin{aligned} \hat{K}^0 &\equiv \hat{K}^z = \sum_n \hat{k}_n^0 \\ \hat{K}^x &= \sum_n \hat{k}_n^x \equiv \sum_n \frac{\hat{k}_n^+ + \hat{k}_n^-}{2} \\ \hat{K}^y &= \sum_n \hat{k}_n^y \equiv \sum_n \frac{\hat{k}_n^+ - \hat{k}_n^-}{2i} \end{aligned} \quad (\text{II.22})$$

which fulfils the standard SU(2) commutation algebra

$$[\hat{K}^x, \hat{K}^y] = i\hat{K}^z \quad (\text{II.23})$$

### II.3.B) The Hilbert space

The model we are considering thus reduces to the known problem of  $N$  coupled spin. Therefore the Hilbert space can be decomposed into irreducible subspaces with a good total pseudo-spin. The state in which all the particles occupied the lower level pertain to the unique subspace associated with the maximum pseudo-spin  $J = N/2$ . We note this state  $|J, -J\rangle$  while the other members of the considered multiplet are  $|J, M\rangle$ . It should be noticed that since the Hamiltonian is completely written in terms of the pseudo-spin operators  $\hat{K}^i$  the Hamiltonian does not couple subspace with different total pseudo-spin.

In each subspace all the operators can be computed using the pseudo-spin properties

$$\begin{aligned} K^0 |J, M\rangle &= M |J, M\rangle \\ K^\pm |J, M\rangle &= \sqrt{J(J+1) - M(M\pm 1)} |J, M\pm 1\rangle \end{aligned} \quad (\text{II.24})$$

Therefore this model can be easily exactly solved providing the exact solution we need to test the approximations discussed in this chapter.

If we neglect the residual interaction,  $V=0$  the ground state of the system is naturally  $|J, -J\rangle$  which energy is nothing but  $-\varepsilon N/2$ . In this state all the particles are occupying the lowest accessible orbital. This is the analogous of the Hartree-Fock ground state. In the following we will use this state to construct the coherent states.

### II.3.C) Coherent states of SU(2)

For this model the coherent states are naturally provided by the application of a SU(2) unitary transformation on the Hartree-Fock ground state which is equivalent to the rotation group. Therefore the parameters  $\mathbf{Z}$  are nothing but the rotation angles. In the present case using the Euler angles we can define

$$|\psi(\mathbf{Z})\rangle = \hat{R}(\mathbf{Z})|\psi(0)\rangle = e^{-i\alpha\hat{K}^z} e^{-i\beta\hat{K}^y} e^{-i\gamma\hat{K}^z} |\psi(0)\rangle \quad (\text{II.25})$$

but if we assume that  $|\psi(0)\rangle = |J, -J\rangle$  then the rotation of the angle  $\gamma$  only modify the phase

and so can be omitted. Then the parameters of the coherent state are only the two Euler angles  $\mathbf{z} = (\alpha, \beta)$

As explained in the section II.1) it is often convenient to introduce the inverse transformation of the operators according to the relation II.3). In particular we only need to transform the  $\hat{\mathbf{K}}$  operators. Since  $\hat{\mathbf{K}}$  is a vector a simple geometrical analysis shows that

$$\begin{pmatrix} \hat{K}^x(\mathbf{Z}) \\ \hat{K}^y(\mathbf{Z}) \\ \hat{K}^z(\mathbf{Z}) \end{pmatrix} = \begin{pmatrix} \cos \alpha \cos \beta & -\sin \alpha & \cos \alpha \sin \beta \\ \sin \alpha \cos \beta & \cos \alpha & \sin \alpha \sin \beta \\ -\sin \beta & 0 & \cos \beta \end{pmatrix} \begin{pmatrix} \hat{K}^x \\ \hat{K}^y \\ \hat{K}^z \end{pmatrix} \quad (\text{II.26})$$

Therefore it is easy to compute  $\langle \hat{\mathbf{K}} \rangle_{\mathbf{z}}$  as

$$\begin{pmatrix} \langle \hat{K}^x \rangle_{\mathbf{z}} \\ \langle \hat{K}^y \rangle_{\mathbf{z}} \\ \langle \hat{K}^z \rangle_{\mathbf{z}} \end{pmatrix} = \begin{pmatrix} \langle J, -J | \hat{K}^x(\mathbf{Z}) | J, -J \rangle \\ \langle J, -J | \hat{K}^y(\mathbf{Z}) | J, -J \rangle \\ \langle J, -J | \hat{K}^z(\mathbf{Z}) | J, -J \rangle \end{pmatrix} = \begin{pmatrix} -J \cos \alpha \sin \beta \\ -J \sin \alpha \sin \beta \\ -J \cos \beta \end{pmatrix} \quad (\text{II.27})$$

These three relations gives the correspondence between  $\langle \hat{\mathbf{K}} \rangle_{\mathbf{z}}$  and the parameters  $\mathbf{z} = (\alpha, \beta)$ . It should be noticed that the  $\langle \hat{\mathbf{K}} \rangle_{\mathbf{z}}$  is a vector of norm J therefore only two angles are needed to define it completely.

### II.3.D) Mean-field solution

Now we can study the dynamics of the system assuming that the wave functions are restricted to coherent states (II.25). The evolution of the  $\mathbf{z} = (\alpha, \beta)$  or of the averaged value  $\langle \hat{\mathbf{K}} \rangle_{\mathbf{z}}$  state are obtained using the generalised Ehrenfest equation (II.18).

$$\begin{pmatrix} \frac{\partial}{\partial t} \langle \hat{K}^x \rangle_{\mathbf{z}} \\ \frac{\partial}{\partial t} \langle \hat{K}^y \rangle_{\mathbf{z}} \\ \frac{\partial}{\partial t} \langle \hat{K}^z \rangle_{\mathbf{z}} \end{pmatrix} = - \begin{pmatrix} \langle [\hat{\mathbf{H}}, \hat{K}^x] \rangle_{\mathbf{z}} \\ \langle [\hat{\mathbf{H}}, \hat{K}^y] \rangle_{\mathbf{z}} \\ \langle [\hat{\mathbf{H}}, \hat{K}^z] \rangle_{\mathbf{z}} \end{pmatrix} = \begin{pmatrix} \varepsilon \langle \hat{K}^y \rangle_{\mathbf{z}} \\ \varepsilon \langle \hat{K}^x \rangle_{\mathbf{z}} - V \langle \hat{K}^x \hat{K}^z + \hat{K}^z \hat{K}^x \rangle_{\mathbf{z}} \\ V \langle \hat{K}^x \hat{K}^y + \hat{K}^y \hat{K}^x \rangle_{\mathbf{z}} \end{pmatrix} \quad (\text{II.28})$$

Using the transformation (II.26) we can evaluate the contributions due to the residual interaction using the relations

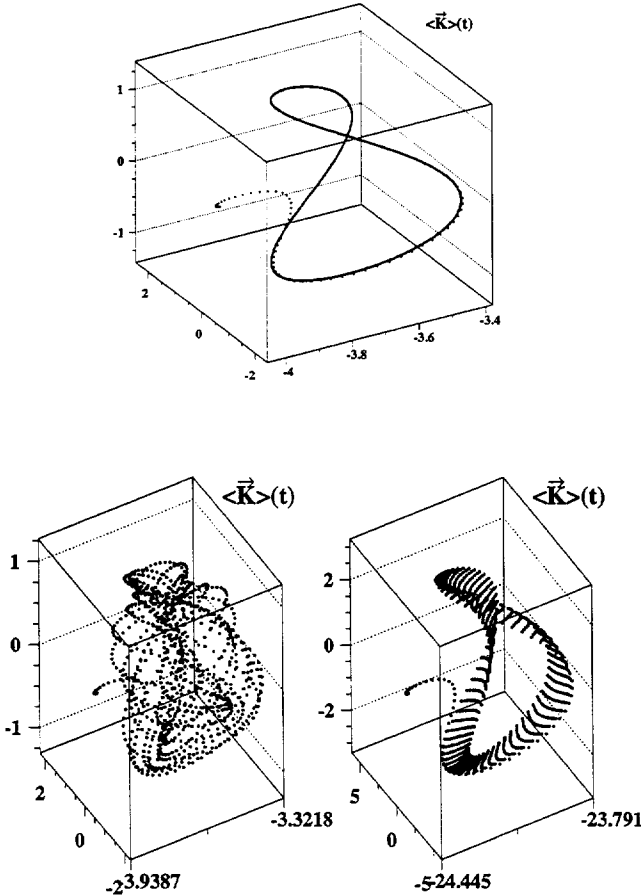
$$\begin{aligned} \langle \hat{K}^x \hat{K}^z + \hat{K}^z \hat{K}^x \rangle_{\mathbf{z}} &= \langle J, -J | \hat{K}^x(\mathbf{Z}) \hat{K}^z(\mathbf{Z}) + \hat{K}^z(\mathbf{Z}) \hat{K}^x(\mathbf{Z}) | J, -J \rangle = (2 - \frac{1}{J}) \langle \hat{K}^x \rangle_{\mathbf{z}} \langle \hat{K}^z \rangle_{\mathbf{z}} \\ \langle \hat{K}^x \hat{K}^y + \hat{K}^y \hat{K}^x \rangle_{\mathbf{z}} &= \langle J, -J | \hat{K}^x(\mathbf{Z}) \hat{K}^y(\mathbf{Z}) + \hat{K}^y(\mathbf{Z}) \hat{K}^x(\mathbf{Z}) | J, -J \rangle = (2 - \frac{1}{J}) \langle \hat{K}^x \rangle_{\mathbf{z}} \langle \hat{K}^y \rangle_{\mathbf{z}} \end{aligned}$$

which leads to the following mean field equations

$$\begin{pmatrix} \frac{\partial}{\partial t} \langle \hat{K}^x \rangle_z \\ \frac{\partial}{\partial t} \langle \hat{K}^y \rangle_z \\ \frac{\partial}{\partial t} \langle \hat{K}^z \rangle_z \end{pmatrix} = \begin{pmatrix} \varepsilon \langle \hat{K}^y \rangle_z \\ \varepsilon \langle \hat{K}^x \rangle_z - V(2 - \frac{1}{J}) \langle \hat{K}^x \rangle_z \langle \hat{K}^0 \rangle_z \\ V(2 - \frac{1}{J}) \langle \hat{K}^x \rangle_z \langle \hat{K}^y \rangle_z \end{pmatrix} \quad (\text{II.29})$$

These equations are highly non linear because the expectation values of two-body terms coming from the residual two-body interaction have been approximated by products of average values of one-body operators (i.e.  $\langle \hat{\mathbf{K}} \rangle_z$ ). In principle the corresponding dynamics could present characteristic behaviours of non-linear systems such as chaos. However, in the simple case studied here if the Hamiltonian is not time dependent the system possesses two constants of motion (the energy and the norm  $|\langle \hat{\mathbf{K}} \rangle_z|^2$ ) and only three degrees of freedom  $\langle \hat{\mathbf{K}} \rangle_z$ . Therefore in this special case the mean-field equation of motion are integrable and so the mean-field dynamics will always be regular.

### II.3.E) Need for stochastic mean-field approaches



**Figure II.2:**

This figure presents the time evolution of the vector  $\langle \hat{\mathbf{K}} \rangle_z$  after a short excitation with an operator  $W(t)\hat{K}^x$ . The upper part correspond to the mean field solution while the two diagrams bellow corresponds to two different total number  $N$ .

In figure II.2 we present the evolution of the Lipkin model after a short excitation with an operator  $W(t)\hat{K}^x$ . One can see that, after the transient period when a time dependent external field is apply, the mean-field approach is rather smooth since it is in fact regular. However, it fails to reproduce the exact trajectory. Indeed, when going from the quantum mechanics to the mean field approach we have replace the average value of two body operators such as

$\langle \hat{K}^i \hat{K}^j \rangle_{\mathbf{z}}$  by essentially the simple product of two average values  $\langle \hat{K}^i \rangle_{\mathbf{z}}$  and  $\langle \hat{K}^j \rangle_{\mathbf{z}}$ . This means that we have disregarded the quantum fluctuations and correlations such as  $\langle \hat{K}^i \hat{K}^j \rangle_{\mathbf{z}} - \langle \hat{K}^i \rangle_{\mathbf{z}} \langle \hat{K}^j \rangle_{\mathbf{z}}$ . In the complete dynamics these quantum terms are introducing fluctuations around the mean field trajectory in such a way that the mean-field trajectory remains close to the exact one only during a finite time.

This illustrates the fact that in mean field approaches we always have only a partial knowledge of the system. Indeed except for some algebraic models the complete description of the system would require an enormous ensemble of expectation values while we have seen that the system is often described through a small subensemble of expectation values of the operators  $\hat{\mathbf{A}} \equiv \{\hat{A}_i\}$  (in the present case the  $\hat{\mathbf{K}} = \{\hat{K}^j\}$ ). This fact imposes a description of the system using statistical mechanics concepts since we must deal with a huge lack of information (i.e., entropy) as for example we ignore all the fluctuations and correlations. Therefore, in general we are forced to introduce a statistical ensemble<sup>1</sup>.

$$\{(|\psi^{(n)}\rangle, p^{(n)})\} \quad (\text{II.30})$$

of Wave functions  $|\psi^{(n)}\rangle$  associated with the probability  $p^{(n)}$ . If we use parametrised wave functions  $|\psi(\mathbf{Z}^{(n)})\rangle$  then we must deal with an ensemble of trajectories  $\mathbf{Z}^{(n)}(t)$  (or equivalently of expectation values  $\langle \hat{\mathbf{A}}^{(n)} \rangle(t)$  in the case of coherent states). The origin of this ensemble is the entropy generated by the lack of information about the system. This missing information strongly influence the dynamics of the observed quantities as can be seen in figure II.2. The aim of stochastic approaches is to restore the disregarded fluctuations and correlations in a statistical way.

### III) Variational evolution of density matrices and dynamics of observables and fluctuations

#### III.1) Concept of density matrix

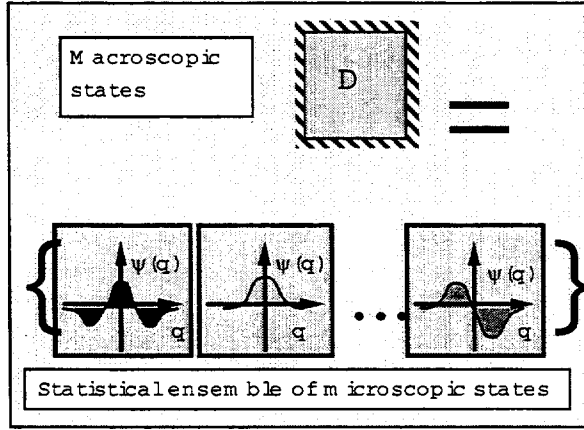
##### III.1.A) Statistical ensemble and density matrix

A very convenient way to take into account the statistical aspect of a description, i.e. the fact that the state of the system is not known exactly but in a statistical way by an ensemble  $\{(|\psi^{(n)}\rangle, p^{(n)})\}$  of Wave functions  $|\psi^{(n)}\rangle$  associated with the probability  $p^{(n)}$ , is to introduce a density matrix

$$\hat{D} = \sum_{(n)} |\psi^{(n)}\rangle p^{(n)} \langle \psi^{(n)}| \quad (\text{III.1})$$

When the wave functions  $|\psi^{(n)}\rangle$  are orthogonal this definition clearly shows that the different possible states are the eigenstates of  $\hat{D}$  while their probabilities are the eigenvalues of  $\hat{D}$ . Therefore, the density matrix does contain all the information about the system.

<sup>1</sup>An alternative route would be to try to describe the system in a coherent way using the generalized generator coordinate state corresponding to a coherent sum over the  $\mathbf{z}$  space:  $|\varphi\rangle = \int d\mathbf{z} \varphi(\mathbf{z}) |\psi(\mathbf{z})\rangle$



**Figure III.1:** Schematic description of a density matrix as a statistical ensemble of different wave functions possibly associated with different probabilities.

The basic concept of a statistical ensemble is that the system might be in many different states  $|\psi^{(n)}\rangle$ . However, if the system happen to be in a given state  $|\psi^{(n)}\rangle$  then it evolves simply with the Schrödinger equation

$$i \frac{d}{dt} |\psi^{(n)}\rangle = \hat{H} |\psi^{(n)}\rangle \quad (\text{III.2})$$

It is essential to understand that its probability  $p^{(n)}$  remains constant

$$\frac{d}{dt} p^{(n)} = 0 \quad (\text{III.3})$$

Using the density matrix it is easy to write a unique equation for the evolution of the statistical ensemble

$$\frac{d}{dt} \hat{D} = \frac{1}{i} [\hat{H}, \hat{D}] \equiv \{\hat{H}, \hat{D}\} \quad (\text{III.4})$$

In this context it is important to remark that the mean values of the expectation values of any operator  $\hat{B}$  reads

$$\langle \hat{B} \rangle = \sum_n p^{(n)} \langle \hat{B} \rangle^{(n)} = \sum_n p^{(n)} \langle \psi^{(n)} | \hat{B} | \psi^{(n)} \rangle = \text{tr} \hat{B} \hat{D} \quad (\text{III.5})$$

### III.1.B) Geometrical interpretation

In the vector space of operators the trace can be interpreted as a scalar product

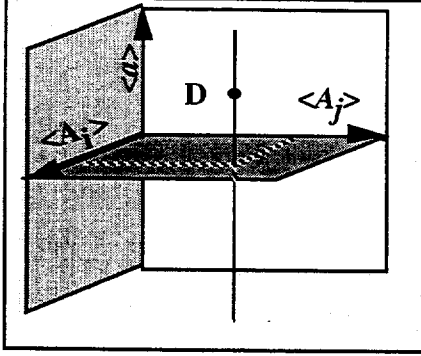
$$\langle \hat{A} | \hat{B} \rangle \equiv \text{tr} \hat{A}^\dagger \hat{B} \quad (\text{III.6})$$

allowing to define distances, orthonormal basis and orthogonal projections. It also connects the space of matrices with its dual space the observables. These geometrical properties will introduce important simplifications in the following discussions.

Let me call  $\hat{A} \equiv \{\hat{A}_t\}$  an ensemble of observables which represents all the information we may have and would like to follow in time

$$\langle \hat{A} \rangle \equiv \{ \langle \hat{A}_\ell \rangle \equiv \text{tr} \hat{A}_\ell \hat{D} \} \quad (\text{III.7})$$

This expression can be understood as the projection of the density matrix on the hyperplane defined by the operators  $\hat{A} \equiv \{ \hat{A}_\ell \}$ .



**Figure III.2:**

Interpretation of the mean values  $\langle \hat{A}_\ell \rangle$  as the orthogonal projection of the density matrix on the axis defined by the matrix  $\hat{A}_\ell$ . Then the description of the state by a reduced ensemble of expectation values can be seen as the projection of the whole density matrix onto the hyper plan defined by the considered operators.

### III.1.C) Minimum entropy density matrix

Since we are in the framework of statistical mechanics it is important to introduce the entropy

$$S = -\text{tr} \hat{D} \log \hat{D} = -\sum_n p^{(n)} \log p^{(n)} \quad (\text{III.8})$$

as a measure of the lack of information associated with the considered reduced description retaining only few expectation values.

If we don't want to bias the considered statistical ensemble the entropy must be maximum in such a way that the density matrix will not content more information than the one provided by the knowledge of the few mean values  $\langle \hat{A} \rangle$ . This is a standard problem in statistical physics to maximise the entropy with constraints. The standard method is to introduce as many Lagrange multipliers  $\mathbf{Z} \equiv \{ Z_\ell \}$  as constraints  $\langle \hat{A} \rangle = \{ \langle \hat{A}_\ell \rangle \}$  and to minimise the modified entropy

$$S' = S + z_0 \langle \hat{I} \rangle + \sum_\ell Z_\ell \langle \hat{A}_\ell \rangle = -\text{tr} \hat{D} \log \hat{D} + z_0 \text{tr} \hat{D} + \sum_\ell Z_\ell \text{tr} \hat{A}_\ell \hat{D} \quad (\text{III.9})$$

where the additional constraint  $z_0 \text{tr} \hat{D}$  has been introduced in order to take care of the normalisation of the probabilities  $p^{(n)}$ . The variation of the modified entropy can be easily computed since the cyclic property of the trace suppresses the non-commutation problems usually encountered when dealing with functions of matrices. Therefore introducing a variation  $\delta \hat{D}$  of the density matrix we get the following variation of the modified entropy

$$\delta S' = -\text{tr} \left( \delta \hat{D} \left( (\log \hat{D} + 1) - z_0 - \sum_\ell Z_\ell \hat{A}_\ell \right) \right) \quad (\text{III.10})$$

Imposing that  $\hat{D}$  is an extremum of  $S'$  means that  $\delta S'$  should be 0 for any variation  $\delta \hat{D}$  and so

$$(\log \hat{D} + 1) - z_0 - \sum_\ell Z_\ell \hat{A}_\ell = 0 \quad (\text{III.11})$$



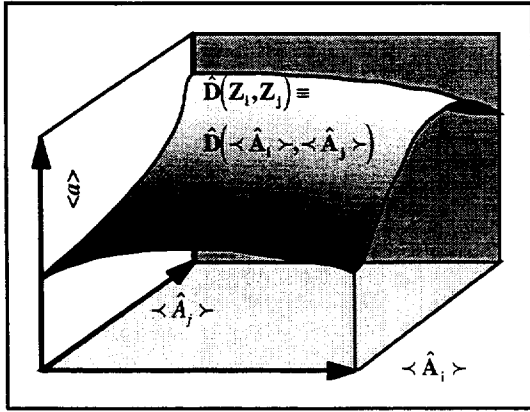
Therefore, the density matrix which maximised the entropy under the constraints  $\langle \hat{A} \rangle$  is [Ba81]:

$$\hat{D}(\mathbf{Z}) = \frac{1}{Z_0} \exp(\mathbf{Z} \cdot \hat{A}) \quad (\text{III.12})$$

where the parameters  $\mathbf{Z} \equiv \{Z_i\}$  are then interpreted as Lagrange multipliers and where  $Z_0 = \text{tr} \exp(\mathbf{Z} \cdot \hat{A})$  is the partition function computed using the unitarity constraint  $\text{tr} \hat{D} = 1$ . The Lagrange multipliers are defined by the constraints  $\langle \hat{A} \rangle \equiv \{\langle \hat{A}_i \rangle\}$  usually written making use of the derivatives of the logarithm of the partition function

$$\langle \hat{A}_i \rangle = \frac{\partial \log Z_0}{\partial Z_i} \quad (\text{III.13})$$

In the space of the matrices, the maximum entropy matrices Eq. (II.12) define a manifold of the same dimension as the hyperplane of the observables  $\hat{A}_i$ .



**Figure III.3:** Schematic illustration of the manifold associated with the maximum entropy under the constraints  $\langle \hat{A}_i \rangle$ . This is the space of the matrices  $\hat{D}(\mathbf{z})$ .

Let us now turn to the problem of hot systems with a temperature  $T = 1/\beta$  where  $-\beta$  is the Lagrange parameter associated to the constraint on the energy  $E = \langle \hat{H} \rangle$ . The equilibrium density matrix corresponds to the maximum of the functional  $S(\mathbf{Z}) - \beta E(\mathbf{Z})$  on the considered space of trial density matrices  $\hat{D}(\mathbf{Z})$  or in an equivalent way as the minimum of the free energy

$$F(\mathbf{Z}) = E(\mathbf{Z}) - T S(\mathbf{Z}) = \langle \hat{H} - T \log \hat{D} \rangle_{\mathbf{Z}} \quad (\text{III.14})$$

However, as soon as  $\hat{H}$  contain a two body interaction, the use of

$$\hat{D}(\beta) = Z_0^{-1} \exp(-\beta \hat{H}) \quad (\text{III.15})$$

becomes untractable. Therefore usually an other type of density matrix is then used as a parametric density matrix and no more the maximum entropy density matrix.

### III.2) Dynamical evolution

#### III.2.A) Variational methods for density matrices

If we now want to address a dynamical problem we have normally to solve the Liouville equation

$$\frac{d}{dt}\hat{D} = \{\hat{H}, \hat{D}\} \quad (\text{III.16})$$

If we want to solve it in a restricted space it has been shown that the solution of the Liouville equation the extremum of the following action [Ba84,Ba85,Ba88]

$$I[\hat{B}, \hat{D}] = \text{tr}\hat{B}(t_1)\hat{D}(t_1) - \int_{t_0}^{t_1} dt \text{tr}\hat{B}(t) \left( \frac{d}{dt}\hat{D}(t) - \{\hat{H}, \hat{D}(t)\} \right) \quad (\text{III.17})$$

where the variational parameters are both the density matrices  $\hat{D}(t)$  and a set of observables  $\hat{B}(t)$ . This variational principle must be complemented by two boundary-conditions: the first one at the initial time  $t_0$  defining the initial density matrix and a second one concerning the observable we want to predict at the final time  $t_1$ . The extremum value of the action (III.17) is then nothing but the mean value  $\langle \hat{B} \rangle$  measured at the final time  $t_1$ . This form of variational principle clearly stress the dual role played by the density matrix and the observables.

If we now restrict our description to an ensemble of observables within a given algebra generated by a set of operators  $\{1, \hat{A}_i\}$

$$\hat{B}(\mathbf{Z}') = \mathbf{Z}'_0 + \mathbf{Z}' \cdot \hat{\mathbf{A}} \quad (\text{III.18})$$

then the maximum entropy argument developed in previous sections shows that we shall use the following parametrised density matrix

$$\hat{D}(\mathbf{Z}) = \exp(\mathbf{Z}_0 + \mathbf{Z} \cdot \hat{\mathbf{A}}) \quad (\text{III.19})$$

Therefore the action  $I[\mathbf{Z}', \mathbf{Z}]$  is a functional of the two sets of parameters  $\mathbf{Z}(t)$  and  $\mathbf{Z}'(t)$ . Since this action is linear in  $\mathbf{Z}'(t)$  the extremum condition on these variables is rather simple and depends only on  $\mathbf{Z}(t)$

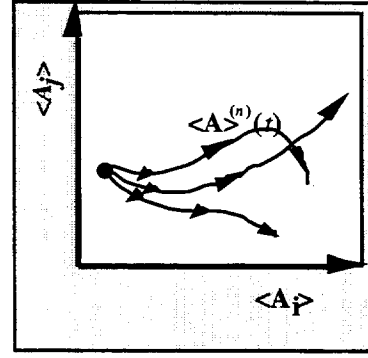
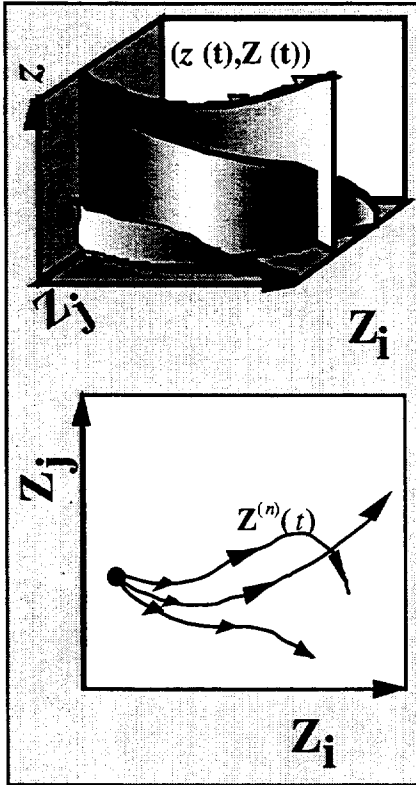
$$\int_{t_0}^{t_1} dt \text{tr} \delta \mathbf{Z}'_i(t) \hat{\mathbf{A}}_i \left( \frac{d}{dt} \hat{D}(\mathbf{z}(t)) - \{\hat{H}, \hat{D}(\mathbf{z}(t))\} \right) = 0 \quad (\text{III.20})$$

Making an integration by part it is easy to show that this condition leads again to a generalised Ehrenfest equation

$$\frac{d}{dt} \langle \hat{\mathbf{A}}_i \rangle_{\mathbf{Z}} = - \langle \{\hat{H}, \hat{\mathbf{A}}_i\} \rangle_{\mathbf{Z}} \quad (\text{III.21})$$

which must be understood as mean-field equations. Indeed, all the mean values are estimated using the parametrised density matrix and thus depend only upon the generalised densities

$$\rho_i = \langle \hat{\mathbf{A}}_i \rangle_{\mathbf{Z}} \quad (\text{III.22})$$



**Figure III.4:**

The variational methods are predicting a unique trajectory  $z_i$ . If we improve the description adding new variables  $z_m$  we will then predict several possible trajectories depending upon the value of the added correlations  $z_m$ . Then, we can define several projected trajectories in the  $z_i$  space. Therefore we must rather follow an ensemble of trajectories  $z_i$  in order to take into account the feedback of the unknown correlation on the dynamics of the considered variables. This is also illustrated in the space of observables by an ensemble of trajectories  $\langle \hat{A}^{(n)}(t) \rangle$ .

### III.2.B) Lack of information and stochastic evolution

The variational methods are predicting a unique trajectory. However, we can always develop a more precise theory by introducing new parameters,  $z_m$ , in the description of our trial states or densities. Most of the time this means that we are introducing new observables,  $\hat{a}_m$ , to characterise the system. Depending upon the different initial value of these new variables, the variational principle will predict different evolution for the whole system. If we now consider the various projections of these trajectories on the old variables  $Z_i(t)$  we will observe an ensemble of projections. These trajectories are different from the unique trajectory predicted when the correlations associated with  $z_m$  were not considered. If we ignore the values of the correlations  $z_m$  we cannot select only one projected trajectory but we must rather consider them all.

Therefore our lack of information about all the possible correlations imposes to consider an ensemble of trajectories. The parameters  $Z_i(t)$  are fluctuating from one "event" to the other. This means that besides the classical equations of motion derived from the variational principle, the  $Z_i$  experience a fluctuating evolution because of the influence of the unknown correlations. To describe this evolution, we will consider in the following stochastic approaches in which the feedback of the unknown correlation is taken into account as a random term "à la Langevin" in the equations of motion.

We will see in the following that the statistical ensemble associated with the density matrices we are considering is not enough to describe the whole dynamics. Indeed, the correlations which are not described may modify the predicted trajectory for the  $\langle \hat{A}_i \rangle(t)$ . Since these correlations are unknown we will be forced to consider an ensemble of correlations and so of trajectories. In fact it is easy to see that the ensemble of density matrices <sup>1</sup>

<sup>1</sup> here the different density matrices are supposed to be equiprobable. It is straightforward to extend this description in order to include different probabilities for the different density matrices.

$$\left\{ \hat{D}(\mathbf{Z}^{(n)}) = \frac{1}{Z_0^{(n)}} \exp(\mathbf{Z}^{(n)} \cdot \hat{\mathbf{A}}) \right\} \quad (\text{III.23})$$

defined using an ensemble of parameters  $\mathbf{Z}^{(n)}$  (or of mean values  $\langle \hat{\mathbf{A}} \rangle^{(n)}$ ) contains many more correlations than any of its members. Indeed the resulting density matrix describing this ensemble of density matrices reads:

$$\hat{D} = \sum_{(n)} \hat{D}(\mathbf{Z}^{(n)}) = \sum_{(n)} \frac{1}{Z_0^{(n)}} \exp(\mathbf{Z}^{(n)} \cdot \hat{\mathbf{A}}) \quad (\text{III.24})$$

and cannot be reduced (in general) to a unique set of parameters  $\mathbf{Z}$ .

### III.3) Example: Mean field for the anharmonic oscillator

The concepts developed above can be illustrated using schematic models such as the one-dimensional anharmonic oscillator excited through a non linear external force as used in reference [Vo95] in order to describe the excitation of multiphonon states. Let us consider the following intrinsic hamiltonian:

$$\hat{H} = \frac{1}{2m} \hat{\mathbf{p}}^2 + \frac{m\omega}{2} \hat{\mathbf{x}}^2 + \frac{\alpha}{3} \hat{\mathbf{x}}^3 + \frac{\beta}{4} \hat{\mathbf{x}}^4 \quad (\text{III.25})$$

for an anharmonic oscillator which we excited through a non-linear time-dependent external field:

$$\hat{\mathbf{W}}(t) = -F(t) \left( \hat{\mathbf{x}} + \frac{\delta}{2} \hat{\mathbf{x}}^2 \right) \quad (\text{III.26})$$

where  $F(t)$  is for example a force simulating the action of the electric field on the transverse degree of freedom of the giant dipole resonance (GDR) during a heavy ion collision. This problem can be solve numerically with an initial condition corresponding to the nucleus in its ground state.

As we have discussed in the present chapter, we can try to describe the dynamics by the mean values  $\langle \hat{\mathbf{x}} \rangle$  and  $\langle \hat{\mathbf{p}} \rangle$  - the mean values associated with the generators of the translation and the Galilean transformation group. The equations of motion for these expectation values are given by the Ehrenfest equations

$$\begin{aligned} \frac{d}{dt} \langle \hat{\mathbf{x}} \rangle &= \frac{1}{m} \langle \hat{\mathbf{p}} \rangle \\ \frac{d}{dt} \langle \hat{\mathbf{p}} \rangle &= m\omega \langle \hat{\mathbf{x}} \rangle + \alpha \langle \hat{\mathbf{x}}^2 \rangle + \beta \langle \hat{\mathbf{x}}^3 \rangle + F(t)(1 + \delta \langle \hat{\mathbf{x}} \rangle) \end{aligned} \quad (\text{III.27})$$

These equations are not a set of closed equations as soon as  $\alpha$  or  $\beta \neq 0$ . This means that classical coherent states are no more a solution of the exact Schrödinger problem.

Applying the minimum information (maximum entropy) argument leads to the simple classical assumption

$$\langle \hat{\mathbf{x}}^n \rangle = \langle \hat{\mathbf{x}} \rangle^n \quad (\text{III.28})$$

where all kinds of quantum fluctuations are neglected. In such a case the equations (III.27) reduce to a set of classical equation of motion. However it is shown in ref. [Vo95] that this approximation is not sufficient and that the introduction of quantum fluctuations is needed in order to understand the observed cross-sections.

#### IV) Projection on relevant observables and stochastic approaches

Another way to consider the problem is to study directly the mean values  $\langle \hat{A} \rangle$  of a set of operators  $\hat{A} \equiv \{\hat{A}_i\}$ . We have discussed in section II.1.B that the knowledge of some mean values is equivalent to the knowledge of the projection of the considered state onto an hyperplane defined by the considered observables. In this sense, we were only able to get a partial description of the system. We have been able to derive a density matrix which was the less biased using a maximum entropy argument. Using the implicit relation between the mean values  $\langle \hat{A} \rangle$  and the Lagrange multipliers  $\mathbf{Z}$  it is possible to write

$$\hat{D}(\mathbf{Z}(\langle \hat{A} \rangle)) = \frac{1}{Z_0(\langle \hat{A} \rangle)} \exp(\mathbf{Z}(\langle \hat{A} \rangle) \cdot \hat{A}) \quad (\text{IV.1})$$

##### IV.1) Evolution of observations

If we want know to predict the evolution of the mean values  $\langle \hat{A} \rangle$  of the  $\hat{A} \equiv \{\hat{A}_i\}$  operators we know that they evolve according to the equation

$$\frac{d}{dt} \langle \hat{A}_i \rangle = - \langle \{ \hat{H}, \hat{A}_i \} \rangle \quad (\text{IV.2})$$

where the mean values are computed using the exact state of the system. However, this equation is in general very difficult or impossible to solve because the right hand side requires the knowledge of a large number of mean values.

##### IV.1.A) Special case of a closed algebra.

If we suppose that the commutators  $\{ \hat{H}, \hat{A}_i \}$  can be expressed as a linear combination of the operators  $\hat{A}_{i'}$ ,

$$\{ \hat{H}, \hat{A}_i \} = \sum_{i'} H_{ii'} \hat{A}_{i'} \quad (\text{IV.3})$$

Then equations (IV.2) leads to a closed set of linear differential equations which can be directly solved

$$\frac{d}{dt} \langle \hat{A}_i \rangle = - \sum_{i'} H_{ii'} \langle \hat{A}_{i'} \rangle \quad (\text{IV.4})$$

However, this simplification will be possible only in few algebraic models and, in general, the commutators  $\{ \hat{H}, \hat{A}_i \}$  cannot be expressed as a linear combination of the operators  $\hat{A}_{i'}$  themselves. Then, the equations (IV.2) do not form a complete set of differential equations in the sense that the mean values  $\langle \hat{A} \rangle$  are not enough information to solve the problem. This is

reasonable since the correlations, which we ignore, do have, in general, an influence on the dynamics of the system.

#### IV.1.B) General formalism.

To solve this problem formally we can always complete the set of operators  $\hat{A}_\ell$  with an ensemble of other operators  $\hat{a}_m$  (which are indeed describing all the possible correlations) in order to be able to express the commutators  $\{\hat{H}, \hat{A}_\ell\}$  and  $\{\hat{H}, \hat{a}_m\}$  as linear combinations of the  $\hat{A}_{\ell'}$  and  $\hat{a}_{m'}$  operators.

$$\begin{cases} \{\hat{H}, \hat{A}_\ell\} = \mathcal{Q}_\ell(\hat{\mathbf{A}}, \hat{\mathbf{a}}) \equiv -\sum_{\ell'} H_{\ell'}^{\ell'} \hat{A}_{\ell'} - \sum_{m'} H_{\ell'}^{m'} \hat{a}_{m'} \\ \{\hat{H}, \hat{a}_m\} = -\mathcal{P}_m(\hat{\mathbf{A}}, \hat{\mathbf{a}}) \equiv -\sum_{\ell'} H_m^{\ell'} \hat{A}_{\ell'} - \sum_{m'} H_m^{m'} \hat{a}_{m'} \end{cases} \quad (\text{IV.5})$$

where the  $\mathcal{Q}_\ell$  and  $\mathcal{P}_m$  are linear functions. It should be noticed that this decomposition is always possible since it is always possible to complete the set of operators  $\hat{A}_\ell$  by an ensemble of new operators  $\hat{a}_m$  to have a basis of the space of the hermitic operators. In such a case, the density matrices associated with the constraints  $\langle \hat{A}_\ell \rangle$  and  $\langle \hat{a}_m \rangle$  describe all the possible states of the considered system since the  $\langle \hat{A}_\ell \rangle$  et  $\langle \hat{a}_m \rangle$  provide a complete information allowing to compute the mean value of any observable.

Using the equation (II.29) we can therefore directly compute the equation of evolution of the various mean values

$$\begin{cases} \frac{d \langle \hat{A}_\ell \rangle}{dt} = -\mathcal{Q}_\ell(\langle \hat{\mathbf{A}} \rangle, \langle \hat{\mathbf{a}} \rangle) = -\sum_{\ell'} H_{\ell'}^{\ell'} \langle \hat{A}_{\ell'} \rangle - \sum_{m'} H_{\ell'}^{m'} \langle \hat{a}_{m'} \rangle \\ \frac{d \langle \hat{a}_m \rangle}{dt} = -\mathcal{P}_m(\langle \hat{\mathbf{A}} \rangle, \langle \hat{\mathbf{a}} \rangle) = -\sum_{\ell'} H_m^{\ell'} \langle \hat{A}_{\ell'} \rangle - \sum_{m'} H_m^{m'} \langle \hat{a}_{m'} \rangle \end{cases} \quad (\text{IV.6})$$

This is a closed set of differential equation since  $\langle \hat{\mathbf{A}} \rangle$  and  $\langle \hat{\mathbf{a}} \rangle$  completely describe the system.

If, at a given time  $t$ , we don't know the correlations  $\langle \hat{\mathbf{a}} \rangle$  but only the collective coordinates  $\langle \hat{\mathbf{A}} \rangle$ , the equations of motion for  $\langle \hat{\mathbf{A}} \rangle$  (the first equation of the set of equations (IV.6)) cannot be solved since they dependent upon the unknown correlations  $\langle \hat{\mathbf{a}} \rangle$ . However we can use the minimum entropy density  $\hat{D}(\mathbf{Z}(\langle \hat{\mathbf{A}} \rangle))$  in order to make an unbiased guess for the mean value of the correlation

$$\overline{\langle \hat{\mathbf{a}} \rangle}(\langle \hat{\mathbf{A}} \rangle) = \text{tr } \hat{\mathbf{a}} \hat{D}(\mathbf{Z}(\langle \hat{\mathbf{A}} \rangle)) \quad (\text{IV.7})$$

It should be noticed that these functions of  $\langle \hat{\mathbf{A}} \rangle$  are always non linear. Introducing the fluctuations defined by

$$\delta \langle \hat{\mathbf{a}} \rangle = \langle \hat{\mathbf{a}} \rangle - \overline{\langle \hat{\mathbf{a}} \rangle}(\langle \hat{\mathbf{A}} \rangle) \quad (\text{IV.8})$$

the equations of motion for the variables  $\langle \hat{\mathbf{A}} \rangle$  becomes

$$\begin{aligned}\frac{d \langle \hat{A}_\ell \rangle}{dt} &= -\mathcal{G}_\ell(\langle \hat{A} \rangle, \overline{\langle \hat{a} \rangle}(\langle \hat{A} \rangle)) - \frac{\delta \mathcal{G}_\ell}{\delta \langle \hat{a} \rangle} \delta \langle \hat{a} \rangle \\ \frac{d \langle \hat{A}_\ell \rangle}{dt} &= -\left( \sum_{\ell'} H_{\ell\ell'}^{\ell'} \langle \hat{A}_{\ell'} \rangle + \sum_{m'} H_{\ell\ell'}^{m'} \overline{\langle \hat{a}_{m'} \rangle}(\langle \hat{A} \rangle) \right) - \sum_{m'} H_{\ell\ell'}^{m'} \delta \langle \hat{a}_{m'} \rangle\end{aligned}\quad (\text{IV.9})$$

The first terms of the right-hand side of equations (IV.9) are nothing but a mean-field term. Indeed, if we neglect the  $\delta \mathcal{G}$  term this equation becomes

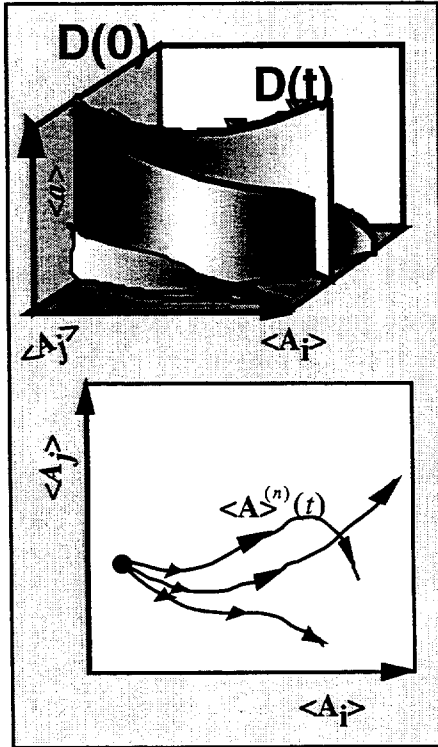
$$\frac{d \langle \hat{A}_\ell \rangle}{dt} = -\mathcal{G}_\ell(\langle \hat{A} \rangle, \overline{\langle \hat{a} \rangle}(\langle \hat{A} \rangle)) = -\langle \{ \hat{H}, \hat{A}_\ell \} \rangle_z \equiv \mathcal{W}_\ell(\langle \hat{A} \rangle) \quad (\text{IV.10})$$

i.e. a mean-field equation where the commutators are estimated using the minimum-entropy density-matrix.

#### IV.1.C) Langevin Approaches

The second term  $\delta \mathcal{G}$  describes the influence of the correlations  $\delta \langle \hat{a} \rangle$  on the dynamics of the mean values  $\langle \hat{A} \rangle$ . If we do not control the value of the correlations  $\delta \langle \hat{a} \rangle$  they will fluctuate from one event to the other so that the  $\delta \mathcal{G}$  term plays the role of a fluctuating force that may have a non zero average value plus a stochastic part.

This description is, in its spirit, identical to the Langevin description of the Brownian motion. The variables  $\langle \hat{A} \rangle$  are somehow equivalent to the coordinate of the pollen particle while the variables  $\delta \langle \hat{a} \rangle$  correspond to the degrees of freedom associated with the molecules of the heat bath.



**Figure IV.1:**

All possible realisations of a system associated with the same initial projection ( $\langle \hat{A} \rangle$ ) on the hyperplane of the observables  $\hat{A}$  but associated with different initial correlations  $\langle \hat{a} \rangle$  will evolve independently leading to different projected trajectories  $\langle \hat{A} \rangle(t)$ . The evolution reduced to the macroscopic variables  $\langle \hat{A} \rangle$  (bottom) will not be deterministic but rather stochastic while the evolution of the whole density matrix is deterministic (top).

Let us now consider an ensemble of realisations of the considered system. In order to take into

account the role of the unknown correlations  $\delta \langle \hat{\mathbf{a}} \rangle$  we can consider that each element of the ensemble of realisations (defined by  $\langle \hat{\mathbf{A}} \rangle^{(n)}$ ) evolve independently according to the equation

$$\frac{d \langle \hat{\mathbf{A}}_t \rangle^{(n)}}{dt} = \mathcal{W}_t(\langle \hat{\mathbf{A}} \rangle^{(n)}) + \delta \mathcal{W}_t^{(n)}(\langle \hat{\mathbf{A}} \rangle^{(n)}) \quad (\text{IV.11})$$

where the  $\delta \mathcal{W}$  term simulates the influence of the correlations in  $\delta \mathcal{G}$ . In the following applications this Langevin term will be either a random force [Ba81, Ba88, La89, Ch89, Co93, Ch94], or a fluctuating collision term as in the Boltzmann-Langevin [Ba87, Be88, Ay88, Ay90, Ra90, Ch91, Bu91, Ch92b].

Let us derive in more details the general structure of the Langevin term. In order to do so, we have to solve the equations for  $\langle \hat{\mathbf{a}}_m \rangle$

$$\frac{d \langle \hat{\mathbf{a}}_m \rangle}{dt} = -\mathcal{G}_m(\langle \hat{\mathbf{A}} \rangle, \overline{\langle \hat{\mathbf{a}} \rangle}(\langle \hat{\mathbf{A}} \rangle)) - \sum_{m'} \mathbf{H}_m^{m'} \delta \langle \hat{\mathbf{a}}_{m'} \rangle \quad (\text{IV.12})$$

This equation can be recasted as an equation for  $\delta \langle \hat{\mathbf{a}}_m \rangle$

$$\begin{aligned} \frac{d \delta \langle \hat{\mathbf{a}}_m \rangle}{dt} &= -\mathcal{G}_m(\langle \hat{\mathbf{A}} \rangle, \overline{\delta \langle \hat{\mathbf{a}} \rangle}(\langle \hat{\mathbf{A}} \rangle)) - \frac{d \overline{\delta \langle \hat{\mathbf{a}} \rangle}(\langle \hat{\mathbf{A}} \rangle)}{dt} - \sum_{m'} \mathbf{H}_m^{m'} \delta \langle \hat{\mathbf{a}}_{m'} \rangle \\ \frac{d \delta \langle \hat{\mathbf{a}}_m \rangle}{dt} &= -\mathcal{L}_m(\langle \hat{\mathbf{A}} \rangle) - \sum_{m'} \mathbf{H}_m^{m'} \delta \langle \hat{\mathbf{a}}_{m'} \rangle \end{aligned} \quad (\text{IV.13})$$

which can be formally solved as

$$\delta \langle \hat{\mathbf{a}} \rangle(t) = - \int_0^t dt' \exp(-\mathbf{H}(t-t')) \mathcal{L}(\langle \hat{\mathbf{A}} \rangle) + \exp(-\mathbf{H}(t-t_0)) \delta \langle \hat{\mathbf{a}} \rangle(t_0) \quad (\text{IV.14})$$

In this expression the first term corresponds to the amount of correlation coming from the coupling with the average dynamics while the second one is associated with the propagation of the initial fluctuations. Using the relation (IV.14) we can have an explicit equation for the fluctuating collision term  $\delta \mathcal{W}$

$$\begin{aligned} \frac{d \langle \hat{\mathbf{A}}_t \rangle}{dt} &= \mathcal{W}_t(\langle \hat{\mathbf{A}} \rangle) \\ &\quad - \sum_m \mathbf{H}_t^m \left( \int_0^t dt' \exp(-\mathbf{H}(t-t')) \mathcal{L}(\langle \hat{\mathbf{A}} \rangle) + \exp(-\mathbf{H}(t-t_0)) \delta \langle \hat{\mathbf{a}} \rangle(t_0) \right)_m \end{aligned} \quad (\text{IV.15})$$

which can be written as

$$\frac{d \langle \hat{\mathbf{A}}_t \rangle}{dt} = \mathcal{W}_t(\langle \hat{\mathbf{A}} \rangle) + \mathcal{K}_t + \delta \mathcal{K}_t \quad (\text{IV.16})$$

where the averaged collision term reads

$$\mathcal{K}_t = - \sum_m \mathbf{H}_t^m \left( \int_0^t dt' \exp(-\mathbf{H}(t-t')) \mathcal{L}(\langle \hat{\mathbf{A}} \rangle) \right)_m \quad (\text{IV.17})$$

while the fluctuating part is given by



$$\delta K_i = -\sum_m H_i^m \left( \exp(-\mathbf{H}(t-t_0)) \right) \delta \langle \hat{\mathbf{a}} \rangle_m(t_0) \quad (\text{IV.18})$$

It should be noticed that these equations are still exact however they exhibit the typical structure of a Langevin dynamics. In these approach the noise is coming from the unknown initial correlations  $\delta \langle \hat{\mathbf{a}} \rangle(t_0)$ . Applying iteratively these equations every time  $\tau$  assuming molecular chaos for the restoration of the fluctuations  $\delta \langle \hat{\mathbf{a}} \rangle(t_0)$  leads to the Boltzmann Langevin theory.

#### IV.2) Evolution close to an equilibrium and Linear response collective behaviours

An important property associated with the non-linearity (or to **the self-consistency**) of the mean-field part of the dynamics is the possible self-organised of the system. An example of this self-organisation is the existence of non-trivial collective modes. To show this fact let us reconsider the generalised stochastic mean-field equations:

$$\frac{d\mathbf{f}^{(n)}}{dt} = \mathcal{W}(\mathbf{f}^{(n)}) + \delta \mathcal{W}^{(n)}(\mathbf{f}^{(n)}) \quad (\text{IV.19})$$

where as before the  $\mathbf{f}^{(n)}$  are either the variables  $\mathbf{z}$  or the mean values  $\langle \hat{\mathbf{A}} \rangle$  and where (n) labels a given trajectory within the considered ensemble.

For a moment let us study only the mean-field part of the dynamics. We will come back to the correlation term  $\delta \mathcal{W}$  right after. The equilibrium (or the ground state)<sup>1</sup>,  $\mathbf{f}_0$ , corresponds to a static solution:  $d\mathbf{f}_0/dt = 0 = \mathcal{W}(\mathbf{f}_0)$ . If we now study the small amplitude motion around this equilibrium we can expand  $\mathbf{f}$  as:

$$\mathbf{f} = \mathbf{f}_0 + \delta \mathbf{f} + \dots \quad (\text{IV.20})$$

Then the linearised equation for  $\delta \mathbf{f}$  simply reads

$$\frac{d\delta \mathbf{f}_t}{dt} = \sum_{t'} \frac{\partial \mathcal{W}_t}{\partial \mathbf{f}_{t'}} \delta \mathbf{f}_{t'} \equiv \sum_{t'} \mathcal{K}_{tt'} \delta \mathbf{f}_{t'} \quad (\text{IV.21})$$

In this equation  $\mathcal{K}$  is the analogue of the RPA approach. Diagonalising this matrix allows to define the collective degrees of freedom<sup>2</sup> of the system such as for example the giant resonances. Moreover, because of the classical structure of the mean-field approximation these collective modes can be often assimilated to vibrations.

If we now turn back to the problem of the propagation induced by the stochastic equation we

<sup>1</sup>we can also extend the present discussion in order to consider a time dependent trajectory  $\mathbf{f}^{(n)}(t)$  and repeat the whole derivation. The main difference is that the RPA matrices are becoming time dependent introducing some additionnal difficulties (see for example reference [Co94]).

<sup>2</sup>The diagonalisation of the RPA matrix is often not enough to define collective motion and one has often to also considers other properties as we will discuss in chapter IV

have to consider the following linearised equation if we assume that the stochastic term is small too:

$$\frac{d \delta f_{\ell}^{(n)}}{dt} = \sum_{\ell'} \mathcal{K}_{\ell\ell'}^{(n)} \delta f_{\ell'}^{(n)} + \delta \mathcal{W}_{\ell}^{(n)} \quad (\text{IV.21})$$

On this equation we can clearly see that the role of the  $\delta \mathcal{W}$  is to agitate the normal mode of the system. In a hot system this is the way that hot giant resonances can be spontaneously excited to reach their thermal equilibrium. In the case of an unstable system the stochastic term will trig the instabilities that will subsequently develop because of the influence of the mean-field.

Equation (II.45) can be easily solved using standard linear response techniques [Ri81, Co94a, Co94, Ch95a, Ay96]. In particular after a simple Fourier transform on the time variable one gets

$$\delta f^{(n)}(\omega) = \frac{1}{\omega + i\eta - \mathcal{K}} \delta \mathcal{W}^{(n)}(\omega) \equiv \mathbf{G}(\omega) \delta \mathcal{W}^{(n)}(\omega) \quad (\text{IV.22})$$

where  $\mathbf{G}$  is the Green's function associated with the linearised problem which can be easily expressed using the eigenvectors and eigen values of the RPA matrix  $\mathcal{K}$ . Then the evolution of  $\delta f^{(n)}$  is given by:

$$\delta f^{(n)}(t) \equiv \int dt' \mathbf{G}(t' - t) \delta \mathcal{W}^{(n)}(t') \quad (\text{IV.23})$$

with

$$\mathbf{G}(t) = \oint_c \frac{d\omega}{2\pi} e^{i\omega t} \mathbf{G}(\omega) \quad (\text{IV.24})$$

where the integral on the frequencies must be performed on a contour which passes below all the poles of  $\mathbf{G}(\omega)$  and which is closed in the upper or lower plane depending upon the sign of  $t' - t$  in order to preserve the causality. The expression for  $\delta f^{(n)}$  will allow us to compute statistical properties such as the two time correlations function:

$$\begin{aligned} \sigma_{\ell_1 \ell_2}(t_1, t_2) &\equiv \langle \delta f_{\ell_1}^{(n)}(t_1) \delta f_{\ell_2}^{(n)}(t_2) \rangle \\ \sigma_{\ell_1 \ell_2}(t_1, t_2) &= \int dt'_1 dt'_2 \mathbf{G}_{\ell_1 \ell'_1}(t'_1 - t_1) \mathbf{G}_{\ell_2 \ell'_2}(t'_2 - t_2) D_{\ell'_1 \ell'_2}(t'_1, t'_2) \end{aligned} \quad (\text{IV.25})$$

as a function of the elementary properties of the fluctuating term such as its correlation which acts as a diffusion term

$$D_{\ell_1 \ell_2}(t_1, t_2) \equiv \langle \delta \mathcal{W}_{\ell_1}^{(n)}(t_1) \delta \mathcal{W}_{\ell_2}^{(n)}(t_2) \rangle \quad (\text{IV.26})$$

Here we have supposed  $\langle \delta \mathcal{W}^{(n)} \rangle = 0$ . Therefore at the first order the fluctuations do not affect the averaged dynamics. However, it should be noticed that if we go to the second order for the calculation of  $\delta f^{(n)}(t)$  then new terms involving  $\delta \mathcal{W}^{(n)}(t_1) \delta \mathcal{W}^{(n)}(t_2)$  will appear and so the propagation of the average trajectory will depend upon the diffusion term  $D(t_1, t_2)$

[Ba81].

### ***IV.3) Irreversibility and chaos : Master equations and the restoration of the linearity of Liouville equation***

It is important to notice that the presence of a fluctuating term generates an irreversible dynamic. This is reasonable since our lack of information about correlations can only grow. Indeed, two trajectories initialised with the same projections but with different correlations will always deviate one from the other. This is even more clear if the fluctuating term is assumed to be at random. We will see in the following that indeed the entropy is always increasing some times up to its limit when the disorder is maximum.

On the other hand, the mean-field part (or the deterministic) part of the dynamics is in most situations highly non-linear. Therefore mean-field dynamics are expected to exhibit all the phenomenology of non-linear processes: chaos, bifurcations, ... For example, a nucleus travelling at constant velocity can be seen as a solitary wave (or soliton) solution of the non-linear mean-field equations. The possible existence of a strong chaotic regime might be a serious problem since then the theory may lose its predictive power. Moreover, this apparition of chaos may be thought as a puzzle since the initial equation (the Liouville or the Schrödinger equations) is not presenting such a phenomenology since they are completely linear.

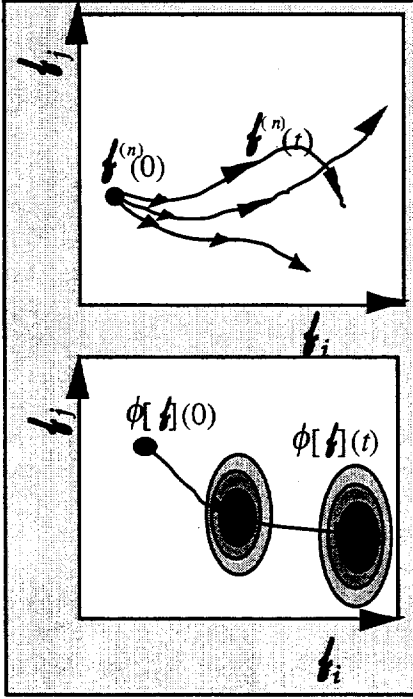
The existence of a fluctuating term provides a natural solution for these problems. Indeed, we have seen in the previous sections that the parametrised or projected approaches are leading to dynamical equations which not only contain a deterministic non-linear average part but also present a fluctuating contribution coming from the unknown correlations. Let us write these equations as

$$\frac{d\mathbf{f}^{(n)}}{dt} = \mathcal{W}(\mathbf{f}^{(n)}) + \delta\mathcal{W}^{(n)}(\mathbf{f}^{(n)}) \quad (\text{IV.27})$$

where the variables  $\mathbf{f}^{(n)}$  are either the parameters  $\mathbf{z}$  or the mean values  $\langle \hat{\mathbf{A}} \rangle$  (or  $\langle \hat{\mathbf{A}} \rangle$ ) from the previous sections. If we now recall that the fluctuating term is coming from the unknown correlations associated with each realisation of the considered system which are independent from one event to another. Therefore, Eq. (II.39) are describing the evolution of an ensemble of independent events (i.e., the evolution of each trajectory  $\mathbf{f}^{(n)}$  just depends on  $\mathbf{f}^{(n)}$  itself but not on the other members of the ensemble).

An alternative way to represent the ensemble of trajectories  $\mathbf{f}^{(n)}$  is to introduce distribution in the  $\mathbf{f}$  space:

$$\phi[\mathbf{f}] = \frac{1}{N} \sum_{n=1}^N \delta[\mathbf{f}^{(n)} - \mathbf{f}] \quad (\text{IV.28})$$



**Figure IV.2:**

Schematic figure showing how to represent an ensemble of trajectories by a time dependent distribution.

This distribution follows a master equation (often approximated by generalised Fokker-Planck equation [Bu91])

$$\frac{\partial \phi}{\partial t} = \mathcal{D}\{\phi\} \quad (\text{IV.29})$$

where  $\mathcal{D}\{\phi\}$  is a linear functional of  $\phi$ . The linearity is a direct consequence of the independence of the various trajectories  $f^{(n)}$ . It is also a direct consequence of the linearity of the initial Liouville equation. Indeed, The Liouville equation (in classical or quantum physics) is intrinsically linear because it describes the evolution of independent events. Indeed, if one considers independent events, then the sum of two sets of events is also a set of events. Therefore the distributions of events are trivially additive showing that the evolution operator in the space of the distributions has to be linear.

This linearity of the functional  $\mathcal{D}\{\phi\}$  implies that the evolution of the distribution of trajectories  $\phi[f]$  is regular even if the underlying individual trajectories were completely chaotic. This is not a paradox, for example everybody knows that a statistical ensemble at equilibrium can be perfectly stable while composed of individual realisations that are often chaotic and even ergodic. Therefore, the stochastic theories are *a priori* more predictive than the deterministic approaches because they give a natural solution to the problem of non linear dynamics (chaos, bifurcations,...) in terms of a statistical distribution of trajectories,  $\phi[f]$ . Intuitively, this remark is trivial: if the stochastic contributions are much bigger than the rounding errors of the computer then these errors will not affect the final distribution. Moreover, since the initial condition of any system can never be defined with absolute accuracy the need to consider an ensemble of realisations is the normal situation to consider in physics.

## V) Example of application - The stochastic mean-field theories.

### V.1) General Formulation.

Let us now take an example: the standard mean field approaches. So first we can introduce the coherent state

$$|\psi(\mathbf{Z})\rangle = \hat{R}(\mathbf{Z})|\psi(\mathbf{0})\rangle = \exp\left(\sum_{ij} i(Z_{ij}^- \hat{K}_{ij}^- + Z_{ij}^0 \hat{K}_{ij}^0 + h.c.)\right) |\psi(\mathbf{0})\rangle \quad (\text{V.1})$$

associated with the algebra of pair of particles

$$\begin{cases} \hat{K}_{ij}^- = \hat{c}_i \hat{c}_j \\ \hat{K}_{ij}^0 = \hat{c}_i^+ \hat{c}_j \end{cases} \quad (\text{V.2})$$

where  $\hat{c}_i^+$  and  $\hat{c}_i$  are particle (or quasi particle) creation and annihilation operators. The state  $|\psi(\mathbf{0})\rangle$  can be the vacuum of particles or already a vacuum of quasi particles. This state is nothing but an independent particle state as described by the Thouless theorem and it can be considered as the vacuum of new creation operators related to the  $\hat{c}$  and  $\hat{c}^+$  operators through a regular Bogoliubov transformation [Ri81, Be92, Ch95a].

This state can be characterised by the expectation values of the algebra operators, the so called normal and abnormal densities:

$$\begin{cases} \rho_{ji} = \langle \hat{K}_{ij}^0 \rangle_{\mathbf{Z}} = \langle \hat{c}_i^+ \hat{c}_j \rangle_{\mathbf{Z}} \\ \kappa_{ji} = \langle \hat{K}_{ij}^- \rangle_{\mathbf{Z}} = \langle \hat{c}_i \hat{c}_j \rangle_{\mathbf{Z}} \end{cases} \quad (\text{V.3})$$

In such a context the ground state is obtained by minimising the energy  $E(\mathbf{Z})$  (or  $E(\rho, \kappa)$ ) [Ri81, Be92, Ch95a]

If we now assume that we don't have a pure state but a state for which we know these densities only as statistical average then we can use the same definitions for  $\rho$  and  $\kappa$  only replacing the expectation values  $\langle \dots \rangle$  by statistical averages  $\langle \dots \rangle$ . The density matrix which maximise the entropy under the constraints  $\rho$  and  $\kappa$  is given by

$$\hat{D}(\mathbf{Z}) = \frac{1}{Z_0} \exp\left(\sum_{ij} (Z_{ij}^- \hat{K}_{ij}^- + Z_{ij}^0 \hat{K}_{ij}^0 + h.c.)\right) \quad (\text{V.4})$$

The equilibrium states can be computed maximising the adapted thermodynamical potentials such as the free-energy  $F(\mathbf{Z})$  (or  $F(\rho, \kappa)$ ) [Ri81, Be92, Ch95a].

In order to predict the evolution of the system we can use the analogue of the Ehrenfest equations

$$\frac{d}{dt} \langle \hat{A}_t \rangle = -\langle \{ \hat{H}, \hat{A}_t \} \rangle \quad (\text{V.5})$$

where  $\langle \dots \rangle$  is either the quantum expectation value  $\langle \dots \rangle$  or the statistical average  $\langle \dots \rangle$ . If we

substitute  $\hat{A}_i \equiv \hat{K}_{ij}^e$  in equations (V.5) we can get the equation of motion for the densities  $\rho$  and  $\kappa$ . However, in general the right hand side of equation (V.5) cannot be expressed only in terms of  $\rho$  and  $\kappa$  (see for example [Ch89, Be92, Ch95a]). However it is possible to have an approximate expression by estimating the right hand side of equation (V.5) on either the coherent states or the minimum entropy density matrix:

$$\begin{cases} \frac{d}{dt}\rho_{ji} = -\langle \{ \hat{H}, \hat{c}_i^\dagger \hat{c}_j \} \rangle_z = \mathcal{W}_{ji}^0(\rho, \kappa) \\ \frac{d}{dt}\kappa_{ji} = -\langle \{ \hat{H}, \hat{c}_i \hat{c}_j \} \rangle_z = \mathcal{W}_{ji}^-(\rho, \kappa) \end{cases} \quad (V.6)$$

These are the mean-field equations (time dependent Hartree-Fock-Bogoliubov equations). However, one must not forget that these equations differ from the equations (V.5) because of the lack of all the correlations which are not described by one-body densities  $\rho$  and  $\kappa$ , and which are not contained in the coherent state or parametrised density matrix. Therefore, we must in fact solve the following equation

$$\begin{cases} \frac{d}{dt}\rho_{ij} = -\langle \{ \hat{H}, \hat{c}_j^\dagger \hat{c}_i \} \rangle = \mathcal{W}_{ij}^0(\rho, \kappa) + \delta\mathcal{W}_{ij}^0(\rho, \kappa) \\ \frac{d}{dt}\kappa_{ij} = -\langle \{ \hat{H}, \hat{c}_j \hat{c}_i \} \rangle = \mathcal{W}_{ij}^-(\rho, \kappa) + \delta\mathcal{W}_{ij}^-(\rho, \kappa) \end{cases} \quad (V.7)$$

which contains a fluctuating term introduced to take care of the difference between Eq (V.5) and (V.6).

## V.2) TDHF and beyond.

Let us take an example in which  $\hat{H}$  contains only a two-body interaction

$$\hat{H} = \sum_{ij} \varepsilon_{ij} \hat{c}_i^\dagger \hat{c}_j + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k \quad (V.8)$$

and let us consider the case where only the operators  $\hat{K}_{ij}^0$  are taken into account (i.e., cases for which the abnormal density is kept zero). The commutator between  $\hat{H}$  and  $\hat{K}_{ij}^0$  reads

$$i\{\hat{H}, \hat{c}_i^\dagger \hat{c}_j\} = \sum_k \varepsilon_{ki} \hat{c}_k^\dagger \hat{c}_j - \varepsilon_{jk} \hat{c}_i^\dagger \hat{c}_k + \frac{1}{2} \sum_{klm} V_{klmi} \hat{c}_k^\dagger \hat{c}_l^\dagger \hat{c}_m \hat{c}_j - V_{jklm} \hat{c}_i^\dagger \hat{c}_k^\dagger \hat{c}_m \hat{c}_l \quad (V.9)$$

Therefore, the part of the commutator coming from the two-body interaction cannot be expressed as a linear combination of the  $\hat{K}_{ij}^0$  operators. Therefore, the right hand side of equation (V.7) will contained the mean value of a two body operator which can be expressed as

$$\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l \rangle = \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l \rangle_z + \sigma_{klij} = \rho_{li} \rho_{kj} - \rho_{ki} \rho_{lj} + \sigma_{klij} \quad (V.10)$$

where  $\sigma_{klij}$  correspond to the two body correlations while  $\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l \rangle_z = \rho_{li} \rho_{kj} - \rho_{ki} \rho_{lj}$  represents the minimum biased two-body density when only the one-body density  $\rho$  is known. Then the equation of motion for  $\rho$  becomes

$$\frac{d}{dt}\rho_{ij} = -\langle \{ \hat{H}, \hat{c}_j^\dagger \hat{c}_i \} \rangle = \{\mathbf{W}, \rho\}_{ij} + \delta\mathcal{W}_{ij}(\sigma) \quad (V.11)$$

where  $\mathbf{w}$  is the mean-field Hamiltonian

$$\mathbf{w}_{ij} = \varepsilon_{ij} + \sum_{kl} V_{ijkl} \rho_{lk} \quad (\text{V.12})$$

The term  $\delta\mathcal{W}(\sigma)$  represents the effect of the two body correlations on the dynamics of the one body density. This term will always be approximated since it is impossible to know all the possible correlations. In the following applications this Langevin term will be either a fluctuating mean-field term [Ba81, Ba88, La89, Ch89] or directly a random force like in the transport equations associated with the Brownian dynamics [Co93, Ch94], or to a fluctuating collision term as in the Boltzmann-Langevin approach [Ba87, Be88, Ay88, Ay90, Ra90, Ch91, Bu91, Ch92b]. In this paper we will present briefly these different methods, more complete discussions can be found in the cited literature.

### ***V.3) Iterative Time Smoothing and Brownian approximation.***

The simplest idea is to suppose that we have absolutely no information about the fluctuating term except may be its global magnitude. For example, in ref. [Ba81], Balian and Vénéroni have proposed to add a random noise in the mean-field Hamiltonian. For sake of simplicity they even assumed that the additional random Hamiltonian was commuting with the mean-field Hamiltonian. In such a way only the single particle energies were fluctuating.

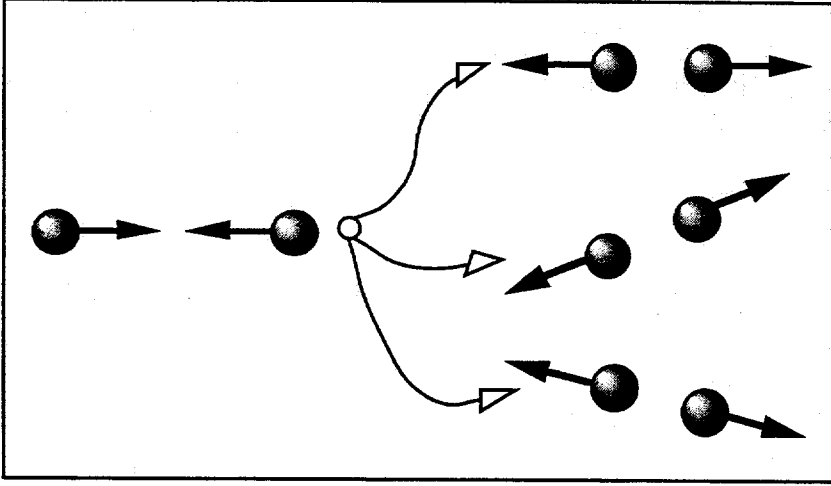
Computing the trajectory averaged over the whole fluctuating ensemble leads to the so-called ITS (iterative time smoothing) equation [Ba81] which have been studied in refs. [Ba88, La89, Ch89]. These approaches are however very phenomenological because the magnitude of the random noise is somehow arbitrary. In references [Ba88, La89, Ch89] the amount of fluctuation and dissipation introduced by the additional fluctuating term have been fitted to reproduce the known width of giant resonances as we will see in the next chapter.

In the semi-classical context the same ideas have been developed in ref. [Co93, Ch94]. Indeed, in ref. [Ch94] we assume that along with the regular mean field the nucleons are experiencing an additional random force coming from the unknown correlations such as the collisions. This would correspond to the transport equation for the pollen particles in a description “a la Langevin” of the Brownian motion. We will also show how the properties of this random force can be derived from more microscopic theories such as the Boltzmann-Langevin approaches which we will be described in the next section.

In the case of unstable system we will show that even simpler stochastic approaches might be used such as a direct introduction of a noise inside the initial condition or even the use of the intrinsic noise of some numerical algorithm [Co93, Co94a, Co94]. These approaches will be discussed in the chapter about phase transitions.

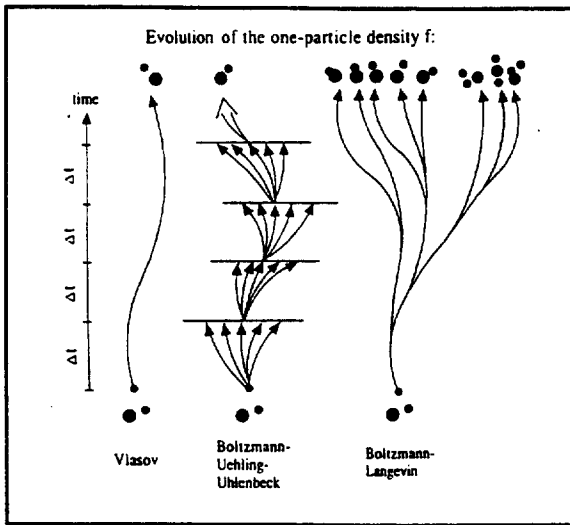
### ***V.4) Boltzmann-Langevin equation.***

Another widely used stochastic mean-field approach is the Boltzmann-Langevin theory [Ba87, Be88, Ay88, Ay90, Ra90, Ch91, Bu91, Ch92b] which can be applied in classical and semi-classical dynamics. This approach is very close from the Boltzmann theory and leads to a fluctuating collision term. The average value of this fluctuating term is nothing but the standard Boltzmann collision term while the difference in the actual collisions experienced by the various trajectories introduces a large degree of stochasticity.



**Figure V.1:**  
Illustration of the collision seen as a stochastic process. The Boltzmann - Langevin theory is nothing but the formal formulation of this random aspect of the collisions.

We can then have a schematic picture of all the approximations involved. In the mean-field approximation only the average evolution is considered. In the Boltzmann approaches, the collisions are taken into account but the fluctuations are averaged out regularly after each collision to be able to define a unique trajectory. Finally, in the Boltzmann-Langevin approaches every branching induced by the collision is followed over the whole time interval. Therefore one deals with a large ensemble of trajectories.



**Figure V.2:**  
Schematic illustration of the different approximations from the mean field to the full Boltzmann-Langevin approaches. Among all these approximations only the stochastic approach is presenting strong many-body correlations because it provides an ensemble of events that can be very different one from the other.

#### V.4.A) Derivation through the BBGKY hierarchy.

In ref. [Ay90] the Boltzmann-Langevin equation is derived using the hierarchy of many body operators (from the one-body to the A-body) operators computing the Ehrenfest equations for this ensemble of observations leads to the well-known BBGKY hierarchy. If we keep only the one-body operators for the final description of the system and if we disregard all the other many-body observables but the two-body operators which will be eliminated according to the procedure describe in section IV the authors of ref. [Ay90] obtain an explicit description of the stochastic evolution of the one-body density. This is a rather straightforward but lengthy application of the formalism described in section IV; For a more details we strongly suggest that the reader consults the reference [Ay90]. In this article we will rather discuss an alternative way to derive the very same equation using simpler arguments.



#### V.4.B) Heuristic derivation using fluctuating collision numbers

The authors of ref.[Ra90,Bu91] developed a more intuitive approach simply based upon the Boltzmann picture of collisions. In addition to the usual mean field evolution they consider that the inclusion of direct two-body collisions subjects the individual nucleons to irregular forces which in turn produce random changes in the one-body phase-space density  $f$ . Consequently, in such a scenario, the dynamical evolution exhibits a continual branching and the temporal distribution of  $f$  is no longer a single trajectory but an ever widening bundle of trajectories. The task is to treat this diffusive behavior within the framework of transport theory.

For this purpose they consider an ensemble of identical many-body systems, labelled by  $n \in [1, N]$ . If we assume that the systems have been prepared in the same manner, so that their one-body phase-space densities  $f^{(n)}(\mathbf{r}, \mathbf{p}, t=0)$  are all equal (at the initial time), they are generally different at the many-body level. Due to the stochastic nature of the residual two-body interaction, the individual many-body systems evolve differently and it is convenient to write the phase-space density of an individual system  $n$  in the form

$$f^{(n)}(\mathbf{r}, \mathbf{p}, t) = f(\mathbf{r}, \mathbf{p}, t) + \delta f^{(n)}(\mathbf{r}, \mathbf{p}, t) \quad (\text{V.13})$$

Here  $f(\mathbf{r}, \mathbf{p}, t)$  is the average of the one-particle phase-space densities for all the individual systems in the ensemble,

$$f(\mathbf{r}, \mathbf{p}, t) \equiv \langle f^{(n)}(\mathbf{r}, \mathbf{p}, t) \rangle \equiv \frac{1}{N} \sum_n f^{(n)}(\mathbf{r}, \mathbf{p}, t) \quad (\text{V.14})$$

where we have introduced the notation  $\langle \dots \rangle$  to denote the ensemble average. The quantity  $\delta f^{(n)}(\mathbf{r}, \mathbf{p}, t)$  denotes the deviation of the phase-space density for the individual system from the ensemble average; by definition its ensemble average vanishes,  $\langle \delta f^{(n)}(\mathbf{r}, \mathbf{p}, t) \rangle = 0$

In order to characterise the fluctuations of  $f^{(n)}$  away from the ensemble average  $f$  it is convenient to introduce the following correlation function for the one-particle phase-space occupancy,

$$\sigma(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}', t) \equiv \langle f^{(n)}(\mathbf{r}, \mathbf{p}, t) f^{(n)}(\mathbf{r}', \mathbf{p}', t) \rangle - \langle f^{(n)}(\mathbf{r}, \mathbf{p}, t) \rangle \langle f^{(n)}(\mathbf{r}', \mathbf{p}', t) \rangle \quad (\text{V.15})$$

$$\sigma(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}', t) \equiv \langle \delta f^{(n)}(\mathbf{r}, \mathbf{p}, t) \delta f^{(n)}(\mathbf{r}', \mathbf{p}', t) \rangle \quad (\text{V.16})$$

From now on we will omit the time argument  $t$  in order to simplify the notation. Here we will mainly concentrate on one-body observables. Such observables have an expectation value for each of the  $N$  systems and these are generally different, because the associated one-body densities  $f^{(n)}$  differ. For a standard one-body observable of the form  $\hat{A}(\mathbf{r}, \mathbf{p})$ , the expectation value for the system  $n$  is :

$$\langle \hat{A} \rangle^{(n)}(t) = \int \frac{d\mathbf{r} d\mathbf{p}}{h^3} \hat{A}(\mathbf{r}, \mathbf{p}) f^{(n)}(\mathbf{r}, \mathbf{p}, t) \quad (\text{V.17})$$

and the expectation value calculated with the ensemble-average phase-space density is simply given by :

$$\langle \hat{A} \rangle(t) = \frac{1}{N} \sum_n \langle \hat{A} \rangle^{(n)}(t) = \int \frac{d\mathbf{r} d\mathbf{p}}{h^3} \hat{A}(\mathbf{r}, \mathbf{p}) f(\mathbf{r}, \mathbf{p}, t) \quad (\text{V.18})$$

The covariance between two standard one-body observables  $\hat{A}$  and  $\hat{B}$  can be expressed in terms of the correlation function :

$$\sigma_{AB} = \langle \hat{A}\hat{B} \rangle(t) - \langle \hat{A} \rangle(t) \langle \hat{B} \rangle(t) = \int \frac{d\mathbf{r}d\mathbf{p}}{h^3} \frac{d\mathbf{r}'d\mathbf{p}'}{h^3} \hat{A}(\mathbf{r},\mathbf{p})\hat{B}(\mathbf{r}',\mathbf{p}')\sigma(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}',t) \quad (\text{V.19})$$

The stochastic contribution to the evolution of the phase-space occupancy is relatively easy to treat when the random force is given in terms of the Uehling-Uhlenbeck collision term, which is generated by a stochastic sequence of individual transitions in the system. The mean number of transitions in which nucleons are scattered from two phase-space elements around the locations  $s_1, s_2, s \equiv (\mathbf{r}, \mathbf{p})$  into two other phase-space elements around  $s_1', s_2'$ , is given by

$$dv_{1,2;1',2'} = f_1 f_2 \bar{f}_{1'} \bar{f}_{2'} \delta(\mathbf{r}) \Omega(\mathbf{p}) ds_1 ds_2 ds_{1'} ds_{2'} \quad (\text{V.20})$$

Here  $f_i \equiv f(\mathbf{r}_i, \mathbf{p}_i)$  is the phase-space occupancy at one of the initial locations and  $\bar{f}_i \equiv 1 - f(\mathbf{r}_i, \mathbf{p}_i)$  are the Pauli blocking factors expressing the availability at the final locations. Moreover, the phase-space elements  $ds \equiv d\mathbf{r}d\mathbf{p}/h^D$  where  $D$  is the dimension of the physical space. The elementary transition rate incorporates energy-momentum conservation and can be related to the cross section of the colliding nucleons,

$$\int W(\mathbf{p}) \frac{d\mathbf{p}_1 d\mathbf{p}_2}{h^{2D}} = v_{1,2} \int d\Omega_{1',2'} \frac{d\sigma}{d\Omega} \quad (\text{V.21})$$

where  $\Omega_{1',2'}$  represents the direction of relative motion after the collision and  $v_{1,2}$  is the relative speed of the two colliding nucleons. Since the collisions are regarded as random processes analogous to a random walk, the number of transitions actually occurring during a time step  $\Delta t$  fluctuates according to the corresponding Poisson distribution:

$$v_{1,2;1',2'}^{(n)} = v_{1,2;1',2'} + \Delta v_{1,2;1',2'}^{(n)},$$

where the average is nothing but the Boltzmann collision term

$$v_{1,2;1',2'} = \int_{\Delta 1, \Delta 2; \Delta 1', \Delta 2'} dv_{1,2;1',2'} \Delta t$$

while the fluctuation are following the Poisson relation<sup>1</sup>

$$\langle \Delta v_{1,2;1',2'}^{(n)} \Delta v_{1',2';1'',2''}^{(n)} \rangle = v_{1,2;1',2'} \delta_{(1,2;1',2'),(1',2';1'',2'')}$$

The stochastic nature of the two-body interaction causes each individual many-body system to evolve differently, and will generate an entire bundle of dynamical trajectories  $f^{(n)}$  which can be described by the following distribution

$$\phi[f] = \frac{1}{N} \sum_{n=1}^N \delta[f^{(n)} - f] \quad (\text{V.22})$$

which gives the probability that a randomly selected system  $n$  has the specified occupancy function  $f$ .

<sup>1</sup> It should be noticed the relation between the average and the variance of the actual collision number can be considered as a microscopic realisation of the collision-dissipation theorem.

Since the two-body collision rate is assumed to depend only on  $f^{(n)}$  at the actual time  $t$ , the evolution of each system of the ensemble is a typical Markovian process, i.e. it does not depend on the particular history experienced by the system. In transport theory, the Markovian evolution of the distribution  $\phi(f)$  is given by a master equation which expresses the rates of transition between one density  $f$  and another  $f'$ . Under suitable smoothness conditions, the master equation can be recasted as a differential equation of the Fokker-Planck type,

$$\frac{d}{dt}\phi[f] = \sum_{k=1} \int ds_1 \dots ds_k \frac{\partial^k}{\partial f(s_1) \dots \partial f(s_k)} (\alpha_k[f](s_1, \dots, s_k) \phi[f]) \quad (\text{V.23})$$

Since the stochastic collisional process is of two-body form, only four phase-space locations are involved and the sum can be stopped at the fourth order. If we consider only one-body observables, the Fokker-Planck equation can be truncated at the second order. The transport coefficients can be derived from the early growth rate of the  $n$ -body correlations. Here we'll discuss only the first and second order.

It is instructive to perform a moment expansion of the distribution  $\phi[f]$ . The first moment is the mean trajectory is given by

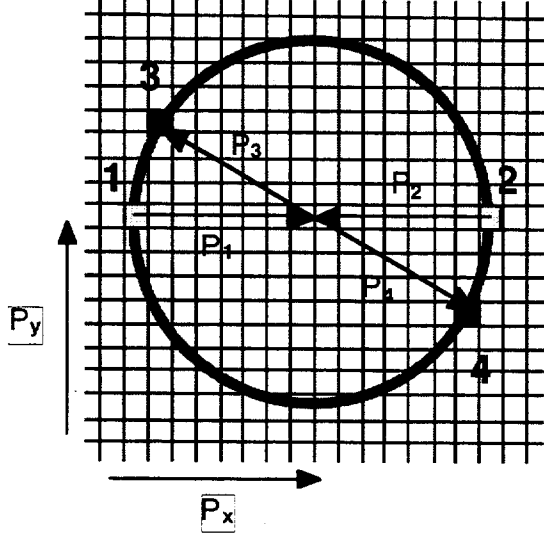
$$\langle f \rangle = \frac{1}{N} \sum_{n=1}^N f^{(n)} \equiv \int D[f] f \phi[f] \quad (\text{V.24})$$

the integral being a functional integral over the phase-space density  $f$ . The time evolution of  $\langle f \rangle$  can readily be obtained from the Fokker-Planck equation via a partial integration that eliminates all the higher-order terms,

$$\frac{d}{dt} \langle f \rangle = \int D[f] \alpha_1[f] \phi[f] \equiv \langle \alpha_1[f] \rangle \equiv \alpha_1[\langle f \rangle] \quad (\text{V.25})$$

The last relation represents the mean-trajectory approximation, in which the ensemble average of the coefficient  $\alpha_1[f]$  is replaced by its value for the average distribution  $\langle f \rangle$ . This approximation is valid when the distribution  $\phi[f]$  is relatively narrow.

In particular, it is accurate for the early evolution when the distribution  $\phi[f]$  has been prepared so as to be concentrated around a single phase-space density  $f_0$ , i.e.  $\phi[f] = \delta[f_0 - f]$ . Thus the initial average rate of change of  $f$  is given by the corresponding value of  $\alpha_1[f]$  and therefore this quantity is called the *drift coefficient*.



**Figure V.3:** Schematic illustration of the kinematics of the collision of the cell 1 with the cell 2 leading to the cells 3 and 4 on the sphere of constant momentum and energy.

There are two distinct contributions to the mean evolution, namely the Vlasov evolution of  $f$  in its mean field and the dissipative evolution arising from the two-body collisions. The former contribution is relatively trivial and will be left out of our further discussion; of course it should be properly included in any actual calculation. As for the contributions from the collisions, they fall into two categories : the *loss* term, for which the specified phase-space location  $(\mathbf{r}, \mathbf{p})$  corresponds to the initial state of one of the colliding nucleons, and the *gain* term, for which the specified phase-space location represents one of the two final states. Therefore, the drift coefficient  $\alpha_1[f]$  can be written as

$$\alpha_1[f](s) = \bar{f}(s)W^+(s) - f(s)W^-(s) \quad (\text{V.26})$$

where the coefficients  $W^+(s)$  and  $W^-(s)$  are given through the relations

$$\begin{aligned} f(s)W^-(s) &= \frac{1}{2} \int dv_{1,2;1',2'} \delta(s_1 - s) \\ \bar{f}(s)W^+(s) &= \frac{1}{2} \int dv_{1,2;1',2'} \delta(s_{1'} - s) \end{aligned} \quad (\text{V.27})$$

Here  $dv_{1,2;1',2'}$  is the collision number discussed above and the factor of one-half compensates for the double counting.

The deviations of the individual trajectories around the mean is conveniently characterised by the covariance

$$\sigma(s, s') = \langle f(s)f(s') \rangle - \langle f(s) \rangle \langle f(s') \rangle = \int D[f] \delta f(s) \delta f(s') \phi[f] \quad (\text{V.28})$$

Performing two partial integrations of the Fokker-Planck equation, we obtain its time evolution

$$\begin{aligned} \frac{d}{dt} \sigma(s, s') &= \int D[f] \alpha_2[f](s, s') \phi[f] \\ &+ \int D[f] \int ds'' \left( \frac{\partial \alpha_1[f](s)}{\partial s''} \delta f(s'') \delta f(s') + (s \leftrightarrow s') \right) \phi[f] \end{aligned} \quad (\text{V.29})$$

If the initial distribution is narrow, the above relation reduces to

$$\frac{d}{dt}\sigma(s, s', t_0) = \alpha_2[f_0](s, s') \quad (\text{V.30})$$

The coefficient  $\alpha_2[f_0](s, s')$  thus expresses the early accumulation of the covariance between the two phase-space locations  $s$  and  $s'$ , and it is related to the *diffusion coefficient* by  $\alpha_2(s, s') = 2D(s, s')$ . Just as the drift coefficient, the diffusion coefficient can be determined by considering the early growth of the fluctuations of an initially narrow distribution, using the above relation.

In ref. [Ra90] it has been shown that is useful to split the covariance into the diagonal and out of diagonal part,

$$\sigma(s, s') = \sigma^2(s)\delta(s - s') + \sigma_{\text{cov}}(s, s') \quad (\text{V.31})$$

In this decomposition, the quantity  $\sigma^2(s)$  represents the variance in the occupancy of a given elementary phase-space cell at the location  $s$  whereas the remaining part  $\sigma_{\text{cov}}(s, s')$  expresses the correlation between the occupancy of the two different cells located at  $s$  and  $s'$ . These two quantities are related by the unitarity relation,

$$\sigma^2(s) = -\int ds' \sigma_{\text{cov}}(s, s') \quad (\text{V.32})$$

coming from the conservation of particle number. It then follows that the corresponding diffusion coefficient can also be decomposed in its diagonal part and a covariant part; these two part being related by a unitarity sum rule.

The latter can be obtained from a consideration of the early growth of the covariance  $\sigma_{\text{cov}}(s, s')$  for an initially narrow distribution,

$$\begin{aligned} \alpha_2^{\text{cov}}[f](s, s') &= \bar{f}(s)\bar{f}(s')W^{++}(s, s') + f(s)f(s')W^{--}(s, s') \\ &\quad - f(s)\bar{f}(s')W^{+-}(s, s') - \bar{f}(s)f(s')W^{-+}(s, s') \end{aligned} \quad (\text{V.33})$$

where the following quantities have been introduced

$$\begin{aligned} f(s)f(s')W^{--}(s, s') &= \frac{1}{2} \int dv_{1,2;1',2'} \delta(s_1 - s)\delta(s_2 - s') \\ \bar{f}(s)\bar{f}(s')W^{++}(s, s') &= \frac{1}{2} \int dv_{1,2;1',2'} \delta(s_1 - s)\delta(s_2 - s') \\ \bar{f}(s)f(s')W^{+-}(s, s') &= \frac{1}{2} \int dv_{1,2;1',2'} \delta(s_1 - s)\delta(s_1 - s') \\ f(s)\bar{f}(s')W^{-+}(s, s') &= \frac{1}{2} \int dv_{1,2;1',2'} \delta(s_1 - s)\delta(s_1' - s') \end{aligned} \quad (\text{V.34})$$

The unitarity relation then yields the diagonal diffusion coefficient,

$$\alpha_2^2[f](s) = \bar{f}(s)W^{+}(s) + f(s)W^{-}(s) \quad (\text{V.35})$$

These results derived above for the first and second moments can be used to obtain equations of motion in the case when the bundle of trajectories is relatively well confined to the neighbourhood of the mean trajectory. In this simple case the integrals can be evaluated approximately on the basis of the mean trajectory only. For the first moment we obtain the following closed equation,

$$\frac{d}{dt} \langle f \rangle \cong \alpha_1 [\langle f \rangle] = \langle \bar{f} \rangle W^+(s) - \langle f \rangle W^-(s) \quad (\text{V.36})$$

In the following the arguments  $\langle f \rangle$  are often omitted in the  $W$  coefficients, in order to simplify the formulae.

The time derivative of the second moment is more complicated,

$$\frac{d}{dt} \sigma(s, s') \approx \alpha_2 [\langle f \rangle](s, s') + \int ds'' \frac{\partial \alpha_1(s)}{\partial f(s'')} \sigma(s'', s') + \{s \leftrightarrow s'\} \quad (\text{V.37})$$

Thus, in order to obtain the equation for the second moment of the distribution  $\phi[f]$ , one needs to calculate the derivative of  $\alpha_1$  with respect to the value of  $f$  at the phase-space location  $s$ . This can be accomplished from the expression of  $\alpha_1$ . Therefore, using the equations above we arrive at a closed form for the evolution of the covariance,

$$\begin{aligned} \frac{d}{dt} \sigma_{\text{cov}}(s, s') = & f(s)f(s')W^-(s, s') + \bar{f}(s)\bar{f}(s')W^{++}(s, s') \\ & - f(s)\bar{f}(s')W^{+-}(s, s') - \bar{f}(s)f(s')W^{-+}(s, s') \\ & + \bar{f}(s)\sigma^2(s') (W^{+-}(s, s') - W^{++}(s, s')) \\ & - f(s)\sigma^2(s') (W^-(s, s') - W^{-+}(s, s')) \\ & + \int ds'' \sigma_{\text{cov}}(s'', s') (\bar{f}(s) (W^{+-}(s, s'') - W^{++}(s, s'')) - f(s) (W^-(s, s'') - W^{-+}(s, s''))) \\ & + \sigma_{\text{cov}}(s, s') (W^+(s) + W^-(s)) \\ & + s \leftrightarrow s' \end{aligned} \quad (\text{V.38})$$

Introducing the combinations

$$\begin{aligned} Z^-(s, s') &= f(s')W^-(s, s') - \bar{f}(s')W^{-+}(s, s') \\ Z^+(s, s') &= \bar{f}(s')W^{++}(s, s') - f(s')W^{+-}(s, s') \\ Z(s, s') &= Z^-(s, s') + Z^+(s, s') \end{aligned} \quad (\text{V.39})$$

and using the unitarity relation to eliminate the variance, the expression above can be simplified,

$$\begin{aligned} \frac{d}{dt} \sigma_{\text{cov}}(s, s') &= f(s)Z^-(s, s') + \bar{f}(s)Z^+(s, s') \\ &+ \int ds'' \sigma_{\text{cov}}(s'', s) Z(s'', s') + \sigma_{\text{cov}}(s, s') Z(s', s'') - \sigma_{\text{cov}}(s', s'') Z(s'', s') \\ &+ s \leftrightarrow s' \end{aligned} \quad (\text{V.40})$$

The equation of evolution of the variance  $\sigma^2$  can be derived from the above result by performing the integration over  $s'$ ,

$$\frac{d}{dt}\sigma^2(s) = f(s)W^-(s) + \bar{f}(s)\bar{f}(s')W^+(s) - 2\sigma^2(s)(W^+(s) + W^-(s)) \quad (\text{V.41})$$

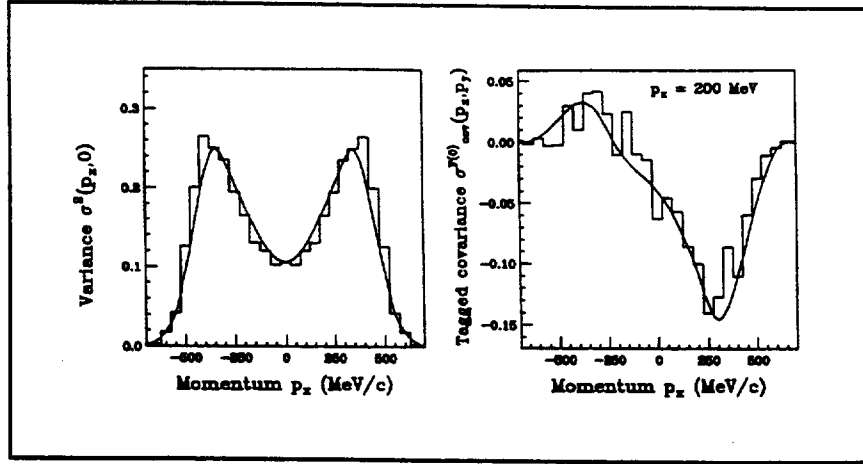
It is easy to show that the deviation  $\Delta = \sigma^2 - f\bar{f}$  evolves according to

$$\frac{d}{dt}\Delta(s) = -\Delta(s)(W^+(s) + W^-(s)) \quad (\text{V.42})$$

This equation shows that  $f\bar{f}$  is the instantaneous equilibrium value towards which  $\sigma^2$  will relax in the course of time. Moreover,  $\Delta = 0$  is a solution to this equation and so the variance  $\sigma^2$  remains equal to  $f\bar{f}$  provided that this condition is fulfilled at the initial time. The relation  $\sigma^2 = f\bar{f}$  is recognised as the standard result for the variance of the Fermi-Dirac occupancy at equilibrium. In a quantum-mechanical description, this result can be derived by considering an ensemble of Slater determinants whose orbitals are either entirely vacant or fully occupied.

#### V.4.C) Test of the approach.

In the case of a fermion gas we have demonstrated that the Boltzmann Langevin approach provides a good statistical limit as far as mean values, correlations and fluctuations are concerned [Ch91, Bu91, Bu94].



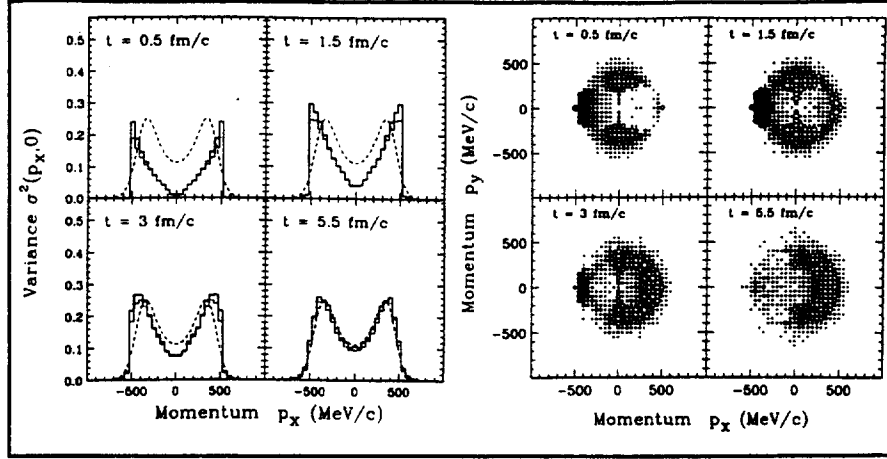
**Figure V.4:**

Figure extracted from references [Ch91, Bu91, Bu94] showing that the Boltzmann-Langevin approach correctly describes the thermalisation of a fermion gas. The left part shows the fluctuations of the occupation of the phase space while the left part presents the correlations of a second particle with a particle detected in the forward direction. The histogram is the asymptotic result of our Boltzmann-Langevin simulations starting from a highly non equilibrated system while the solid line presents the thermodynamical predictions.

Moreover, it has been shown that the Boltzmann-Langevin simulations correctly describe the dynamics of fluctuations. For example, references [Ch91, Bu91] study the thermalisation of two colliding Fermi fluids. We show that the fluctuations of  $f(\mathbf{p}, t)$  in phase space follows the relation

$$\sigma^2(\mathbf{p}, t) = f(\mathbf{p}, t)(1 - f(\mathbf{p}, t)) \quad (\text{V.43})$$

which is what is expected in the case of a fermion fluid.



**Figure V.5:**

Boltzmann-Langevin simulation of the collision of two Fermi fluids. The left part shows the fluctuations in phase space as function of time. The thick histograms are the result of the simulations while the dashed line represents the thermodynamical limit. The thin histograms correspond to the fluctuation  $\sigma^2(p, t) = f(p, t)(1 - f(p, t))$ . The right part presents the correlation in phase space associated with the detection of a forward particle.

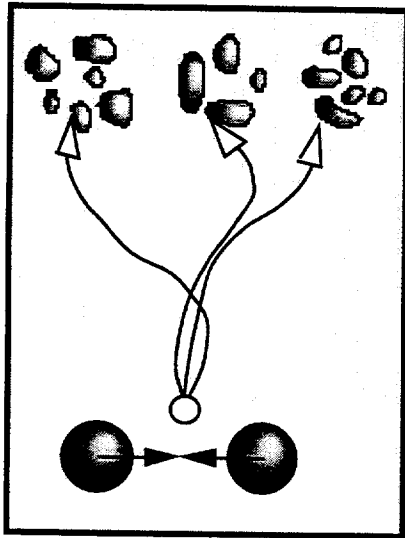
The Boltzmann-Langevin theory appears therefore well founded and promising as far as the possibility to describe fluctuations in a dynamical system is concerned. In the chapters devoted to the problem of instabilities and phase transitions we will apply this theory to the catastrophic dynamics associated with spinodal decomposition.

### V.5) Application of the Boltzmann-Langevin approaches to phase transition

Let us now consider the problem of liquid-gas phase transitions, spontaneous symmetry breaking, multifragmentation and nuclear collisions.

During the multifragmentation of atomic nuclei it seems that identical (or almost identical) initial conditions are leading to very different partitions of the system in interaction (see fig. V.5). In such a case it is necessary to develop approaches that are able to describe the observed extra-ordinary diversity of the final channels. On the other hand the multifragmentation being characterised by the formation of relatively large fragments, one may think that the mean field plays an important role to organise the system in nuclei. Indeed, the mean field (i.e., the long range part of the bare nucleon-nucleon interaction) is at the origin of the cohesion of the nuclei. Moreover, it has been shown that mean-field approaches or one-body approaches including "à la Boltzmann" collision terms were providing excellent descriptions of many aspects of heavy ion reactions around the Fermi energy (see for example [Be88] and references therein).





**Figure V.6:**

Illustration of the fact that heavy ion reactions may lead to a large variety of final partitions even starting with almost identical initial conditions.

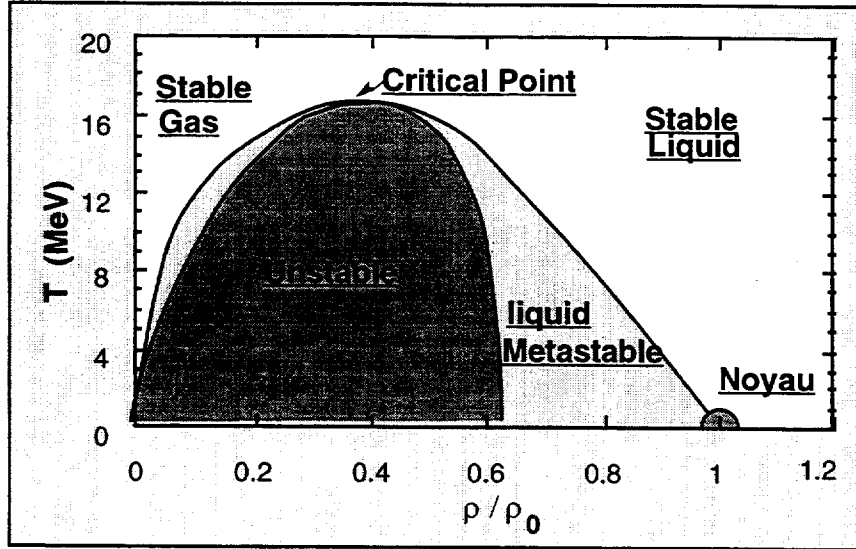
The problem with bare mean-field approaches is that they are unable to break spontaneously symmetries. Therefore, they cannot describe phenomena where bifurcations, instabilities or chaos occurs. However, since few years, many tests and studies have been performed showing that the stochastic extensions of mean-field approaches were good candidates for the description of catastrophic processes. Indeed, the presence of a source of stochasticity allows to explore a large variety of evolutions. Therefore, such approaches may provide valuable descriptions of the dynamics of phase transitions (at least in the case of first-order phase transitions for which the mean-field is known to give a reasonable description of equilibrium properties).

We will see that this description of the dynamics of first order phase transitions in infinite and finite system is now partial achieved. An important conclusion is that in some specific cases we have shown that well-defined collective motions were initiating the self-organisation of the unstable matter in fragments. We will see that in the case of finite systems the possible signals kept from this early fragmentation stage can inform us on the possible occurrence of a liquid-gas phase transition in nuclei. This is a little analogous to the fact that the observation of the stable compression monopole mode provides a direct information on the nuclear equation of state and in particular on the nuclear incompressibility.

In this chapter, as a continuation of the study of hot giant resonances we will discuss now the properties of collective compression modes when they become unstable because the system lies deep enough in the liquid-gas region. We will illustrate the validity of the considered stochastic approach by studying the case of a classical Van der Waals Gas. We will then discuss the role of the dynamics in the cluster formation far from the spinodal zone.

### V.5.A) Phase Diagram.

Let us first recall that nuclei are understood as a Fermi liquid [Bo67, Bo75, Ri81] and since we can also observe nucleon gas we expect the existence of at least one liquid-gas phase transition (see fig. V.6)



**Figure V.7:**

Illustration of the nuclear matter phase-diagram presenting a Fermi-liquid Fermi-gas phase transition. It should be noticed that the nucleus in its ground state is on the coexistence line because it is in equilibrium with its vapour at 0 vapour saturation pressure.

As matter of fact, the nuclear forces are known to have a long range attractive force and a short range repulsive hard core analogous to a Van der Waals interaction. Therefore, we expect the same phenomenology as far as the phase transitions are concerned.

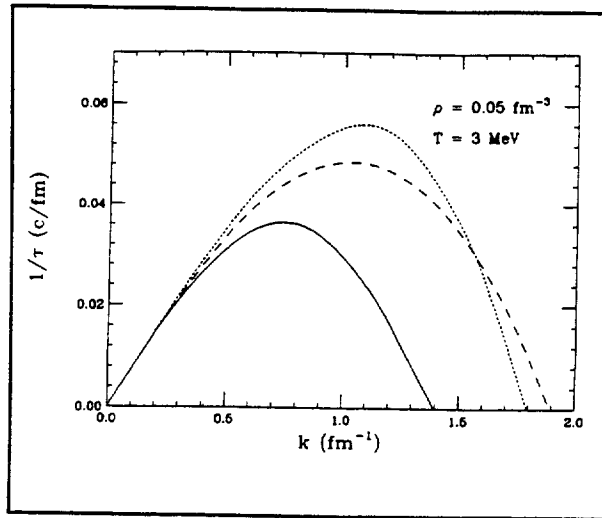
The phase diagram of nuclear matter is still partially unknown because it is very difficult to extract unambiguous information from the experimental observation. Indeed, it is only possible to create in laboratory tiny short-lived fragments of excited matter. However, it is generally believed that during a nuclear collision the system may explore a large portion of the nuclear phase diagram and that the observed copious fragment production might be related to a liquid-gas phase transition.

In particular, it is generally believed and shown by one-body approaches that the system may enter deep in the liquid-gas coexistence region and even in the spinodal zone that is the region where the system is mechanically unstable against infinitesimal density fluctuations. Considering the involved size and time scales this is certainly an adequate region for the nuclear multifragmentation.

### V.5.B) Instability of zero-sound

In the spinodal region the density fluctuations are spontaneously amplified. This region can be investigated by studying the evolution of small density undulations. In particular we can solve the linear response of the considered system in particular solving the RPA equations. In the spinodal region some modes do not oscillate but are simply amplified because of the instability. These modes have an imaginary eigenfrequency (see for example references [Co94a, Co94, Ay95]). This frequency is the inverse of the instability growth time.

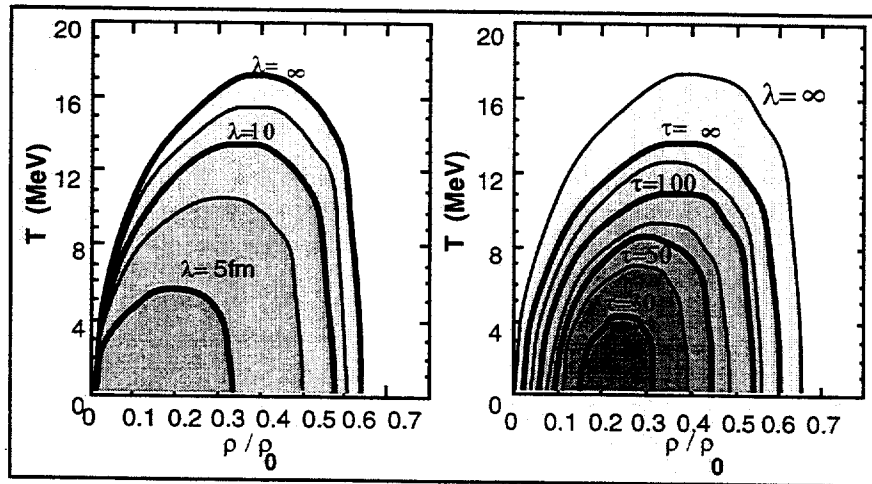
Figure V.7 presents an example a RPA result extracted from reference [Ay95]. This calculation is performed for the infinite nuclear matter at 3 MeV temperature and at about one third of the saturation density. This figure presents the imaginary RPA frequencies as a function of the wave number  $k$  of the considered perturbation. The slope at the origin is the imaginary zero sound velocity as predicted by the Landau theory of Fermi liquids [Fe71, Pe88, Pi89]. The most important characteristic of this dispersion relation is that it presents a strong maximum at a given wave number followed by an ultraviolet cut-off after which the modes are stables. These properties are directly related to the range of the nuclear force and to the nucleon zero-point motion (see [Ay95]). This can be easily understood: when the wave length of the oscillations is shorter than the range of the attractive part of the potential or than the zero point motion of the nucleons it will be washed out in the mean-field and so the corresponding fluctuations will not be amplified.



**Figure V.8**

RPA dispersion relation calculated for a realistic interaction [Ay95] (solid line); the dashed line corresponds to a semi-classical result while the dotted line is associated with a RPA calculation for a zero range force.

The most unstable wave length appears to be around 10 fm. It should be noticed that this wave length does not evolve much in the spinodal region except nearby the spinodal boarder where it rapidly diverges. The limit of the spinodal region corresponds to infinite minimum time of instability and associated wave length. From this point of view this limit has no real meaning for a dynamic evolution of a small system over a finite time. Indeed, such a small system cannot wait an infinite time for the fluctuations to develop and cannot afford infinite wave length because of its limited dimensions.



**Figure V.9:**

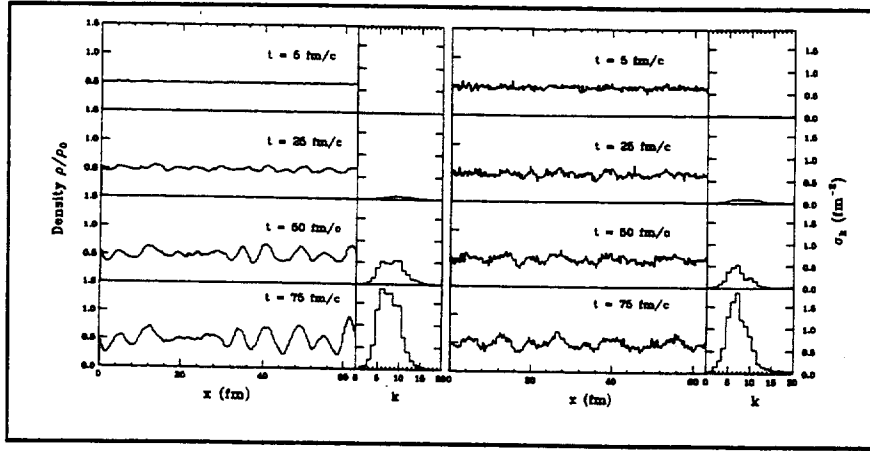
Spinodal zone as a function of the wave length (left) and as a function of the instability time (in fm/c) for a wave length  $\lambda = 10$  fm (right).

By solving the RPA equations for various physical conditions of density and pressure we can define for each wave length a limit of instability (fig V.8) [Co94]. We can observe on the figure that this region reduces with the considered wave length and indeed small wave length appears to be always stable. This figure can also be interpreted as a limit of instability as a function of the size of the system because at least one oscillation inside the system is needed to make the system unstable. The same ideas apply for the time scales. Indeed, for a given wave length one can define a region in which the instability time is shorter than a given time (see Fig. V.8). If now the dynamics of the reaction, such as the expansion of the system, impose a given time scale, one should consider the associated region of instability to discuss the possibility to observe the exponential amplification of the small fluctuations and the formation of fragments through spinodal decomposition.

In fact, if we introduce two typical time and size scales: 10 fm and 100 fm/c one can observe an instability region rather large: approximately one half of the spinodal zone associated with an infinite time of instability for an infinite wave length. Therefore, the above considerations impose a reduction of the instability region but do not imply a strong modification of the spinodal scenario.

### V.5.C) Spontaneous symmetry breaking and stochastic approaches .

In the spinodal region the system does present instabilities. However, in a regular mean-field approach this does not mean that instabilities will develop because there is no mean to break an initial symmetry. To describe this spontaneous symmetry breaking one can use the recently developed stochastic approaches. Figure V.9 shows some results obtained using two versions of such approaches: an application of the Boltzmann-Langevin theory [Bu92, Bu95] and a simplified treatment (see refs. [Co93, Ch94]).



**Figure V.10:**

*Simulation of the evolution of a piece of nuclear matter in two-dimension (see [Bu92, Bu95]). The left part presents a simulation performed according to the Boltzmann-Langevin theory solved on a lattice grid. It should be notice that in absence of a fluctuation source the initial symmetry by translation is always preserved and the system remains in an unstable equilibrium situation. When the stochastic source is taken into account the symmetry is broken and the system can develop clusters after a catastrophic evolution towards multifragmentation. The right part presents the simulation using a simplified stochastic approach as described in ref. [Co93, Ch94]. This comparison shows that in the case of strong instabilities the detailed structure of the source of fluctuation is not important the dynamics being dominated by the amplification of the unstable modes.*

In ref. [Co94a, Co94, Ay96] it is shown that the onset of the instabilities can be described according to the stochastic linear response theory as described in chapter II.4:

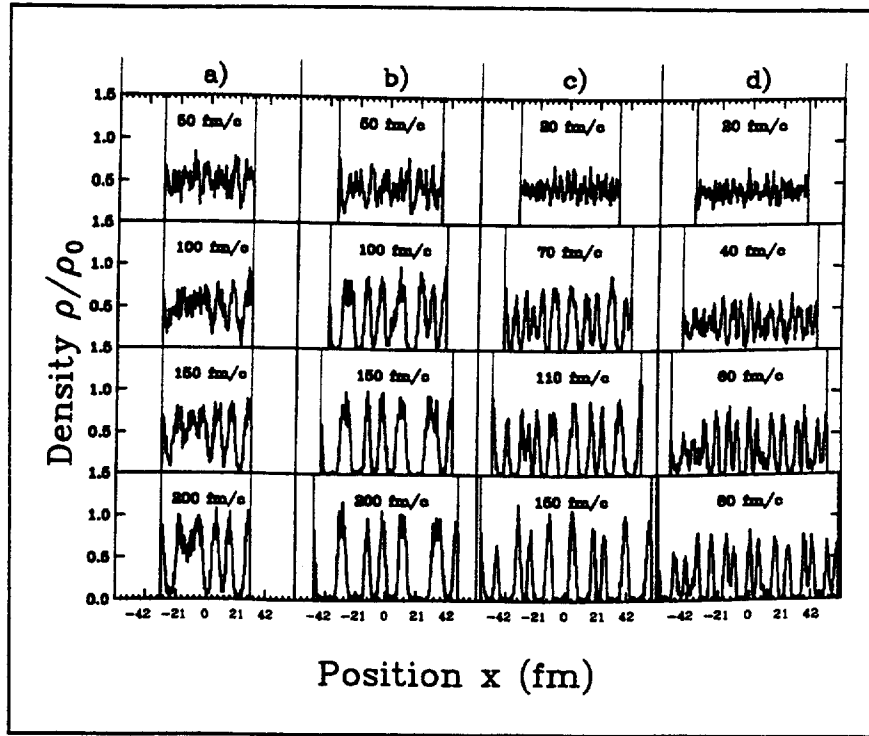
$$\frac{d\delta f_v^{(n)}(t)}{dt} = -i\omega_v \delta f_v^{(n)}(t) + \delta \mathcal{W}_v^{(n)}(t) \quad (\text{V.45})$$

which means that each RPA mode,  $v$ , of frequency  $\omega_v$  is agitated in the event  $n$  by the noise source  $\delta \mathcal{W}_v^{(n)}(t)$ . Therefore after a time  $t$  it is associated with the amplitude  $\delta f_v^{(n)}(t)$ . If we now consider an ensemble of trajectories we can measure the typical fluctuation by the correlation  $\sigma_v(t) = \langle \delta f_v^{(n)}(t) \delta f_v^{(n)}(t) \rangle$ . It is easy to show that this quantity evolve according to the so-called Lalime's equation

$$\frac{d\sigma_v}{dt} = -2i\omega_v\sigma_v + 2D_v \quad (\text{V.46})$$

where  $D_v$  is a diffusion coefficient measuring the strength of the fluctuation source. On the equation the various roles played by the noise and the vibration frequency, are clear: the fluctuation source excites the various modes which are then propagated according to the restoring force related with  $\omega_v$ . When this frequency contains a negative imaginary part the fluctuations are damped and so the system can reach an equilibrium. Conversely when the system presents a positive imaginary energy the fluctuations are amplified and no equilibrium is possible. In the case of the spinodal instabilities we have shown that this linear approach was valid until rather large times ( $t \approx 100 \text{ fm} / c$ ) and that the chaos was playing a minor role. Therefore the peak of  $\sigma_v(t)$  presented in figure VII.6 is a direct image of the peak in the dispersion relation (fig. VII.4). This means that the most unstable wave length introduces a scale for the fragment partition of the system.

Similar calculations can be apply to finite size and expanding systems. Figure VII.7 shows some example of such calculations for periodic systems in expansion. One can see again that the dynamics is dominated by the appearance of a given scale associated with the most unstable wave length. Moreover this wave length is almost independent of the expansion velocity. The main effect is therefore that the fragmentation of a more dilute system is characterised by the apparition of more fragments which are then smaller (see [Co95] for more details).

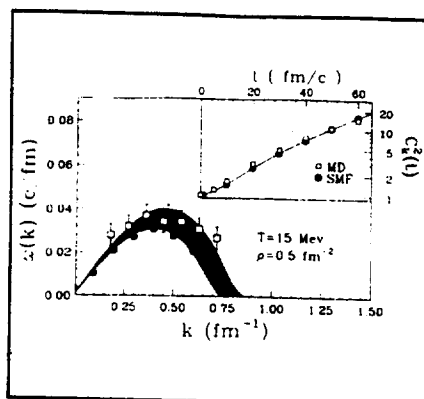


**Figure V.11:** Time evolution of a piece of nuclear matter expanding at various velocities. The vertical lines correspond to the time dependent boundary conditions (see ref. [Co95]).

From these different studies, one can conclude that the fragmentation of a system initialised in the spinodal region is initiated by the amplification of unstable zero sound waves. These modes are characterised by typical size and time scales. These modes tend to favour the partition of the system in close mass fragments with the absence of light clusters.

### V.5.D) Case of a classical system:

These ideas can be easily tested in the case of a classical Van der Waals gas. In ref. [Ja96] the stochastic simulations are compared with an exact numerical solution of the classical N-body problem. This comparison has been performed by fitting an effective density dependent mean-field potential to the volume energy of the considered classical gas. This allows to define a phase diagram in the mean field approach which was found to be rather closed from the exact one. As far as the dynamical evolution is concerned an important ingredient is the existence of a finite range for the interaction. Indeed far from the critical point this gives a scale to the fragmentation process. This range in the mean field potential has been fitted on the surface energy of the classical gas.

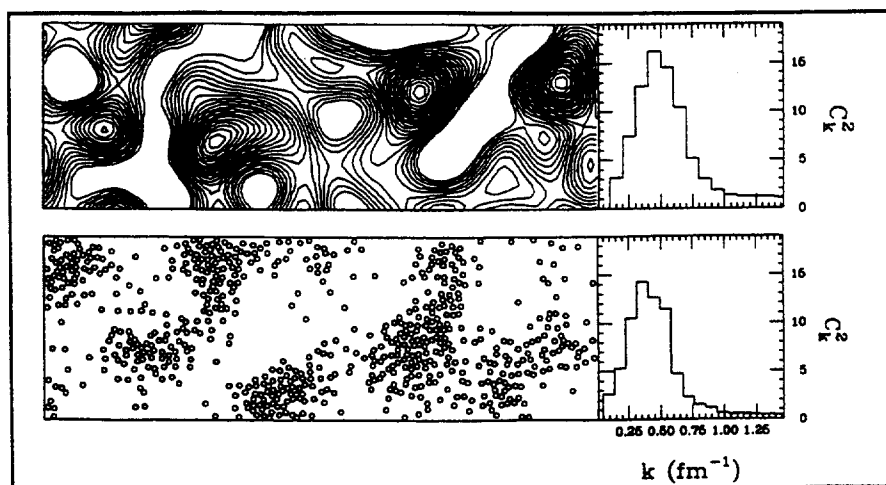


**Figure V.12:**

Classical dispersion relation computed for a classical Van der Waals gas in two dimensions initialised deep in its spinodal region: at the critical density and at the half of the critical temperature. The squares correspond to the exact simulation while the dots are the mean-field simulations. The shade area corresponds to the predictions of the mean-field linear response theory. The inserted figure shows the time evolution of the most unstable mode both for the exact simulation and for the mean-field approach.

Figure VII.8 presents an example of a classical dispersion relation extracted from the exact many-body dynamics. As in the nuclear case, we observe that the dispersion relation is dominated by a typical scale directly related to the range of the considered forces. As can be seen from the comparison presented on figure VII.8, the mean-field simulation and the linear response approach give a very accurate description of the observed mode which should be then interpreted as unstable zero-sound waves.

The dynamics of the phase transition can be studied solving the exact many-body dynamics as shown in figure VII.9 in the case of one event. It can be also simulated using a classical version of the Boltzmann-Langevin theory and such an example is also presented in figure VII.9. The qualitative comparison of these two events shows striking similarities:



**Figure V.13:**

Left part: distribution of the matter for two dynamical simulations of the spinodal

decomposition of a piece of infinite nuclear matter; top: an exact classical many-body evolution; bottom: a stochastic mean field simulation. The left part shows the Fourier analysis of the fluctuations normalised to the time 0 and computed over 100 events such as those presented on the left.

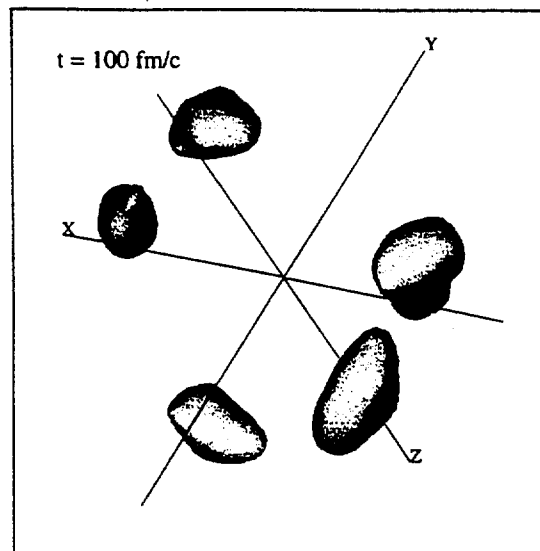
To study quantitatively these dynamics, one should consider an ensemble of events and compute statistical quantities. Figure VII.8 and VII.9 present the fluctuations associated with the different modes, i.e., the ensemble average of the square of the Fourier transform of the density fluctuations. Again one can observe a very good agreement between the exact simulations and the stochastic mean-field approximation. This shows that the stochastic mean-field approaches can also be used in the case of very strong instabilities.

It is important to notice that the classical liquid-gas phase transition is initiated by the presence of unstable collective zero-sound waves which lead to a self organisation of the system in fragments. Moreover, far from the spinodal line these zero-sound instabilities are dominated by typical wave length that are strongly related to the range of the nuclear forces. This characteristic wave length is correctly predicted by the linear response to the mean-field. This wave length dominates the density fluctuation and so it will strongly influence the size of the produced fragments. This type of evolution is already well known for many physical systems such as for example the binary alloys [Bi87, Gu83].

The presented results provide a microscopic understanding of the dynamics of a phase transition and they demonstrate the validity of the stochastic mean-field approaches.

#### V.5.E) Spinodal instabilities and multifragmentation

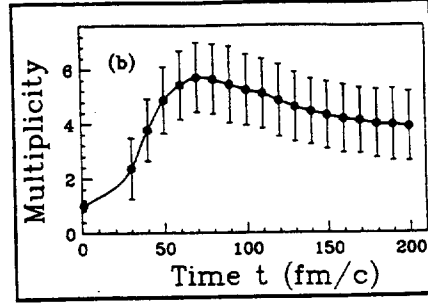
We can now study the fragmentation of a hot and diluted nucleus lying deep inside the spinodal zone of instabilities. We have considered masses, charges, densities, temperatures, spins, expansion,... as predicted by one-body dynamic approaches [Co92,Gu96]. To describe the spontaneous symmetry breaking associated with the fragmentation of hot spherical sources we have used the recently developed stochastic approaches.



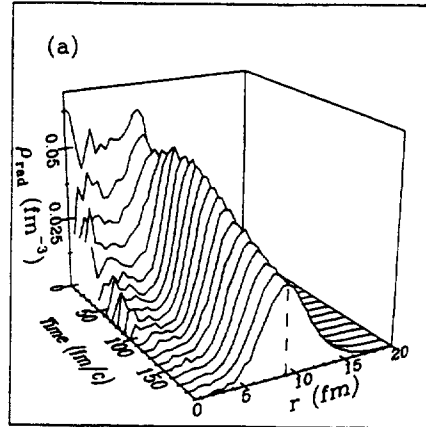
**Figure V.14:** A typical event of spinodal decomposition for an initial nucleus with a mass 210, a temperature  $T=3$  MeV and an initial density of half the normal density. The isosurface at a density of  $0.13 \text{ fm}^{-3}$  is presented.

Figure VII.10 presents one of the many predicted partitions of a large hot and diluted nucleus containing 210 nucleons that has been fragmented in 5 pieces under the influence of spinodal instabilities. This is a rather typical event the average multiplicity computed over 400 simulation being sharply peaked on the production of 5 fragments (see figure VII.11). Indeed, the multiplicity rapidly grows up to 5/6 fragments when the fragments are formed and then it slightly reduces to 4/5 fragments because of the final state interaction induces some coalescence effects.

This dominant multiplicity is clearly linked to the occurrence of spinodal instabilities since this is topologically the optimum way to have undulations in a finite system with an average distance between density lobes, compatible with the most unstable wave length of 10 fm.

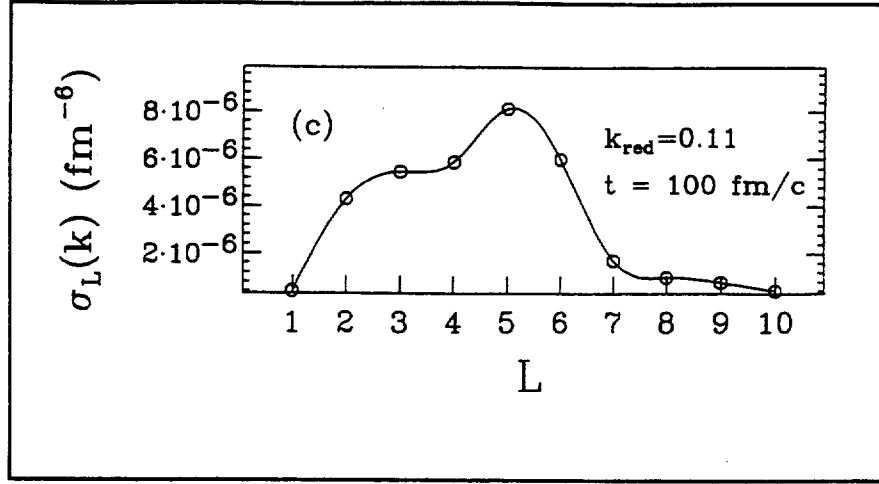


**Figure V.15:** Fragment multiplicity computed over an ensemble of approximately 400 events similar to the one shown in figure VII.12. The vertical bars correspond to one standard fluctuation.



**Figure V.16:** Radial density as a function of time computed over 400 events.





**Figure V.17:** Distribution of fluctuations as a function of the multipolarity  $L$ .

These characteristics are better seen on figures VII.12 et VII.13. On the first hand we observe in figure VII.12 radial oscillations associated with a wave length around 10 fm. In average the matter gets concentrated close to the surface and a hole is produced at the centre of the nucleus. It should be noticed that this production of bubble-like shapes is, in this approach, directly connected with spinodal instabilities.

To get a deeper insight into the characteristic of the unstable modes in finite nuclei, we have performed an analysis in terms of spherical harmonics projecting the fluctuations on the modes defined by

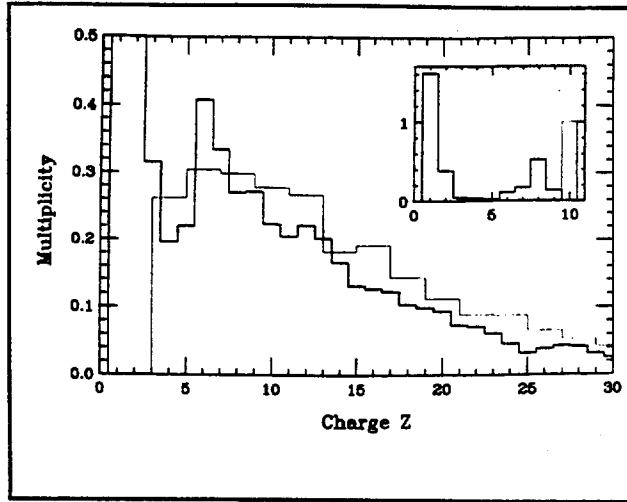
$$j_L(kr)Y_{LM}(\Omega) \quad (V.47)$$

, i.e., on the modes corresponding to the multipole expansion of the plane waves that are the unstable degrees of freedom in an infinite system. This analysis shows that these projections are strongly peaked at wave numbers that, taking into account the  $L$  dependence of the Bessel Function, correspond to a distance between two radial maxima around 10 fm. Moreover, this strong peaking of the  $k$ -dependent projection demonstrates that the actual fluctuation resembles to a Bessel function, i.e., to the multipole expansion of a plane wave with 10 fm wave length.

On the other hand, if for this  $k_L$  of maximum instability we draw the  $L$ -dependence of the measured fluctuation (figure VII.13) we can observe that the multipolarity 5 dominates the instabilities. As a matter of fact, this multipolarity  $L=5$  corresponds to a distance of 10 fm between two maxima of density fluctuation inducing the fragmentation of the system in approximately 5 equal pieces. For this multipolarity the most unstable radial  $k$  corresponds to  $k=0.6 \text{ fm}^{-1}$  that is exactly the most unstable wave number of the infinite matter system at the considered temperature and density.

In conclusion we have seen that a large enough finite system is developing instabilities very close to the one predicted for the equivalent infinite nuclear matter. Therefore, one may hope that studying the spinodal decomposition of finite system may directly provide information on the nuclear equation of state.

#### V.5.F Partitions of nuclei due to spinodal instabilities.



**Figure V.18** Charge distribution of the fragments associated with a spinodal decomposition. The thin line corresponds to the primary distribution while the thick line is associated with the final partition. The insert corresponds to the decay of an excited Ne.

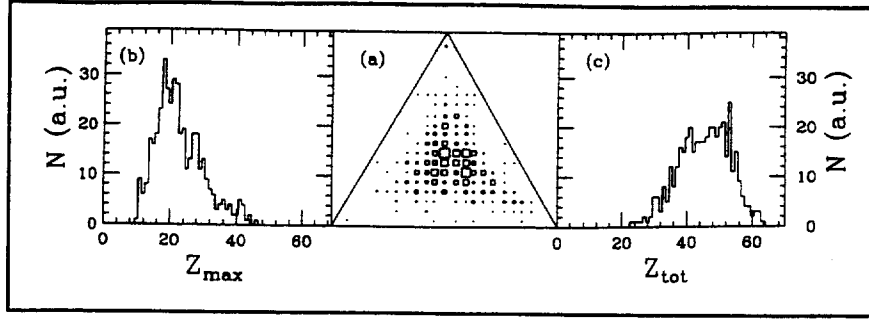
Using the stochastic mean field approaches we can now directly compute the various characteristics of the multifragmentation events such as the various partitions or the fragment velocities. For example figure VII.14 shows the primary charge distribution computed right after the multifragmentation of the system. One can observe that the primary distribution is strongly influenced by the properties of spinodal instabilities. Indeed, the small wave length being stable the spinodal instabilities are unable to produce small clusters. Conversely, the dynamics is dominated by the most unstable wave length around 10 fm and consequently the primary charge distribution is peaked around the Ne-like nuclei. However, it should not be forgotten that the large scale behaviour is not affected by the existence of an intrinsic range.

In particular, one can observe a large mass tail coming from

- i) the beating of different modes
- ii) the presence of large wave length instabilities
- iii) the coalescence effects due to the residual interaction between fragments before the complete disassembly of the system.

The predicted fragments are still hot when they are formed. Starting with a 3MeV initial temperature the fragment temperature appears to be around 4MeV. This temperature may seem rather low compared with initial available energy in the reactions leading to the formation of the dilute system we have considered. However, it should be noticed that this initial energy has been spend in pre-equilibrium particles, in surface energy, in expansion velocity and in residual excitation energy. Since the fragments are still hot, the deexcitation phase must be taken into account before any comparison with experimental observations. However, we can see on figure VII.14 that the characteristics of the initial fragments are not completely washed out by the secondary decay process. This is because the formed hot fragments are decaying through the emission of few particles leaving behind a residue with a mass close to original mass (see the final fragment distribution on figure VII.14).

However this charge distribution is only a global information and one should look for more exclusive information. Some more exclusive observables are discussed in ref. [Gu96] in order to characterise better the various partitions of the system and are shown in figure VII.15.



**Figure V.19** Charge distribution of the largest fragments of each event associated with a spinodal decomposition (left) and of the sum of the three largest fragments (right). In the centre a Dalitz plot is presented for the 3 largest charges.

In conclusion we can observe that the spinodal decomposition is characterised, in a finite system by the occurrence of a typical scale associated with the wave length of the most unstable modes in nuclear matter. An expected consequence is the existence of a favoured initial partition in approximately equal mass pieces with a lack of primary small fragments. Moreover, our simulations of the spinodal decomposition seem to indicate that the above signals are partly preserved by the secondary decay steps.

An other characteristic is given by the time needed to form the fragments from an already diluted source (to have the total multifragmentation time one must then add the time needed to reach the spinodal zone). The instability times are predicted to be around 30 to 50 fm/c therefore about 100 fm/c are needed to get separated fragments. These short time scales indicate the presence of instabilities because they are the fastest way to form fragments.

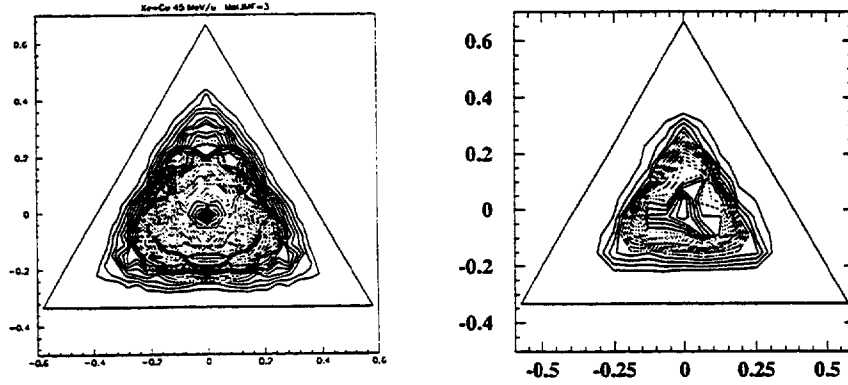
### V.5.G A first comparison with experiments.

Some experimental data are already pleading in favour of the spinodal decomposition scenario for the time scales, for the favoured partition in equal mass fragments and even for the quenching. However, before entering this discussion, we would like to stress that more experimental and theoretical studies are needed prior to conclude about the observation of spinodal decomposition in nuclei. However, almost all the one-body approaches are predicting that the composite system should enter the spinodal zone. We will see that stochastic mean-field simulations of subsequent spinodal decomposition are able to describe correctly various aspects of multifragmentation events from central collisions.

First, let us discuss the results obtained for the **Xe + Cu** reaction at 45 MeV per nucleon [Br94]. Using kinematical constraints, the authors of these articles were able to separate central reactions for which they observed that 3 fold events are dominated by partitions of the composite system in equal mass fragments. For example, figure VII.16 presents a Dalitz plot obtained in the experiment which is showing that the three observed fragments have approximately identical masses. The total charge distribution is also plotted in the same figure. It is strongly peaked around 35 demonstrating that the 3 fragments have charges around 12. These features are well reproduced by our theoretical calculation performed as follow:

- i) the reaction is first treated within a regular one-body approach using the BUU code based on a lattice hamiltonian method as described in ref. [Gu96]. This calculation is performed until the system runs across instabilities. From this point and on, the bare mean field cannot be applied anymore and one should take into account correlations and fluctuations. It should be noticed that during the first stage of the reaction, the inclusion of the fluctuations was not crucial because the mean-field dynamics complemented with a collision term was representing a reasonable ensemble average.
- ii) The unstable dynamics is simulated using a stochastic mean-field approach as described

- in reference [Gu96] which corresponds to the addition of specific noise to the BUU dynamics. This simulation is followed until fragments are formed
- iii) Finally, when the fragments are formed they are still hot and their decay may take a very long time. However, this slow process is well described by statistical decay approaches. Therefore, instead of simulating this decay within the mean-field approach which does not predict correctly the particle and fragment evaporation, we prefer to use a statistical model. This part that includes both the fragments classical trajectory and the evaporation process is simulated using the code SIMON developed by D. Durant.

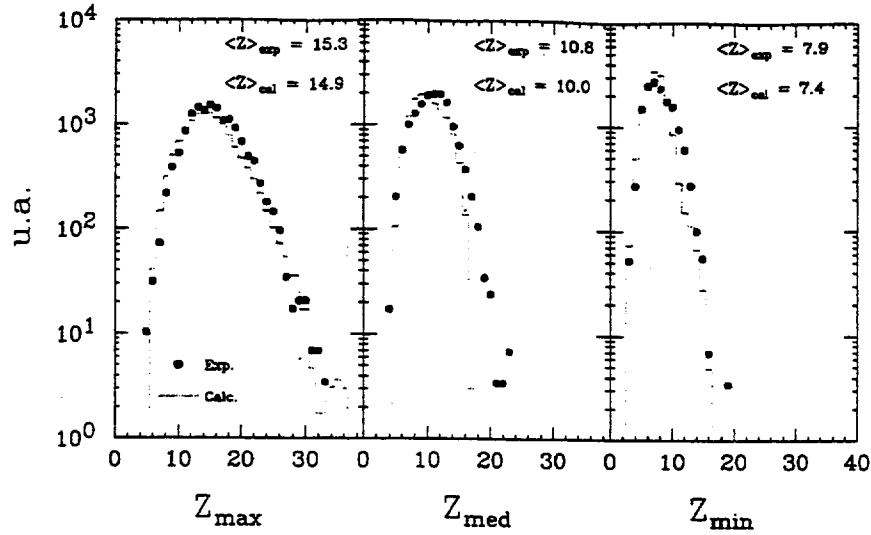


**Figure V.20** Dalitz plot for the three largest fragments observed in the  $\text{Xe} + \text{Cu}$  reaction at 45 MeV per nucleon [Br94] and in the stochastic mean-field simulations.

Figure VII.16 also presents the theoretical prediction for the mass partition and the mass distribution. We can see that the theory production of equal mass fragments with a total mass close to the experimental one. Only the width of the total mass distribution is underestimated by 20 %. However, this might be related to fluctuation in temperature and size of the initial composite source that has not been taken into account in the actual theoretical calculation. The comparison can be performed in more details looking at the mass distribution of the ordered 3 largest fragments (see fig VII.17). One can see that the theoretical prediction nicely reproduces the experimental distributions.

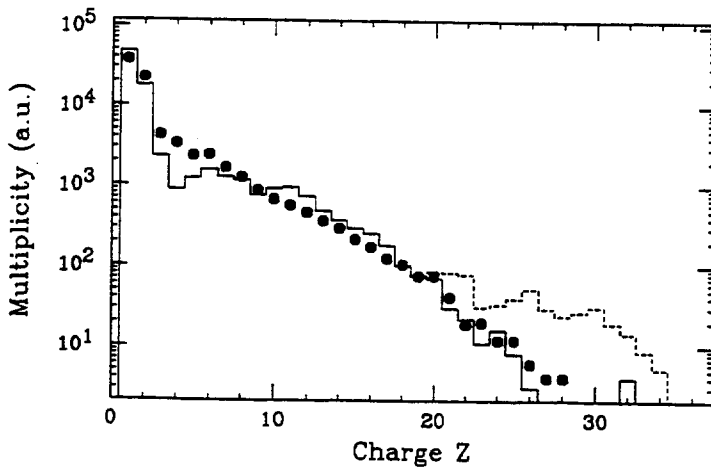
Finally, the theoretical simulations are also able to reproduce the kinematical observables in particular the observed peaking at 120 degrees of the fragment relative angle that was understood as a confirmation of the partition of the system in 3 equal-mass fragments.

It should be noticed that all the other models of multifragmentation were unable to describe these experimental data (see ref. [Br94] for more details). Therefore, the success of our ab initio calculation with no fitting parameter can be seen as a strong indication about the validity of the proposed scenario.

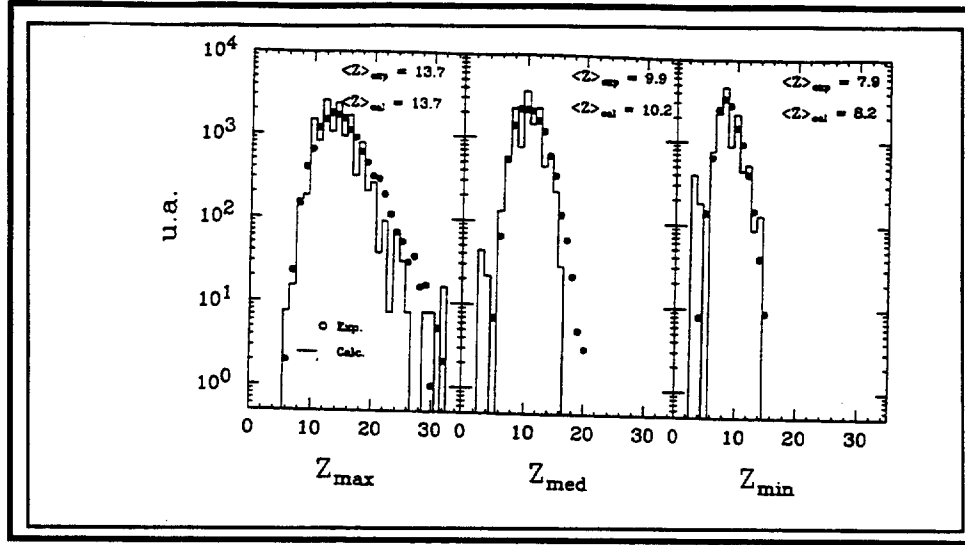


**Figure V.21** Charge distribution of the three largest fragments of each event associated with a spinodal decomposition from the left to the right in increasing size order.

We have also performed a comparison with the recent results of the INDRA collaboration [Ma95] concerning events with the formation of a composite source in the Xe+Sn reaction at 50 MeV per nucleon. Indeed, also in this case our one body approaches are predicting the formation of a composite system diving deep in the spinodal region. Figure VII.18 presents the fragment charge distribution associated with these events while Figure VII.19 displays the individual charge distributions of the 3 largest fragments. One can see a rather good agreement between experiment and theory. In particular the tail at large  $Z$  is well reproduced by the theory. We would like to recall that this tail is coming from both the mode beating and the final state interaction between fragments. On the other hand, the charge distributions of the 3 largest fragments are well reproduced both in centre position and in global shape (and width). In conclusion, while more studies are certainly needed to compare more characteristics of the multifragmentation events with the spinodal decomposition scenario, the presented results are very encouraging. Stochastic mean-field approaches can be now applied for realistic simulation in 3D. These dynamic approaches are now able to compete with multifragmentation models and can be directly compared with experiments.



**Figure V.22:** The fragment charge distribution Xe+Sn reaction at 50 MeV per nucleon. The dots are the experimental results from ref. [Ma95] and the solid line the theoretical predictions of the stochastic mean-field simulations filtered using the experimental selection. The dashed line being the unfiltered theoretical result.



**Figure V.23** Charge distribution of the three largest fragments of each event associated with a spinodal decomposition from the left to the right in increasing size order.

## VI) Conclusions and perspectives

In these lectures we have presented derivations and justifications of generalised mean field approaches. We have emphasised the physical importance of the concept of observables and observations. We introduced variational methods for both wave functions and density matrices. We present projection concept in order to justify the random part of the dynamics of the pertinent observations. For all these different concepts we have provided simple examples.

We have then presented the Boltzmann-Langevin approach and we have discussed its properties. Through an ensemble of simulation we have illustrate the power of such a new kind of approaches. Finally we have discussed the implications of these concepts for first order phase transitions and spontaneous symmetry breaking.

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