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François Golse

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On the Dynamics of Large Particle Systems in the Mean Field Limit

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In memory of Seiji Ukai (1940-2012)

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Chapter 1

On the Dynamics of Large Particle Systems in the Mean Field Limit

The general purpose of all the mean field equations considered below is to describe the dynamics of a very large number of identical particles, assuming that the interaction between particles is known exactly. For instance, at a temperature of 273 K and a pressure of $1.01 \cdot 10^5$ Pa, the number of molecules of any ideal gas to be found in a volume of $2.24 \cdot 10^{-2}$ m³ is the Avogadro number, i.e. $6.02 \cdot 10^{23}$. This is typically what we have in mind when we think of a number of particles so large that the dynamics of each individual particle cannot be exactly determined. Thus, in order to be of any practical interest, these mean field models should be set on (relatively) low dimensional spaces. In any case, they should involve fewer degrees of freedom (of the order of a few units) than the total number of degrees of freedom of the whole particle system.

To be more precise: in classical mechanics, the number of degrees of freedom of a single point particle moving without constraint in the d -dimensional Euclidean space \mathbf{R}^d is d . The *single-particle phase space* is the set $\mathbf{R}^d \times \mathbf{R}^d$ of pairs of all possible positions and momenta of an unconstrained single point particle in \mathbf{R}^d .

For a system of N identical point particles moving without constraint in the d -dimensional Euclidean space \mathbf{R}^d , the number of degrees of freedom is therefore dN . The space $(\mathbf{R}^d \times \mathbf{R}^d)^N$ of $2N$ -tuples of all possible positions and momenta of the N point particles is the *N -particle phase space*.

Thus, the laws of motion of classical mechanics (Newton's second law) written for each molecule of a monatomic gas enclosed in a container form a system of differential equations set on the N -particle phase space, where N is the total number of gas molecules to be found in the container. With N of the order of the Avogadro number, this is of little practical interest. In the kinetic theory of gases, the evolution of the same gas is described by the Boltzmann equation,

an integro-differential equation set on the single-particle phase space. Although the kinetic theory of gases will not be discussed in these notes, all the mean field limits considered below will involve the same reduction of the N -particle phase space to the single-particle phase space.

Here is a (by no means exhaustive) list of typical examples of mean field equations:

(a) the particles are the ions and the electrons in a plasma; the interaction is the Coulomb electrostatic force; in that case, the mean field equation is the Vlasov-Poisson system of the kinetic theory of plasmas;

(b) the particles are the nuclei and the electrons in a molecule; the interaction is again the Coulomb electrostatic force; the corresponding mean field model in this context is the Hartree equation or the system of Hartree-Fock equations in atomic physics;

(c) the particles are vortices in an incompressible fluid in space dimension 2; the interaction is given by the Helmholtz potential; the corresponding mean field model is the vorticity formulation of the Euler equations of incompressible fluid mechanics

All these models are obtained as approximations of the system of equations of motion for each particle in the limit when the number of particles involved tends to infinity. Rigorous justifications of these approximations are based on various mathematical formalisms that are introduced and discussed below.

Excellent references on the issues discussed above are [88, 90, 26]

1.1 Examples of mean field models in classical mechanics

In this section, we consider the examples mentioned above in which the motion of each particle is described in the formalism of classical mechanics, i.e. examples (a) and (c). All these examples have a common structure, to be discussed later, which involves the Liouville equation recalled below.

1.1.1 The Liouville equation

The Liouville equation governs the evolution of the distribution function for a system of particles subject to an external force field.

The notion of distribution function is fundamental in the kinetic theories of gases and plasmas, and more generally in statistical mechanics. It was introduced by Maxwell in one of his most famous articles¹.

The distribution function of a system of identical point particles is $f \equiv f(t, x, v)$, that is the number density of particles that are located at the position

¹*Illustrations of the Dynamical Theory of Gases*, Philosophical Magazine (1860); reprinted in “The Scientific Papers of James Clerk Maxwell”, edited by W.D. Niven, Cambridge University Press, 1890; pp. 377–409.

x and have instantaneous velocity v at time t . In other words, the number of particles to be found at time t in an infinitesimal volume $dx dv$ of the single-particle phase space centered at (x, v) is $\simeq f(t, x, v) dx dv$.

Assume that a particle located at the position x with instantaneous velocity v at time t is subject to some external (or imposed) force field $F(t, x, v)$. As a consequence of Newton's second law of classical mechanics, the distribution function f of the system of particles under consideration satisfies the Liouville equation

$$\partial_t f + v \cdot \nabla_x f + \frac{1}{m} \operatorname{div}_v (F(t, x, v) f) = 0,$$

where $m > 0$ is the particle mass. The Liouville equation is a partial differential equation (PDE) of order 1, whose solution can be expressed by the method of characteristics.

To the PDE of order 1 above, one associates the system of ordinary differential equations (ODE)

$$\begin{cases} \dot{X} = V, \\ \dot{V} = \frac{1}{m} F(t, X, V), \end{cases}$$

with the usual notation

$$\dot{\phi}(t) = \frac{d\phi}{dt}(t).$$

These ODEs are referred to as the “equations of characteristics” for the Liouville equation. Denote by $t \mapsto (X(t, t_0, x, v), V(t, t_0, x, v))$ the solution of this ODE system such that

$$X(t_0, t_0, x, v) = x, \quad V(t_0, t_0, x, v) = v;$$

the map $(t, t_0, x, v) \mapsto (X(t, t_0, x, v), V(t, t_0, x, v))$ will be henceforth referred to as “the characteristic flow” associated to the Liouville equation above.

One immediately recognizes in the system of ODEs above the equations of motion of classical mechanics for a particle of mass m subject to the force field $F \equiv F(t, x, v)$ (the first equality being the definition of the velocity, while the second is Newton's second law).

Assume that the force field F is such that the characteristic flow (X, V) is globally defined (i.e. defined on $\mathbf{R} \times \mathbf{R} \times \mathbf{R}^d \times \mathbf{R}^d$). This characteristic flow is used as follows to express the solution of the Cauchy problem

$$\begin{cases} \partial_t f + v \cdot \nabla_x f + \frac{1}{m} \operatorname{div}_v (F(t, x, v) f) = 0, & x, v \in \mathbf{R}^d \times \mathbf{R}^d, t \in \mathbf{R}, \\ f|_{t=0} = f^{in}. \end{cases}$$

For each test function² $\phi \in C_c^1(\mathbf{R}^d \times \mathbf{R}^d)$, and for each $t \in \mathbf{R}$, one has

$$\iint_{\mathbf{R}^d \times \mathbf{R}^d} f(t, x, v) \phi(x, v) dx dv = \iint_{\mathbf{R}^d \times \mathbf{R}^d} f^{in}(x, v) \phi((X, V)(t, 0, x, v)) dx dv,$$

²For each topological space X and each finite dimensional vector space E on \mathbf{R} , we designate by $C(X, E)$ the set of continuous functions defined on X with values in E , and by $C_c(X, E)$ the set of functions belonging to $C(X, E)$ whose support is compact in X . For each $n, k \geq 1$, we denote by $C_c^k(\mathbf{R}^n, E)$ the set of functions of class C^k defined on \mathbf{R}^n with values in E whose support is compact in \mathbf{R}^n . We also denote $C(X) := C(X, \mathbf{R})$, $C_c(X) := C_c(X, \mathbf{R})$ and $C_c^k(\mathbf{R}^n) := C_c^k(\mathbf{R}^n, \mathbf{R})$.

and this completely determines the distribution function $f(t, x, v)$.

Exercise: Deduce from the equality above an explicit formula giving $f(t, x, v)$ in terms of f^{in} and of the characteristic flow (X, V) .

For a concise discussion of the method of characteristics (and a solution of the exercise above), see chapter 1, section 1, in [17].

1.1.2 The Vlasov-Poisson system

Our first example of a mean field kinetic model is the Vlasov-Poisson system used in plasma physics.

Consider a system of identical point particles with mass m and charge q . The electrostatic (Coulomb) force exerted on any such particle located at the position $x \in \mathbf{R}^3$ by another particle located at the position $y \neq x$ is

$$\frac{q^2}{4\pi\epsilon_0} \frac{x - y}{|x - y|^3},$$

where ϵ_0 is the dielectric permittivity of vacuum. This force is indeed repulsive, as it is of the form $\lambda(x - y)$ with $\lambda > 0$.

More generally, the electrostatic force exerted on a particle located at the position x by a cloud of particles with number density $\rho(t, y)$ (which means that, at time t , approximately $\rho(t, y)dy$ particles are to be found in any infinitesimal volume element dy centered at y) is

$$F(t, x) := \frac{q^2}{4\pi\epsilon_0} \int_{\mathbf{R}^3} \frac{x - y}{|x - y|^3} \rho(t, y) dy.$$

Recall that

$$G(x) = \frac{1}{4\pi|x|}, \quad x \in \mathbf{R}^3 \setminus \{0\}$$

is the solution of

$$\begin{cases} -\Delta G = \delta_0 & \text{in } \mathcal{D}'(\mathbf{R}^3), \\ G(x) \rightarrow 0 & \text{as } |x| \rightarrow \infty, \end{cases}$$

where δ_0 designates the Dirac measure at the origin.

Thus the electrostatic force F is given by

$$F(t, x) = qE(t, x),$$

where $E \equiv E(t, x)$ is the electric field, i.e.

$$E(t, x) = -\nabla_x \phi(t, x)$$

with electrostatic potential ϕ given by

$$\phi(t, \cdot) = \frac{q}{\epsilon_0} G \star \rho(t, \cdot).$$

In particular

$$\begin{aligned} -\Delta\phi(t, \cdot) &= -\frac{q}{\epsilon_0}\Delta(G \star \rho(t, \cdot)) = -\frac{q}{\epsilon_0}(\Delta G) \star \rho(t, \cdot) \\ &= \frac{q}{\epsilon_0}\delta_0 \star \rho(t, \cdot) = \frac{q}{\epsilon_0}\rho(t, \cdot). \end{aligned}$$

The Vlasov-Poisson system describes the motion of a system of identical charged point particles accelerated by the electrostatic force created by their own distribution of charges — referred to as the “self-consistent electrostatic force”. It consists of the Liouville equation governing the evolution of the distribution function, coupled to the Poisson equation satisfied by the self-consistent electrostatic potential as follows:

$$\left\{ \begin{array}{l} (\partial_t + v \cdot \nabla_x)f(t, x, v) - \frac{q}{m}\nabla_x\phi(t, x) \cdot \nabla_v f(t, x, v) = 0, \\ -\Delta_x\phi(t, x) = \frac{1}{\epsilon_0}q\rho_f(t, x), \\ \rho_f(t, x) = \int_{\mathbf{R}^3} f(t, x, v)dv. \end{array} \right.$$

Exercise: Let $f \equiv f(t, x, v)$ and $\phi \equiv \phi(t, x)$ be a solution of the Vlasov-Poisson system. To avoid technicalities, we assume that f and ϕ belong to $C^\infty(\mathbf{R}_+ \times \mathbf{R}^3 \times \mathbf{R}^3)$ and $C^\infty(\mathbf{R}_+ \times \mathbf{R}^3)$ respectively, and that, for each $t \geq 0$, the functions $(x, v) \mapsto f(t, x, v)$ and $x \mapsto \phi(t, x)$ belong to the Schwartz class³ $\mathcal{S}(\mathbf{R}^3 \times \mathbf{R}^3)$ and $\mathcal{S}(\mathbf{R}^3)$ respectively.

1) Prove that

$$\begin{aligned} \partial_t \rho_f(t, x) + \operatorname{div}_x \int_{\mathbf{R}^3} v f(t, x, v) dv &= 0, \\ \partial_t \int_{\mathbf{R}^3} m v f(t, x, v) dv + \operatorname{div}_x \int_{\mathbf{R}^3} m v^{\otimes 2} f(t, x, v) dv \\ &\quad + q \rho_f(t, x) \nabla_x \phi(t, x) = 0, \\ \partial_t \int_{\mathbf{R}^3} \frac{1}{2} m |v|^2 f(t, x, v) dv + \operatorname{div}_x \int_{\mathbf{R}^3} v \frac{1}{2} m |v|^2 f(t, x, v) dv \\ &\quad + \nabla_x \phi(t, x) \cdot \int_{\mathbf{R}^3} q v f(t, x, v) dv = 0. \end{aligned}$$

These three equalities are respectively the local conservation laws of mass, momentum and energy.

³For each $n \geq 1$, the Schwartz class $\mathcal{S}(\mathbf{R}^n)$ is the set of real-valued C^∞ functions defined on \mathbf{R}^n all of whose partial derivatives are rapidly decreasing at infinity:

$$\mathcal{S}(\mathbf{R}^n) := \{f \in C^\infty(\mathbf{R}^n) \text{ s.t. } |x|^m \partial^\alpha f(x) \rightarrow 0 \text{ as } |x| \rightarrow \infty \text{ for all } m \geq 1 \text{ and } \alpha \in \mathbf{N}^n\}.$$

2) Prove the global conservation of mass (or equivalently of the total number of particles)

$$\frac{d}{dt} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(t, x, v) dx dv = 0.$$

3) Prove that, for each $\psi \in C^2(\mathbf{R}^3)$, one has

$$\Delta \psi \nabla \psi = \operatorname{div}((\nabla \psi)^{\otimes 2}) - \frac{1}{2} \nabla |\nabla \psi|^2$$

and conclude that

$$\frac{d}{dt} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} mv f(t, x, v) dx dv = 0.$$

(This is the global conservation of momentum).

4) Prove the global conservation of energy:

$$\frac{d}{dt} \left(\iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{1}{2} m |v|^2 f(t, x, v) dx dv + \frac{1}{2} \epsilon_0 \int_{\mathbf{R}^3} |\nabla_x \phi(t, x)|^2 dx \right) = 0.$$

(Hint: the term

$$\int_{\mathbf{R}^3} \phi(t, x) \operatorname{div}_x \left(\int_{\mathbf{R}^3} qv f(t, x, v) dv \right) dx$$

can be simplified by using the result in question 1).)

The Vlasov-Poisson system above is written in the case of a single species of identical charged particles. In reality, a plasma is a globally neutral system, and therefore involves many different species of particles. Denoting by $f_k \equiv f_k(t, x, v)$ for $k = 1, \dots, M$ the distribution function of the k th species in a system of M different kinds of particles, the Vlasov-Poisson describes the motion of this system of particles submitted to the self-consistent electrostatic force resulting from the distribution of charges of all the particles in that system:

$$\left\{ \begin{array}{l} (\partial_t + v \cdot \nabla_x) f_k(t, x, v) - \frac{q_k}{m_k} \nabla_x \phi(t, x) \cdot \nabla_v f_k(t, x, v) = 0, \quad k = 1, \dots, M, \\ -\Delta_x \phi(t, x) = \frac{1}{\epsilon_0} \sum_{k=1}^M q_k \rho_k(t, x), \\ \rho_k(t, x) = \int_{\mathbf{R}^3} f_k(t, x, v) dv. \end{array} \right.$$

Here m_k and q_k designate respectively the mass and the charge of particles of the k th species. In practice, considering systems of particles of different species in the Vlasov-Poisson system does not involve additional mathematical difficulties. Therefore, we shall consider only the (unphysical) case of a single species of particles in our mathematical discussion of this system.

There is a huge literature on the Vlasov-Poisson system, which is of considerable importance in plasma physics. The global existence and uniqueness of classical solutions of the Cauchy problem for the Vlasov-Poisson system was obtained by Ukai-Okabe [94] in the 2-dimensional case, and independently by Lions-Perthame [68] and Pfaffelmoser [79] in the 3-dimensional case. For a presentation of the mathematical analysis of this system, the interested reader is referred to [41, 17, 84].

1.1.3 The Euler equation for two-dimensional incompressible fluids

The Euler equation for an incompressible fluid with constant density (set to 1 in the sequel without loss of generality) governs the evolution of the unknown velocity field $u \equiv u(t, x) \in \mathbf{R}^2$ and of the unknown pressure field $p \equiv p(t, x) \in \mathbf{R}$ in the fluid, assumed to fill the Euclidean plane \mathbf{R}^2 . It takes the form

$$\partial_t u(t, x) + (u \cdot \nabla_x)u(t, x) + \nabla_x p(t, x) = 0, \quad \operatorname{div}_x u(t, x) = 0.$$

The pressure field p can be viewed as the Lagrange multiplier associated to the constraint $\operatorname{div}_x u = 0$.

There is another formulation of the Euler equation in which the pressure field is eliminated. To the velocity field $u \equiv u(t, x) \in \mathbf{R}^2$, one associates its scalar vorticity field $\omega \equiv \omega(t, x)$ defined as follows

$$\omega(t, x) := \partial_{x_1} u_2(t, x) - \partial_{x_2} u_1(t, x).$$

The vorticity field satisfies

$$\partial_t \omega + \operatorname{div}_x (u\omega) = 0.$$

One can check that the Euler equation is (formally) equivalent to the system

$$\begin{cases} \partial_t \omega + \operatorname{div}_x (u\omega) = 0, \\ \operatorname{div}_x u = 0, \\ \omega = \operatorname{div}_x (Ju), \end{cases}$$

where J designates the rotation of an angle $-\frac{\pi}{2}$:

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

There is yet another formulation of this system, where the velocity field u is represented in terms of a stream function. Indeed, since $\operatorname{div}_x u = 0$, there exists a stream function $\phi \equiv \phi(t, x)$ such that

$$u(t, x) = J\nabla_x \phi(t, x).$$

The vorticity field ω is related to the stream function ϕ as follows:

$$\omega = \operatorname{div}_x (Ju) = \operatorname{div}_x (J^2 \nabla_x \phi) = -\Delta_x \phi,$$

so that the vorticity formulation of the Euler equation becomes

$$\begin{cases} \partial_t \omega + \operatorname{div}_x(\omega J \nabla_x \phi) = 0, \\ -\Delta_x \phi = \omega. \end{cases}$$

In this last system, the unknown is the pair (ω, ϕ) ; once the stream function ϕ is known, the velocity field u is obtained as the spatial gradient of ϕ rotated of an angle $-\frac{\pi}{2}$.

There is an obvious analogy between this formulation of the Euler equation and the Vlasov-Poisson system: the vorticity field ω is the analogue of the distribution function f in the Vlasov-Poisson system, the stream function is the analogue of the electrostatic potential in the Vlasov-Poisson system, and the velocity field u is the analogue of the electric field in the Vlasov-Poisson system. There is however a subtle difference between both systems: the equations of characteristics associated to the vorticity formulation of the Euler equations are

$$J\dot{X} = -\nabla_x \phi(t, X),$$

while those corresponding with the Vlasov-Poisson system are

$$\ddot{X} = -\frac{q}{m} \nabla_x \phi(t, X),$$

(after eliminating $V = \dot{X}$). The first ODE system is of order 1, while the second is of order 2, because the gradient of the solution of the Poisson equation is a velocity field in the vorticity formulation of the Euler equation, while it is an acceleration field in the case of the Vlasov-Poisson system.

An excellent reference on the Euler equations of incompressible fluids and on issues related to the mean field limit is [71].

1.1.4 The Vlasov-Maxwell system

Observe that magnetic effects are not taken into account in the Vlasov-Poisson system. Yet charged particles in motion generate both an electric and a magnetic field; on the other hand, the electric and magnetic fields both act on charged particles via the Lorentz force. Studying magnetized plasmas (such as tokamak plasmas, or the solar wind, for instance) requires using the Vlasov-Maxwell, instead of the Vlasov-Poisson system.

The unknown in the Vlasov-Maxwell system is the triple (f, E, B) , where $E \equiv E(t, x) \in \mathbf{R}^3$ and $B \equiv B(t, x) \in \mathbf{R}^3$ are respectively the electric and the magnetic fields, while $f \equiv f(t, x, \xi)$ is the particle distribution function. Notice that the velocity variable v is replaced with the momentum ξ in the distribution function. In other words, $f(t, x, \xi)$ is the phase space density of particles located at the position x at time t , with momentum ξ . The momentum and the velocity are related as follows. The relativistic energy of a particle of mass m with momentum ξ is

$$e(\xi) := \sqrt{m^2 c^4 + c^2 |\xi|^2},$$

where c is the speed of light (notice that $e(0) = mc^2$, the energy at rest of a particle with mass m). Then

$$v(\xi) = \nabla e(\xi) = \frac{c^2 \xi}{\sqrt{m^2 c^4 + c^2 |\xi|^2}}.$$

The (relativistic) Vlasov-Maxwell system takes the form

$$\left\{ \begin{array}{l} \partial_t f + v(\xi) \cdot \nabla_x f + q(E + v(\xi) \times B) \cdot \nabla_\xi f = 0, \\ \operatorname{div}_x B = 0, \quad \partial_t B + \operatorname{rot}_x E = 0, \\ \operatorname{div}_x E = \frac{1}{\epsilon_0} q \rho_f, \quad \frac{1}{c^2} \partial_t E - \operatorname{rot}_x B = -\mu_0 q j_f, \\ \rho_f = \int_{\mathbf{R}^3} f d\xi, \quad j_f = \int_{\mathbf{R}^3} v(\xi) f d\xi. \end{array} \right.$$

The first equation in this system is the relativistic Liouville equation governing f ; the term

$$q(E(t, x) + v(\xi) \times B(t, x))$$

is the Lorentz force field at time t and position x exerted by the electromagnetic field (E, B) on a particle with charge q and momentum ξ . The second and third equations are respectively the equation expressing the absence of magnetic monopoles and the Faraday equation, while the fourth and fifth equations are respectively the Gauss equation (as in electrostatics) and the Maxwell-Ampère equation. Since the source terms in the Maxwell system are the charge density $q\rho_f$ and the current density qj_f , the Lorentz force in the Liouville equation is the self-consistent Lorentz force, i.e. the electromagnetic force generated by the motion of the charged particles accelerated by this force itself.

For the same reason as in the case of the Vlasov-Poisson system, the case of a single species of charged particles is somewhat unrealistic. Physically relevant models in plasma physics involve different species of particles so as to maintain global neutrality of the particle system.

Exercise: Following the discussion in the previous section, write the relativistic Vlasov-Maxwell system for a system of M species of particles with masses m_k and charges q_k , for $k = 1, \dots, M$. Write the local conservation laws of mass, momentum and energy for the resulting system, following the analogous discussion above in the case of the Vlasov-Poisson system.

For more information on the Vlasov-Maxwell system, see [41, 17, 84].

1.2 A general formalism for mean field limits in classical mechanics

We first introduce a formalism for mean field limits in classical mechanics that encompasses all the examples discussed above.

Consider a system of N particles, whose state at time t is defined by phase space coordinates $\hat{z}_1(t), \dots, \hat{z}_N(t) \in \mathbf{R}^d$. For instance, z_j is the position x_j of the j th vortex center in the case of the two dimensional Euler equations for incompressible fluids, and the phase space dimension is $d = 2$. In the case of the Vlasov-Poisson system, the phase space is $\mathbf{R}^3 \times \mathbf{R}^3 \simeq \mathbf{R}^6$, so that $d = 6$, and $z_j = (x_j, v_j)$, where x_j and v_j are respectively the position and the velocity of the j th particle.

The interaction between the i th and the j th particle is given by $K(\hat{z}_i, \hat{z}_j)$, where

$$K : \mathbf{R}^d \times \mathbf{R}^d \rightarrow \mathbf{R}^d$$

is a map whose properties will be discussed below.

The evolution of $\hat{z}_1(t), \dots, \hat{z}_N(t) \in \mathbf{R}^d$ is governed by the system of ODEs

$$\frac{d\hat{z}_i}{dt}(t) = \sum_{\substack{j=1 \\ j \neq i}}^N K(\hat{z}_i(t), \hat{z}_j(t)), \quad i, j = 1, \dots, N.$$

Problem: to describe the behavior of $\hat{z}_1(t), \dots, \hat{z}_N(t) \in \mathbf{R}^d$ in the large N limit and in some appropriate time scale.

First we need to rescale the time variable, and introduce a new time variable \hat{t} so that, in new time scale, the action on any one of the N particles due to the $N - 1$ other particles is of order 1 as $N \rightarrow +\infty$. In other words, the new time variable \hat{t} is chosen so that

$$\frac{d\hat{z}_i}{d\hat{t}} = O(1) \text{ for each } i = 1, \dots, N \text{ as } N \rightarrow \infty.$$

The action on the i th particle of the $N - 1$ other particles is

$$\sum_{\substack{j=1 \\ j \neq i}}^N K(\hat{z}_i, \hat{z}_j),$$

and it obviously contains $N - 1$ terms of order 1 (assuming each term $K(\hat{z}_i, \hat{z}_j)$ to be of order 1, for instance). Set $\hat{t} = t/N$, then

$$\frac{d\hat{z}_i}{d\hat{t}} = \frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^N K(\hat{z}_i, \hat{z}_j).$$

From now on, we drop hats on all variables and consider as our starting point the rescaled problem

$$\dot{z}_i(t) = \frac{1}{N} \sum_{\substack{j=1 \\ j \neq i}}^N K(z_i(t), z_j(t)), \quad i = 1, \dots, N.$$

At this point, we introduce an important assumption on the interaction kernel: the action of the j th particle on the i th particle must exactly balance the action of the i th particle on the j th particle. When the interaction is a force, this is precisely Newton's third law of mechanics. Thus we assume that the interaction kernel satisfies

$$K(z, z') = -K(z', z), \quad z, z' \in \mathbf{R}^d.$$

We have assumed here that the interaction kernel K is defined on the whole $\mathbf{R}^d \times \mathbf{R}^d$ space; in particular, the condition above implies that K vanishes identically on the diagonal, i.e.

$$K(z, z) = 0, \quad z \in \mathbf{R}^d.$$

Hence the restriction $j \neq i$ can be removed in the summation that appears on the right hand side of the ODEs governing the N -particle dynamics: since $K(z_i(t), z_i(t)) = 0$ for all $i = 1, \dots, N$, one has

$$\dot{z}_i(t) = \frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)) \quad i = 1, \dots, N.$$

At this point, we can explain the key idea in the mean field limit: if the points $z_j(t)$ for $j = 1, \dots, N$ are “distributed at time t under the probability measure $f(t, dz)$ ” in the large N limit, then, one expects that

$$\frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)) \rightarrow \int_{\mathbf{R}^d} K(z_i(t), z') f(t, dz') \quad \text{as } N \rightarrow +\infty.$$

This suggests replacing the N -particle system of differential equations with the single differential equation

$$\dot{z}(t) = \int_{\mathbf{R}^d} K(z(t), z') f(t, dz').$$

Here $f(t, dz)$ is unknown, as is $z(t)$, so that it seems that this single differential equation is insufficient to determine both these unknowns.

But one recognizes in the equality above the equation of characteristics for the mean field PDE

$$\partial_t f + \operatorname{div}_z (f \mathcal{K} f) = 0,$$

where the notation \mathcal{K} designates the integral operator defined by the formula

$$\mathcal{K}f(t, z) := \int_{\mathbf{R}^d} K(z, z')f(t, dz').$$

Now, this is a single PDE (in fact an integro-differential equation) for the single unknown f .

A priori f is a time dependent Borel probability measure on \mathbf{R}^d , so that the mean field PDE is to be understood in the sense of distributions on \mathbf{R}^d . In other words,

$$\frac{d}{dt} \int_{\mathbf{R}^d} \phi(z)f(t, dz) = \int_{\mathbf{R}^d} \mathcal{K}f(t, z) \cdot \nabla \phi(z)f(t, dz)$$

for each test function⁴ $\phi \in C_b^1(\mathbf{R}^d)$.

A very important mathematical object in the mathematical theory of the mean field limit is the empirical measure, which is defined below.

Definition 1.2.1 *To each N -tuple $Z_N = (z_1, \dots, z_N) \in (\mathbf{R}^d)^N \simeq \mathbf{R}^{dN}$, one associates its empirical measure*

$$\mu_{Z_N} := \frac{1}{N} \sum_{j=1}^N \delta_{z_j}.$$

The empirical measure of a N -tuple $Z_N \in (\mathbf{R}^d)^N$ is a Borel probability measure on \mathbf{R}^d . As we shall see in the next section, the N -tuple

$$t \mapsto Z_N(t) = (z_1(t), \dots, z_N(t))$$

is a solution of the N -particle ODE system

$$\dot{z}_i(t) = \frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)), \quad i = 1, \dots, N$$

if and only if the empirical measure $\mu_{Z_N(t)}$ is a solution of the mean field PDE

$$\partial_t \mu_{Z_N(t)} + \operatorname{div}_z (\mu_{Z_N(t)} \mathcal{K} \mu_{Z_N(t)}) = 0.$$

⁴For each topological space X and each finite dimensional vector space E on \mathbf{R} , we denote by $C_b(X, E)$ the set of continuous functions defined on X with values in E that are bounded on X . For each $n, k \geq 1$, we denote by $C_b^k(\mathbf{R}^n, E)$ the set of functions of class C^k defined on \mathbf{R}^n with values in E all of whose partial derivatives are bounded on \mathbf{R}^n : for each norm $|\cdot|_E$ on E , one has

$$C_b^k(\mathbf{R}^n, E) := \{f \in C^k(\mathbf{R}^n, E) \text{ s.t. } \sup_{x \in \mathbf{R}^n} |\partial^\alpha f(x)|_E < \infty \text{ for each } \alpha \in \mathbf{N}^n\}.$$

We also denote $C_b(X) := C_b(X, \mathbf{R})$ and $C_b^k(\mathbf{R}^n) := C_b^k(\mathbf{R}^n, \mathbf{R})$.

We conclude this section with a few exercises where the reader can verify that the formalism introduced here encompasses the two main examples of mean-field theories presented above, i.e. the two dimensional Euler equation and the Vlasov-Poisson system.

Exercise:

- 1) Compute $\Delta \ln |x|$ in the sense of distributions on \mathbf{R}^2 (answer: $2\pi\delta_0$).
- 2) Define

$$K(x, x') := -\frac{1}{2\pi} \frac{J(x - x')}{|x - x'|^2}, \quad x \neq x' \in \mathbf{R}^2,$$

where J designates the rotation of an angle $-\frac{\pi}{2}$:

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

For each $\omega \equiv \omega(t, x)$ belonging to $C_b^1(\mathbf{R}_+ \times \mathbf{R}^2)$ such that $\text{supp}(\omega(t, \cdot))$ is compact for each $t \geq 0$, prove that the vector field u defined by

$$u(t, x) := \int_{\mathbf{R}^2} K(x, x') \omega(x') dx'$$

is of class C_b^1 on $\mathbf{R}_+ \times \mathbf{R}^2$ and satisfies

$$\text{div}_x u(t, x) = 0, \quad \text{div}_x (Ju)(t, x) = \omega(t, x).$$

- 3) Conclude that the two dimensional Euler equation for incompressible fluids can be put in the formalism described in the present section, except for the fact that the interaction kernel K is singular on the diagonal of $\mathbf{R}^2 \times \mathbf{R}^2$.

Exercise: Let (f, ϕ) be a solution of the Vlasov-Poisson system satisfying the same assumptions as in the exercise of section 1.1.2. Assume further that

$$\iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(0, x, v) dx dv = 1, \quad \text{and} \quad \iint_{\mathbf{R}^3 \times \mathbf{R}^3} v f(0, x, v) dx dv = 0.$$

- 1) Prove that

$$\iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(t, x, v) dx dv = 1 \quad \text{and} \quad \iint_{\mathbf{R}^3 \times \mathbf{R}^3} v f(t, x, v) dx dv = 0 \quad \text{for all } t \geq 0.$$

- 2) Set $z = (x, v)$ and

$$K(z, z') = K(x, v, x', v') := \left(v - v', \frac{q^2}{4\pi\epsilon_0 m} \frac{x - x'}{|x - x'|^3} \right).$$

Prove that

$$\iint_{\mathbf{R}^3 \times \mathbf{R}^3} K(x, v, x', v') f(t, x', v') dx' dv' = \left(v, -\frac{q}{m} \nabla_x \phi(t, x) \right),$$

where

$$-\Delta_x \phi(t, x) = \frac{q}{\epsilon_0} \int_{\mathbf{R}^3} f(t, x, v) dv.$$

- 3) Conclude that the Vlasov-Poisson system can be put in the formalism described in the present section, except for the fact that the interaction kernel K is singular on the set $\{(x, v, x', v') \in (\mathbf{R}^3)^4 \text{ s.t. } x = x'\}$.

1.3 The mean field characteristic flow

Henceforth we assume that the interaction kernel $K : \mathbf{R}^d \times \mathbf{R}^d \rightarrow \mathbf{R}^d$ satisfies the following assumptions.

First K is skew-symmetric:

$$(HK1) \quad K(z, z') = -K(z', z) \quad \text{for all } z, z' \in \mathbf{R}^d.$$

Besides, $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d; \mathbf{R}^d)$, with bounded partial derivatives of order 1. In other words, there exists a constant $L \geq 0$ such that

$$(HK2) \quad \sup_{z' \in \mathbf{R}^d} |\nabla_z K(z, z')| \leq L, \quad \text{and} \quad \sup_{z \in \mathbf{R}^d} |\nabla_{z'} K(z, z')| \leq L.$$

Applying the mean value theorem shows that assumption (HK2) implies that K is Lipschitz continuous in z uniformly in z' (and conversely):

$$\begin{cases} \sup_{z' \in \mathbf{R}^d} |K(z_1, z') - K(z_2, z')| \leq L|z_1 - z_2|, \\ \sup_{z \in \mathbf{R}^d} |K(z, z_1) - K(z, z_2)| \leq L|z_1 - z_2|. \end{cases}$$

Assumption (HK2) also implies that K grows at most linearly at infinity:

$$|K(z, z')| \leq L(|z| + |z'|), \quad z, z' \in \mathbf{R}^d.$$

Notice also that the integral operator \mathcal{K} can be extended to the set of Borel probability measures⁵ on \mathbf{R}^d with finite moment of order 1, i.e.

$$\mathcal{P}_1(\mathbf{R}^d) := \left\{ p \in \mathcal{P}(\mathbf{R}^d) \text{ s.t. } \int_{\mathbf{R}^d} |z| p(dz) < \infty \right\},$$

in the obvious manner, i.e.

$$\mathcal{K}p(z) := \int_{\mathbf{R}^d} K(z, z') p(dz').$$

The extended operator \mathcal{K} so defined maps $\mathcal{P}_1(\mathbf{R}^d)$ into the class $\text{Lip}(\mathbf{R}^d; \mathbf{R}^d)$ of Lipschitz continuous vector fields on \mathbf{R}^d .

With the assumptions above, one easily arrives at the existence and uniqueness theory for the N -body ODE system.

Theorem 1.3.1 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d; \mathbf{R}^d)$ satisfies assumptions (HK1-HK2). Then*

a) for each $N \geq 1$ and each N -tuple $Z_N^{in} = (z_1^{in}, \dots, z_N^{in})$, the Cauchy problem for the N -particle ODE system

$$\begin{cases} \dot{z}_i(t) = \frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)), & i = 1, \dots, N, \\ z_i(0) = z_i^{in}, \end{cases}$$

⁵Henceforth, the set of Borel probability measures on \mathbf{R}^d will be denoted by $\mathcal{P}(\mathbf{R}^d)$.

has a unique solution of class C^1 on \mathbf{R}

$$t \mapsto Z_N(t) = (z_1(t), \dots, z_N(t)) =: T_t Z_N^{in};$$

b) the empirical measure $f(t, dz) := \mu_{T_t Z_N^{in}}$ is a weak solution of the Cauchy problem for the mean field PDE

$$\begin{cases} \partial_t f + \operatorname{div}_z (f \mathcal{K} f) = 0, \\ f|_{t=0} = f^{in}. \end{cases}$$

Statement a) follows from the Cauchy-Lipschitz theorem. Statement b) follows from the method of characteristics for the transport equation. For the sake of being complete, we sketch the main steps in the proof of statement b), and leave the details as an exercise to be treated by the reader.

Exercise: Let $b \equiv b(t, y) \in C([0, \tau]; \mathbf{R}^d)$ be such that $D_y b \in C([0, \tau]; \mathbf{R}^d)$ and

$$(H) \quad |b(t, y)| \leq \kappa(1 + |y|)$$

for all $t \in [0, \tau]$ and $y \in \mathbf{R}^d$, where κ is a positive constant.

1) Prove that, for each $t \in [0, \tau]$, the Cauchy problem for the ODE

$$\begin{cases} \dot{Y}(s) = b(s, Y(s)), \\ Y(t) = y, \end{cases}$$

has a unique solution $s \mapsto Y(s, t, y)$. What is the maximal domain of definition of this solution? What is the regularity of the map Y viewed as a function of the 3 variables s, t, y ?

2) What is the role of assumption (H)?

3) Prove that, for each $t_1, t_2, t_3 \in [0, \tau]$ and $y \in \mathbf{R}^d$, one has

$$Y(t_3, t_2, Y(t_2, t_1, y)) = Y(t_3, t_1, y).$$

4) Compute

$$\partial_t Y(s, t, y) + b(t, y) \cdot \nabla_y Y(s, t, y).$$

5) Let $f^{in} \in C^1(\mathbf{R}^d)$. Prove that the Cauchy problem for the transport equation

$$\begin{cases} \partial_t f(t, y) + b(t, y) \cdot \nabla_y f(t, y) = 0, \\ f|_{t=0} = f^{in}, \end{cases}$$

has a unique solution $f \in C^1([0, \tau] \times \mathbf{R}^d)$, and that this solution is given by the formula

$$f(t, y) = f^{in}(Y(0, t, y)).$$

6) Let μ^{in} be a Borel probability measure on \mathbf{R}^d . Prove that the push-forward measure⁶

$$\mu(t) := Y(t, 0, \cdot) \# \mu^{in}$$

⁶Given two measurable spaces (X, \mathcal{A}) and (Y, \mathcal{B}) , a measurable map $\Phi : (X, \mathcal{A}) \rightarrow (Y, \mathcal{B})$ and a measure m on (X, \mathcal{A}) , the push-forward of m under Φ is the measure on (Y, \mathcal{B}) defined by the formula

$$\Phi \# m(B) = m(\Phi^{-1}(B)), \quad \text{for all } B \in \mathcal{B}.$$

is a weak solution of

$$\begin{cases} \partial_t \mu + \operatorname{div}_y(\mu b) = 0, \\ \mu|_{t=0} = \mu^{in}. \end{cases}$$

Hint: for $\phi \in C_c^1(\mathbf{R}^d)$, compute

$$\frac{d}{dt} \int_{\mathbf{R}^d} \phi(Y(t, 0, y)) \mu^{in}(dy).$$

7) Prove that the unique weak solution⁷ $\mu \in C([0, \tau], w - \mathcal{P}(\mathbf{R}^d))$ of the Cauchy problem considered in 6) is the push-forward measure defined by the formula

$$\mu(t) := Y(t, 0, \cdot) \# \mu^{in}$$

for each $t \in [0, \tau]$. (Hint: for $\phi \in C_c^1(\mathbf{R}^d)$, compute

$$\frac{d}{dt} \langle Y(0, t, \cdot) \# \mu(t), \phi \rangle$$

in the sense of distributions on $(0, \tau)$.)

For a solution of this exercise, see chapter 1, section 1 of [17].

Our next step is to formulate and solve a new problem that will contain both the N -particle ODE system in the mean-field scaling and the mean-field PDE.

Theorem 1.3.2 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies assumptions (HK1-HK2). For each $\zeta^{in} \in \mathbf{R}^d$ and each Borel probability measure $\mu^{in} \in \mathcal{P}_1(\mathbf{R}^d)$, there exists a unique solution denoted by*

$$\mathbf{R} \ni t \mapsto Z(t, \zeta^{in}, \mu^{in}) \in \mathbf{R}^d$$

of class C^1 of the problem

$$\begin{cases} \partial_t Z(t, \zeta^{in}, \mu^{in}) = (\mathcal{K}\mu(t))(Z(t, \zeta^{in}, \mu^{in})), \\ \mu(t) = Z(t, \cdot, \mu^{in}) \# \mu^{in}, \\ Z(0, \zeta^{in}, \mu^{in}) = \zeta^{in}. \end{cases}$$

Notice that the ODE governing the evolution of $t \mapsto Z(t, \zeta^{in}, \mu^{in})$ is set in the single-particle phase space \mathbf{R}^d , and not in the N -particle phase space, as is the case of the ODE system studied in Theorem 1.3.1.

Obviously, the ODE appearing in Theorem 1.3.2 is precisely the equation of characteristics for the mean field PDE. Henceforth, we refer to this ODE as the equations of “mean field characteristics”, and to its solution Z as the “mean field characteristic flow”.

How the mean field characteristic flow Z and the flow T_t associated to the N -particle ODE system are related is explained in the next proposition.

⁷We designate by $w - \mathcal{P}(\mathbf{R}^d)$ the set $\mathcal{P}(\mathbf{R}^d)$ equipped with the weak topology of probability measures, i.e. the topology defined by the family of semi-distances

$$d_\phi(\mu, \nu) := \left| \int_{\mathbf{R}^d} \phi(z) \mu(dz) - \int_{\mathbf{R}^d} \phi(z) \nu(dz) \right|$$

as ϕ runs through $C_b(\mathbf{R}^d)$.

Proposition 1.3.3 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies assumptions (HK1-HK2). For each $Z_N^{in} = (z_1^{in}, \dots, z_N^{in})$, the solution*

$$T_t Z_N^{in} = (z_1(t), \dots, z_N(t))$$

of the N -body problem and the mean field characteristic flow $Z(t, \zeta^{in}, \mu^{in})$ satisfy

$$z_i(t) = Z(t, z_i^{in}, \mu_{Z_N^{in}}), \quad i = 1, \dots, N,$$

for all $t \in \mathbf{R}$.

Proof of Proposition 1.3.3. Define

$$\zeta_i(t) := Z(t, z_i^{in}, \mu_{Z_N^{in}}), \quad i = 1, \dots, N.$$

Then⁸

$$\mu(t) = Z(t, \cdot, \mu_{Z_N^{in}}) \# \mu_{Z_N^{in}} = \frac{1}{N} \sum_{j=1}^N \delta_{\zeta_j(t)}$$

for all $t \in \mathbf{R}$. Therefore, ζ_i satisfies

$$\dot{\zeta}_i(t) = (\mathcal{K}\mu(t))(\zeta_i(t)) = \frac{1}{N} \sum_{j=1}^N K(\zeta_i(t), \zeta_j(t)), \quad i = 1, \dots, N,$$

for all $t \in \mathbf{R}$. Moreover

$$\zeta_i(0) = Z(0, z_i^{in}, \mu^{in}) = z_i^{in}, \quad i = 1, \dots, N.$$

Therefore, by uniqueness of the solution of the N -particle equation (Theorem 1.3.1), one has

$$\zeta_i(t) = z_i(t),$$

for all $i = 1, \dots, N$ and all $t \in \mathbf{R}$. ■

The proof of Theorem 1.3.2 is a simple variant of the proof of the Cauchy-Lipschitz theorem.

⁸The reader should be aware of the following subtle point. In classical references on distribution theory, such as [53], the Dirac mass is viewed as a distribution, therefore as an object that generalizes the notion of function. There is a notion of pull-back of a distribution under a C^∞ diffeomorphism such that the pull-back of the Dirac mass at y_0 with a C^∞ diffeomorphism $\chi: \mathbf{R}^N \rightarrow \mathbf{R}^N$ satisfying $\chi(x_0) = y_0$ is

$$\delta_{y_0} \circ \chi = |\det(D\chi(x_0))|^{-1} \delta_{x_0}.$$

This notion is not to be confused with the push-forward under χ of the Dirac mass at δ_{x_0} viewed as a probability measure, which, according to the definition in the previous footnote is

$$\chi \# \delta_{x_0} = \delta_{y_0}.$$

In particular

$$\chi \# \delta_{x_0} \neq \delta_{x_0} \circ \chi^{-1}$$

unless χ has Jacobian determinant 1 at x_0 .

Proof of Theorem 1.3.2. Let $\mu^{in} \in \mathcal{P}_1(\mathbf{R}^d)$, and denote

$$C_1 := \int_{\mathbf{R}^d} |z| \mu^{in}(dz).$$

Let

$$X := \left\{ v \in C(\mathbf{R}^d; \mathbf{R}^d) \text{ s.t. } \sup_{z \in \mathbf{R}^d} \frac{|v(z)|}{1+|z|} < \infty \right\},$$

which is a Banach space for the norm

$$\|v\|_X := \sup_{z \in \mathbf{R}^d} \frac{|v(z)|}{1+|z|}.$$

By assumption (HK2) on the interaction kernel K , for each $v, w \in X$, one has

$$\begin{aligned} & \left| \int_{\mathbf{R}^d} K(v(z), v(z')) \mu^{in}(dz') - \int_{\mathbf{R}^d} K(w(z), w(z')) \mu^{in}(dz') \right| \\ & \leq L \int_{\mathbf{R}^d} (|v(z) - w(z)| + |v(z') - w(z')|) \mu^{in}(dz') \\ & \leq L \|v - w\|_X (1 + |z|) + L \|v - w\|_X \int_{\mathbf{R}^d} (1 + |z'|) \mu^{in}(dz') \\ & = L \|v - w\|_X (1 + |z| + 1 + C_1) \\ & \leq L \|v - w\|_X (2 + C_1)(1 + |z|). \end{aligned}$$

Define a sequence $(Z_n)_{n \geq 0}$ by induction, as follows:

$$\begin{cases} Z_{n+1}(t, \zeta) = \zeta + \int_0^t \int_{\mathbf{R}^d} K(Z_n(s, \zeta), Z_n(s, \zeta')) \mu^{in}(d\zeta') ds, & n \geq 0, \\ Z_0(t, \zeta) = \zeta. \end{cases}$$

One checks by induction with the inequality above that, for each $n \in \mathbf{N}$,

$$\|Z_{n+1}(t, \cdot) - Z_n(t, \cdot)\|_X \leq \frac{((2 + C_1)L|t|)^n}{n!} \|Z_1(t, \cdot) - Z_0(t, \cdot)\|_X.$$

Since

$$\begin{aligned} |Z_1(t, \zeta) - \zeta| &= \left| \int_0^t \int_{\mathbf{R}^d} K(\zeta, \zeta') \mu^{in}(d\zeta') ds \right| \\ &\leq \int_0^{|t|} \int_{\mathbf{R}^d} L(|\zeta| + |\zeta'|) \mu^{in}(d\zeta') ds \\ &= \int_0^{|t|} L(|\zeta| + C_1) ds \leq L(1 + C_1)(1 + |\zeta|)|t|, \end{aligned}$$

one has

$$\|Z_{n+1}(t, \cdot) - Z_n(t, \cdot)\|_X \leq \frac{((2 + C_1)L|t|)^{n+1}}{n!}.$$

Thus, for each $\tau > 0$,

$$Z_n(t, \cdot) \rightarrow Z(t, \cdot) \quad \text{in } X \text{ uniformly on } [-\tau, \tau],$$

where $Z \in C(\mathbf{R}; X)$ satisfies

$$Z(t, \zeta) = \zeta + \int_0^t \int_{\mathbf{R}^d} K(Z(s, \zeta), Z(s, \zeta')) \mu^{in}(d\zeta') ds$$

for all $t \in \mathbf{R}$ and all $\zeta \in \mathbf{R}^d$.

If Z and $\tilde{Z} \in C(\mathbf{R}; X)$ satisfy the integral equation above, then

$$Z(t, \zeta) - \tilde{Z}(t, \zeta) = \int_{\mathbf{R}^d} (K(Z(s, \zeta), Z(s, \zeta')) - K(\tilde{Z}(s, \zeta), \tilde{Z}(s, \zeta'))) \mu^{in}(d\zeta'),$$

so that, for all $t \in \mathbf{R}$, one has

$$\|Z(t, \cdot) - \tilde{Z}(t, \cdot)\|_X \leq L(2 + C_1) \left| \int_0^t \|Z(s, \cdot) - \tilde{Z}(s, \cdot)\|_X ds \right|.$$

This implies that

$$\|Z(t, \cdot) - \tilde{Z}(t, \cdot)\|_X = 0$$

by Gronwall's inequality, so that $Z = \tilde{Z}$. Hence the integral equation has only one solution $Z \in C(\mathbf{R}; X)$.

Since $Z \in C(\mathbf{R}_+; X)$, $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies (HK2) and $\mu^{in} \in \mathcal{P}_1(\mathbf{R}^d)$, the function

$$s \mapsto \int_{\mathbf{R}^d} K(Z(s, \zeta), Z(s, \zeta')) \mu^{in}(d\zeta')$$

is continuous on \mathbf{R} .

Using the integral equation shows that the function $t \mapsto Z(t, \zeta)$ is of class C^1 on \mathbf{R} and satisfies

$$\begin{cases} \partial_t Z(t, \zeta) = \int_{\mathbf{R}^d} K(Z(t, \zeta), Z(t, \zeta')) \mu^{in}(d\zeta'), \\ Z(0, \zeta) = \zeta. \end{cases}$$

Substituting $z' = Z(t, \zeta')$ in the integral above, one has

$$\int_{\mathbf{R}^d} K(Z(t, \zeta), Z(t, \zeta')) \mu^{in}(d\zeta') = \int_{\mathbf{R}^d} K(Z(t, \zeta), z') Z(t, \cdot) \# \mu^{in}(dz')$$

so that the element Z of $C(\mathbf{R}; X)$ so constructed is the unique solution of the mean field characteristic equation. ■

References for this and the previous section are [20, 75].

1.4 Dobrushin's stability estimate and the mean field limit

1.4.1 The Monge-Kantorovich distance

For each $r > 1$, we denote by $\mathcal{P}_r(\mathbf{R}^d)$ the set of Borel probability measures on \mathbf{R}^d with a finite moment of order r , i.e. satisfying

$$\int_{\mathbf{R}^d} |z|^r \mu(dz) < \infty.$$

Given $\mu, \nu \in \mathcal{P}_r(\mathbf{R}^d)$, we define $\Pi(\mu, \nu)$ to be the set of Borel probability measures π on $\mathbf{R}^d \times \mathbf{R}^d$ with first and second marginals μ and ν respectively. Equivalently, for each $\pi \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$,

$$\pi \in \Pi(\mu, \nu) \Leftrightarrow \iint_{\mathbf{R}^d \times \mathbf{R}^d} (\phi(x) + \psi(y)) \pi(dxdy) = \int_{\mathbf{R}^d} \phi(x) \mu(dx) + \int_{\mathbf{R}^d} \psi(y) \nu(dy)$$

for each $\phi, \psi \in C(\mathbf{R}^d)$ such that $\phi(z) = O(|z|^r)$ and $\psi(z) = O(|z|^r)$ as $|z| \rightarrow \infty$.

Probability measures belonging to $\Pi(\mu, \nu)$ are sometimes referred to as “couplings of μ and ν ”.

Exercise: Check that, if μ and $\nu \in \mathcal{P}_r(\mathbf{R}^d)$ for some $r > 0$, then one has $\Pi(\mu, \nu) \subset \mathcal{P}_r(\mathbf{R}^d \times \mathbf{R}^d)$.

With these elements of notation, we now introduce the notion of Monge-Kantorovich distance.

Definition 1.4.1 For each $r \geq 1$ and each $\mu, \nu \in \mathcal{P}_r(\mathbf{R}^d)$, the Monge-Kantorovich distance $\text{dist}_{MK,r}(\mu, \nu)$ between μ and ν is defined by the formula

$$\text{dist}_{MK,r}(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \left(\iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y|^r \pi(dxdy) \right)^{1/r}.$$

These distances also go by the name of “Kantorovich-Rubinstein distances” or “Wasserstein distances” — although the minimization problem in the right hand side of the formula defining $\text{dist}_{MK,r}$ had been considered for the first time by Monge⁹ and systematically studied by Kantorovich.

We shall use the Monge-Kantorovich distances only as a convenient tool for studying the stability of the mean field characteristic flow. Therefore, we shall not attempt to present the mathematical theory of these distances and refer instead to the C. Villani's books [95, 96] for a very detailed discussion of this topic.

However, it is useful to know the following property that is special to the case $r = 1$.

⁹Monge's original problem was to minimize over the class of all Borel measurable transportation maps $T : \mathbf{R}^d \rightarrow \mathbf{R}^d$ such that $T\#\mu = \nu$ the transportation cost

$$\int_{\mathbf{R}^d} |x - T(x)| \mu(dx).$$

Proposition 1.4.2 *The Monge-Kantorovich distance with exponent 1 is also given by the formula*

$$\text{dist}_{MK,1}(\mu, \nu) = \sup_{\substack{\phi \in \text{Lip}(\mathbf{R}^d) \\ \text{Lip}(\phi) \leq 1}} \left| \int_{\mathbf{R}^d} \phi(z) \mu(dz) - \int_{\mathbf{R}^d} \phi(z) \nu(dz) \right|,$$

with the notation

$$\text{Lip}(\phi) := \sup_{x \neq y \in \mathbf{R}^d} \frac{|\phi(x) - \phi(y)|}{|x - y|}.$$

for the Lipschitz constant of ϕ .

The proof of this proposition is based on a duality argument in optimization: see for instance Theorems 1.14 and 7.3 (i) in [95].

1.4.2 Dobrushin's estimate

As explained in Proposition 1.3.3, the mean field characteristic flow contains all the relevant information about both the mean field PDE and the N -particle ODE system.

Dobrushin's approach to the mean field limit is based on the idea of proving the stability of the mean field characteristic flow $Z(t, \zeta^{in}, \mu^{in})$ in *both* the initial position in phase space ζ^{in} and the initial distribution μ^{in} . As we shall see, the Monge-Kantorovich distance is the best adapted mathematical tool to measure this stability.

Dobrushin's idea ultimately rests on the following key computation. Let $\zeta_1^{in}, \zeta_2^{in} \in \mathbf{R}^d$, and let $\mu_1^{in}, \mu_2^{in} \in \mathcal{P}_1(\mathbf{R}^d)$. Then

$$\begin{aligned} Z(t, \zeta_1, \mu_1^{in}) - Z(t, \zeta_2, \mu_2^{in}) &= \zeta_1 - \zeta_2 \\ &+ \int_0^t \int_{\mathbf{R}^d} K(Z(s, \zeta_1, \mu_1^{in}), z') \mu_1(s, dz') ds \\ &- \int_0^t \int_{\mathbf{R}^d} K(Z(s, \zeta_2, \mu_2^{in}), z') \mu_2(s, dz') ds. \end{aligned}$$

Since $\mu_j(t) = Z(t, \cdot, \mu_j^{in}) \# \mu_j^{in}$ for $j = 1, 2$, each inner integral on the right hand side of the equality above can be expressed as follows:

$$\begin{aligned} \int_{\mathbf{R}^d} K(Z(s, \zeta_j, \mu_j^{in}), z') \mu_j(s, dz') \\ = \int_{\mathbf{R}^d} K(Z(s, \zeta_j, \mu_j^{in}), Z(s, \zeta_j', \mu_j^{in})) \mu_j^{in}(d\zeta_j') \end{aligned}$$

for $j = 1, 2$. Therefore, for each coupling $\pi^{in} \in \mathcal{P}_1(\mu_1^{in}, \mu_2^{in})$, one has

$$\begin{aligned} & \int_{\mathbf{R}^d} K(Z(s, \zeta_1, \mu_1^{in}), Z(s, \zeta'_1, \mu_1^{in})) \mu_1^{in}(d\zeta'_1) \\ & - \int_{\mathbf{R}^d} K(Z(s, \zeta_2, \mu_2^{in}), Z(s, \zeta'_2, \mu_2^{in})) \mu_2^{in}(d\zeta'_2) \\ & = \iint_{\mathbf{R}^d \times \mathbf{R}^d} (K(Z(s, \zeta_1, \mu_1^{in}), Z(s, \zeta'_1, \mu_1^{in})) \\ & \quad - K(Z(s, \zeta_2, \mu_2^{in}), Z(s, \zeta'_2, \mu_2^{in}))) \pi^{in}(d\zeta'_1, d\zeta'_2), \end{aligned}$$

so that

$$\begin{aligned} Z(t, \zeta_1, \mu_1^{in}) - Z(t, \zeta_2, \mu_2^{in}) &= \zeta_1 - \zeta_2 \\ &+ \int_0^t \iint_{\mathbf{R}^d \times \mathbf{R}^d} (K(Z(s, \zeta_1, \mu_1^{in}), Z(s, \zeta'_1, \mu_1^{in})) \\ & \quad - K(Z(s, \zeta_2, \mu_2^{in}), Z(s, \zeta'_2, \mu_2^{in}))) \pi^{in}(d\zeta'_1, d\zeta'_2) ds. \end{aligned}$$

This last equality is the key observation in Dobrushin's argument, which explains the role of couplings of μ_1^{in} and μ_2^{in} in this problem, and therefore why it is natural to use the Monge-Kantorovich distance.

After this, the end of the argument is plain sailing. By assumption (HK2) on the interaction kernel K , for all $a, a', b, b' \in \mathbf{R}^d$, one has

$$\begin{aligned} |K(a, a') - K(b, b')| &\leq |K(a, a') - K(b, a')| + |K(b, a') - K(b, b')| \\ &\leq L|a - b| + L|a' - b'|. \end{aligned}$$

Therefore

$$\begin{aligned} & |Z(t, \zeta_1, \mu_1^{in}) - Z(t, \zeta_2, \mu_2^{in})| \\ & \leq |\zeta_1 - \zeta_2| + L \int_0^t |Z(s, \zeta_1, \mu_1^{in}) - Z(s, \zeta_2, \mu_2^{in})| ds \\ & + L \int_0^t \iint_{\mathbf{R}^d \times \mathbf{R}^d} |Z(s, \zeta'_1, \mu_1^{in}) - Z(s, \zeta'_2, \mu_2^{in})| \pi^{in}(d\zeta'_1, d\zeta'_2) ds. \end{aligned}$$

It is convenient at this point to introduce the notation

$$D[\pi](s) := \iint_{\mathbf{R}^d \times \mathbf{R}^d} |Z(s, \zeta'_1, \mu_1^{in}) - Z(s, \zeta'_2, \mu_2^{in})| \pi(d\zeta'_1, d\zeta'_2)$$

for each $\pi \in \mathcal{P}_1(\mathbf{R}^d \times \mathbf{R}^d)$. Thus, the previous inequality becomes

$$\begin{aligned} & |Z(t, \zeta_1, \mu_1^{in}) - Z(t, \zeta_2, \mu_2^{in})| \leq |\zeta_1 - \zeta_2| \\ & + L \int_0^t |Z(s, \zeta_1, \mu_1^{in}) - Z(s, \zeta_2, \mu_2^{in})| ds + L \int_0^t D[\pi^{in}](s) ds. \end{aligned}$$

Integrating both sides of the inequality above with respect to $\pi^{in}(d\zeta_1 d\zeta_2)$ leads to

$$\begin{aligned} D[\pi^{in}](t) &\leq \iint_{\mathbf{R}^d \times \mathbf{R}^d} |\zeta_1 - \zeta_2| \pi^{in}(d\zeta_1 d\zeta_2) + 2L \int_0^t D[\pi^{in}](s) ds \\ &= D[\pi^{in}](0) + 2L \int_0^t D[\pi^{in}](s) ds. \end{aligned}$$

By Gronwall's inequality, we conclude that, for all $t \in \mathbf{R}$, one has

$$D[\pi^{in}](t) \leq D[\pi^{in}](0) e^{2L|t|}.$$

Now we can state Dobrushin's stability theorem.

Theorem 1.4.3 (Dobrushin) *Assume that $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies (HK1-HK2). Let $\mu_1^{in}, \mu_2^{in} \in \mathcal{P}_1(\mathbf{R}^d)$. For all $t \in \mathbf{R}$, let*

$$\begin{cases} \mu_1(t) = Z(t, \cdot, \mu_1^{in}) \# \mu_1^{in}, \\ \mu_2(t) = Z(t, \cdot, \mu_2^{in}) \# \mu_2^{in}, \end{cases}$$

where Z is the mean field characteristic flow defined in Theorem 1.3.2.

Then, for all $t \in \mathbf{R}$, one has

$$\text{dist}_{MK,1}(\mu_1(t), \mu_2(t)) \leq e^{2L|t|} \text{dist}_{MK,1}(\mu_1^{in}, \mu_2^{in}).$$

Proof. We have seen that, for all $\mu_1^{in}, \mu_2^{in} \in \mathcal{P}_1(\mathbf{R}^d)$ and all $\pi^{in} \in \Pi(\mu_1^{in}, \mu_2^{in})$, one has

$$D[\pi^{in}](t) \leq D[\pi^{in}](0) e^{2L|t|}$$

for all $t \in \mathbf{R}$.

Since $Z(t, \cdot, \mu_j^{in}) \# \mu_j^{in} = \mu_j(t)$ for $j = 1, 2$, the map

$$\Phi_t : (\zeta_1, \zeta_2) \mapsto (Z(t, \zeta_1, \mu_1^{in}), Z(t, \zeta_2, \mu_2^{in}))$$

satisfies

$$\Phi_t \# \pi^{in} = \pi(t) \in \Pi(\mu_1(t), \mu_2(t))$$

for all $t \in \mathbf{R}$, since $\pi^{in} \in \Pi(\mu_1^{in}, \mu_2^{in})$.

Thus

$$\begin{aligned} \text{dist}_{MK,1}(\mu_1(t), \mu_2(t)) &= \inf_{\pi \in \Pi(\mu_1(t), \mu_2(t))} \iint_{\mathbf{R}^d \times \mathbf{R}^d} |\zeta_1 - \zeta_2| \pi(d\zeta_1 d\zeta_2) \\ &\leq \inf_{\pi^{in} \in \Pi(\mu_1^{in}, \mu_2^{in})} \iint_{\mathbf{R}^d \times \mathbf{R}^d} |Z(t, \zeta_1, \mu_1^{in}) - Z(t, \zeta_2, \mu_2^{in})| \pi^{in}(d\zeta_1 d\zeta_2) \\ &= \inf_{\pi^{in} \in \Pi(\mu_1^{in}, \mu_2^{in})} D[\pi^{in}](t) \leq e^{2L|t|} \inf_{\pi^{in} \in \Pi(\mu_1^{in}, \mu_2^{in})} D[\pi^{in}](0) \\ &= e^{2L|t|} \text{dist}_{MK,1}(\mu_1^{in}, \mu_2^{in}) \end{aligned}$$

which concludes the proof. ■

The discussion in this section is inspired from [29]; see also [71]. The interested reader is also referred to the very interesting paper [69] where Monge-Kantorovich distances with exponents different from 1 are used in the same context — see also [48].

1.4.3 The mean field limit

The mean field limit of the N -particle system is a consequence of Dobrushin's stability theorem, as explained below.

Theorem 1.4.4 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d)$ and satisfies assumptions (HK1-HK2). Let f^{in} be a probability density on \mathbf{R}^d such that*

$$\int_{\mathbf{R}^d} |z| f^{in}(z) dz < \infty.$$

Then the Cauchy problem for the mean field PDE

$$\begin{cases} \partial_t f(t, z) + \operatorname{div}_z(f(t, z) \mathcal{K} f(t, z)) = 0, & z \in \mathbf{R}^d, t \in \mathbf{R}, \\ f|_{t=0} = f^{in} \end{cases}$$

has a unique weak solution $f \in C(\mathbf{R}; L^1(\mathbf{R}^d))$.

For each $N \geq 1$, let $\mathfrak{Z}(N) = (z_{1,N}^{in}, \dots, z_{N,N}^{in}) \in (\mathbf{R}^d)^N$ be such that

$$\mu_{\mathfrak{Z}(N)} = \frac{1}{N} \sum_{j=1}^N \delta_{z_{j,N}^{in}}$$

satisfies

$$\operatorname{dist}_{MK,1}(\mu_{\mathfrak{Z}(N)}, f^{in}) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Let $t \mapsto T_t \mathfrak{Z}(N) = (z_{1,N}(t), \dots, z_{N,N}(t)) \in (\mathbf{R}^d)^N$ be the solution of the N -particle ODE system with initial data $\mathfrak{Z}(N)$, i.e.

$$\begin{cases} \dot{z}_i(t) = \frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)), & i = 1, \dots, N, \\ z_i(0) = z_i^{in}. \end{cases}$$

Then¹⁰

$$\mu_{T_t \mathfrak{Z}(N)} \rightarrow f(t, \cdot) \mathcal{L}^d \quad \text{as } N \rightarrow \infty$$

in the weak topology of probability measures, with convergence rate

$$\operatorname{dist}_{MK,1}(\mu_{T_t \mathfrak{Z}(N)}, f(t, \cdot) \mathcal{L}^d) \leq e^{2L|t|} \operatorname{dist}_{MK,1}(\mu_{\mathfrak{Z}(N)}, f^{in}) \rightarrow 0$$

as $N \rightarrow \infty$ for each $t \in \mathbf{R}$.

Proof. By Theorem 1.3.2 and questions 6 and 7 in the exercise on the method of characteristics before Theorem 1.3.2, one has

$$f(t, \cdot) \mathcal{L}^d = Z(t, \cdot, f^{in} \mathcal{L}^d) \# f^{in} \mathcal{L}^d$$

for all $t \in \mathbf{R}$. This implies in particular the uniqueness of the solution of the Cauchy problem in $C(\mathbf{R}; L^1(\mathbf{R}^d))$ for the mean field PDE.

¹⁰The notation \mathcal{L}^d designates the Lebesgue measure on \mathbf{R}^d .

By Proposition 1.3.3,

$$\mu_{T_t \mathfrak{Z}(N)} = Z(t, \cdot, \mu_{\mathfrak{Z}(N)}) \# \mu_{\mathfrak{Z}(N)}$$

for all $t \in \mathbf{R}$.

By Dobrushin's stability estimate,

$$\text{dist}_{MK,1}(\mu_{T_t \mathfrak{Z}(N)}, f(t, \cdot) \mathcal{L}^d) \leq e^{2L|t|} \text{dist}_{MK,1}(\mu_{\mathfrak{Z}(N)}, f^{in})$$

for all $t \in \mathbf{R}$, and since we have chosen $\mathfrak{Z}(N)$ so that

$$\text{dist}_{MK,1}(\mu_{\mathfrak{Z}(N)}, f^{in}) \rightarrow 0$$

as $N \rightarrow \infty$, we conclude that

$$\text{dist}_{MK,1}(\mu_{T_t \mathfrak{Z}(N)}, f(t, \cdot) \mathcal{L}^d) \rightarrow 0$$

as $N \rightarrow \infty$ for each $t \in \mathbf{R}$.

As for weak convergence, pick $\phi \in \text{Lip}(\mathbf{R}^d)$; then

$$\begin{aligned} & \left| \int_{\mathbf{R}^d} \phi(z) \mu_{T_t \mathfrak{Z}(N)}(dz) - \int_{\mathbf{R}^d} \phi(z) f(t, z) dz \right| \\ &= \left| \iint_{\mathbf{R}^d \times \mathbf{R}^d} (\phi(x) - \phi(y)) \pi(dxdy) \right| \\ &\leq \iint_{\mathbf{R}^d \times \mathbf{R}^d} |\phi(x) - \phi(y)| \pi(dxdy) \\ &\leq \text{Lip}(\phi) \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y| \pi(dxdy) \end{aligned}$$

for each $\pi \in \Pi(\mu_{T_t \mathfrak{Z}(N)}, f(t, \cdot) \mathcal{L}^d)$. Thus

$$\begin{aligned} & \left| \int_{\mathbf{R}^d} \phi(z) \mu_{T_t \mathfrak{Z}(N)}(dz) - \int_{\mathbf{R}^d} \phi(z) f(t, z) dz \right| \\ &\leq \text{Lip}(\phi) \inf_{\pi \in \Pi(\mu_{T_t \mathfrak{Z}(N)}, f(t, \cdot) \mathcal{L}^d)} \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y| \pi(dxdy) \\ &= \text{Lip}(\phi) \text{dist}_{MK,1}(\mu_{T_t \mathfrak{Z}(N)}, f(t, \cdot) \mathcal{L}^d) \rightarrow 0 \end{aligned}$$

for each $t \in \mathbf{R}$ as $N \rightarrow \infty$. (Notice that the inequality above is an obvious consequence of the definition of $\text{dist}_{MK,1}$, so that the equality in Proposition 1.4.2 is not needed here.)

This is true in particular for each $\phi \in C_c^1(\mathbf{R}^d)$, and since $C_c^1(\mathbf{R}^d)$ is dense in $C_c(\mathbf{R}^d)$, we conclude that

$$\int_{\mathbf{R}^d} \phi(z) \mu_{T_t \mathfrak{Z}(N)}(dz) \rightarrow \int_{\mathbf{R}^d} \phi(z) f(t, z) dz$$

as $N \rightarrow \infty$ for each $\phi \in C_c(\mathbf{R}^d)$. Since

$$\int_{\mathbf{R}^d} \mu_{T_t \mathfrak{Z}(N)}(dz) = \int_{\mathbf{R}^d} f(t, z) dz = 1$$

for all $t \in \mathbf{R}$, we conclude that the convergence above holds for each $\phi \in C_b(\mathbf{R}^d)$, which means that

$$\mu_{T_t \mathfrak{Z}(N)} \rightarrow f(t, \cdot) \mathcal{L}^d$$

as $N \rightarrow \infty$ in the weak topology of probability measures, by applying Theorem 6.8 in chapter II of [70], sometimes referred to as the ‘‘portmanteau theorem’’.

■

The theorem above is the main result on the mean field limit in [75, 20, 29].

1.4.4 On the choice of the initial data

In practice, using Theorem 1.4.4 as a rigorous justification of the mean field limit requires being able to generate N -tuples of the form $\mathfrak{Z}(N) = (z_{1,N}^{in}, \dots, z_{N,N}^{in}) \in (\mathbf{R}^d)^N$ such that

$$\mu_{\mathfrak{Z}(N)} = \frac{1}{N} \sum_{j=1}^N \delta_{z_{j,N}^{in}}$$

satisfies

$$\text{dist}_{MK,1}(\mu_{\mathfrak{Z}(N)}, f^{in}) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Assume that f^{in} is a probability density on \mathbf{R}^d such that

$$\int_{\mathbf{R}^d} |z|^2 f(z) dz < \infty.$$

Let $\Omega := (\mathbf{R}^d)^{\mathbf{N}^*}$, the set of sequences of points in \mathbf{R}^d indexed by \mathbf{N}^* . Let \mathcal{F} be the σ -algebra on Ω generated by cylinders, i.e. by sets of the form

$$\prod_{n \geq 1} B_n \quad \text{with } B_n \text{ Borel set in } \mathbf{R}^d$$

and $B_n = \mathbf{R}^d$ for all but finitely many n .

Finally, we endow the measurable space (Ω, \mathcal{F}) with the probability measure $\mathbf{P} := (f^{in})^{\otimes \infty}$, defined on the set of cylinders of Ω by the formula

$$\mathbf{P} \left(\prod_{n \geq 1} B_n \right) = \prod_{n \geq 1} f^{in}(B_n).$$

(Notice that $f^{in}(B_n) = 1$ for all but finitely many n , since $B_n = \mathbf{R}^d$ except for finitely many n .)

Theorem 1.4.5 *For each $\mathbf{z}^{in} = (z_k^{in})_{k \geq 1} \in \Omega$, let $Z_N^{in} = (z_1^{in}, \dots, z_N^{in})$. Then*

$$\text{dist}_{MK,1}(\mu_{Z_N^{in}}, f^{in} \mathcal{L}^d) \rightarrow 0$$

as $N \rightarrow \infty$ for \mathbf{P} -a.e. $\mathbf{z}^{in} \in \Omega$.

Proof. For $\phi \in C_c(\mathbf{R}^d)$ or $\phi(z) = |z|$, consider the sequence of random variables on (Ω, \mathcal{F}) defined by

$$Y_n(\mathbf{z}) = \phi(z_n),$$

where

$$\mathbf{z} := (z_1, \dots, z_n, \dots) \in \Omega.$$

The random variables Y_n are identically distributed, since

$$\mathbf{P}(Y_n \geq a) = \int_{\mathbf{R}^d} \mathbf{1}_{\phi(z) \geq a} f^{in}(z) dz$$

is independent of n .

The random variables Y_n are also independent, since for all $N \geq 1$ and all $g_1, \dots, g_N \in C_b(\mathbf{R})$, one has

$$\mathbf{E}^{\mathbf{P}}(g_1(Y_1) \dots g_N(Y_N)) = \prod_{k=1}^N \int_{\mathbf{R}^d} g_k(\phi(z)) f^{in}(z) dz = \prod_{k=1}^N \mathbf{E}^{\mathbf{P}}(g_k(Y_k)).$$

Finally, the random variables Y_n have finite variance since

$$\mathbf{E}^{\mathbf{P}}(|Y_n|^2) = \int_{\mathbf{R}^d} |z|^2 f^{in}(z) dz < \infty.$$

By the strong law of large numbers (see Theorem 3.27 in [21]), one has

$$\left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi \right\rangle = \frac{1}{N} \sum_{k=1}^N Y_k \rightarrow \mathbf{E}^{\mathbf{P}}(Y_1) = \int_{\mathbf{R}^d} \phi(z) f^{in}(z) dz$$

for \mathbf{P} -a.e. \mathbf{z} .

Since $C_c(\mathbf{R}^d)$ is separable, one can assume that the \mathbf{P} -negligible set is the same for all $\phi \in C_c(\mathbf{R}^d)$, and take its union with the one corresponding to $\phi(z) = |z|$. This means precisely that

$$\frac{1}{N} \sum_{k=1}^N \delta_{z_k} \rightarrow f^{in} \mathcal{L}^d$$

weakly in $\mathcal{P}_1(\mathbf{R}^d)$ for \mathbf{P} -a.e. $\mathbf{z} \in \Omega$. One concludes the proof with the lemma below. ■

Lemma 1.4.6 *The Monge-Kantorovich distance $\text{dist}_{MK,1}$ metricizes the topology of weak convergence on $\mathcal{P}_1(\mathbf{R}^d)$. In other words, given a sequence $(\mu_n)_{n \geq 1}$ of elements of $\mathcal{P}_1(\mathbf{R}^d)$ and $\mu \in \mathcal{P}_1(\mathbf{R}^d)$, the two following statements are equivalent:*

- (1) $\text{dist}_{MK,1}(\mu_n, \mu) \rightarrow 0$ as $n \rightarrow \infty$;
- (2) $\mu_n \rightarrow \mu$ weakly in $\mathcal{P}(\mathbf{R}^d)$ as $n \rightarrow \infty$ and

$$\sup_n \int_{\mathbf{R}^d} |z| \mathbf{1}_{|z| \geq R} \mu_n(dz) \rightarrow 0 \quad \text{as } R \rightarrow \infty.$$

For a proof of Lemma 1.4.6, see [95].

Exercise: The reader is invited to verify the fact that one can choose the \mathbf{P} -negligible set that appears in the proof of Theorem 1.4.5 to be the same for all $\phi \in C_c(\mathbf{R}^d)$ and for $\phi(z) = |z|$. Here is an outline of the argument.

a) Let $R > 0$; let E_R be the set of real-valued continuous functions defined on $[-R, R]^d$ that vanish identically on $\partial[-R, R]^d$, equipped with the sup-norm

$$\|\phi\| := \sup_{x \in [-R, R]^d} |\phi(x)|.$$

Prove that E_R is a separable Banach space.

Denote by \mathcal{N}_ϕ be the set of $\mathbf{z} \in \Omega$ such that

$$\left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi \right\rangle$$

does not converge to

$$\int_{\mathbf{R}^d} \phi(z) f^{in}(z) dz$$

as $N \rightarrow \infty$. Let $R > 0$ and let $(\phi_n)_{n \geq 1}$ be a dense sequence of elements of E_R , extended by 0 to \mathbf{R}^d . Define

$$\mathcal{N}_R := \bigcup_{n \geq 1} \mathcal{N}_{\phi_n}.$$

b) Prove that

$$\left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi \right\rangle \rightarrow \int_{\mathbf{R}^d} \phi(z) f^{in}(z) dz$$

as $N \rightarrow \infty$ for all $\phi \in E_R$ and all $\mathbf{z} \notin \mathcal{N}_R$. (Hint: pick $\phi \in E_R$ and $\epsilon > 0$, and choose $m := m(\phi, \epsilon)$ such that $\|\phi - \phi_m\| < \epsilon$. With the decomposition

$$\begin{aligned} \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi \right\rangle - \int_{\mathbf{R}^d} \phi(z) f^{in}(z) dz &= \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi - \phi_m \right\rangle \\ &+ \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi_m \right\rangle - \int_{\mathbf{R}^d} \phi_m(z) f^{in}(z) dz \\ &+ \int_{\mathbf{R}^d} (\phi_m(z) - \phi(z)) f^{in}(z) dz, \end{aligned}$$

prove that

$$\left| \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{z_k}, \phi \right\rangle - \int_{\mathbf{R}^d} \phi(z) f^{in}(z) dz \right| < 3\epsilon$$

for all $\mathbf{z} \notin \mathcal{N}_R$ provided that $N \geq N_0 = N_0(\epsilon, \phi)$.

c) Complete the proof of Theorem 1.4.5.

Thus, using Theorem 1.4.4 to prove the mean field limit requires choosing

$$\mathfrak{Z}(N) = (z_{1,N}^{in}, \dots, z_{N,N}^{in}) \in (\mathbf{R}^d)^N$$

for each $N \geq 1$ so that

$$\text{dist}_{MK,1}(\mu_{\mathfrak{Z}(N)}, f^{in} \mathcal{L}^d) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Theorem 1.4.5 provides us with a strategy for making this choice, which is to draw an infinite sequence z_j^{in} at random and independently with distribution $f^{in} \mathcal{L}^d$, and to set $z_{j,N}^{in} := z_j^{in}$. This strategy avoids the unpleasant task of having to change the first terms in $\mathfrak{Z}(N)$ as $N \rightarrow \infty$.

Since Dobrushin's estimate bounds $\text{dist}_{MK,1}(f(t, \cdot) \mathcal{L}^d, \mu_{T_t \mathfrak{Z}(N)})$ in terms of $\text{dist}_{MK,1}(f^{in} \mathcal{L}^d, \mu_{\mathfrak{Z}(N)})$, having an explicit bound on $\text{dist}_{MK,1}(f^{in} \mathcal{L}^d, \mu_{\mathfrak{Z}(N)})$ would provide us with a quantitative error estimate for the mean field limit. Such a bound will be given below — see Theorem 1.6.4.

More details on the topics discussed in the present section are to be found in [20], as well as a precise statement concerning the behavior of fluctuations around the mean field limit — in some sense, the asymptotic behavior at next order after the mean field limit (see Theorem 3.5 in [20]).

1.5 The BBGKY hierarchy and the mean field limit

In the previous derivation of the mean field limit of the N -particle system with interaction kernel K satisfying assumptions (HK1)-(HK2), we benefited from a happy circumstance, i.e. the fact that the empirical measure built on any solution of the N -particle ODE system is an *exact* solution of the mean field PDE. This is why the mean field limit was reduced to the stability of the solution of the mean field PDE in terms of its initial data, which follows from Dobrushin's stability estimate.

However, there are other situations in statistical mechanics where the empirical measure built on solutions of the N -particle ODE system may not be an exact solution of the target equation — the best known example of this being the Boltzmann equation of the kinetic theory of gases. There are various examples of such situations where the mean field limit can nevertheless be justified rigorously — see for instance [73], and [92] in the case of random dynamics.

There are also situations where there is no clear notion of empirical measure — think for instance to the N -body problem in quantum mechanics: in that case, it is impossible to exactly localize any one of the N particles in phase space, according to the Heisenberg uncertainty principle.

In the present section, we present another approach to the mean field limit of N -particle systems, that is, in some sense, more systematic than the method based on empirical measure and that can be applied to a greater variety of situations (including quantum models, as we shall see later).

1.5.1 N -particle distributions

The state at time t of a system of N identical particles located at the positions $z_1(t), \dots, z_N(t)$ in the single-particle phase space \mathbf{R}^d was described in the previous section by means of the empirical measure

$$\mu_{Z_N(t)} := \frac{1}{N} \sum_{i=1}^N \delta_{z_i(t)},$$

where $Z_N(t) := (z_1(t), \dots, z_N(t))$. The empirical is a probability measure in the single-particle phase space \mathbf{R}^d as mentioned above. This measure is parametrized by the element $Z_N(t)$ of the N -particle phase space $(\mathbf{R}^d)^N$.

Another way of describing the state of the same system of N particles at time t is to use its N -particle distribution function, that is

$$F_N(t, z_1, \dots, z_N).$$

More generally, one could think of the N -particle distribution as being a probability measure on the N -body phase space $(\mathbf{R}^d)^N$

$$F_N(t, dz_1 \dots dz_N).$$

The meaning of this N -particle distribution is as follows. Let $A_j \subset \mathbf{R}^d$ be Borel measurable sets for $j = 1, \dots, N$; then, the joint probability at time t to have particle 1 in A_1 , particle 2 in A_2 ... and particle N in A_N is

$$\int_{A_1} \int_{A_2} \dots \int_{A_N} F(t, dz_1 dz_2 \dots dz_N).$$

Now, we are interested in situations where all the particles in the N -particle system considered are identical. (For example, all electrons in the universe are identical; ions of any given species in a plasma are identical too.) Therefore, for any permutation $\sigma \in \mathfrak{S}_N$, the joint probability of having particle 1 in A_1 , particle 2 in A_2 ... and particle N in A_N is equal to the joint probability of having particle 1 in $A_{\sigma^{-1}(1)}$, particle 2 in $A_{\sigma^{-1}(2)}$... and particle N in $A_{\sigma^{-1}(N)}$. This is indeed obvious since it is impossible to distinguish particle 1 from particle $\sigma^{-1}(1)$, particle 2 from particle $\sigma^{-1}(2)$... and particle N from particle $\sigma^{-1}(N)$. Thus

$$\begin{aligned} & \int_{A_1} \int_{A_2} \dots \int_{A_N} F(t, dz_1 dz_2 \dots dz_N) \\ &= \int_{A_{\sigma^{-1}(1)}} \int_{A_{\sigma^{-1}(2)}} \dots \int_{A_{\sigma^{-1}(N)}} F(t, dz_1 dz_2 \dots dz_N). \end{aligned}$$

Equivalently

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} \mathbf{1}_{A_1 \times A_2 \times \dots \times A_N}(z_1, z_2, \dots, z_N) F(t, dz_1 dz_2 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} \mathbf{1}_{A_1 \times A_2 \times \dots \times A_N}(z_{\sigma(1)}, z_{\sigma(2)}, \dots, z_{\sigma(N)}) F(t, dz_1 dz_2 \dots dz_N). \end{aligned}$$

For $\sigma \in \mathfrak{S}_N$, define

$$S_\sigma : (z_1, \dots, z_N) \mapsto (z_{\sigma(1)}, \dots, z_{\sigma(N)}).$$

The equality above is recast as

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} \mathbf{1}_{A_1 \times A_2 \times \dots \times A_N}(z_1, z_2, \dots, z_N) F(t, dz_1 dz_2 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} \mathbf{1}_{A_1 \times A_2 \times \dots \times A_N} \circ S_\sigma(z_1, \dots, z_N) F(t, dz_1 dz_2 \dots dz_N) \end{aligned}$$

for all A_1, A_2, \dots, A_N Borel subsets of \mathbf{R}^d . This is equivalent to the equality

$$S_\sigma \# F(t, \cdot) = F(t, \cdot)$$

for all $\sigma \in \mathfrak{S}_N$.

Obviously, when F is a probability density instead of a probability measure, the condition

$$S_\sigma \# F(t, \cdot) \mathcal{L}^{dN} = F(t, \cdot) \mathcal{L}^{dN}$$

for all $\sigma \in \mathfrak{S}_N$ is equivalent to the condition

$$F(t, z_{\sigma(1)}, \dots, z_{\sigma(N)}) = F(t, S_\sigma(z_1, \dots, z_N)) = F(t, z_1, \dots, z_N)$$

for all $\sigma \in \mathfrak{S}_N$ and for all $z_1, \dots, z_N \in \mathbf{R}^d$. In other words, the function

$$(z_1, \dots, z_N) \mapsto F(t, z_1, \dots, z_N)$$

is symmetric.

1.5.2 Marginal distributions of symmetric N -particle distributions

There is however one serious difficulty in considering N -particle distributions in the context of the mean field limit. Indeed, this limit assumes that $N \rightarrow \infty$, so that one would have to deal with “functions of infinitely many variables” in this limit, which does not make much sense at first sight¹¹.

A traditional way of circumventing this difficulty is by considering the string of marginal distributions of the N -particle distribution. Before giving precise definitions, let us explain the idea in simple geometrical terms.

Consider a sphere centered at the origin in the 3 dimensional Euclidean space. The only missing information in order to completely define this sphere is its diameter. In other words, the sphere is completely determined as soon as one knows its orthogonal projection on any axis passing through the origin. However, if one does not know a priori that the object is a sphere, its orthogonal

¹¹This last statement is not completely correct, as P.-L. Lions recently proposed a well defined mathematical object that would play the role of a “symmetric function of infinitely many variables that is slowly varying in each variable”: see [67] and section 1.7.3 below.

projections on each axis passing through the origin is not enough in order to reconstruct completely the object, since they will not distinguish between a ball centered at the origin and its boundary that is a sphere of equal radius.

The situation that we consider here is slightly more complicated, since the group of symmetries is not the orthogonal group, but the group generated by the reflections exchanging two coordinate axis in the N dimensional Euclidean space. Knowing the orthogonal projection of a set that is invariant under the action of this group on the first coordinate axis is again not sufficient as it will not distinguish between a sphere of radius r centered at the origin and the (hyper)cube of side $2r$ centered at the origin with edges parallel to the coordinate axis. Knowing the orthogonal projection on any one of the planes defined by two coordinate axis removes this ambiguity.

Considering marginals of an N -particle distribution is the analogous operation on probability measures. Denote by $\mathcal{P}_{sym}((\mathbf{R}^d)^N)$ the set of symmetric probability measures on the N -particle phase space, i.e.

$$\mathcal{P}_{sym}((\mathbf{R}^d)^N) := \{P \in \mathcal{P}((\mathbf{R}^d)^N) \mid S_\sigma \# P = P \text{ for all } \sigma \in \mathfrak{S}_N\},$$

where we recall that S_σ is the transformation on $(\mathbf{R}^d)^N$ defined by

$$S_\sigma(z_1, \dots, z_N) = (z_{\sigma(1)}, \dots, z_{\sigma(N)})$$

for all $\sigma \in \mathfrak{S}_N$ and all $z_1, \dots, z_N \in \mathbf{R}^d$.

Definition 1.5.1 *For each $N \in \mathbf{N}^*$, each $P_N \in \mathcal{P}_{sym}((\mathbf{R}^d)^N)$ and each $k \in \{1, \dots, N\}$, the k -particle marginal of P_N is the element of $\mathcal{P}_{sym}((\mathbf{R}^d)^k)$ defined by the formula*

$$\int_{(\mathbf{R}^d)^k} \phi(z_1, \dots, z_k) P_{N:k}(dz_1 \dots dz_k) = \int_{(\mathbf{R}^d)^N} \phi(z_1, \dots, z_k) P_N(dz_1 \dots dz_N)$$

for each test function $\phi \in C_b((\mathbf{R}^d)^k)$. We shall systematically use the convention

$$P_{N:k} = 0 \quad \text{whenever } j > N.$$

If

$$P_N(dz_1 \dots dz_N) = F_N(z_1, \dots, z_N) dz_1 \dots dz_N$$

where F_N is a symmetric probability density on $(\mathbf{R}^d)^N$, then, for each $k = 1, \dots, N$, one has

$$P_{N:k}(dz_1 \dots dz_k) = F_{N:k}(z_1, \dots, z_k) dz_1 \dots dz_k$$

with

$$F_{N:k}(z_1, \dots, z_k) = \int_{(\mathbf{R}^d)^{N-k}} F_N(z_1, \dots, z_N) dz_{k+1} \dots dz_N.$$

Obviously, $F_{N:k}$ is also a symmetric probability density on $(\mathbf{R}^d)^k$.

The following elementary exercise confirms the analogy between the orthogonal projections of a subset of the Euclidean space on the subspaces generated by the coordinate axis and the marginal distributions associated to a symmetric probability on the N -particle phase space.

Exercise: Consider for each $N \in \mathbf{N}^*$ and each $k = 1, \dots, N$ the orthogonal projection

$$\mathbf{P}_N^k : (\mathbf{R}^d)^N \ni (z_1, \dots, z_N) \mapsto (z_1, \dots, z_k) \in (\mathbf{R}^d)^k.$$

Check that, for each $P_N \in \mathcal{P}_{sym}((\mathbf{R}^d)^N)$, one has

$$P_{N:k} = \mathbf{P}_N^k \# P_N,$$

and that

$$(P_{N:k})_{:j} = P_{N:j} \quad \text{for all } j, k \text{ such that } 1 \leq j \leq k \leq N.$$

An important example of symmetric N -particle distributions is the case of *factorized distributions*. Given a probability density f on \mathbf{R}^d , we consider for each $N \in \mathbf{N}^*$ the N -particle probability density F_N defined by the formula

$$F_N(z_1, \dots, z_N) := \prod_{j=1}^N f(z_j).$$

This N -particle probability density is denoted as follows:

$$F_N = f^{\otimes N}.$$

Obviously $F_N = f^{\otimes N}$ is a symmetric N -particle probability distribution, and its marginals are also factorized distributions, since

$$F_N = f^{\otimes N} \Rightarrow F_{N:k} = f^{\otimes k}$$

for all $k = 1, \dots, N$.

There is a very nice characterization of factorized distributions in terms of entropy. We shall not use it in the sequel. Nevertheless, it is important to know it, and we leave it as an exercise.

Exercise: For each probability density f on \mathbf{R}^d and each $N \in \mathbf{N}^*$, define

$$E_N(f) = \{F_N \text{ symmetric probability density on } (\mathbf{R}^d)^N \text{ s.t. } F_{N:1} = f\}.$$

We want to prove that $F_N = f^{\otimes N}$ realizes

$$\inf_{F_N \in E_N(f)} \int_{(\mathbf{R}^d)^N} F_N \ln F_N(z_1, \dots, z_N) dz_1 \dots dz_N.$$

1) Let $a = (a_1, \dots, a_d) \in (\mathbf{R}_+^*)^d$ satisfy $a_1 + \dots + a_d = 1$, and consider

$$M(a) := \{A = A^T \in M_d(\mathbf{R}_+^*) \text{ s.t. } (1, \dots, 1) \cdot A = a\}.$$

Find the critical points of the function

$$H : M(a) \ni A \mapsto \sum_{i,j=1}^d A_{ij} \ln A_{ij} \in \mathbf{R}.$$

2) Prove that, for each $x, y > 0$

$$\phi(x, y) := x \ln \left(\frac{x}{y} \right) - x + y \geq 0,$$

with equality if and only if $x = y$.

3) Express in terms of $\phi(A_{ij}, a_i a_j)$ the quantity

$$\sum_{i,j=1}^d (A_{ij} \ln A_{ij} - a_i a_j \ln(a_i a_j)).$$

4) Find

$$\inf_{A \in M(a)} H(A).$$

5) Using the intuition provided by questions 1-4, solve the minimization problem

$$\inf_{F_N \in E_N(f)} \int_{(\mathbf{R}^d)^N} F_N \ln F_N(z_1, \dots, z_N) dz_1 \dots dz_N.$$

References for this and the previous section are chapter 3 in [17] and chapter 3 in [26].

1.5.3 The N -particle Liouville equation

We have explained above how the state of a system of N identical particles is described by a symmetric probability measure on the N -particle phase space. Our next task is to define the evolution of such a probability measure, knowing that the positions of the particles in phase space are governed by the system of N -particle ODEs

$$\begin{cases} \dot{z}_i(t) = \frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)), & i = 1, \dots, N, \\ z_i(0) = z_i^{in}. \end{cases}$$

As explained in Theorem 1.3.1, whenever $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies assumptions (HK1-HK2), the system of ODEs above generates a flow on the N -particle phase space $(\mathbf{R}^d)^N$ denoted by T_t and defined by the formula

$$T_t(z_1^{in}, \dots, z_N^{in}) := (z_1(t), \dots, z_N(t))$$

for all $t \in \mathbf{R}$.

Given a N -particle symmetric probability measure $F_N^{in} \in \mathcal{P}_{sym}((\mathbf{R}^d)^N)$, we set

$$F_N(t) := T_t \# F_N^{in}, \quad t \in \mathbf{R}.$$

This formula defines $F_N(t)$ as the unique weak solution in $C(\mathbf{R}; w - \mathcal{P}((\mathbf{R}^d)^N))$ of the Cauchy problem for the N -particle Liouville equation

$$\begin{cases} \partial_t F_N + \frac{1}{N} \sum_{i,j=1}^N \operatorname{div}_{z_i} (F_N K(z_i, z_j)) = 0, & z_1, \dots, z_N \in \mathbf{R}^d, t \in \mathbf{R}, \\ F_N|_{t=0} = F_N^{in}. \end{cases}$$

Exercise: Check this, by using the method of characteristics as in the exercise following the statement of Theorem 1.3.1. (For the solution, see chapter 1 in [17]).

As explained above, it is important that the probability measure in the N -particle phase space describing the state of a system of identical particles should be symmetric. Whether this symmetry property is propagated by the flow of the N -particle Liouville equation is therefore a very natural question. The answer to that question is given by the following proposition.

Proposition 1.5.2 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies the assumptions (HK1)-(HK2) so that the N -particle ODE system defines a unique flow T_t on $(\mathbf{R}^d)^N$ as proved in Theorem 1.3.1. For each $\sigma \in \mathfrak{S}_N$ we denote as above by S_σ the transformation on $(\mathbf{R}^d)^N$ defined by*

$$S_\sigma(z_1, \dots, z_N) = (z_{\sigma(1)}, \dots, z_{\sigma(N)})$$

for all $z_1, \dots, z_N \in \mathbf{R}^d$.

1) For all $\sigma \in \mathfrak{S}_N$ and all $t \in \mathbf{R}$, one has

$$T_t S_\sigma = S_\sigma T_t,$$

viz.

$t \mapsto (z_{\sigma(1)}(t), \dots, z_{\sigma(N)}(t))$ is the solution of the N -particle ODE system with initial condition $(z_{\sigma(1)}^{in}, \dots, z_{\sigma(N)}^{in})$;

2) For each $F_N^{in} \in \mathcal{P}((\mathbf{R}^d)^N)$ and all $t \in \mathbf{R}$, the probability measure

$$F_N(t) := T_t \# F_N^{in}$$

is symmetric if F_N^{in} is symmetric, i.e.

$$S_\sigma \# F_N(t) = F_N(t) \quad \text{for all } t \in \mathbf{R},$$

if

$$S_\sigma \# F_N^{in} = F_N^{in}.$$

Proof. An elementary computation shows that

$$t \mapsto (z_{\sigma(1)}(t), \dots, z_{\sigma(N)}(t))$$

satisfies the same N -particle ODE system as

$$t \mapsto (z_1(t), \dots, z_N(t)).$$

By uniqueness of the solution of the Cauchy problem for this ODE system (Theorem 1.3.1), this is therefore the unique solution of that problem with initial data $(z_{\sigma(1)}^{in}, \dots, z_{\sigma(N)}^{in})$. In other words,

$$T_t S_\sigma(z_1^{in}, \dots, z_N^{in}) = (z_{\sigma(1)}(t), \dots, z_{\sigma(N)}(t)) = S_\sigma T_t(z_1^{in}, \dots, z_N^{in})$$

for all $(z_1^{in}, \dots, z_N^{in}) \in (\mathbf{R}^d)^N$ and all $t \in \mathbf{R}$, which proves statement 1).

As for statement 2), observe that

$$\begin{aligned} S_\sigma \# F_N(t) &= S_\sigma \# (T_t \# F_N^{in}) = (S_\sigma T_t) \# F_N^{in} \\ &= (T_t S_\sigma) \# F_N^{in} = T_t \# (S_\sigma \# F_N^{in}) = T_t \# F_N^{in} = F_N(t) \end{aligned}$$

for all $t \in \mathbf{R}$ and all $\sigma \in \mathfrak{S}_N$, which is precisely the desired relation. ■

Finally, we discuss the growth of $F_N(t, z_1, \dots, z_N)$ as $|z_1| + \dots + |z_N| \rightarrow \infty$.

Lemma 1.5.3 *Under the assumptions (HK1)-(HK2) on the interaction kernel K , one has*

$$\|T_t(z_1^{in}, \dots, z_N^{in})\|_1 \leq e^{2L|t|} \|(z_1^{in}, \dots, z_N^{in})\|_1$$

with the notation

$$\|(z_1, \dots, z_N)\|_1 = |z_1| + \dots + |z_N|.$$

In particular, if $F_N^{in} \in \mathcal{P}_1((\mathbf{R}^d)^N)$, then $T_t \# F_N^{in} \in \mathcal{P}_1((\mathbf{R}^d)^N)$, and one has

$$\begin{aligned} &\int_{(\mathbf{R}^d)^N} \|(z_1, \dots, z_N)\|_1 T_t \# F_N^{in}(dz_1 \dots dz_N) \\ &\leq e^{2L|t|} \int_{(\mathbf{R}^d)^N} \|(z_1, \dots, z_N)\|_1 F_N^{in}(dz_1 \dots dz_N) \end{aligned}$$

for all $t \in \mathbf{R}$.

Proof. Observe that

$$\begin{aligned} \frac{d}{dt} \|(z_1(t), \dots, z_N(t))\|_1 &= \frac{1}{N} \sum_{i,j=1}^N K(z_i(t), z_j(t)) \cdot \frac{z_i(t)}{|z_i(t)|} \\ &\leq \frac{1}{N} \sum_{i,j=1}^N |K(z_i(t), z_j(t))| \\ &\leq \frac{1}{N} \sum_{i,j=1}^N L(|z_i(t)| + |z_j(t)|) \\ &= \sum_{i=1}^N L \left(|z_i(t)| + \frac{1}{N} \|(z_1(t), \dots, z_N(t))\|_1 \right) \\ &= 2L \|(z_1(t), \dots, z_N(t))\|_1, \end{aligned}$$

and conclude by the Gronwall inequality.

Moreover, if $F_N^{in} \in \mathcal{P}_1((\mathbf{R}^d)^N)$, then

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} \|(z_1, \dots, z_N)\|_1 T_t \# F_N^{in}(dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} \|T_t(z_1, \dots, z_N)\|_1 F_N^{in}(dz_1 \dots dz_N) \\ &\leq e^{2L|t|} \int_{(\mathbf{R}^d)^N} \|(z_1, \dots, z_N)\|_1 F_N^{in}(dz_1 \dots dz_N) < \infty, \end{aligned}$$

so that $T_t \# F_N^{in} \in \mathcal{P}_1((\mathbf{R}^d)^N)$. ■

1.5.4 The BBGKY hierarchy

The curious designation for this procedure finds its origin in the names of N.N. Bogoliubov, M. Born, H.S. Green, J.G. Kirkwood and J. Yvon, who introduced it in various contexts.

Before presenting the BBGKY hierarchy in detail, we first discuss the main reason for considering it in the first place.

As explained above, the N -particle distribution F_N is defined on the N -particle phase space $(\mathbf{R}^d)^N$, whose dimension increases as $N \rightarrow \infty$. In other words, the number of variables in F_N goes to infinity with N , so that the exact nature of the limiting object associated with F_N is not entirely obvious. Therefore, we seek to describe the behavior of F_N in the large N limit by considering instead its first marginal $F_{N:1}$ in that limit. By doing so, we avoid the problem of having the number of variables going to infinity with N , at the expense of losing some amount of information by reducing F_N to $F_{N:1}$.

To fulfill this program, it would be desirable to know the evolution of $F_{N:1}$, typically by means of a PDE in the 1-particle phase space to be satisfied by $F_{N:1}$.

Unfortunately, because of the interaction modeled by the kernel K , it is impossible to find a closed equation for $F_{N:1}$. Instead, the equation for $F_{N:1}$ deduced from the N -particle Liouville equation involves $F_{N:2}$. Again it is impossible to find a closed equation governing the evolution of $F_{N:2}$ when $N > 2$, as the pairwise interaction between particles will involve $F_{N:3}$ in the equation for $F_{N:2}$ deduced from the N -particle Liouville equation. By the same token, one can check that it is impossible to derive from the N -particle Liouville equation a closed system of equations for *finitely many* — i.e. $m < N$ — of the marginals $F_{N:k}$.

Even though the system of PDEs governing the evolution of the marginal distributions $F_{N:k}$ cannot be put in closed form, these equations are nevertheless interesting, and we explain how to derive them below.

We start from the N -particle Liouville equation satisfied by F_N :

$$\partial_t F_N + \frac{1}{N} \sum_{i,j=1}^N \operatorname{div}_{z_i} (K(z_i, z_j) F_N) = 0.$$

That $t \mapsto F_N(t)$ is a weak solution of this equation means that, for each $\Phi \equiv \Phi(z_1, \dots, z_N)$ in $C_b^1((\mathbf{R}^d)^N)$, one has

$$\begin{aligned} & \partial_t \int_{(\mathbf{R}^d)^N} \Phi_N(z_1, \dots, z_N) F_N(t, dz_1 \dots dz_N) \\ &= \frac{1}{N} \sum_{i,j=1}^N \int_{(\mathbf{R}^d)^N} K(z_i, z_j) \nabla_{z_i} \Phi(z_1, \dots, z_N) F_N(t, dz_1 \dots dz_N) \end{aligned}$$

in the sense of distributions on \mathbf{R} .

We first seek an equation for the first marginal $F_{N:1}$. Let $\phi \in C_b^1(\mathbf{R}^d)$; writing the weak formulation of the N -particle Liouville equation for the test function $\Phi(z_1, \dots, z_N) = \phi(z_1)$, we see that

$$\begin{aligned} & \partial_t \int_{(\mathbf{R}^d)^N} \phi(z_1) F_N(t, dz_1 \dots dz_N) \\ &= \frac{1}{N} \sum_{j=2}^N \int_{(\mathbf{R}^d)^N} K(z_1, z_j) \cdot \nabla \phi(z_1) F_N(t, dz_1 \dots dz_N). \end{aligned}$$

(Notice that the term associated to $j = 1$ in the summation on the right hand side of the equality above vanishes identically since K vanishes on the diagonal by assumption (HK1).)

In the term

$$\int_{(\mathbf{R}^d)^N} K(z_1, z_j) \cdot \nabla \phi(z_1) F_N(t, dz_1 \dots dz_N)$$

we exchange the variables z_2 and z_j . Denoting by $\sigma_{2j} \in \mathfrak{S}_N$ the transposition exchanging 2 and j , one has

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} K(z_1, z_j) \cdot \nabla \phi(z_1) F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} K(z_1, z_2) \cdot \nabla \phi(z_1) S_{\sigma_{2j}} F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} K(z_1, z_2) \cdot \nabla \phi(z_1) F_N(t, dz_1 \dots dz_N). \end{aligned}$$

by symmetry of $F_N(t)$.

Therefore

$$\begin{aligned} & \partial_t \int_{(\mathbf{R}^d)^N} \phi(z_1) F_N(t, dz_1 \dots dz_N) \\ &= \frac{N-1}{N} \int_{(\mathbf{R}^d)^N} K(z_1, z_2) \cdot \nabla \phi(z_1) F_N(t, dz_1 \dots dz_N). \end{aligned}$$

The integral on the left hand side of the equality above is recast as follows:

$$\int_{(\mathbf{R}^d)^N} \phi(z_1) F_N(t, dz_1 \dots dz_N) = \int_{\mathbf{R}^d} \phi(z_1) F_{N:1}(t, dz_1).$$

By the same token, the integral on the right hand side becomes

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} K(z_1, z_2) \cdot \nabla \phi(z_1) F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^2} K(z_1, z_2) \cdot \nabla \phi(z_1) F_{N:2}(t, dz_1 dz_2). \end{aligned}$$

Thus, for each $\phi \in C_b^1(\mathbf{R}^d)$, one has

$$\partial_t \int_{\mathbf{R}^d} \phi(z_1) F_{N:1}(t, dz_1) = \frac{N-1}{N} \int_{(\mathbf{R}^d)^2} K(z_1, z_2) \cdot \nabla \phi(z_1) F_{N:2}(t, dz_1 dz_2),$$

which is the weak formulation of

$$\partial_t F_{N:1} + \frac{N-1}{N} \operatorname{div}_{z_1} \int_{\mathbf{R}^d} K(z_1, z_2) F_{N:2}(\cdot, dz_2) = 0.$$

Equivalently

$$\partial_t F_{N:1} + \frac{N-1}{N} \operatorname{div}_{z_1} [K(z_1, z_2) F_{N:2}]_{:1} = 0,$$

where $K(z_1, z_2) F_{N:2}$ designates the Radon measure defined on $(\mathbf{R}^d)^2$ as the linear functional on bounded continuous functions given by the formula

$$\langle K(z_1, z_2) F_{N:2}, \psi \rangle := \int_{(\mathbf{R}^d)^2} \psi(z_1, z_2) K(z_1, z_2) F_{N:2}(dz_1 dz_2),$$

while $[K(z_1, z_2) F_{N:2}]_{:1}$ designates the Radon measure defined on \mathbf{R}^d by the formula

$$\langle [K(z_1, z_2) F_{N:2}]_{:1}, \phi \rangle := \int_{(\mathbf{R}^d)^2} \phi(z_1) K(z_1, z_2) F_{N:2}(dz_1 dz_2).$$

(Equivalently,

$$[K(z_1, z_2) F_{N:2}]_{:1} := \mathbf{P}_2^1 \# [K(z_1, z_2) F_{N:2}]$$

where we recall that \mathbf{P}_2^1 is the orthogonal projection defined by the formula $\mathbf{P}_2^1(z_1, z_2) := z_1$.)

In any case, as anticipated, the equation for the first marginal distribution $F_{N:1}$ involves the second marginal distribution $F_{N:2}$.

We next proceed to derive the equations satisfied by the sequence of marginal distributions $F_{N:j}$ for $j = 2, \dots, N$; this derivation will proceed as in the case $j = 1$, except for one additional term.

For $1 < j < N$, we write the weak formulation of the N -particle Liouville equation with test function $\Phi(z_1, \dots, z_N) = \phi(z_1, \dots, z_j)$, where $\phi \in C_b((\mathbf{R}^d)^j)$.

Thus

$$\begin{aligned} & \partial_t \int_{(\mathbf{R}^d)^N} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) \\ &= \frac{1}{N} \sum_{l=1}^j \sum_{k=j+1}^N \int_{(\mathbf{R}^d)^N} K(z_l, z_k) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) \\ & \quad + \frac{1}{N} \sum_{l=1}^j \sum_{k=1}^j \int_{(\mathbf{R}^d)^N} K(z_l, z_k) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N). \end{aligned}$$

Notice that the range of the index l is limited to $\{1, \dots, j\}$ since the test function ϕ does not depend on the variables z_{j+1}, \dots, z_N . The range of the index k remains $\{1, \dots, N\}$, and we have decomposed it into $\{1, \dots, j\}$ and $\{j+1, \dots, N\}$. This decomposition is quite natural, as the sum involving $k, l \in \{1, \dots, j\}$ accounts for the pairwise interactions between the j particles whose state is described by $F_{N:j}$, while the sum involving $l \in \{1, \dots, j\}$ and $k \in \{j+1, \dots, N\}$ accounts for the pairwise interactions between each one of the j particles whose state is described by $F_{N:j}$ and the $N-j$ other particles in the system.

As in the case $j=1$,

$$\int_{(\mathbf{R}^d)^N} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) = \int_{(\mathbf{R}^d)^j} \phi(z_1, \dots, z_j) F_{N:j}(t, dz_1 \dots dz_j),$$

and by the same token, if $1 \leq k, l \leq j$

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} K(z_l, z_k) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^j} K(z_l, z_k) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_{N:j}(t, dz_1 \dots dz_j). \end{aligned}$$

If $1 \leq l \leq j < k \leq N$, denote by $\sigma_{j+1,k} \in \mathfrak{S}_N$ the transposition exchanging $j+1$ and k . Then

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} K(z_l, z_k) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} K(z_l, z_{j+1}) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) S_{\sigma_{j+1,k}} F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^N} K(z_l, z_{j+1}) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) \end{aligned}$$

by symmetry of $F_N(t)$. Then

$$\begin{aligned} & \int_{(\mathbf{R}^d)^N} K(z_l, z_{j+1}) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_N(t, dz_1 \dots dz_N) \\ &= \int_{(\mathbf{R}^d)^{j+1}} K(z_l, z_{j+1}) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_{N:j+1}(t, dz_1 \dots dz_{j+1}). \end{aligned}$$

Finally, we obtain the equality

$$\begin{aligned} & \frac{d}{dt} \int_{(\mathbf{R}^d)^j} \phi(z_1, \dots, z_j) F_{N:j}(t, dz_1 \dots dz_j) \\ &= \frac{1}{N} \sum_{k,l=1}^j \int_{(\mathbf{R}^d)^j} K(z_l, z_k) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_{N:j}(t, dz_1 \dots dz_j) \\ &+ \frac{N-j}{N} \sum_{l=1}^j \int_{(\mathbf{R}^d)^{j+1}} K(z_l, z_{j+1}) \cdot \nabla_{z_l} \phi(z_1, \dots, z_j) F_{N:j+1}(t, dz_1 \dots dz_{j+1}) \end{aligned}$$

to be verified for each $\phi \in C_b^1((\mathbf{R}^d)^j)$.

This is the weak formulation of the equation

$$\begin{aligned} \partial_t F_{N:j} + \frac{N-j}{N} \sum_{l=1}^j \operatorname{div}_{z_l} \int_{\mathbf{R}^d} K(z_l, z_{j+1}) F_{N:j+1}(\cdot, dz_{j+1}) \\ + \frac{1}{N} \sum_{k,l=1}^j \operatorname{div}_{z_l} (K(z_l, z_k) F_{N:j}) = 0. \end{aligned}$$

Equivalently

$$\begin{aligned} \partial_t F_{N:j} + \frac{N-j}{N} \sum_{l=1}^j \operatorname{div}_{z_l} [K(z_l, z_{j+1}) F_{N:j+1}]_{:j} \\ + \frac{1}{N} \sum_{k,l=1}^j \operatorname{div}_{z_l} (K(z_l, z_k) F_{N:j}) = 0, \end{aligned}$$

where $K(z_l, z_{j+1}) F_{N:j+1}$ designates the Radon measure defined on $(\mathbf{R}^d)^{j+1}$ as the linear functional on bounded continuous functions given by the formula

$$\begin{aligned} & \langle K(z_l, z_{j+1}) F_{N:j+1}, \psi \rangle \\ &:= \int_{(\mathbf{R}^d)^{j+1}} \psi(z_1, \dots, z_{j+1}) K(z_l, z_{j+1}) F_{N:j+1}(dz_1 \dots dz_{j+1}), \end{aligned}$$

while $[K(z_l, z_{j+1}) F_{N:j+1}]_{:j}$ designates the Radon measure defined on $(\mathbf{R}^d)^j$ by the formula

$$\begin{aligned} & \langle [K(z_l, z_{j+1}) F_{N:j+1}]_{:j}, \phi \rangle \\ &:= \int_{(\mathbf{R}^d)^j} \phi(z_1, \dots, z_j) K(z_l, z_{j+1}) F_{N:j+1}(dz_1 \dots dz_{j+1}). \end{aligned}$$

Equivalently,

$$[K(z_l, z_{j+1}) F_{N:j+1}]_{:j} := \mathbf{P}_{j+1}^j \# [K(z_l, z_{j+1}) F_{N:j+1}],$$

where we recall that \mathbf{P}_{j+1}^j is the orthogonal projection defined by the formula

$$\mathbf{P}_{j+1}^j(z_1, \dots, z_{j+1}) := (z_1, \dots, z_j).$$

The equation obtained in the case $j = N$ is nothing but the N -particle Liouville equation itself since $F_{N:N} = F_N$ and $F_{N:j} = 0$ for all $j > N$: thus

$$\partial_t F_{N:N} + \frac{1}{N} \sum_{k,l=1}^N \operatorname{div}_{z_l} (K(z_l, z_k) F_{N:N}) = 0.$$

We summarize the above lengthy computations in the following theorem, where the notation $\mathcal{P}_{1,\text{sym}}((\mathbf{R}^d)^N)$ designates

$$\mathcal{P}_{1,\text{sym}}((\mathbf{R}^d)^N) = \mathcal{P}_1((\mathbf{R}^d)^N) \cap \mathcal{P}_{\text{sym}}((\mathbf{R}^d)^N).$$

Theorem 1.5.4 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies (HK1-HK2). Let $F_N^{\text{in}} \in \mathcal{P}_{1,\text{sym}}((\mathbf{R}^d)^N)$, and let $F_N(t) = T_t \# F_N^{\text{in}}$ for all $t \in \mathbf{R}$, where T_t is the flow defined on $(\mathbf{R}^d)^N$ by the N -particle ODE system as in Theorem 1.3.1. The sequence of marginal distributions $F_{N:j}$ of F_N with $j = 1, \dots, N$ is a weak solution of the string of equations*

$$\left\{ \begin{array}{l} \partial_t F_{N:1} + \frac{N-1}{N} \operatorname{div}_{z_1} [K(z_1, z_2) F_{N:2}]_{:1} = 0, \\ \partial_t F_{N:j} + \frac{N-j}{N} \sum_{l=1}^j \operatorname{div}_{z_l} [K(z_l, z_{j+1}) F_{N:j+1}]_{:j} \\ \quad + \frac{1}{N} \sum_{k,l=1}^j \operatorname{div}_{z_l} (K(z_l, z_k) F_{N:j}) = 0, \quad j = 2, \dots, N-1, \\ \partial_t F_{N:N} + \frac{1}{N} \sum_{k,l=1}^N \operatorname{div}_{z_l} (K(z_l, z_k) F_{N:N}) = 0, \end{array} \right.$$

and satisfies the initial conditions

$$F_{N:j}|_{t=0} = F_{N:j}^{\text{in}}, \quad j = 1, \dots, N.$$

This string of equations bears the name of *BBGKY hierarchy* for the N -particle system whose dynamics is defined by the ODE system

$$\dot{z}_i(t) = \frac{1}{N} \sum_{j=1}^N K(z_i(t), z_j(t)), \quad 1 \leq i \leq N.$$

In spite of all the (somewhat) technical computations involved in the derivation of the BBGKY hierarchy, the careful reader will notice that

a) the BBGKY hierarchy is a consequence of the N -particle Liouville equation, but

b) it contains the N -particle Liouville equation (which is the last equation in the hierarchy).

This observation might cast some doubts as to the interest of considering the BBGKY hierarchy instead of the Liouville equation itself, since both contain exactly the same amount of information.

References for this section are chapters 3-4 in [26], [88, 90], chapter 3 in [17] and [10].

1.5.5 The mean field hierarchy and factorized distributions

In the present section, our discussion of the mean field limit becomes purely formal.

Our aim is to pass to the limit in each equation in the BBGKY hierarchy as $N \rightarrow \infty$, keeping $j \geq 1$ fixed. Assume that $F_{N:j} \rightarrow F_j$ as $N \rightarrow \infty$ (in some sense to be made precise) for all $j \geq 1$. Then, in the limit as $N \rightarrow \infty$

$$\frac{N-j}{N} \int_{\mathbf{R}^d} K(z_l, z_{j+1}) F_{N:j+1}(dz_{j+1}) \rightarrow \int_{\mathbf{R}^d} K(z_l, z_{j+1}) F_{j+1}(dz_{j+1}),$$

while

$$\frac{1}{N} K(z_l, z_k) F_{N:j} \rightarrow 0,$$

so that

$$\partial_t F_j + \sum_{l=1}^j \operatorname{div}_{z_l} \int_{\mathbf{R}^d} K(z_l, z_{j+1}) F_{j+1}(dz_{j+1}) = 0, \quad j \geq 1.$$

This hierarchy of equations is henceforth referred to as *the mean field hierarchy*, or *the Vlasov hierarchy*. The similarities between this mean field hierarchy and the BBGKY hierarchy are striking. Yet there is an important difference: the mean field hierarchy is an *infinite* hierarchy of equations — unlike the BBGKY hierarchy, which contains only N equations, where N is the total number of particles. The physical meaning of this infinite hierarchy of equations will be explained in section 1.7.2.

However, this infinite hierarchy is directly related to the mean field equation by the following observation.

Proposition 1.5.5 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies assumptions (HK1)-HK2). Let f^{in} be a smooth (at least C^1) probability density on \mathbf{R}^d such that*

$$\int_{\mathbf{R}^d} |z| f^{in}(z) dz < \infty.$$

Assume that the Cauchy problem for the mean field equation

$$\begin{cases} \partial_t f(t, z) + \operatorname{div}_z \left(f(t, z) \int_{\mathbf{R}^d} K(z, z') f(t, z') dz' \right) = 0, \\ f|_{t=0} = f^{in}, \end{cases}$$

has a classical (at least of class C^1) solution $f \equiv f(t, z)$. Set $f_j(t, \cdot) = f(t, \cdot)^{\otimes j}$, i.e.

$$f_j(t, z_1, \dots, z_j) = \prod_{k=1}^j f(t, z_k)$$

for each $t \in \mathbf{R}$ and each $z_1, \dots, z_j \in \mathbf{R}^d$.

Then the sequence $(f_j)_{j \geq 1}$ is a solution of the infinite mean field hierarchy

$$\partial_t f_j(z_1, \dots, z_j) + \sum_{l=1}^j \operatorname{div}_{z_l} \int_{\mathbf{R}^d} K(z_l, z_{j+1}) f_{j+1}(z_1, \dots, z_{j+1}) dz_{j+1} = 0$$

for all $j \geq 1$.

Proof. Since f is of class C^1 at least, one has

$$\begin{aligned} \partial_t f_j(t, z_1, \dots, z_j) &= \sum_{k=1}^j \prod_{\substack{l=1 \\ l \neq k}}^j f(t, z_l) \partial_t f(t, z_k) \\ &= - \sum_{k=1}^j \prod_{\substack{l=1 \\ l \neq k}}^j f(t, z_l) \operatorname{div}_{z_k} \left(f(t, z_k) \int_{\mathbf{R}^d} K(z_k, z') f(t, z') dz' \right) \\ &= - \sum_{k=1}^j \operatorname{div}_{z_k} \left(\prod_{l=1}^j f(t, z_l) \int_{\mathbf{R}^d} K(z_k, z') f(t, z') dz' \right) \\ &= - \sum_{k=1}^j \operatorname{div}_{z_k} \left(\int_{\mathbf{R}^d} K(z_k, z') f_{j+1}(t, z_1, \dots, z_j, z') dz' \right), \end{aligned}$$

which is precisely the j -th equation in the mean field hierarchy. ■

This crucial observation suggests the following strategy to prove the mean field limit by the method of hierarchies.

Choose factorized initial data for N -particle Liouville equation: given f^{in} a probability density on \mathbf{R}^d such that

$$\int_{\mathbf{R}^d} |z| f(t, z) dz < \infty,$$

define

$$F_N^{in} = (f^{in})^{\otimes N} \quad \text{for each } N \geq 1,$$

i.e.

$$F_N^{in}(t, z_1, \dots, z_N) = \prod_{k=1}^N f^{in}(t, z_k).$$

Let F_N be the solution of the Cauchy problem for the N -particle Liouville equation

$$\begin{cases} \partial_t F_N + \frac{1}{N} \sum_{k,l=1}^N \operatorname{div}_{z_k} (F_N K(z_k, z_l)) = 0, \\ F_N|_{t=0} = (f^{in})^{\otimes N}, \end{cases}$$

with that initial data.

Assume that one can prove

- a) that $F_{N;j} \rightarrow F_j$ (in some sense to be made precise) for each $j \geq 1$, where F_j is a solution of the infinite hierarchy, and
- b) that the Cauchy problem for the infinite hierarchy has a unique solution.

Let f be a solution of the mean field PDE with initial data f^{in} .

Since the sequence $f_j := f^{\otimes j}$ (for $j \geq 1$) is a solution of the infinite mean field hierarchy with initial data $(f^{in})^{\otimes j}$ by Proposition 1.5.5, statement b) implies that it is *the* solution of the infinite hierarchy for that initial data. Therefore

$$F_{N;j} \rightarrow F_j = f^{\otimes j} \quad \text{as } N \rightarrow \infty \text{ for all } j \geq 1.$$

In particular, for $j = 1$, one finds that the solution F_N of the Liouville equation satisfies

$$F_{N;1} \rightarrow f \quad \text{as } N \rightarrow \infty.$$

In other words, the first marginal of the solution of the N -particle Liouville equation with factorized initial data converges to the solution of the mean field PDE in the large N limit.

This is precisely the strategy outlined by Cercignani [25] for justifying rigorously the Boltzmann equation in the case of the hard sphere gas.

Notice that, in this approach, one needs to know that the Cauchy problem for the mean field PDE is well-posed (i.e. that it has a unique solution for each initial data in some appropriate functional space). On the contrary, in the previous approach based on the notion of empirical measure, the existence of a solution of the Cauchy problem for the mean field PDE is a consequence of the existence for finitely many particles and of the mean field limit itself, and the uniqueness of that solution is a consequence of Dobrushin's estimate.

The reader might be under the impression that proving the uniqueness of the solution of the Cauchy problem for the infinite mean field hierarchy is a matter of pure routine, since the mean field hierarchy is a linear problem, at variance with the mean field PDE, which is nonlinear. This is obviously wrong, since the uniqueness of the solution of the infinite mean field hierarchy implies the uniqueness of the solution of the mean field PDE. In fact, the uniqueness property for the infinite mean field hierarchy is a very strong property and proving it is by no means obvious. See [89] and section 1.7.2 for a precise

discussion of this point — as well as of the physical meaning of the infinite mean field hierarchy.

However, the strategy described in the present section (starting from the N -particle Liouville equation, deriving the BBGKY hierarchy, passing to the limit to arrive at an infinite hierarchy of equations and concluding with the uniqueness of the solution of the infinite hierarchy with given initial data) has been used successfully in a greater variety of problems than the mean field limit considered in this course. For instance, the only rigorous derivation of the Boltzmann equation of the kinetic theory of gases known to this date (proposed by Lanford [65]) follows exactly these steps¹² — see also chapter 3 of [17] and chapters 2-4 of [26] for an account of this fundamental result. The recent paper [37] extends Lanford's result to short range potentials other than hard spheres, and gives a more detailed presentation of the Boltzmann-Grad limit than all previous references, even in the hard sphere case.

1.6 Chaotic sequences, empirical measures and BBGKY hierarchies

Our discussion of BBGKY hierarchies shows the importance of the following property of symmetric N -particle probability measures F_N :

$$F_{N:j} \rightarrow f^{\otimes j} \quad \text{weakly as } N \rightarrow \infty \text{ for all } j \geq 1 \text{ fixed.}$$

Of course, if ϕ is a probability density on \mathbf{R}^d , one has

$$\Phi_N = \phi^{\otimes N} \Rightarrow \Phi_{N:j} = \phi^{\otimes j}.$$

But if ψ is another probability density on \mathbf{R}^d , defining

$$\tilde{\Phi}_N = \frac{1}{N} \sum_{k=1}^N \phi^{\otimes(k-1)} \otimes \psi \otimes \phi^{\otimes(N-k)},$$

which is in general a non-factorized symmetric probability density on $(\mathbf{R}^d)^N$, then

$$\tilde{\Phi}_{N:j} = \frac{N-j}{N} \phi^{\otimes j} + \frac{1}{N} \sum_{k=1}^j \phi^{\otimes(k-1)} \otimes \psi \otimes \phi^{\otimes(j-k)} \rightarrow \phi^{\otimes j}$$

for all $j \geq 1$ as $N \rightarrow \infty$.

Thus, the property above can be verified, in the limit as $N \rightarrow \infty$, by sequences of N -particle probability measures that are not factorized exactly for each finite $N \geq 1$.

¹²For the case of the Boltzmann-Grad limit for a system of N hard spheres, the infinite hierarchy cannot be derived rigorously from the Liouville equation by passing to the limit in the sense of distributions in each equation of the (finite) BBGKY hierarchy: see the discussion on pp. 74–75 in [26]. The infinite Boltzmann hierarchy is derived by a different, more subtle procedure that is the core of the Lanford proof — see section 4.4 in [26].

Definition 1.6.1 Let p be a probability measure on \mathbf{R}^d . A sequence P_N of symmetric N -particle probability measures on $(\mathbf{R}^d)^N$ for all $N \geq 1$ is said to be chaotic, and more precisely p -chaotic, if

$$P_{N:j} \rightarrow p^{\otimes j} \quad \text{weakly in } \mathcal{P}((\mathbf{R}^d)^j)$$

as $N \rightarrow \infty$, for all $j \geq 1$ fixed.

The notion of chaotic sequences appeared in the context of the derivation of kinetic equations from particle dynamics, for the first time in [58]. Perhaps the reason for this terminology is that this property corresponds to asymptotic independence of the N -particles in the large N limit.

1.6.1 Chaotic sequences and empirical measures

We begin our discussion of chaotic sequences with a characterization of chaotic sequences in terms of empirical measures.

Theorem 1.6.2 Let $p \in \mathcal{P}(\mathbf{R}^d)$, and let $P_N \in \mathcal{P}_{sym}((\mathbf{R}^d)^N)$ for each $N \geq 1$. Then the two following properties are equivalent:

(a) for each $j \geq 1$

$$P_{N:j} \rightarrow p^{\otimes j}$$

weakly in $\mathcal{P}((\mathbf{R}^d)^j)$ as $N \rightarrow \infty$;

(b) for each $\phi \in C_b(\mathbf{R}^d)$ and each $\epsilon > 0$,

$$P_N(\{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - p, \phi \rangle| \geq \epsilon\}) \rightarrow 0$$

as $N \rightarrow \infty$, where we recall that

$$\mu_{Z_N} := \frac{1}{N} \sum_{k=1}^N \delta_{z_k}$$

with $Z_N = (z_1, \dots, z_N)$.

In very informal terms,

$$P_{N:j} \rightarrow p^{\otimes j}$$

weakly in $\mathcal{P}((\mathbf{R}^d)^j)$ as $N \rightarrow \infty$ for all $j \geq 1$ if and only if

$$P_N \rightarrow \delta_p$$

“weakly in $\mathcal{P}(\mathcal{P}(\mathbf{R}^d))$ ” as $N \rightarrow \infty$. In this statement, each N -tuples Z_N is identified with the corresponding empirical measure μ_{Z_N} and P_N is viewed as a probability measure on $\mathcal{P}(\mathbf{R}^d)$ that is concentrated on the set of N -particle empirical measures. This identification goes back to Grünbaum [47] and is discussed in section 1.7.3 below.

Remark: Observe that property (a) is equivalent to
(a') $P_{N:1} \rightarrow p$ and $P_{N:2} \rightarrow p \otimes p$ weakly in $\mathcal{P}(\mathbf{R}^d)$ and $\mathcal{P}((\mathbf{R}^d)^2)$ as $N \rightarrow \infty$.

In fact, as we shall see, the proof given below establishes that (a') \Rightarrow (b) \Rightarrow (a).

Proof. First we prove that property (a) implies property (b).

Applying Bienaymé-Chebyshev's inequality shows that

$$P_N(\{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - p, \phi \rangle| \geq \epsilon\}) \leq \frac{1}{\epsilon^2} \mathbf{E}^{P_N} |\langle \mu_{Z_N} - p, \phi \rangle|^2.$$

Then we compute

$$\begin{aligned} & \mathbf{E}^{P_N} |\langle \mu_{Z_N} - p, \phi \rangle|^2 \\ &= \mathbf{E}^{P_N} \left(\frac{1}{N} \sum_{j=1}^N \phi(z_j) \right)^2 + \mathbf{E}^{P_N} \langle p, \phi \rangle^2 - 2 \mathbf{E}^{P_N} \left(\langle p, \phi \rangle \frac{1}{N} \sum_{j=1}^N \phi(z_j) \right) \\ &= \mathbf{E}^{P_N} \left(\frac{1}{N} \sum_{j=1}^N \phi(z_j) \right)^2 + \langle p, \phi \rangle^2 - 2 \langle p, \phi \rangle \mathbf{E}^{P_N} \frac{1}{N} \sum_{j=1}^N \phi(z_j). \end{aligned}$$

Observe that, by symmetry of P_N , one has

$$\mathbf{E}^{P_N} (\phi(z_j) \phi(z_k)) = \begin{cases} \mathbf{E}^{P_N} (\phi(z_1) \phi(z_2)) & \text{if } j \neq k, \\ \mathbf{E}^{P_N} (\phi(z_1)^2) & \text{if } j = k. \end{cases}$$

Thus

$$\begin{aligned} \mathbf{E}^{P_N} \left(\frac{1}{N} \sum_{j=1}^N \phi(z_j) \right)^2 &= \frac{1}{N^2} \sum_{j,k=1}^N \mathbf{E}^{P_N} (\phi(z_j) \phi(z_k)) \\ &= \frac{1}{N} \mathbf{E}^{P_N} (\phi(z_1)^2) + \frac{N-1}{N} \mathbf{E}^{P_N} (\phi(z_1) \phi(z_2)) \\ &= \frac{1}{N} \langle P_{N:1}, \phi^2 \rangle + \frac{N-1}{N} \langle P_{N:2}, \phi \otimes \phi \rangle \\ &\rightarrow \langle p^{\otimes 2}, \phi^{\otimes 2} \rangle = \langle p, \phi \rangle^2 \end{aligned}$$

as $N \rightarrow \infty$ by (a), while

$$\begin{aligned} \mathbf{E}^{P_N} \left(\frac{1}{N} \sum_{j=1}^N \phi(z_j) \right) &= \frac{1}{N} \sum_{j=1}^N \mathbf{E}^{P_N} (\phi(z_j)) \\ &= \frac{1}{N} \sum_{j=1}^N \mathbf{E}^{P_N} (\phi(z_1)) = \langle P_{N:1}, \phi \rangle \rightarrow \langle p, \phi \rangle \end{aligned}$$

as $N \rightarrow \infty$, again by (a).

Therefore, property (a) implies that

$$\mathbf{E}^{P_N} |\langle \mu_{Z_N} - p, \phi \rangle|^2 \rightarrow \langle p, \phi \rangle^2 + \langle p, \phi \rangle^2 - 2\langle p, \phi \rangle^2 = 0$$

as $N \rightarrow \infty$, and therefore

$$P_N(\{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - p, \phi \rangle| \geq \epsilon\}) \leq \frac{1}{\epsilon^2} \cdot o(1)$$

by Bienaymé-Chebyshev's inequality, which is precisely property (b).

Next we prove that, conversely, property (b) implies property (a).

Step 1: let us prove first that property (b) implies that $P_{N:1} \rightarrow p$ weakly as $N \rightarrow \infty$.

Let $\phi \in C_b(\mathbf{R}^d)$. Denote

$$\begin{aligned} U_N^\epsilon(\phi) &:= \{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - p, \phi \rangle| > \epsilon\}, \\ V_N^\epsilon(\phi) &:= (\mathbf{R}^d)^N \setminus U_N^\epsilon(\phi). \end{aligned}$$

Then

$$\begin{aligned} &|\mathbf{E}^{P_N} \langle \mu_{Z_N}, \phi \rangle - \langle p, \phi \rangle| = |\mathbf{E}^{P_N} \langle \mu_{Z_N} - p, \phi \rangle| \\ &\leq \mathbf{E}^{P_N} (|\langle \mu_{Z_N} - p, \phi \rangle| \mathbf{1}_{U_N^\epsilon(\phi)}) + \mathbf{E}^{P_N} (|\langle \mu_{Z_N} - p, \phi \rangle| \mathbf{1}_{V_N^\epsilon(\phi)}). \end{aligned}$$

Obviously

$$\mathbf{E}^{P_N} (|\langle \mu_{Z_N} - p, \phi \rangle| \mathbf{1}_{U_N^\epsilon(\phi)}) \leq 2\|\phi\|_{L^\infty} P_N(U_N^\epsilon(\phi)),$$

and

$$\mathbf{E}^{P_N} (|\langle \mu_{Z_N} - p, \phi \rangle| \mathbf{1}_{V_N^\epsilon(\phi)}) \leq \epsilon.$$

By (b), there exists $N(\epsilon, \phi)$ such that

$$N > N(\epsilon, \phi) \Rightarrow P_N(U_N^\epsilon(\phi)) < \epsilon,$$

so that

$$|\mathbf{E}^{P_N} \langle \mu_{Z_N}, \phi \rangle - \langle p, \phi \rangle| \leq (2\|\phi\|_{L^\infty} + 1)\epsilon.$$

On the other hand

$$\mathbf{E}^{P_N} (\langle \mu_{Z_N}, \phi \rangle) = \mathbf{E}^{P_N} \left(\frac{1}{N} \sum_{j=1}^N \phi(z_j) \right) = \mathbf{E}^{P_N} (\phi(z_1)) = \langle P_{N:1}, \phi \rangle,$$

so that

$$N > N(\epsilon, \phi) \Rightarrow |\langle P_{N:1}, \phi \rangle - \langle p, \phi \rangle| \leq (2\|\phi\|_{L^\infty} + 1)\epsilon.$$

which concludes step 1.

Step 2: next we prove that property (b) implies that $P_{N:j} \rightarrow p^{\otimes j}$ weakly as $N \rightarrow \infty$, for all $j > 1$.

Let $\phi \in C_b(\mathbf{R}^d) \setminus \{0\}$. Let $\mathcal{E}_N^j := \{1, \dots, N\}^{\{1, \dots, j\}}$ (the set of maps from $\{1, \dots, j\}$ to $\{1, \dots, N\}$) and let \mathcal{A}_N^j be the set of one-to-one elements of \mathcal{E}_N^j . Then

$$\begin{aligned} \mathbf{E}^{P_N}(\langle \mu_{Z_N}^{\otimes j}, \phi^{\otimes j} \rangle) &= \mathbf{E}^{P_N} \left(\frac{1}{N^j} \sum_{s \in \mathcal{E}_N^j} \phi(z_{s(1)}) \dots \phi(z_{s(j)}) \right) \\ &= \frac{1}{N^j} \sum_{s \in \mathcal{A}_N^j} \mathbf{E}^{P_N}(\phi(z_{s(1)}) \dots \phi(z_{s(j)})) \\ &\quad + \frac{1}{N^j} \sum_{s \in \mathcal{E}_N^j \setminus \mathcal{A}_N^j} \mathbf{E}^{P_N}(\phi(z_{s(1)}) \dots \phi(z_{s(j)})). \end{aligned}$$

For $s \in \mathcal{A}_N^j$, one has

$$\mathbf{E}^{P_N}(\phi(z_{s(1)}) \dots \phi(z_{s(j)})) = \mathbf{E}^{P_N}(\phi(z_1) \dots \phi(z_j)) = \langle P_{N;j}, \phi^{\otimes j} \rangle$$

by symmetry of P_N , while, for all $s \in \mathcal{E}_N^j$

$$|\mathbf{E}^{P_N}(\phi(z_{s(1)}) \dots \phi(z_{s(j)}))| \leq \|\phi\|_{L^\infty}^j.$$

Now, for all j fixed

$$\begin{cases} \#\mathcal{A}_N^j = N(N-1) \dots (N-j+1) \sim N^j \text{ as } N \rightarrow \infty, \\ \#(\mathcal{E}_N^j \setminus \mathcal{A}_N^j) = N^j - N(N-1) \dots (N-j+1) = o(N^j), \end{cases}$$

so that

$$\left| \mathbf{E}^{P_N} \langle \mu_{Z_N}^{\otimes j}, \phi^{\otimes j} \rangle - \langle P_{N;j}, \phi^{\otimes j} \rangle \right| \leq 2 \frac{N^j - \#\mathcal{A}_N^j}{N^j} \|\phi\|_{L^\infty}^j.$$

Introduce

$$\begin{cases} X_N^\epsilon(j, \phi) = \{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle| > \epsilon\}, \\ Y_N^\epsilon(j, \phi) = (\mathbf{R}^d)^N \setminus X_N^\epsilon(j, \phi). \end{cases}$$

Observe that

$$\langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle = \sum_{k=1}^j \langle \mu_{Z_N}, \phi \rangle^{k-1} \langle \mu_{Z_N} - p, \phi \rangle \langle p, \phi \rangle^{j-k},$$

so that

$$|\langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle| \leq j \|\phi\|_{L^\infty}^{j-1} |\langle \mu_{Z_N} - p, \phi \rangle|.$$

Therefore, property (b) implies that

$$P_N(X_N^\epsilon(j, \phi)) \leq P_N(U_N^{\epsilon/j \|\phi\|_{L^\infty}^{j-1}}(\phi)) \rightarrow 0$$

as $N \rightarrow \infty$ for all $j > 1$, all $\epsilon > 0$ and all $\phi \in C_b(\mathbf{R}^d) \setminus \{0\}$.

In particular, for each $j \geq 1$, there exists $N_j(\epsilon, \phi) \geq j$ such that

$$N > N_j(\epsilon, \phi) \Rightarrow P_N(X_N^\epsilon(j, \phi)) < \epsilon.$$

Thus

$$\begin{aligned} |\mathbf{E}^{P_N} \langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle| &\leq \mathbf{E}^{P_N} (|\langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle| \mathbf{1}_{X_N^\epsilon(j, \phi)}) \\ &\quad + \mathbf{E}^{P_N} (|\langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle| \mathbf{1}_{Y_N^\epsilon(j, \phi)}) \\ &\leq 2\|\phi\|_{L^\infty}^j P_N(X_N^\epsilon(j, \phi)) + \epsilon \end{aligned}$$

so that

$$N > N_j(\epsilon, \phi) \Rightarrow |\mathbf{E}^{P_N} \langle \mu_{Z_N}^{\otimes j} - p^{\otimes j}, \phi^{\otimes j} \rangle| < (2\|\phi\|_{L^\infty}^j + 1)\epsilon.$$

Therefore, for each $\epsilon > 0$ and each $j > 1$, and for all $N > N_j(\epsilon, \phi)$, one has

$$\begin{aligned} |\langle p^{\otimes j} - P_{N:j}, \phi^{\otimes j} \rangle| &\leq |\mathbf{E}^{P_N} (\langle p^{\otimes j} - \mu_{Z_N}^{\otimes j}, \phi^{\otimes j} \rangle)| \\ &\quad + |\mathbf{E}^{P_N} (\langle \mu_{Z_N}^{\otimes j}, \phi^{\otimes j} \rangle) - \langle P_{N:j}, \phi^{\otimes j} \rangle| \\ &\leq (2\|\phi\|_{L^\infty}^j + 1)\epsilon + 2\frac{N^j - \#\mathcal{A}_N^j}{N^j} \|\phi\|_{L^\infty}^j, \end{aligned}$$

and since $N^j - \#\mathcal{A}_N^j = o(N^j)$ as $N \rightarrow \infty$,

$$\overline{\lim}_{N \rightarrow \infty} |\langle p^{\otimes j} - P_{N:j}, \phi^{\otimes j} \rangle| \leq (2\|\phi\|_{L^\infty}^j + 1)\epsilon.$$

Since this holds for each $\epsilon > 0$, we conclude that

$$\langle P_{N:j}, \phi^{\otimes j} \rangle \rightarrow \langle p^{\otimes j}, \phi^{\otimes j} \rangle \quad \text{as } N \rightarrow \infty.$$

This property holds for each $\phi \in C_b(\mathbf{R}^d) \setminus \{0\}$ so that, by a classical density argument, we conclude that the sequence P_N is p -chaotic. ■

Exercise: The purpose of this exercise is to complete the “classical density argument” used at the end of the proof of Theorem 1.6.2. For each $\Phi \in C((\mathbf{R}^d)^j)$, denote by $S_j\Phi$ the element of $C((\mathbf{R}^d)^j)$ defined by the formula

$$S_j\Phi(z_1, \dots, z_j) := \frac{1}{j!} \sum_{\sigma \in \mathfrak{S}_j} \Phi(z_{\sigma(1)}, \dots, z_{\sigma(j)}).$$

Finally, for each $\phi_1, \dots, \phi_j \in C(\mathbf{R}^d)$, we denote by $\phi_1 \otimes \dots \otimes \phi_j$ the function

$$\phi_1 \otimes \dots \otimes \phi_j : (z_1, \dots, z_j) \mapsto \phi_1(z_1) \dots \phi_j(z_j),$$

and by $\phi^{\otimes j}$ the j -fold tensor product of ϕ with itself.

a) Prove that

$$S_j(\phi_1 \otimes \dots \otimes \phi_j) = \frac{1}{j!} \frac{\partial^j}{\partial X_1 \dots \partial X_j} (X_1 \phi_1 + \dots + X_j \phi_j)^{\otimes j}.$$

b) Prove that, for each $Q \in \mathcal{P}_{sym}((\mathbf{R}^d)^j)$ and each $\Phi \in C_b((\mathbf{R}^d)^j)$, one has

$$\langle Q, \Phi \rangle = \langle Q, S_j \Phi \rangle.$$

c) Let¹³ $\Phi \in C_0((\mathbf{R}^d)^j)$ and $\epsilon > 0$. Prove that there exists $\alpha_1, \dots, \alpha_n \in \mathbf{R}$ and a jn -tuple $(\phi_{i,m})_{1 \leq i \leq j, 1 \leq m \leq n}$ of elements of $C_0(\mathbf{R}^d)$ such that

$$\left\| \Phi - \sum_{m=1}^n \alpha_m \phi_{1,m} \otimes \dots \otimes \phi_{j,m} \right\| < \epsilon,$$

where

$$\|\Psi\| = \sup_{z_1, \dots, z_j \in \mathbf{R}^d} |\Psi(z_1, \dots, z_j)|.$$

(Hint: apply the Stone-Weierstrass theorem.)

d) Let $Q \in \mathcal{P}_{sym}((\mathbf{R}^d)^j)$ and $(Q_N)_{N \geq 1}$ be a sequence of elements of $\mathcal{P}_{sym}((\mathbf{R}^d)^j)$ such that

$$\langle Q_N, \phi^{\otimes j} \rangle \rightarrow \langle Q, \phi^{\otimes j} \rangle$$

as $N \rightarrow \infty$ for each $\phi \in C_0(\mathbf{R}^d)$. Prove that

$$\langle Q_N, \Phi \rangle \rightarrow \langle Q, \Phi \rangle$$

as $N \rightarrow \infty$ for each $\Phi \in C_0((\mathbf{R}^d)^j)$.

e) Conclude that

$$\langle Q_N, \Phi \rangle \rightarrow \langle Q, \Phi \rangle$$

as $N \rightarrow \infty$ for each $\Phi \in C_b((\mathbf{R}^d)^j)$. (Hint: apply Theorem 6.8 in chapter II of [70].)

References for this section are chapter 1, section 2 in [92], and chapter 4, section 6 in [26].

1.6.2 From Dobrushin's theorem to the BBGKY hierarchy

In the proof of the mean-field limit based on the notion of empirical measure, one proves the stability of the limiting, mean field PDE in the weak topology of probability measures on the single-particle phase space. The method based on the BBGKY hierarchy involves the N -particle phase space, and the need for considering marginals of the N -particle distribution in the limit as $N \rightarrow \infty$. Perhaps the best way to understand the relation between these two approaches of the same problem is to think of the nature of the N -particle empirical measure. Indeed

$$\mu_{Z_N}(dz)$$

¹³For each locally compact topological space X and each finite dimensional vector space E on \mathbf{R} , we denote by $C_0(X, E)$ the set of continuous functions on X with values in E that converge to 0 at infinity. We set $C_0(X) := C_0(X, E)$.

is a symmetric *function* of the N variables $Z_N = (z_1, \dots, z_N)$, defined on the N -particle phase space $(\mathbf{R}^d)^N$, and with values in the set of *probability measures on the single-particle phase space* \mathbf{R}^d — in the notation above, z is the variable in the single-particle phase space.

Already the characterization of chaotic sequences in terms of empirical measures obtained in the previous section clarifies the respective roles of the single particle phase space and of the N -particle phase space in this limit. The N -particle symmetric distribution function F_N can be viewed as a probability on $\mathcal{P}(\mathbf{R}^d)$ concentrated on the set of empirical measures — in other words, the N -tuple Z_N is, up to permutations of its N components, identified with the empirical measure μ_{Z_N} . (This idea can be found in [47] and will be discussed in more detail in section 1.7.3 below.)

Although this is a static picture, it provides the right point of view in order to unify the two approaches of the mean field limit presented above, i.e. the approach based on empirical measures and Dobrushin's estimate, and the one based on the BBGKY hierarchy. More precisely, we shall prove that the sequence $F_N(t)$ of solutions of the N -particle Liouville equation with factorized initial data is $f(t)\mathcal{L}^d$ -chaotic for each $t \in \mathbf{R}$, where f is the solution of the mean field PDE.

The proof of this result goes as follows.

Since F_N^{in} is factorized, it is of course chaotic (factorized probability measures being the first example of chaotic measures). But in fact, F_N^{in} satisfies a stronger estimate than property (b) in Theorem 1.6.2, in terms of the Monge-Kantorovich distance $\text{dist}_{MK,2}$ (see Theorem 1.6.4 below). This estimate is propagated for all $t \in \mathbf{R}$ by Dobrushin's inequality, involving the weaker distance $\text{dist}_{MK,1}$. The resulting bound implies that property (b) in Theorem 1.6.2 holds for $F_N(t)$ for all t with $p := f(t)\mathcal{L}^d$. Applying Theorem 1.6.2, we conclude that $F_N(t)$ is $f(t)\mathcal{L}^d$ -chaotic.

Our main result in this section is summarized in the following statement.

Theorem 1.6.3 *Assume that the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ satisfies assumptions (HK1)-(HK2). Let f^{in} be a probability density on \mathbf{R}^d such that*

$$\int_{\mathbf{R}^d} |z|^{d+5} f(z) dz < \infty.$$

Let $F_N^{in} = (f^{in} \mathcal{L}^d)^{\otimes N}$, and let $F_N(t) = T_t \# F_N^{in}$ be the solution of the N -particle Liouville equation

$$\begin{cases} \partial_t F_N + \frac{1}{N} \sum_{j=1}^N \text{div}_{z_i} (K(z_i, z_j) F_N) = 0, \\ F_N|_{t=0} = F_N^{in}. \end{cases}$$

Then, for each $j \geq 1$

$$F_{N;j}(t) \rightarrow (f(t, \cdot) \mathcal{L}^d)^{\otimes j}$$

weakly in $\mathcal{P}((\mathbf{R}^d)^j)$ as $N \rightarrow \infty$, where the probability density $f(t, \cdot)$ is the solution of the mean field PDE

$$\begin{cases} \partial_t f(t, z) + \operatorname{div}_z \left(f(t, z) \int_{\mathbf{R}^d} K(z, z') f(t, z') dz' \right) = 0, \\ f|_{t=0} = f^{in}. \end{cases}$$

The rather stringent moment condition on the initial single-particle density f^{in} comes from the following important result from statistics, that can be viewed as a quantitative variant of the law of large numbers.

Theorem 1.6.4 (Horowitz-Karandikar) *For all $p \in \mathcal{P}(\mathbf{R}^d)$ such that*

$$a := \langle p, |z|^{d+5} \rangle < \infty,$$

one has

$$\int_{(\mathbf{R}^d)^N} \operatorname{dist}_{MK,2}(\mu_{Z_N}, p)^2 p^{\otimes N}(dZ_N) \leq \frac{C(a, d)^2}{N^{2/(d+4)}},$$

where $C(a, d)$ is a positive constant that depends only on a and the space dimension d .

References for this result are the original article [57], and the monograph [82].

Taking this estimate for granted, we give the proof of Theorem 1.6.3.

Proof of Theorem 1.6.3. By the Cauchy-Schwarz inequality, for all $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^d)$ and all $\pi \in \Pi(\mu, \nu)$, one has

$$\iint_{\mathbf{R}^d} |x - y| \pi(dxdy) \leq \left(\iint_{\mathbf{R}^d} |x - y|^2 \pi(dxdy) \right)^{1/2}.$$

Taking the infimum of both sides of the inequality above as π runs through $\Pi(\mu, \nu)$ shows that

$$\operatorname{dist}_{MK,1}(\mu, \nu) \leq \operatorname{dist}_{MK,2}(\mu, \nu).$$

Hence

$$\int_{(\mathbf{R}^d)^N} \operatorname{dist}_{MK,1}(\mu_{Z_N}, f^{in} \mathcal{L}^d)^2 (f^{in})^{\otimes N}(Z_N)(dZ_N) \leq \frac{C(a, d)}{N^{2/(d+4)}}.$$

Since $F_N(t) = T_t \# F_N^{in}$, one has

$$\begin{aligned} & F_N(t)(\{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - f(t) \mathcal{L}^d, \phi \rangle| \geq \epsilon\}) \\ &= F_N^{in}(\{Z_N^{in} \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{T_t Z_N^{in}} - f(t) \mathcal{L}^d, \phi \rangle| \geq \epsilon\}). \end{aligned}$$

For each $\pi \in \Pi(\mu_{T_t Z_N^{in}}, f(t)\mathcal{L}^d)$,

$$\begin{aligned} |\langle \mu_{T_t Z_N^{in}} - f(t)\mathcal{L}^d, \phi \rangle| &= \left| \iint_{\mathbf{R}^d \times \mathbf{R}^d} (\phi(x) - \phi(y)) \pi(dx dy) \right| \\ &\leq \text{Lip}(\phi) \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y| \pi(dx dy). \end{aligned}$$

Taking the inf of both sides of this inequality as π runs through the set of couplings $\Pi(\mu_{T_t Z_N^{in}}, f(t)\mathcal{L}^d)$ shows that

$$|\langle \mu_{T_t Z_N^{in}} - f(t)\mathcal{L}^d, \phi \rangle| \leq \text{Lip}(\phi) \text{dist}_{MK,1}(\mu_{T_t Z_N^{in}}, f(t)\mathcal{L}^d).$$

By Proposition 1.4.2 and Dobrushin's inequality (Theorem 1.4.3),

$$\begin{aligned} |\langle \mu_{T_t Z_N^{in}} - f(t)\mathcal{L}^d, \phi \rangle| &\leq \text{Lip}(\phi) \text{dist}_{MK,1}(\mu_{T_t Z_N^{in}}, f(t)\mathcal{L}^d) \\ &\leq \text{Lip}(\phi) e^{2L|t|} \text{dist}_{MK,1}(\mu_{Z_N^{in}}, f^{in}\mathcal{L}^d). \end{aligned}$$

Therefore

$$\begin{aligned} &F_N(t)(\{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - f(t)\mathcal{L}^d, \phi \rangle| \geq \epsilon\}) \\ &\leq F_N^{in}(\{Z_N^{in} \in (\mathbf{R}^d)^N \text{ s.t. } \text{dist}_{MK,1}(\mu_{Z_N^{in}}, f^{in}\mathcal{L}^d) \geq e^{-2L|t|}\epsilon/\text{Lip}(\phi)\}). \end{aligned}$$

Applying the Horowitz-Karandikar theorem recalled above and the Bienaymé-Chebyshev inequality shows that

$$\begin{aligned} &F_N^{in}(\{Z_N^{in} \in (\mathbf{R}^d)^N \text{ s.t. } \text{dist}_{MK,1}(\mu_{Z_N^{in}}, f^{in}\mathcal{L}^d) \geq e^{-2L|t|}\epsilon/\text{Lip}(\phi)\}) \\ &\leq \frac{e^{4L|t|} \text{Lip}(\phi)^2}{\epsilon^2} \int_{(\mathbf{R}^d)^N} \text{dist}_{MK,1}(\mu_{Z_N^{in}}, f^{in}\mathcal{L}^d)^2 (f^{in})^{\otimes N}(Z_N) dZ_N \\ &\leq \frac{e^{4L|t|} \text{Lip}(\phi)^2}{\epsilon^2} \frac{C(a, d)^2}{N^{2/(d+4)}}. \end{aligned}$$

Hence

$$F_N(t)(\{Z_N \in (\mathbf{R}^d)^N \text{ s.t. } |\langle \mu_{Z_N} - f(t)\mathcal{L}^d, \phi \rangle| \geq \epsilon\}) \rightarrow 0$$

as $N \rightarrow \infty$ for each $\phi \in L^\infty \cap \text{Lip}(\mathbf{R}^d)$. By density of $L^\infty \cap \text{Lip}(\mathbf{R}^d)$ in $C_b(\mathbf{R}^d)$ and the implication (b) \Rightarrow (a) in Theorem 1.6.2, we conclude that

$$F_{N;j}(t) \rightarrow (f(t)\mathcal{L}^d)^{\otimes j}$$

weakly in $\mathcal{P}((\mathbf{R}^d)^j)$ as $N \rightarrow \infty$ for all $j \geq 1$.

In particular

$$F_{N;1}(t) \rightarrow f(t)\mathcal{L}^d$$

weakly in $\mathcal{P}(\mathbf{R}^d)$ as $N \rightarrow \infty$, where $f(t, \cdot)$ is the solution of the mean field PDE, and this concludes the proof. \blacksquare

1.7 Further results on mean field limits in classical mechanics

1.7.1 Propagation of chaos and quantitative estimates

Following carefully our proof in the previous section, the convergence result stated in Theorem 1.6.3 could obviously have been formulated as a quantitative estimate of the form

$$\text{dist}_{MK,1}(P_{N:j}(t), (f(t)\mathcal{L}^d)^{\otimes j}) \leq \epsilon_j(N),$$

where $\epsilon_j(N) \rightarrow 0$ for each $j \geq 1$ in the limit as $N \rightarrow \infty$. Such an estimate would obviously imply Theorem 1.6.3 since the Monge-Kantorovich distance $\text{dist}_{MK,1}$ metrizes the weak topology on $\mathcal{P}_1(\mathbf{R}^n)$ for all $n \geq 1$ — see Theorem 6.9 in [96], although what is needed here is a consequence of Proposition 1.4.2.

In fact, there is another approach of Theorem 1.6.3 which is perhaps worth mentioning, since it provides additional information on the relation between the approach with the empirical measure and the approach based on BBGKY hierarchies.

Specifically, one can prove that, if $F_N^{in} \in \mathcal{P}_{1,sym}((\mathbf{R}^d)^N)$ and if $t \mapsto F_N(t)$ is the solution of the Cauchy problem for the N -particle Liouville equation with initial data F_N^{in} , assuming that the interaction kernel K satisfies the assumptions (HK1-HK2), then

$$\int_{(\mathbf{R}^d)^N} \mu_{T_t Z_N^{in}}^{\otimes m} F_N^{in}(dZ_N^{in}) = \frac{N!}{(N-m)!N^m} F_{N:m}(t) + R_{N,m}(t)$$

where T_t is the flow defined by the N -particle ODE system, while $R_{N,m}(t)$ is a positive Radon measure on $(\mathbf{R}^d)^m$ whose total mass satisfies

$$\langle R_{N,m}(t), 1 \rangle = 1 - \frac{N!}{(N-m)!N^m} \leq \frac{m(m-1)}{2N}.$$

This explicit formula, which can be found in [44] expresses the m -th marginal of the N -particle distribution $F_N(t)$ in terms of the empirical measure of the N -particle system at time t , i.e. $\mu_{T_t Z_N^{in}}$, up to an error that vanishes as $N \rightarrow \infty$.

With this formula, one easily arrives at the following quantitative estimate for the propagation of chaos in the mean field problem. Assume that the initial data is factorized, i.e.

$$F_N^{in} = (f^{in} \mathcal{L}^d)^{\otimes N}$$

and that

$$a := \int_{\mathbf{R}^d} |z|^{d+5} f^{in}(z) dz < \infty.$$

Then

$$\|P_{N:m}(t) - (f(t)\mathcal{L}^d)^{\otimes m}\|_{W^{-1,1}((\mathbf{R}^d)^m)} \leq m \left(\frac{m-1}{N} + e^{2L|t|} \frac{C(a,d)}{N^{1/(d+4)}} \right).$$

for all $t \in \mathbf{R}$ and all $N \geq m \geq 1$. In particular, for $m = 1$, one has

$$\text{dist}_{MK,1}(P_{N:1}(t), f(t)\mathcal{L}^d) \leq C(a, d)e^{2L|t|}/N^{1/(d+4)}.$$

This estimate can be found in [44]; it is established independently and in a slightly different manner in [73].

In fact, the idea of obtaining quantitative estimates for the propagation of chaos in various situations of non equilibrium classical statistical mechanics has been systematically pursued in the reference [73], which bears on a more general class of models than the one considered so far in the present notes. In particular, the discussion in [73] applies to situations where the empirical measure of the N -particle system is *not an exact weak solution* of the limiting mean field equation.

1.7.2 Infinite hierarchies and statistical solutions

While the physical content of the BBGKY hierarchy is transparent (it is the string of equations satisfied by the marginals of the N -particle distribution), the physical meaning of the infinite mean field hierarchy is somewhat less obvious. We discuss this point in the present section.

Consider the Cauchy problem for the mean field PDE:

$$\begin{cases} \partial_t f + \text{div}_z(f\mathcal{K}f) = 0, \\ f|_{t=0} = f^{in}, \end{cases}$$

where we recall that

$$\mathcal{K}f(t, z) := \int_{\mathbf{R}^d} K(z, z')f(t, dz'),$$

and where the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$ is assumed to satisfy conditions (HK1-HK2).

Denote by $G_t : \mathcal{P}_1(\mathbf{R}^d) \mapsto \mathcal{P}_1(\mathbf{R}^d)$ the nonlinear 1-parameter group defined by

$$G_t f^{in} := f(t, \cdot)$$

where f is the unique solution of the Cauchy problem above.

The notion of statistical solutions of the mean field PDE is defined by analogy with the case of an ODE. Consider the Cauchy problem for an ODE with unknown $t \mapsto x(t) \in \mathbf{R}^n$ in the form

$$\begin{cases} \dot{x}(t) = v(x(t)), \\ x(0) = x_0. \end{cases}$$

Assuming that $v \in \text{Lip}(\mathbf{R}^n, \mathbf{R}^n)$, the Cauchy-Lipschitz theorem provides the existence of a global solution flow $X : \mathbf{R} \times \mathbf{R}^n \rightarrow \mathbf{R}^n$, so that the map

$$t \mapsto X(t, x_0)$$

is the solution of the ODE above satisfying $X(0, x_0) = x_0$. The flow X corresponds with a completely deterministic notion of solution: knowing the initial condition x_0 exactly determines the solution $t \mapsto X(t, x_0)$ for all times. Suppose that, instead of knowing exactly the initial condition x_0 , one is given a probability distribution μ_0 on the set \mathbf{R}^n of initial data x_0 . In other words, μ_0 can be regarded as a “statistical initial condition” for the Cauchy problem above. With the flow X and the statistical initial condition μ_0 , one defines

$$\mu(t) := X(t, \cdot) \# \mu_0, \quad t \in \mathbf{R}.$$

Applying the method of characteristics (see the exercise following Theorem 1.3.1) shows that

$$\begin{cases} \partial_t \mu(t) + \operatorname{div}(\mu(t)v) = 0, \\ \mu(0) = \mu_0. \end{cases}$$

In other words, we recover the well-known fact that solutions of the transport equation (a 1st order PDE) can be viewed as statistical solutions of the ODE defined by the characteristic field of the transport operator. The idea of considering the time-dependent probability $\mu(t)$ (or distribution function, when $\mu(t)$ is absolutely continuous with respect to the Lebesgue measure on the single-particle phase space) instead of the deterministic solution $X(t, x_0)$ for each initial data x_0 lies at the core of the kinetic theory of gases.

Let us return to the problem of defining a notion of statistical solution of the mean field PDE recalled above. First we need a probability measure ν_0 on the space of initial conditions f^{in} , in this case on $\mathcal{P}_1(\mathbf{R}^d)$: this probability ν_0 will be the statistical initial condition for the mean field PDE. By analogy with the case of the simple ODE presented above, we define

$$\nu(t) := G_t \# \nu_0, \quad t \in \mathbf{R}.$$

The next question is to find the analogue of the transport equation satisfied by $\mu(t)$.

First we need to have a better grasp on $\nu(t)$. One way to understand the formula above expressing $\nu(t)$ as the push-forward of ν_0 under the map G_t defined by the mean field evolution is to write

$$\int_{\mathcal{P}_1(\mathbf{R}^d)} \mathcal{F}(p) \nu(t, dp) = \int_{\mathcal{P}_1(\mathbf{R}^d)} \mathcal{F}(G_t p) \nu_0(dp)$$

for some appropriate class of continuous (in some sense to be defined) functions \mathcal{F} on $\mathcal{P}_1(\mathbf{R}^d)$. Certainly this class of functions should contain “polynomials” on $\mathcal{P}_1(\mathbf{R}^d)$, i.e. linear combinations of “monomials”. A monomial of degree k on $\mathcal{P}(\mathbf{R}^d)$ is an expression of the form

$$M_{k, \phi}(p) := \int_{(\mathbf{R}^d)^k} \phi(z_1, \dots, z_k) p(dx_1) \dots p(dx_k) = \langle p^{\otimes k}, \phi \rangle$$

where $\phi \in C_b((\mathbf{R}^d)^k)$ — without loss of generality one can assume that ϕ is symmetric in the variables z_1, \dots, z_k .

Specializing the formula above to the case $\mathcal{F} = M_{j,\phi}$ as ϕ runs through $C_b((\mathbf{R}^d)^j)$ results in the equality

$$\int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes j} \nu(t, dp) = \int_{\mathcal{P}_1(\mathbf{R}^d)} (G_t p)^{\otimes j} \nu_0(dp).$$

Defining

$$F_j(t) := \int_{\mathcal{P}_1(\mathbf{R}^d)} (G_t p)^{\otimes j} \nu_0(dp), \quad j \geq 1,$$

we claim that the sequence $(F_j)_{j \geq 1}$ is a solution of the infinite mean field hierarchy. Indeed, for each initial single particle probability distribution $p \in \mathcal{P}_1(\mathbf{R}^d)$, the sequence $((G_t p)^{\otimes j})_{j \geq 1}$ is a solution of the infinite mean field hierarchy, which is a sequence of linear equations. Therefore $(F_j)_{j \geq 1}$ is also a solution of the infinite mean field hierarchy, being an average under ν_0 of solutions of this hierarchy.

There is another formulation of this observation. Set $\Omega := (\mathbf{R}^d)^{\mathbf{N}^*}$, equipped with its product topology and the associated Borel σ -algebra $\mathcal{B}(\Omega)$. For each $p \in \mathcal{P}_1(\mathbf{R}^d)$, we denote by $p^{\otimes \infty}$ the unique Borel probability measure defined on Ω by the formula

$$p^{\otimes \infty} \left(\prod_{k \geq 1} E_k \right) = \prod_{k \geq 1} p(E_k)$$

for each sequence $(E_k)_{k \geq 1}$ of Borel subsets of \mathbf{R}^d such that $E_k = \mathbf{R}^d$ for all but finitely many k s. Notice that

$$(p^{\otimes \infty})_{:j} = p^{\otimes j}, \quad j \geq 1.$$

Define

$$\mathbf{F}(t) := \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes \infty} \nu(t, dp) = \int_{\mathcal{P}_1(\mathbf{R}^d)} (G_t p)^{\otimes \infty} \nu_0(dp);$$

then, for each $j \geq 1$ and each $t \in \mathbf{R}$,

$$\mathbf{F}(t)_{:j} = F_j(t)$$

so that $(\mathbf{F}(t)_{:j})_{j \geq 1}$ is a solution of the infinite mean field hierarchy. Let us write the j th equation of the infinite mean field hierarchy in terms of $\mathbf{F}(t)$:

$$\partial_t \mathbf{F}(t)_{:j} + \sum_{i=1}^j \operatorname{div}_{z_i} (\mathbf{F}(t)_{:j+1} K(z_i, z_{j+1}))_{:j} = 0.$$

This equality is equivalent to the following weak formulation: for each test function $\psi_j \in C_c^1((\mathbf{R}^d)^j)$

$$\begin{aligned} \partial_t \langle \mathbf{F}(t), \psi_j \rangle &= \partial_t \langle \mathbf{F}(t)_{:j}, \psi_j \rangle = \sum_{i=1}^j \langle \mathbf{F}(t)_{:j+1}, K(z_i, z_{j+1}) \cdot \nabla_{z_i} \psi_j \rangle \\ &= \left\langle \mathbf{F}(t), \sum_{i=1}^j K(z_i, z_{j+1}) \cdot \nabla_{z_i} \psi_j \right\rangle \end{aligned}$$

This suggests the following definition. We denote by $\mathcal{P}_{sym}(\Omega)$ the set of Borel probability measures μ on Ω such that

$$U_\sigma \# \mu = \mu$$

for each $N > 1$ and each $\sigma \in \mathfrak{S}_N$, where

$$U_\sigma(z_1, z_2, \dots) := (z_{\sigma(1)}, \dots, z_{\sigma(N)}, z_{N+1}, z_{N+2}, \dots).$$

Definition 1.7.1 (Spohn [89]) *Let $I \subset \mathbf{R}$ be an interval. A map*

$$I \ni t \mapsto \mathbf{P}(t) \in \mathcal{P}_{sym}(\Omega)$$

is a measure-valued solution of the mean field hierarchy if and only if, for each $j \in \mathbf{N}^$ and each¹⁴ $\psi_j \in C_0^1((\mathbf{R}^d)^j)$, the map $t \mapsto \langle \mathbf{P}(t), \psi_j \rangle$ is of class C^1 on the interval I and*

$$\partial_t \langle \mathbf{P}(t), \psi_j \rangle = \partial_t \langle \mathbf{P}(t)_{:j}, \psi_j \rangle = \left\langle \mathbf{P}(t), \sum_{i=1}^j K(z_i, z_{j+1}) \cdot \nabla_{z_i} \psi_j \right\rangle$$

for all $t \in I$.

With this definition, the map $\mathbf{R} \ni t \mapsto \mathbf{F}(t) \in \mathcal{P}_{sym}(\Omega)$ defined above is a measure-valued solution of the mean-field hierarchy satisfying the initial condition

$$\mathbf{F}(0) = \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes \infty} \nu_0(dp).$$

This observation raises two natural questions:

- a) are measure-valued solutions of the mean-field hierarchy uniquely determined by their initial data?
- b) are all the measure-valued solutions of the mean-field hierarchy defined by statistical solutions of the mean field PDE?

A first useful tool in answering these questions is the following result.

Theorem 1.7.2 (Hewitt-Savage [52]) *For each $\mathbf{P} \in \mathcal{P}_{sym}(\Omega)$, there exists a unique Borel probability measure π on $\mathcal{P}(\mathbf{R}^d)$ such that*

$$\mathbf{P} = \int_{\mathcal{P}(\mathbf{R}^d)} p^{\otimes \infty} \pi(dp).$$

¹⁴For each $n, k \geq 1$ and each finite dimensional vector space E on \mathbf{R} , we denote by $C_0^k(\mathbf{R}^n, E)$ the set of functions of class C^k defined on \mathbf{R}^n with values in E all of whose partial derivatives converge to 0 at infinity. In other words,

$$C_0^k(\mathbf{R}^n, E) := \{f \in C^k(\mathbf{R}^n, E) \text{ s.t. } \partial^\alpha f(x) \rightarrow 0 \text{ as } |x| \rightarrow \infty \text{ for each } \alpha \in \mathbf{N}^n\}.$$

We denote $C_0^k(\mathbf{R}^n) := C_0^k(\mathbf{R}^n, \mathbf{R})$.

The Hewitt-Savage theorem is often quoted and used as follows. Given $(P_j)_{j \geq 1}$ a sequence of probability measures such that $P_j \in \mathcal{P}_{sym}((\mathbf{R}^d)^j)$ satisfying the compatibility condition

$$(CC) \quad P_{k:j} = P_j \quad \text{for each } k > j \geq 1,$$

by the Kolmogorov extension theorem [91], there exists a unique probability measure $\mathbf{P} \in \mathbf{P}_{sym}(\Omega)$ such that

$$\mathbf{P}_{:j} = P_j \quad \text{for each } j \in \mathbf{N}^*.$$

Therefore, by the Hewitt-Savage theorem, there exists a unique Borel probability measure π on $\mathcal{P}(\mathbf{R}^d)$ such that

$$P_j = \int_{\mathcal{P}(\mathbf{R}^d)} p^{\otimes j} \pi(dp).$$

With this, we can answer the questions a) and b) above.

First we consider the problem of admissible initial data. In view of the discussion above, the initial data for the mean field hierarchy can be equivalently either a sequence $(F_j^{in})_{j \geq 1}$ such that $F_j^{in} \in \mathcal{P}_{1,sym}((\mathbf{R}^d)^j)$ for $j \geq 1$ and satisfying the compatibility conditions (CC), or a unique element $\mathbf{F}^{in} \in \mathcal{P}(\Omega)$ such that

$$\mathbf{F}_{:j}^{in} = F_j, \quad j \geq 1,$$

or a unique Borel probability measure ν^{in} on $\mathcal{P}_1(\mathbf{R}^d)$ such that

$$F_j^{in} = \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes j} \nu^{in}(dp), \quad j \geq 1,$$

or equivalently

$$\mathbf{F}^{in} = \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes \infty} \nu^{in}(dp).$$

The same reasoning applies for each instant of time $t \neq 0$. A solution at time t of the infinite mean field hierarchy is a sequence $(P_j(t))_{j \geq 1}$ that satisfies in particular $P_j(t) \in \mathcal{P}_{1,sym}((\mathbf{R}^d)^j)$ for $j \geq 1$ together with the compatibility condition (CC). Equivalently, this defines a unique probability measure $\mathbf{P}(t) \in \mathcal{P}_{sym}(\Omega)$ such that $\mathbf{P}(t)_{:j} = P_j(t)$ for each $j \geq 1$, or a unique Borel probability measure $\pi(t)$ on $\mathcal{P}(\mathbf{R}^d)$ such that

$$P_j(t) = \int_{\mathcal{P}(\mathbf{R}^d)} p^{\otimes j} \pi(t, dp), \quad j \geq 1,$$

or equivalently

$$\mathbf{P}(t) = \int_{\mathcal{P}(\mathbf{R}^d)} p^{\otimes \infty} \pi(t, dp).$$

The following important result was proved by H. Spohn [89]. It answers questions a) and b) above.

Theorem 1.7.3 *Under the assumptions (HK1-HK2) on the interaction kernel $K \in C^1(\mathbf{R}^d \times \mathbf{R}^d, \mathbf{R}^d)$, for each Borel probability measure ν^{in} on $\mathcal{P}_1(\mathbf{R}^d)$, the only measure-valued solution of the infinite mean field hierarchy with initial data*

$$\mathbf{F}^{in} = \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes \infty} \nu^{in}(dp)$$

is

$$\mathbf{F}(t) = \int_{\mathcal{P}_1(\mathbf{R}^d)} (G_t p)^{\otimes \infty} \nu^{in}(dp), \quad t \in \mathbf{R}.$$

In other words, Spohn's theorem proves that the only measure valued solution of the infinite mean field hierarchy is the statistical solution of the mean field PDE

$$\nu(t) := G_t \# \nu^{in}, \quad t \in \mathbf{R},$$

where ν^{in} is the initial probability measure on the space $\mathcal{P}_1(\mathbf{R}^d)$ of initial data for the mean field PDE such that the initial condition for the mean field hierarchy is the element of $\mathcal{P}_{sym}(\Omega)$ given by

$$\mathbf{F}^{in} = \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes \infty} \nu^{in}(dp),$$

or equivalently the sequence

$$F_j^{in} = \int_{\mathcal{P}_1(\mathbf{R}^d)} p^{\otimes j} \nu^{in}(dp) \in \mathcal{P}_{sym}((\mathbf{R}^d)^j), \quad j \geq 1.$$

Notice that, in the case where $\nu^{in} = \delta_{f^{in}}$, one has

$$\mathbf{F}^{in} = (f^{in})^{\otimes \infty}, \text{ or equivalently } F_j^{in} = (f^{in})^{\otimes j} \text{ for all } j \geq 1,$$

and

$$\mathbf{F}(t) = (G_t f^{in})^{\otimes \infty}, \text{ or equivalently } F_j(t) = (G_t f^{in})^{\otimes j} \text{ for all } j \geq 1.$$

In other words the statistical solution $\nu(t)$ of the mean field PDE at time t is given by the formula

$$\nu(t) = \delta_{f(t)} = \delta_{G_t f^{in}} = G_t \# \delta_{f^{in}}.$$

That the statistical solution $\nu(t)$ is a Dirac measure for each $t \in \mathbf{R}$, knowing that $\nu(0) = \nu^{in}$ is a Dirac measure, is equivalent to the propagation of chaos in the context of the mean field limit.

Therefore, Spohn's theorem contains as a particular case the uniqueness theorem with factorized initial data which justifies the validity of the mean field limit in the approach with the BBGKY hierarchy.

But more generally, Spohn's theorem shows that solutions of the infinite mean field hierarchy coincide with the notion of statistical solutions of the mean

field PDE. This important piece of information clarifies the meaning of the infinite hierarchy.

Spohn's uniqueness theorem can also be combined with the following uniform stability result on the BBGKY hierarchy to produce a quantitative stability estimate on statistical solutions of the mean field PDE. The following quantitative stability estimate uses the following variant of Monge-Kantorovich distance. For each $P \in \mathcal{P}_{1, \text{sym}}((\mathbf{R}^d)^M)$ and $Q \in \mathcal{P}_{1, \text{sym}}((\mathbf{R}^d)^N)$, consider

$$\text{Dist}_{MK,1}(P, Q) = \inf_{\rho \in \Pi(P, Q)} \iint_{\mathbf{R}^{dM} \times \mathbf{R}^{dN}} \text{dist}_{MK,1}(\mu_{X_M}, \mu_{Y_N}) \rho(dX_M, dY_N).$$

In this formula, P and Q are viewed as Borel probability measures on $\mathcal{P}_1(\mathbf{R}^d)$ concentrated on the set of M - and N -particle empirical measures respectively.

Theorem 1.7.4 *Let $M, N \geq 1$, and let $P_M^{\text{in}} \in \mathcal{P}_{1, \text{sym}}((\mathbf{R}^d)^M)$ and $Q_N^{\text{in}} \in \mathcal{P}_{1, \text{sym}}((\mathbf{R}^d)^N)$. Assume that the interaction kernel K satisfies the conditions (HK1-HK2). Let $t \mapsto P_M(t)$ and $t \mapsto Q_N(t)$ be respectively the solutions of the M -particle and the N -particle Liouville equations with initial data P_M^{in} and Q_N^{in} respectively. Then*

a) for each $t \in \mathbf{R}$, one has

$$\text{Dist}_{MK,1}(P_M(t), Q_N(t)) \leq e^{2L|t|} \text{Dist}_{MK,1}(P_M^{\text{in}}, Q_N^{\text{in}}).$$

b) for each $t \in \mathbf{R}$, each $m, M, N \in \mathbf{N}^*$ such that $M, N \geq m$, and for each bounded and Lipschitz continuous function ϕ_m defined on $(\mathbf{R}^d)^m$, one has

$$\begin{aligned} & | \langle P_{M:m}(t) - Q_{N:m}(t), \phi_m \rangle | \\ & \leq m \left(e^{2L|t|} \text{Lip}(\phi_m) \text{Dist}_{MK,1}(P_M^{\text{in}}, Q_N^{\text{in}}) + (m-1) \|\phi_m\|_{L^\infty} \left(\frac{1}{M} + \frac{1}{N} \right) \right). \end{aligned}$$

For a proof of this result, see [44].

Notice however that Spohn's uniqueness theorem for the infinite mean field hierarchy, even in the particular case of factorized initial data, is more than what is needed to justify the mean field limit. It would be enough to prove the uniqueness of those solutions of the infinite hierarchy that are limits of the sequence of marginals of N -particle distributions as $N \rightarrow \infty$. This weaker uniqueness property follows from Theorem 1.7.4, without using Spohn's uniqueness theorem.

1.7.3 Symmetric functions of infinitely many variables

In various places in this notes — and especially in the last theorem — we encountered the idea of viewing elements of $\mathcal{P}_{\text{sym}}((\mathbf{R}^d)^N)$ as Borel probability measures on $\mathcal{P}(\mathbf{R}^d)$ concentrated on the set of empirical measures.

In fact, the identification

$$(\mathbf{R}^d)^N / \mathfrak{S}_N \ni (z_1, \dots, z_N) \mapsto \mu_{Z_N} := \frac{1}{N} \sum_{k=1}^N \delta_{z_k} \in \mathcal{P}_{\text{sym}}(\mathbf{R}^d)$$

can be found in [47] (see especially p. 330 there).

This point of view was pushed much further by P.-L. Lions. He constructed a complete mathematical framework for handling continuous symmetric functions of infinitely many variables that depend weakly on each variable, and used it systematically in his 2007-2008 lectures at the Collège de France on mean field games [67]. This remarkable circle of ideas also appears in the recent work of Mischler, Mouhot and Wennberg (see [72] and [73]) on the mean field limit and on quantitative estimates on the propagation of chaos in classical statistical mechanics.

We introduce, for each $X, Y \in Q^N$, the notation

$$d_{LP}(X, Y) := \inf\{\epsilon > 0 \text{ s.t. } \#\{k = 1, \dots, N \mid |x_k - y_k| > \epsilon\} < N\epsilon\}.$$

This quantity is related to the Levy-Prokhorov distance dist_{LP} on Borel probability measures on Q in the following manner:

$$\text{dist}_{LP}(\mu_X, \mu_Y) = \inf_{\sigma \in \mathfrak{S}_N} d_{LP}(X, Y_\sigma),$$

where $Y_\sigma := (y_{\sigma(1)}, \dots, y_{\sigma(N)})$. We recall the definition of the Levy-Prokhorov distance dist_{LP} on $\mathcal{P}(Q)$:

$$\text{dist}_{LP}(P_1, P_2) := \inf\left\{\epsilon > 0 \mid \inf_{\pi \in \Pi(P_1, P_2)} \iint_{Q \times Q} \mathbf{1}_{|x-y| > \epsilon} \pi(dx dy) < \epsilon\right\}.$$

We also recall that the Levy-Prokhorov distance metrizes the weak topology on $\mathcal{P}(Q)$, so that $(\mathcal{P}(Q), \text{dist}_{LP})$ is a compact metric space — see for instance [14].

Lions' key observation is summarized in the following theorem.

Theorem 1.7.5 (P.-L. Lions [67]) *Let Q be a compact metric space and consider, for each $N \geq 1$, a symmetric function $u_N \in C(Q^N)$. Assume that*

$$\sup_{N \geq 1} \sup_{(z_1, \dots, z_N) \in Q^N} |u_N(z_1, \dots, z_N)| < \infty,$$

and that

$$\sup\{|u_N(X) - u_N(Y)| \text{ s.t. } X, Y \in Q^N \text{ and } d_{LP}(X, Y) < \epsilon\} \rightarrow 0$$

uniformly in $N \geq 1$ as $\epsilon \rightarrow 0$. Then there exists $U \in C(\mathcal{P}(Q))$ and a subsequence u_{N_k} of u_N such that

$$\sup_{Z \in Q^{N_k}} |u_{N_k}(Z) - U(\mu_Z)| \rightarrow 0 \text{ as } N_k \rightarrow \infty.$$

This point of view is obviously dual of the Hewitt-Savage theorem quoted above. In fact, as noticed by P.-L. Lions, it leads to a very simple proof of the Hewitt-Savage theorem. Lions' argument [67] is sketched below.

Consider a sequence $(P_j)_{j \geq 1}$ of probability measures satisfying the compatibility condition (CC) above. Lions' idea is to consider

$$C(\mathcal{P}(Q)) \ni U \mapsto L(U) := \lim_{N \rightarrow \infty} \int_{Q^N} U(\mu_{Z_N}) P_N(dZ_N) \in \mathbf{R}.$$

That the limit on the right hand side of the equality above exists follows from considering the case of a monomial. Indeed, when $U = M_{k,\phi}$ with the notation used in the previous section, i.e.

$$U(\mu) = M_{k,\phi}(\mu) := \int_{Q^k} \phi(x_1, \dots, x_k) \mu^{\otimes k}(dx_1 \dots dx_k)$$

where $\phi \in C(Q^k)$, a straightforward computation shows that

$$\int_{Q^N} M_{k,\phi}(\mu_{Z_N}) P_N(dZ_N) = \int_{Q^k} \phi(z_1, \dots, z_k) P_k(dz_1 \dots dz_k) + O(1/N).$$

Hence

$$L(M_{k,\phi}) = \int_{Q^k} \phi(z_1, \dots, z_k) P_k(dz_1 \dots dz_k)$$

for all $k \geq 1$ and all $\phi \in C(Q^k)$.

The set of polynomials, i.e. of linear combinations of monomials, is a subalgebra of $C(\mathcal{P}(Q))$ since

$$M_{k,\phi}(\mu) M_{l,\psi}(\mu) = M_{k+l,\phi \otimes \psi}(\mu)$$

with

$$\phi \otimes \psi(x_1, \dots, x_{k+l}) := \phi(x_1, \dots, x_k) \psi(x_{k+1}, \dots, x_{k+l}).$$

We also use the convention

$$M_{0,1} = 1.$$

This subalgebra is dense in $C(\mathcal{P}(Q))$ for the topology of uniform convergence by the Stone-Weierstrass theorem.

Since

$$\left| \int_{Q^N} U(\mu_{Z_N}) P_N(dZ_N) \right| \leq \sup_{\mu \in \mathcal{P}(Q)} |U(\mu)|,$$

for each¹⁵ $U \in C(\mathcal{P}(Q))$, and since the limit

$$L(M_{k,\phi}) := \lim_{N \rightarrow \infty} \int_{Q^N} M_{k,\phi}(\mu_{Z_N}) P_N(dZ_N) = \int_{Q^k} \phi(z_1, \dots, z_k) P_k(dz_1 \dots dz_k)$$

exists for each $k \geq 1$ and each $\phi \in C(Q^k)$, we conclude that this limit exists for each $U \in C(\mathcal{P}(Q))$.

¹⁵Since $(\mathcal{P}(Q), \text{dist}_{LP})$ is compact, any element U of $C(\mathcal{P}(Q))$ is bounded on $\mathcal{P}(Q)$, so that

$$\sup_{\mu \in \mathcal{P}(Q)} |U(\mu)| < \infty.$$

Since obviously $L \geq 0$ (being the limit of linear functionals defined by P_N which is a positive measure), and since

$$L(1) = \int_{Q^N} P_N(dZ_N) = 1 \quad \text{for each } N \geq 1$$

we conclude that the linear functional L is represented by a unique probability measure $\pi \in \mathcal{P}(\mathcal{P}(Q))$, i.e.

$$L(U) = \int_{\mathcal{P}(Q)} U(\mu)\pi(d\mu).$$

Specializing to monomials

$$\begin{aligned} L(M_{k,\phi}) &= \int_{Q^k} \phi(z_1, \dots, z_k) P_k(dz_1 \dots dz_k) = \int_{\mathcal{P}(Q)} M_{k,\phi}(\mu)\pi(d\mu) \\ &= \int_{\mathcal{P}(Q)} \left(\int_{Q^k} \phi(z_1, \dots, z_k) \mu^{\otimes k}(dz_1 \dots dz_k) \right) \pi(d\mu) \\ &= \int_{Q^k} \phi(z_1, \dots, z_k) \left(\int_{\mathcal{P}(Q)} \mu^{\otimes k}(dz_1 \dots dz_k) \pi(d\mu) \right) \end{aligned}$$

and this means that

$$P_k = \int_{\mathcal{P}(Q)} \mu^{\otimes k} \pi(d\mu)$$

with the unique probability measure π defined above. This is precisely the representation formula in the Hewitt-Savage theorem.

1.7.4 The case of singular interaction kernels

The method for proving the mean field limit presented above is based on Dobrushin's estimate and, as such, is limited to cases where the interaction kernel k is Lipschitz continuous in both its arguments. This is most annoying since many interaction kernels of physical interest are singular on the diagonal. All the examples presented in the first section (i.e. the Vlasov-Poisson system and the vorticity formulation of the Euler equation for incompressible fluids in two space dimensions) involve the fundamental solution of the Laplacian, leading to interaction kernels that become singular as the distance between the two interacting particles vanishes. Obtaining rigorous derivations of both models as the mean field limit of large particle systems remains an important open problem.

However, some remarkable results have been obtained in this direction.

In the case of the vorticity formulation of the two-dimensional Euler equation for incompressible fluids, the mean field limit for the dynamics of a large number of vortex centers is analogous to the convergence problem for vortex methods in the numerical analysis of the Euler equation. These methods approximate the vorticity field $\omega \equiv \omega(t, x)$ as follows:

$$\omega(t, \cdot) \simeq \sum_{k=1}^N \omega_k \delta_{x_k(t)},$$

where ω_k is the (constant) intensity of the vortex centered at $x_k(t)$. (Notice the slight difference with the mean-field limit discussed above, where each vortex would have the same intensity $\omega_k = 1/N$.) The motion of the vortex centers $x_k(t)$ is governed by the following ODE system:

$$\dot{x}_k(t) = \sum_{\substack{l=1 \\ l \neq k}}^N \omega_l K_\epsilon(x_k(t) - x_l(t)), \quad k = 1, \dots, N,$$

where K_ϵ is an approximation of the vortex interaction kernel

$$K(x) = -\frac{1}{2\pi} \frac{Jx}{|x|^2},$$

(with J standing for the rotation of an angle $-\frac{\pi}{2}$).

In one variant of these methods, called “the vortex blob method”, the interaction potential is truncated near the singularity at the origin so as to remain smooth as the distance between interacting vortices vanishes. The method based on Dobrushin’s estimate presented above for proving the mean field limit applies without modification to the convergence of the vortex blob method. See chapter 5 in [71] for more details on this topic.

In another variant of these methods, called “the vortex point method”, there is no regularization of the interaction kernel, i.e. one takes $K_\epsilon = K$ in the system of ODEs above governing the motion of vortices. The vorticity field $\omega \equiv \omega(t, x)$ is approximated as follows

$$\omega(t, \cdot) \simeq \omega^h(t, \cdot) := \sum_{k \in \mathbf{Z}^2} \omega_k^h \delta_{x_k^h(t)},$$

where $h > 0$, and the vortex centers satisfy

$$\begin{cases} \dot{x}_k^h(t) = \sum_{\substack{l \in \mathbf{Z}^2 \\ l \neq k}}^N \omega_l^h K(x_l^h(t) - x_k^h(t)), \\ x_k^h(0) = hk, \quad k \in \mathbf{Z}^2, \end{cases}$$

while the vortex intensities are chosen so that

$$\omega_k^h = \omega(0, hk), \quad k \in \mathbf{Z}^2.$$

The convergence of the vortex point method for initial data in the Schwartz class $\mathcal{S}(\mathbf{R}^2)$ of infinitely differentiable functions with rapidly decaying derivatives of all orders has been proved in [45] — see also [46, 86, 48]. The key argument is a control of the minimal distance between vortex centers in Proposition 1 of [48].

One should also mention recent attempts to justify the derivation of the Vlasov-Poisson system as the mean field limit of the Liouville equation for a large number of identical point particles with (unmollified) Coulomb interaction: see [49, 50]. These papers prove the mean field limit and the propagation of chaos for large systems of point particles with singular interaction force field of order $O(d^{-\alpha})$ for $\alpha \leq 1$, where d designates the distance between the two interacting particles.

1.7.5 From particle systems to the Vlasov-Maxwell system

There are several difficulties in adapting the method for proving the mean field limit presented above to the case of the Vlasov-Maxwell system; see [43] for a detailed discussion of this problem.

First, the source term in the system of Maxwell's equations is not a probability distribution — as in the case of the Vlasov-Poisson system, where the electric field $E \equiv E(t, x)$ is given by

$$E(t, x) = -\nabla_x \phi_f(t, x), \quad \text{with } -\Delta_x \phi_f(t, x) = \rho_f(t, x).$$

(We recall that

$$\rho_f(t, x) := \int_{\mathbf{R}^3} f(t, x, v) dv$$

so that $\rho_f(t, \cdot)$ is a probability distribution on \mathbf{R}^3 if $f(t, \cdot, \cdot)$ is a probability distribution on $\mathbf{R}^3 \times \mathbf{R}^3$, which can be assumed without loss of generality since the total particle number is invariant under the Vlasov-Poisson dynamics.)

In the case of the Vlasov-Maxwell system, the source term in Maxwell's equations is the 4-vector (ρ_f, j_f) , defined as follows:

$$\rho_f(t, x) := \int_{\mathbf{R}^3} f(t, x, \xi) d\xi, \quad j_f(t, x) := \int_{\mathbf{R}^3} v(\xi) f(t, x, \xi) d\xi.$$

This difficulty is handled by an idea introduced in earlier works on Vlasov-Maxwell type systems [16, 15]. The idea is to represent the solution of Maxwell's equations for the electromagnetic field in terms of a *single momentum distribution* of electromagnetic potential, as follows. Consider the Cauchy problem for the wave equation

$$\begin{cases} \square_{t,x} u_f(t, x, \xi) = f(t, x, \xi), \\ u_f|_{t=0} = \partial_t u_f|_{t=0} = 0, \end{cases}$$

where $\square_{t,x} := \partial_t^2 - \Delta_x$ is the d'Alembert operator in the variables t and x . In other words, the momentum variable is a simple parameter in the wave equation above. The self-consistent electromagnetic field in the Vlasov-Maxwell system is represented as

$$\begin{aligned} E(t, x) &= -\partial_t \int_{\mathbf{R}^d} v(\xi) u_f(t, x, \xi) d\xi - \nabla_x \int_{\mathbf{R}^d} u_f(t, x, \xi) d\xi \\ &\quad - \partial_t A_0(t, x) - \nabla_x \phi_0(t, x), \\ B(t, x) &= \text{rot}_x \int_{\mathbf{R}^d} v(\xi) u_f(t, x, \xi) d\xi + \text{rot}_x A_0(t, x), \end{aligned}$$

where $\phi_0 \equiv \phi_0(t, x) \in \mathbf{R}$ and $A_0 \equiv A_0(t, x) \in \mathbf{R}^3$ are respectively a scalar and a vector potential satisfying

$$\square_{t,x} \phi_0 = 0, \quad \text{and } \square_{t,x} A_0 = 0,$$

together with appropriate initial conditions so that the formulas above for E and B match the prescribed initial conditions in the Cauchy problem for the Vlasov-Maxwell system.

With this representation for the electromagnetic field in the Vlasov-Maxwell system, the source term in the field equation is now f itself, a probability distribution in the single particle phase space $\mathbf{R}_x^3 \times \mathbf{R}_\xi^3$ whenever $f|_{t=0}$ is a probability distribution, since the integral

$$\iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(t, x, \xi) dx d\xi$$

is an invariant of the dynamics defined by the Vlasov-Maxwell equations.

A second difficulty is that the solution of the Cauchy problem for the wave equation defining u_f involves the space-time convolution with Kirchoff's kernel (the forward fundamental solution of the d'Alembert operator): see for instance [87]. This formula is equivalent to the retarded potential formula for solving the system of Maxwell's equations. At variance with the solution of the Poisson equation

$$-\Delta_x \phi_f(t, x) = \rho_f(t, x),$$

the formula giving the solution u_f of the wave equation above in terms of f is not local in the time variable t . Physically, this is due to the fact that the electromagnetic field is propagated at the speed of light $c > 0$ in the Vlasov-Maxwell system, while the electrostatic field in the Vlasov-Poisson system is propagated instantaneously — in other words, the speed of light is considered as infinite in the Vlasov-Poisson system. It remains to check that this difference in structure between the Vlasov-Poisson and the Vlasov-Maxwell systems does not rule out the possibility of an estimate *à la* Dobrushin.

This second difficulty was partially handled in an earlier work [31] for the simpler Vlasov-d'Alembert system

$$\begin{cases} (\partial_t + v(\xi) \cdot \nabla_x) f(t, x, \xi) - \nabla_x \phi_f(t, x) \cdot \nabla_\xi f(t, x, \xi) = 0, \\ \square_{t,x} \phi_f(t, x) = \rho_f(t, x), \end{cases}$$

where ρ_f is defined in terms of f as above, and $v(\xi) = \nabla_\xi \sqrt{1 + |\xi|^2}$ as in the Vlasov-Maxwell system.

A third difficulty — albeit a less essential one — is to choose a regularization procedure for the interaction potential that does not destroy the delicate invariance properties of the Vlasov-Maxwell system. Let $\chi_\epsilon \equiv \chi_\epsilon(x)$ be a regularizing sequence in \mathbf{R}^3 , chosen so that the function χ_ϵ is even for each $\epsilon > 0$. The Vlasov-Maxwell system is regularized by replacing the momentum distribution of electromagnetic potential u_f with the solution of the Cauchy problem

$$\begin{cases} \square_{t,x} u_f^\epsilon(t, x, \xi) = \chi_\epsilon \star_x \chi_\epsilon \star_x f(t, x, \xi), \\ u_f|_{t=0} = \partial_t u_f|_{t=0} = 0, \end{cases}$$

where \star_x designates the convolution product in the x variable. This regularization procedure, originally due to E. Horst, is such that both the conservation

of the total particle number and the conservation of some variant of the total energy are satisfied by the mollified system (see [83]).

The interested reader is referred to [43] for a complete discussion of the material presented in this section.

1.8 The mean field problem in quantum mechanics

1.8.1 The N -body problem in quantum mechanics

At variance with classical mechanics, the N -body problem in quantum mechanics is a PDE, and not a system of ODEs. The state at time t of a system of N identical point particles is defined by its N -body wave function

$$\Psi_N \equiv \Psi_N(t, x_1, \dots, x_N) \in \mathbf{C}, \quad x_1, \dots, x_N \in \mathbf{R}^d.$$

We assume that the reader is more or less familiar with the formalism of quantum mechanics, and we shall not attempt to recall more than a few basic facts. An excellent introduction to quantum mechanics can be found in [12].

The meaning of the wave function is such that $|\Psi(x_1, \dots, x_N)|^2$ is the (joint) probability density of having particle 1 at the position x_1 , particle 2 at the position x_2, \dots , and particle N at the position x_N at time t . This implies the

normalization¹⁶

$$\int_{(\mathbf{R}^d)^N} |\Psi_N(t, x_1, \dots, x_N)|^2 dx_1 \dots dx_N = 1,$$

that is satisfied for all $t \in \mathbf{R}$.

We assume that the interaction between a particle at position x and a particle at position y is given by a 2-body potential $V(x-y) \in \mathbf{R}$. Henceforth, we assume that V is even, so that the force exerted by the particle at position y on the particle at position x , i.e. $-\nabla V(x-y)$, exactly balances the force exerted by the particle at position x on the particle at position y , i.e. $-\nabla V(y-x)$. (Indeed, ∇V is odd since V is even.)

With these data, we can write the Schrödinger equation governing the N -body wave function for a system of N identical particles of mass m with 2-body interaction given by the potential V :

$$i\hbar\partial_t\Psi_N = -\frac{\hbar^2}{2m}\sum_{k=1}^N\Delta_{x_k}\Psi_N + \sum_{1\leq k<l\leq N}V(x_k-x_l)\Psi_N,$$

¹⁶This normalization condition is not satisfied by “generalized eigenfunctions” of an operator with continuous spectrum. Consider the two following examples, where $\mathfrak{H} = L^2(\mathbf{R})$.

(a) Let $\mathcal{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$ (the quantum harmonic oscillator), which has discrete spectrum only. The sequence of eigenvalues of \mathcal{H} is $n + \frac{1}{2}$ with $n \in \mathbf{N}$. Besides $\text{Ker}(H - (n + \frac{1}{2})I) = \mathbf{C}h_n$ for each $n \in \mathbf{N}$, with

$$h_n(x) := \frac{1}{\sqrt{2^n n! \pi^{1/4}}} e^{-x^2/2} H_n(x), \quad \text{where } H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

The function H_n is the n th Hermite polynomial, and the sequence $(h_n)_{n \geq 0}$ is a Hilbert basis of \mathfrak{H} . In particular one has the orthonormality condition

$$\int_{\mathbf{R}} h_n(x) h_m(x) dx = \delta_{mn}, \quad \text{for all } m, n \geq 0$$

where δ_{mn} is the Kronecker symbol (i.e. $\delta_{mn} = 0$ if $m \neq n$ and $\delta_{mn} = 1$ if $m = n$).

(b) Let $P = -i\frac{d}{dx}$ (the momentum operator), which has continuous spectrum only. The spectrum of P is the real line \mathbf{R} , and the generalized eigenfunctions of P are the functions $e_k : x \mapsto e_k(x) := e^{i2\pi kx}$. For each $k \in \mathbf{R}$, one has $Pe_k = 2\pi k e_k$ but $e_k \notin \mathfrak{H}$. However one has the “formula” analogous to the orthonormality condition in case (a):

$$\int_{\mathbf{R}} \overline{e_k(x)} e_l(x) dx = \delta_0(k-l)$$

where δ_0 is the Dirac mass at the origin. The integrand on the left hand side of the equality above is not an element of $L^1(\mathbf{R})$, and the integral is not a Lebesgue integral. The identity above should be understood as the Fourier inversion formula on the class $\mathcal{S}'(\mathbf{R})$ of tempered distributions on the real line \mathbf{R} .

In the case (a), if the system is in an eigenstate corresponding with the eigenvalue $n + \frac{1}{2}$ of the operator \mathcal{H} , its wave function is of the form $\psi = \omega h_n$ with $|\omega| = 1$, so that $\|\psi\|_{\mathfrak{H}} = 1$.

In the case (b), if the system is in an eigenstate corresponding with the element k of the spectrum of the operator P , it cannot be described by any wave function in \mathfrak{H} , but only by a generalized eigenfunction of P , that does not belong to \mathfrak{H} .

In the discussion below, we shall never consider quantum states described by generalized eigenfunctions as in (b), but only quantum states corresponding with normalized wave functions.

where \hbar is the reduced Planck constant.

The N -body Schrödinger equation above is a PDE which is the analogue in quantum mechanics of Newton's second law

$$\begin{cases} m\dot{x}_k = \xi_k, \\ \dot{\xi}_k = -\sum_{\substack{l=1 \\ l \neq k}}^N \nabla V(x_k - x_l), \end{cases} \quad k = 1, \dots, N$$

in classical mechanics.

The question of existence and uniqueness of a solution of the Schrödinger equation of N -particle quantum dynamics is settled by the following remarkable result. (Without loss of generality, we assume that $\hbar^2/m = 1$.)

Theorem 1.8.1 (Kato) *Assume that the space dimension is $d = 3$. If, for some $R > 0$,*

$$V|_{B(0,R)} \in L^2(B(0,R)) \quad \text{and} \quad V|_{\mathbf{R}^3 \setminus B(0,R)} \in L^\infty(\mathbf{R}^3 \setminus B(0,R)),$$

then, for all $N \geq 1$, the unbounded operator

$$\mathcal{H}_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} + \sum_{1 \leq k < l \leq N} V(x_k - x_l)$$

has a self-adjoint extension on $\mathfrak{H}_N := L^2((\mathbf{R}^3)^N)$ and generates a unitary group $e^{-it\mathcal{H}_N}$ on \mathfrak{H}_N .

See chapter V, §5.3 in [60] and [59] for a proof of this result.

This result is the analogue in quantum mechanics of the existence and uniqueness of the solution of the Cauchy problem for the motion equations in classical mechanics that follow from the Cauchy-Lipschitz theorem. Observe that applying the Cauchy-Lipschitz theorem to the system of ODEs resulting from Newton's second law applied to each particle would require V to have Lipschitz continuous first order derivatives. The assumptions on the regularity of the potential in Kato's result are obviously much less stringent — for instance, the Coulomb potential $V(z) = C/|z|$ obviously satisfies these assumptions. (That the Coulomb potential satisfies the assumptions in Kato's theorem is of course very satisfying since most computations in atomic physics involve the Coulomb interaction between the electrons and the nuclei in atoms and molecules.)

As in the case of classical mechanics, our goal is to study the behavior of $\Psi_N(t) = e^{-it\mathcal{H}_N} \Psi_N^{in}$ in the limit as $N \rightarrow \infty$, under appropriate scaling assumptions involving the interaction potential V and the particle number N .

First we need to define the analogue of the mean field scaling used in the case of classical mechanics. Our argument for choosing this scaling is based on considering the energy of the particle system.

In quantum mechanics, the energy of a system of N identical point particles of mass m with pairwise interaction described in terms of the real-valued 2-body potential V is

$$\begin{aligned} & \sum_{k=1}^N \int_{(\mathbf{R}^d)^N} \frac{\hbar^2}{2m} |\nabla_{x_k} \Psi_N(x_1, \dots, x_N)|^2 dx_1 \dots, dx_N \\ & + \sum_{1 \leq k < l \leq N} \int_{(\mathbf{R}^d)^N} V(x_k - x_l) |\Psi_N(x_1, \dots, x_N)|^2 dx_1 \dots, dx_N, \end{aligned}$$

where the first term is the kinetic energy, while the second term is the potential energy.

Pick a typical length scale L and energy scale E in the system of N particles under consideration. We introduce the dimensionless space variables and potential as follows:

$$\hat{x}_k = \frac{x_k}{L}, \quad \hat{V}(\hat{x}_k - \hat{x}_l) = \frac{1}{E} V(x_k - x_l).$$

Likewise, the N -particle wave function is scaled as

$$\hat{\Psi}_N(\hat{t}, \hat{x}_1, \dots, \hat{x}_N) = L^{dN/2} \Psi_N(t, x_1, \dots, x_N),$$

where T is a time scale to be defined later, and where

$$\hat{t} = \frac{t}{T}$$

is the dimensionless time variable.

Observe that

$$\int |\hat{\Psi}_N(\hat{t}, \hat{x}_1, \dots, \hat{x}_N)|^2 d\hat{x}_1 \dots d\hat{x}_N = \int |\Psi_N(t, x_1, \dots, x_N)|^2 dx_1 \dots dx_N = 1$$

with this scaling.

With these dimensionless quantities, the kinetic and potential energies become respectively

$$\begin{aligned} \text{Kinetic energy} &= \sum_{k=1}^N \int_{(\mathbf{R}^d)^N} \frac{\hbar^2}{2mL^2} |\nabla_{\hat{x}_k} \hat{\Psi}_N|^2 d\hat{x}_1 \dots d\hat{x}_N, \\ \text{Potential energy} &= \sum_{1 \leq k < l \leq N} \int_{(\mathbf{R}^d)^N} E \hat{V}(\hat{x}_k - \hat{x}_l) |\hat{\Psi}_N|^2 d\hat{x}_1 \dots d\hat{x}_N. \end{aligned}$$

Observe that there are N terms in the kinetic energy, while the potential energy involves $\frac{1}{2}N(N-1)$ terms. Therefore, we scale the system so that the kinetic energy and the potential energy are of same order of magnitude, by choosing E and L so that

$$\frac{\hbar^2}{mL^2} = NE.$$

Thus

$$\begin{aligned} & -\frac{\hbar^2}{2m} \sum_{k=1}^N \Delta_{x_k} \Psi_N + \sum_{1 \leq k < l \leq N} V(x_k - x_l) \Psi_N \\ & = L^{-dN/2} \frac{\hbar^2}{mL^2} \left(-\frac{1}{2} \sum_{k=1}^N \Delta_{\hat{x}_k} \hat{\Psi}_N + \frac{1}{N} \sum_{1 \leq k < l \leq N} \hat{V}(\hat{x}_k - \hat{x}_l) \hat{\Psi}_N \right). \end{aligned}$$

At this point, we set

$$\hat{H}_N \hat{\Psi}_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{\hat{x}_k} \hat{\Psi}_N + \frac{1}{N} \sum_{1 \leq k < l \leq N} \hat{V}(\hat{x}_k - \hat{x}_l) \hat{\Psi}_N,$$

and define the time scale T as follows:

$$T = \frac{mL^2}{\hbar}.$$

With the rescaled time variable $\hat{t} = t/T$, the N -body Schrödinger equation in mean-field scaling becomes

$$i\partial_{\hat{t}} \hat{\Psi}_N = -\frac{1}{2} \sum_{k=1}^N \Delta_{\hat{x}_k} \hat{\Psi}_N + \frac{1}{N} \sum_{1 \leq k < l \leq N} \hat{V}(\hat{x}_k - \hat{x}_l) \hat{\Psi}_N.$$

Henceforth we drop all hats on variables, and consider as our starting point the scaled equation

$$i\partial_t \Psi_N = -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} \Psi_N + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l) \Psi_N.$$

A formal computation based on the fact that V is real-valued shows that

$$\frac{d}{dt} \int_{(\mathbf{R}^d)^N} |\Psi_N(t, x_1, \dots, x_N)|^2 dx_1 \dots dx_N = 0,$$

so that

$$\int_{(\mathbf{R}^d)^N} |\Psi_N(t, x_1, \dots, x_N)|^2 dx_1 \dots dx_N = 1.$$

for all $t \in \mathbf{R}$.

The rigorous argument is based on Kato's theorem (Theorem 1.8.1) stated above in space dimension $d = 3$: with the notation

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l)$$

the one-parameter group e^{-itH_N} is unitary on $\mathfrak{H}_N = L^2((\mathbf{R}^3)^N)$, so that

$$\int_{(\mathbf{R}^3)^N} |\Psi_N(t, x_1, \dots, x_N)|^2 dx_1 \dots dx_N = \|e^{-itH_N} \Psi_N^{in}\|_{\mathfrak{H}_N}^2 = 1$$

for all $t \in \mathbf{R}$.

1.8.2 The target mean-field equation

The target quantum mean-field equation is the quantum analogue of the Vlasov-Poisson equation.

Its unknown is the single-particle wave function $\psi \equiv \psi(t, x) \in \mathbf{C}$, with $x \in \mathbf{R}^d$

The basic idea in the mean field approximation is the same as in the classical case. Since the probability of finding a particle in an infinitesimal volume element dx at time t is $|\psi(t, x)|^2 dx$, one expects that the action on the k -th particle located at x_k is defined in terms of the potential V by the formula

$$\frac{1}{N} \sum_{\substack{l=1 \\ k \neq l}}^N V(x_k - x_l) \sim \int_{\mathbf{R}^d} V(x_k - z) |\psi(t, z)|^2 dz.$$

This suggests that the target mean-field equation for single-particle wave function obtained as the limit of the N -body Schrödinger equation is

$$i\partial_t \psi(t, x) = -\frac{1}{2} \Delta_x \psi(t, x) + \psi(t, x) \int_{\mathbf{R}^d} V(x - y) |\psi(t, y)|^2 dy.$$

This equation is known as the Hartree equation — and also sometimes referred to as the Schrödinger-Poisson equation when $V(z)$ is the Coulomb potential in space dimension 3. Indeed, if

$$V(z) = \frac{1}{4\pi|z|}, \quad z \in \mathbf{R}^3 \setminus \{0\},$$

the equation above is equivalent to the system

$$\begin{cases} i\partial_t \psi(t, x) = -\frac{1}{2} \Delta_x \psi(t, x) + U(t, x) \psi(t, x), \\ -\Delta_x U(t, x) = |\psi(t, x)|^2. \end{cases}$$

This system is the quantum analogue of the Vlasov-Poisson system.

The Hartree equation has been studied extensively by various authors: see [18, 39]. The following statement is a consequence of Theorem 3.1 in [39].

Proposition 1.8.2 *Assume that V is a real-valued, even element of $L^\infty(\mathbf{R}^d)$. For each $\psi^{in} \in H^k(\mathbf{R}^d)$, there exists a unique mild solution¹⁷ of the Cauchy*

¹⁷A mild solution of the Cauchy problem

$$\begin{cases} \dot{u}(t) = Au(t) + F[u(t)], \\ u|_{t=0} = u^{in}, \end{cases}$$

where A generates a strongly continuous contraction semigroup on a Banach space X and $F : X \rightarrow X$ is a continuous map, is an X -valued continuous function $I \ni t \mapsto u(t) \in X$ defined on $I = [0, \tau]$ with $\tau \in [0, +\infty]$ that is a solution of the integral equation

$$u(t) = e^{tA} u^{in} + \int_0^t e^{(t-s)A} F[u(s)] ds$$

for each $t \in I$.

problem for Hartree's equation

$$\begin{cases} i\partial_t\psi(t, x) = -\frac{1}{2}\Delta_x\psi(t, x) + (V \star_x |\psi|^2)\psi(t, x), & x \in \mathbf{R}^d \\ \psi|_{t=0} = \psi^{in} \end{cases}$$

such that $\psi \in C_b(\mathbf{R}; H^1(\mathbf{R}^d)) \cap C(\mathbf{R}; H^k(\mathbf{R}^2))$. Besides, this solution satisfies the conservation laws of mass and energy, viz.

$$\|\psi(t, \cdot)\|_{L^2(\mathbf{R}^d)} = \text{Const.}$$

and

$$\frac{1}{2}\|\nabla_x\psi(t, \cdot)\|_{L^2(\mathbf{R}^d)}^2 + \frac{1}{2}\iint_{\mathbf{R}^d \times \mathbf{R}^d} V(x-y)|\psi(t, x)|^2|\psi(t, y)|^2 dx dy = \text{Const.}$$

for all $t \in \mathbf{R}$.

1.8.3 The formalism of density matrices

Before studying the N -particle Schrödinger equation in the large N limit, we need another formulation of the quantum N -body problem.

Henceforth we denote by $\langle \cdot | \cdot \rangle$ (or by $\langle \cdot | \cdot \rangle_{\mathfrak{H}_N}$ to avoid ambiguity if needed) the inner product of the Hilbert space $\mathfrak{H}_N := L^2((\mathbf{R}^d)^N)$, and by $|\cdot|$ or $|\cdot|_{\mathfrak{H}_N}$ the associated norm, defined by the formula

$$|\Phi|_{\mathfrak{H}_N} := \langle \Phi | \Phi \rangle_{\mathfrak{H}_N}^{1/2}.$$

To the N -particle wave function $\Psi_N \equiv \Psi_N(x_1, \dots, x_N)$ that is an element of $\mathfrak{H}_N := L^2((\mathbf{R}^d)^N)$, one associates the bounded linear operator D_N on \mathfrak{H} defined as follows:

$$D_N := \text{orthogonal projection on } \mathbf{C}\Psi_N \text{ in } \mathfrak{H}_N,$$

i.e.

$$D_N\Phi_N = \Psi_N \int_{(\mathbf{R}^d)^N} \overline{\Psi_N}\Phi_N(x_1, \dots, x_N) dx_1 \dots dx_N = \langle \Psi_N | \Phi_N \rangle \Psi_N.$$

This linear operator is called the “density matrix” of the N -particle system.

Whenever convenient, we use the notation common in the physics literature

$$D_N := |\Psi_N\rangle\langle\Psi_N|$$

which is the equivalent of

$$D_N := \Psi_N \otimes L_{\Psi_N}, \quad \text{with } L_{\Psi_N} := \langle \Psi_N | \cdot \rangle \in \mathfrak{H}_N^*.$$

Obviously, D_N is an integral operator, whose integral kernel is

$$D_N(x_1, \dots, x_N, y_1, \dots, y_N) = \Psi_N(x_1, \dots, x_N) \overline{\Psi_N(y_1, \dots, y_N)}.$$

In the sequel, we shall sometimes abuse the notation and use the same letter to designate an integral operator and its integral kernel.

Being an orthogonal projection in \mathfrak{H}_N , the operator D_N is self-adjoint and nonnegative:

$$D_N = D_N^* = D_N^2 \geq 0.$$

This property is the quantum analogue of the positivity of the N -particle distribution function in classical statistical mechanics.

The density matrix D_N for a system of identical, indistinguishable particles satisfies the following symmetry: for all $\sigma \in \mathfrak{S}_N$, one has

$$S_\sigma D_N = D_N,$$

where S_σ is the transformation on integral kernels defined by the formula

$$S_\sigma D_N(x_1, \dots, x_N, y_1, \dots, y_N) := D_N(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(N)}, y_{\sigma^{-1}(1)}, \dots, y_{\sigma^{-1}(N)}).$$

This assumption is not to be confused with the condition

$$U_\sigma \Psi_N = \Psi_N,$$

where U_σ is the unitary operator defined on \mathfrak{H}_N by the formula

$$U_\sigma \Psi_N(x_1, \dots, x_N) := \Psi_N(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(N)}).$$

This assumption is an assumption on the *statistics* of particles, i.e. on whether the particles under consideration follow the Bose-Einstein or the Fermi-Dirac statistics. Particles following the Bose-Einstein statistics are called bosons, and the wave function of any system of N identical bosons satisfies the condition

$$U_\sigma \Psi_N = \Psi_N.$$

Particles following the Fermi-Dirac statistics are called fermions, and the wave function of any system of N identical fermions satisfies the condition

$$U_\sigma \Psi_N = (-1)^{\text{sign}(\sigma)} \Psi_N.$$

Exercise: Express $U_{\sigma\sigma'}$ and U_σ^* in terms of U_σ and $U_{\sigma'}$ for all $\sigma, \sigma' \in \mathfrak{S}_N$, and check that U_σ is a unitary operator on \mathfrak{H}_N . Express the transformation S_σ in terms of U_σ for all $\sigma \in \mathfrak{S}_N$.

In fact, whenever

$$U_\sigma \Psi_N = \omega(\sigma) \Psi_N \quad \text{with } \omega(\sigma) \in \mathbf{C} \text{ and } |\omega(\sigma)| = 1$$

one has

$$S_\sigma D_N = D_N.$$

In particular, the density matrix of a system of N identical bosons ($\omega(\sigma) = 1$) or N identical fermions ($\omega(\sigma) = (-1)^{\text{sign}(\sigma)}$) satisfies

$$S_\sigma D_N = D_N.$$

Exercise: Assume that, for some $\Psi_N \in \mathfrak{H}_N$ such that $|\Psi_N| = 1$ and for all $\sigma \in \mathfrak{S}_N$, one has

$$U_\sigma \Psi_N = \omega(\sigma) \Psi_N \quad \text{with } \omega(\sigma) \in \mathbf{C} \text{ and } |\omega(\sigma)| = 1.$$

Compute $\omega(\sigma\sigma')$ in terms of $\omega(\sigma)$ and $\omega(\sigma')$ for all $\sigma, \sigma' \in \mathfrak{S}_N$. Prove that $\omega(\sigma) = \pm 1$ for all $\sigma \in \mathfrak{S}_N$.

Assuming that the time-dependent wave function $\Psi_N(t, \cdot)$ of a system of N identical particles satisfies the N -body Schrödinger equation with initial data Ψ_N^{in} , i.e.

$$\begin{cases} i\partial_t \Psi_N = H_N \Psi_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} \Psi_N + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l) \Psi_N, \\ \Psi_N|_{t=0} = \Psi_N^{in}, \end{cases}$$

our next task is to find the equation satisfied by $D_N := |\Psi_N\rangle\langle\Psi_N|$.

Since e^{-itH_N} is a unitary operator on \mathfrak{H}_N provided that the interaction potential V satisfies the assumptions of Kato's theorem above, one has

$$\begin{aligned} D_N(t) &= |e^{-itH_N} \Psi_N^{in}\rangle\langle e^{-itH_N} \Psi_N^{in}| \\ &= e^{-itH_N} D_N^{in} (e^{-itH_N})^* = e^{-itH_N} D_N^{in} e^{itH_N}, \end{aligned}$$

where

$$D_N^{in} := |\Psi_N^{in}\rangle\langle\Psi_N^{in}|.$$

It is instructive to do the analogous computation in finite dimension (i.e. with matrices). Assume that $A, B \in M_n(\mathbf{C})$, and set

$$M(t) := e^{tA} B e^{-tA}.$$

Then the function $\mathbf{R} \ni t \mapsto M(t) \in M_n(\mathbf{C})$ is obviously of class C^∞ (and even real analytic) and satisfies¹⁸

$$\begin{aligned} \frac{d}{dt} M(t) &= \frac{d}{dt} (e^{tA} B e^{-tA}) = A e^{tA} B e^{-tA} - e^{tA} B A e^{-tA} \\ &= A e^{tA} B e^{-tA} - e^{tA} B e^{-tA} A \\ &= A M(t) - M(t) A = [A, M(t)]. \end{aligned}$$

since A commutes with e^{-tA} .

In view of this elementary computation, we leave it to the reader to verify the following statement.

¹⁸For linear operators A, B on the Hilbert space \mathfrak{H} , we designate by $[A, B]$ their commutator $[A, B] := AB - BA$. There is obviously a difficulty with the domain of $[A, B]$ viewed as an unbounded operator on \mathfrak{H} if A and B are unbounded operators on \mathfrak{H} . This difficulty will be deliberately left aside, as we shall mostly consider $B \mapsto [A, B]$ as an unbounded operator on $\mathcal{L}(\mathfrak{H})$, which is different matter.

Proposition 1.8.3 *Assume that the potential V satisfies the assumptions in Kato's theorem (Theorem 1.8.1), and let $\Psi_N^{in} \in \mathfrak{H}_N = L^2((\mathbf{R}^d)^N)$.*

Let $\Psi_N \equiv \Psi_N(t, x_1, \dots, x_N)$ be the solution of the N -particle Schrödinger equation

$$\begin{cases} i\partial_t \Psi_N = -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} \Psi_N + \sum_{1 \leq k < l \leq N} V(x_k - x_l) \Psi_N, & x_1, \dots, x_N \in \mathbf{R}^d, t \in \mathbf{R}, \\ \Psi_N|_{t=0} = \Psi_N^{in}, \end{cases}$$

i.e.

$$\Psi_N(t, \cdot) = e^{-itH_N} \Psi_N^{in},$$

with scaled Hamiltonian

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_k + \frac{1}{N} \sum_{1 \leq k < l \leq N} V_{kl},$$

where Δ_k designates the Laplacian in the k th variable, while V_{kl} is the operator defined as the multiplication by $V(x_k - x_l)$.

Then the density matrix

$$D_N(t) := |\Psi_N(t, \cdot)\rangle \langle \Psi_N(t, \cdot)| = e^{-itH_N} D_N(0) e^{itH_N}$$

satisfies the von Neumann equation

$$i\dot{D}_N(t) = [H_N, D_N(t)] = -\frac{1}{2} \sum_{k=1}^N [\Delta_k, D_N(t)] + \frac{1}{N} \sum_{1 \leq k < l \leq N} [V_{kl}, D_N].$$

In terms of integral kernels

$$\begin{aligned} & i\partial_t D_N(t, x_1, \dots, x_N, y_1, \dots, y_N) \\ &= -\frac{1}{2} \sum_{k=1}^N (\Delta_{x_k} - \Delta_{y_k}) D_N(t, x_1, \dots, x_N, y_1, \dots, y_N) \\ &+ \frac{1}{N} \sum_{1 \leq k < l \leq N} (V(x_k - x_l) - V(y_k - y_l)) D_N(t, x_1, \dots, x_N, y_1, \dots, y_N). \end{aligned}$$

The fundamental properties of the density matrix are propagated under the flow associated to the von Neumann equation.

Proposition 1.8.4 *Assume that the potential V satisfies the assumptions in Kato's theorem, and let*

$$D_N^{in} = (D_N^{in})^* = (D_N^{in})^2 \geq 0.$$

Then for each $t \in \mathbf{R}$, one has

$$D_N(t) := e^{-itH_N} D_N^{in} e^{itH_N} = D_N(t)^* = D_N(t)^2 \geq 0,$$

with scaled Hamiltonian

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_k + \frac{1}{N} \sum_{1 \leq k < l \leq N} V_{kl}$$

where Δ_k designates the Laplacian in the k th variable, while V_{kl} is the operator defined as the multiplication by $V(x_k - x_l)$.

Likewise, if particles are indistinguishable initially, i.e. if

$$S_\sigma D_N^{in} = D_N^{in},$$

then

$$S_\sigma D_N(t) = D_N(t)$$

for all $t \in \mathbf{R}$.

Proof. First

$$D_N(t)^* = (e^{-itH_N} D_N^{in} e^{itH_N})^* = e^{-itH_N} (D_N^{in})^* e^{itH_N}$$

since H_N is self adjoint, so that $(e^{itH_N})^* = e^{-itH_N}$. Then

$$\begin{aligned} D_N(t)^2 &= (e^{-itH_N} D_N^{in} e^{itH_N})^2 \\ &= e^{-itH_N} (D_N^{in})^2 e^{itH_N} = (e^{-itH_N} D_N^{in} e^{itH_N})^2 = D_N(t)^2. \end{aligned}$$

That $S_\sigma D_N(t) = D_N(t)$ for all $t \in \mathbf{R}$ if $S_\sigma D_N^{in} = D_N^{in}$ is a straightforward consequence of the following lemma.

Lemma 1.8.5 *Let U_σ be the unitary operator defined on \mathfrak{H}_N for each $\sigma \in \mathfrak{S}_N$ by*

$$U_\sigma \Psi_N(x_1, \dots, x_N) := \Psi_N(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(N)}).$$

Then

$$U_\sigma e^{itH_N} = e^{itH_N} U_\sigma$$

for each $t \in \mathbf{R}$ and each $\sigma \in \mathfrak{S}_N$.

Thus, for each $t \in \mathbf{R}$ and each $\sigma \in \mathfrak{S}_N$, one has

$$\begin{aligned} S_\sigma D_N(t) &= U_\sigma D_N(t) U_\sigma^* = U_\sigma e^{-itH_N} D_N^{in} e^{itH_N} U_\sigma^* \\ &= e^{-itH_N} U_\sigma D_N^{in} U_\sigma^* e^{itH_N} = e^{-itH_N} D_N^{in} e^{itH_N} = D_N(t), \end{aligned}$$

provided that

$$S_\sigma D_N^{in} = U_\sigma D_N^{in} U_\sigma^* = D_N^{in}.$$

■
Proof of Lemma 1.8.5. If $\Phi \in C_c^\infty((\mathbf{R}^d)^N)$, one has

$$\Delta_k U_\sigma \Phi = U_\sigma \Delta_{\sigma(k)} \Phi$$

and

$$V_{kl}U_\sigma\Phi = U_\sigma V_{\sigma(k),\sigma(l)}\Phi,$$

so that

$$H_N U_\sigma \Phi = U_\sigma H_N \Phi.$$

Therefore

$$U_\sigma e^{itH_N} = e^{itH_N} U_\sigma$$

for each $t \in \mathbf{R}$ and each $\sigma \in \mathfrak{S}_N$. ■

1.9 Elements of operator theory

We recall that \mathfrak{H} designates a complex, separable Hilbert space \mathfrak{H} , with inner product denoted by $\langle \cdot | \cdot \rangle$ and norm denoted by $|\cdot|$. (To avoid ambiguity, we also use the notation $\langle \cdot | \cdot \rangle_{\mathfrak{H}}$ and $|\cdot|_{\mathfrak{H}}$ whenever needed.) We always assume that the inner product is antilinear in its first argument and linear in its second argument. The set of Hilbert basis of \mathfrak{H} — i.e. the set of orthonormal and total families in \mathfrak{H} — is denoted by $HB(\mathfrak{H})$.

The set of bounded operators on \mathfrak{H} is denoted by $\mathcal{L}(\mathfrak{H})$, with operator norm

$$\|A\| = \sup_{|x|=1} |Ax|.$$

We recall that $\mathcal{L}(\mathfrak{H})$ endowed with the operator norm $\|\cdot\|$ is a Banach algebra — and even a C^* -algebra, since

$$\|A^*A\| = \|A\|^2 \quad \text{for each } A \in \mathcal{L}(\mathfrak{H}).$$

A bounded operator A on \mathfrak{H} is said to be compact if $A(\overline{B(0,1)})$ is relatively compact in \mathfrak{H} . The set of compact operators on \mathfrak{H} is denoted by $\mathcal{K}(\mathfrak{H})$; one easily checks that $\mathcal{K}(\mathfrak{H})$ is a closed (for the operator norm) two-sided ideal in $\mathcal{L}(\mathfrak{H})$.

We recall the following fundamental facts about compact operators:

- if A is a compact operator on \mathfrak{H} , its adjoint A^* is also a compact operator;
- $\mathcal{K}(\mathfrak{H})$ is the operator-norm closure of the set of finite rank operators on \mathfrak{H} .

Next we introduce the trace norm: for each $A \in \mathcal{L}(\mathfrak{H})$

$$\|A\|_1 := \sup_{e,f \in HB(\mathfrak{H})} \sum_{k \geq 0} |\langle Ae_k | f_k \rangle| \in [0, \infty].$$

A bounded operator A on \mathfrak{H} is said to be a trace-class operator if and only if it has finite trace norm. The set of trace-class operators on \mathfrak{H} is denoted by $\mathcal{L}^1(\mathfrak{H})$; in other words,

$$\mathcal{L}^1(\mathfrak{H}) := \{A \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } \|A\|_1 < \infty\}.$$

One easily checks that $\mathcal{L}^1(\mathfrak{H})$ is a two-sided ideal in $\mathcal{L}(\mathfrak{H})$, that $A \mapsto \|A\|_1$ defines a norm on $\mathcal{L}^1(\mathfrak{H})$, and that $\mathcal{L}^1(\mathfrak{H})$ equipped with the trace norm $\|\cdot\|_1$ is a separable Banach space. Besides, the map

$$\mathcal{L}^1(\mathfrak{H}) \ni A \mapsto A^* \in \mathcal{L}^1(\mathfrak{H})$$

is an isometry for the trace norm. The following properties can be checked easily:

- (a) $\mathcal{L}^1(\mathfrak{H}) \subset \mathcal{K}(\mathfrak{H}) \subset \mathcal{L}(\mathfrak{H})$ with $\|A\| \leq \|A\|_1$ for all $A \in \mathcal{L}^1(\mathfrak{H})$, and
- (b) for all $A \in \mathcal{L}^1(\mathfrak{H})$ and $B \in \mathcal{L}(\mathfrak{H})$

$$\|AB\|_1 \text{ and } \|BA\|_1 \leq \|A\|_1 \|B\|, \quad A \in \mathcal{L}^1(\mathfrak{H}) \text{ and } B \in \mathcal{L}(\mathfrak{H}).$$

There is a natural notion of trace for operators in infinite dimensional spaces, that can be defined for each trace-class operator. For each $A \in \mathcal{L}^1(\mathfrak{H})$,

$$\text{trace}(A) := \sum_{k \geq 0} \langle Ae_k | e_k \rangle,$$

for each $(e_k)_{k \geq 0} \in HB(\mathfrak{H})$. We leave it to the reader to check that the expression on the right hand side of the previous equality is independent of the choice of $(e_k)_{k \geq 0} \in HB(\mathfrak{H})$.

Perhaps the most important property of the trace is the following identity: for all $A \in \mathcal{L}^1(\mathfrak{H})$ and $B \in \mathcal{L}(\mathfrak{H})$, the operators AB and BA are both trace-class operators on \mathfrak{H} , and one has

$$\text{trace}(AB) = \text{trace}(BA).$$

Let us recall the notion of polar decomposition of an operator. For each $A \in \mathcal{L}(\mathfrak{H})$, there exists $|A|, U \in \mathcal{L}(\mathfrak{H})$ such that

$$UU^* = U^*U = I, \quad |A| = |A|^* \geq 0 \text{ and } A = |A|U.$$

In this decomposition

$$|A| = \sqrt{AA^*}.$$

Then

$$A \in \mathcal{L}^1(\mathfrak{H}) \Leftrightarrow |A| \in \mathcal{L}^1(\mathfrak{H}) \text{ and } \|A\|_1 = \text{trace}(|A|).$$

The polar decomposition is the analogue of polar coordinates in operator theory: $|A|$ is the analogue of $|z|$ for $z \in \mathbf{C}$, while U is the analogue of $z/|z|$ for $z \in \mathbf{C}^*$.

Exercise: Let $A \in \mathcal{L}^1(\mathfrak{H})$. Prove that $\text{trace}(\sqrt{AA^*}) = \text{trace}(\sqrt{A^*A}) = \|A\|_1$.

The two following facts are important:

- $\mathcal{L}^1(\mathfrak{H})$ is the (topological) dual of $\mathcal{K}(\mathfrak{H})$, with duality defined by the trace as follows

$$\mathcal{L}^1(\mathfrak{H}) \times \mathcal{K}(\mathfrak{H}) \ni (A, K) \mapsto \text{trace}(AK) \in \mathbf{C};$$

- $\mathcal{L}(\mathfrak{H})$ is the (topological) dual of $\mathcal{L}^1(\mathfrak{H})$, with duality defined by the trace as follows

$$\mathcal{L}(\mathfrak{H}) \times \mathcal{L}^1(\mathfrak{H}) \ni (B, A) \mapsto \text{trace}(BA) \in \mathbf{C}.$$

Another important class of bounded operators on \mathfrak{H} is the class of Hilbert-Schmidt operators, denoted by $\mathcal{L}^2(\mathfrak{H})$, defined as follows:

$$A \in \mathcal{L}^2(\mathfrak{H}) \Leftrightarrow A^*A \in \mathcal{L}^1(\mathfrak{H}) \Leftrightarrow AA^* \in \mathcal{L}^1(\mathfrak{H}).$$

The class $\mathcal{L}^2(\mathfrak{H})$ is a closed two-sided ideal in $\mathcal{L}(\mathfrak{H})$. It is a Banach space for the Hilbert-Schmidt norm defined as follows:

$$\|A\|_2 := \|A^*A\|_1^{1/2} = \|AA^*\|_1^{1/2}.$$

One easily checks that

$$\mathcal{L}^1(\mathfrak{H}) \subset \mathcal{L}^2(\mathfrak{H}) \subset \mathcal{K}(\mathfrak{H}).$$

An important particular case is $\mathfrak{H} = L^2(\mathcal{X})$, where \mathcal{X} is a measurable subset of \mathbf{R}^d , equipped with the Lebesgue measure. In that case, a bounded operator A on $L^2(\mathcal{X})$ is a Hilbert-Schmidt operator if and only if it is an integral operator of the form

$$Af(x) = \int_{\mathcal{X}} a(x, y)f(y)dy \quad \text{for all } f \in L^2(\mathcal{X}),$$

with

$$a \in L^2(\mathcal{X} \times \mathcal{X}).$$

In that case

$$\|A\|_2 = \left(\iint_{\mathcal{X} \times \mathcal{X}} |a(x, y)|^2 dx dy \right)^{1/2} = \|a\|_{L^2(\mathcal{X} \times \mathcal{X})}.$$

References for the material presented so far in this section are chapter VI of [22] and chapter XIX, section 1 of [54].

According to the discussion above, each $A \in \mathcal{L}^1(L^2(\mathbf{R}^n))$ is an integral operator with integral kernel $a \in L^2(\mathbf{R}^n \times \mathbf{R}^n)$. The integral kernel of a trace-class operator on $L^2(\mathbf{R}^n)$ has an additional interesting property, recalled below.

Lemma 1.9.1 *If $A \in \mathcal{L}^1(L^2(\mathbf{R}^n))$, its integral kernel $a \equiv a(x, y)$ is such that the map¹⁹*

$$z \mapsto a(x, x + z) \text{ belongs to } C_b(\mathbf{R}_z^n; L^1(\mathbf{R}_x^n)).$$

Exercise. Here is an outline of the proof of Lemma 1.9.1. Let $A \in \mathcal{L}^1(\mathfrak{H})$ with $\mathfrak{H} := L^2(\mathbf{R}^n)$.

1) Prove that the integral kernel a of A can be represented as

$$a(x, y) = \sum_{n \geq 1} \lambda_n e_n(x) \overline{f_n(y)}$$

¹⁹For each topological space X and each vector space E on \mathbf{R} equipped with the norm $\|\cdot\|_E$, we designate by $C(X, E)$ the set of continuous maps from X to E , and we denote

$$C_b(X, E) := \{f \in C(X, E) \text{ s.t. } \sup_{x \in X} \|f(x)\|_E < \infty\}.$$

In other words, $C_b(X, E)$ is the set of bounded continuous functions defined on X with values in E .

with $e_n, f_n \in \mathfrak{H}$ such that $|e_n|_{\mathfrak{H}} = |f_n|_{\mathfrak{H}} = 1$ and with

$$\sum_{n \geq 1} |\lambda_n| < \infty.$$

2) Prove that, for each $\phi \in \mathfrak{H}$, one has

$$\int_{\mathbf{R}^n} |\phi(x+h) - \phi(x)|^2 dx \rightarrow 0$$

as $|h| \rightarrow 0$.

3) Prove that

$$\int_{\mathbf{R}^n} |a(x, x+z) - a(x, x+z')| dx \rightarrow 0 \quad \text{as } |z - z'| \rightarrow 0,$$

and conclude.

In particular, if $A \in \mathcal{L}^1(L^2(\mathbf{R}^n))$, then its integral kernel $a \equiv a(x, y)$ is such that the map $x \mapsto a(x, x)$ is well-defined as an element of $L^1(\mathbf{R}^n)$, and

$$\text{trace}(A) = \int_{\mathbf{R}^n} a(x, x) dx.$$

The converse of this last statement is obviously false: if $A \in \mathcal{L}(\mathfrak{H})$ is an integral operator with integral kernel $a(x, y)$, that the map $x \mapsto a(x, x)$ belongs to $L^1(\mathbf{R}^n)$ does not imply in general that $A \in \mathcal{L}^1(L^2(\mathbf{R}^n))$.

Exercise: Construct an example of operator that belongs to $\mathcal{L}^2(L^2(\mathbf{R}^n))$ but not to $\mathcal{L}^1(L^2(\mathbf{R}^n))$.

In the sequel, we shall need the notion of “partial trace” for a trace-class operator defined on the tensor product of two Hilbert spaces. Let \mathfrak{H}_1 and \mathfrak{H}_2 be two complex, separable Hilbert spaces.

Definition 1.9.2 For each $A \in \mathcal{L}^1(\mathfrak{H}_1 \otimes \mathfrak{H}_2)$, the first partial trace of A , denoted

$$A_{:1} = \text{trace}_1(A) \in \mathcal{L}^1(\mathfrak{H}_1),$$

is the unique element of $\mathcal{L}^1(\mathfrak{H}_1)$ such that

$$\text{trace}_{\mathfrak{H}_1}(A_{:1}B) = \text{trace}_{\mathfrak{H}_1 \otimes \mathfrak{H}_2}(A(B \otimes I_{\mathfrak{H}_2}))$$

holds for each $B \in \mathcal{L}(\mathfrak{H}_1)$, where $I_{\mathfrak{H}_2}$ is the identity on \mathfrak{H}_2 .

The second partial trace of A is the element of $\mathcal{L}^1(\mathfrak{H}_2)$ defined analogously.

Let A be an integral operator with integral kernel $a \equiv a(x_1, x_2, y_1, y_2)$ in the case where $\mathfrak{H}_j = L^2(\mathbf{R}^{n_j})$ for $j = 1, 2$. In that case, $\mathfrak{H}_1 \otimes \mathfrak{H}_2 = L^2(\mathbf{R}^{n_1+n_2})$, and one easily checks that $A_{:1}$ is the integral operator with integral kernel

$$a_{:1}(x_1, y_1) = \int_{\mathbf{R}^{n_2}} a(x_1, z, y_1, z) dz$$

on $\mathfrak{H}_1 = L^2(\mathbf{R}^{n_1})$.

There is an easy generalization of the notion of partial trace to the case of trace-class operators defined on N -fold tensor products of separable Hilbert spaces. Given N complex, separable Hilbert spaces $\mathfrak{H}_1, \dots, \mathfrak{H}_N$ and a trace-class operator $A \in \mathcal{L}^1(\mathfrak{H}_1 \otimes \dots \otimes \mathfrak{H}_N)$, for each $1 \leq k \leq N$, we define

$$A_{:,k} = \text{trace}_k(A)$$

to be the first partial trace $\text{trace}_1(A)$ in the decomposition

$$\mathfrak{H}_1 \otimes \dots \otimes \mathfrak{H}_N \simeq (\mathfrak{H}_1 \otimes \dots \otimes \mathfrak{H}_k) \otimes (\mathfrak{H}_{k+1} \otimes \dots \otimes \mathfrak{H}_N).$$

If one views $A \in \mathcal{L}^1(\mathfrak{H}_1 \otimes \dots \otimes \mathfrak{H}_N)$ such that $A = A^* \geq 0$ and $\text{trace}(A) = 1$ as the operator analogue of an N -particle probability measure, then $A_{:,k}$ is the analogue of its (first) k -particle marginal considered above in our description of the BBGKY hierarchy for the mean field limit in classical statistical mechanics.

More details on partial traces can be found in [7, 8].

Remark: All the quantum states of the N -particle system considered so far are defined by an N -particle wave function $\Psi_N(t, \cdot)$ that belongs to $L^2((\mathbf{R}^d)^N)$ and satisfies the normalization condition $\|\Psi_N(t, \cdot)\|_{L^2((\mathbf{R}^d)^N)} = 1$ for each $t \in \mathbf{R}$. An N -particle density matrix $D_N(t)$ is associated to this N -particle wave function by the formula $D_N(t) := |\Psi_N(t, \cdot)\rangle\langle\Psi_N(t, \cdot)|$, and we have seen that this N -particle density matrix $D_N(t)$ satisfies

$$D_N(t) = D_N(t)^* = D_N(t)^2, \quad \text{and } \text{trace}(D_N(t)) = 1.$$

Conversely, if $D_N(t) \in \mathcal{L}^1(L^2((\mathbf{R}^d)^N))$ satisfies the conditions above, it is an orthogonal projection with rank 1, and therefore there exists $\Phi_N(t, \cdot) \in L^2((\mathbf{R}^d)^N)$ such that $\|\Phi_N(t, \cdot)\|_{L^2((\mathbf{R}^d)^N)} = 1$ and $D_N(t) := |\Phi_N(t, \cdot)\rangle\langle\Phi_N(t, \cdot)|$. Besides, the function $\Phi(t, \cdot)$ is defined uniquely up to multiplication by a complex number of modulus 1.

Such quantum states are referred to as “pure states”.

However, there also exist more general quantum states, that are described by an N -particle density matrix $D_N(t) \in \mathcal{L}^1(L^2((\mathbf{R}^d)^N))$ satisfying

$$D_N(t) = D_N(t)^* \geq 0, \quad \text{and } \text{trace}(D_N(t)) = 1.$$

The condition $D_N(t) = D_N(t)^* \geq 0$ is equivalent to the fact that

$$\langle\Phi_N|D_N(t)\Phi_N\rangle_{L^2((\mathbf{R}^d)^N)} \geq 0 \quad \text{for all } \Phi_N \in L^2((\mathbf{R}^d)^N).$$

Equivalently, the spectrum of $D_N(t)$ consists of nonnegative eigenvalues (since $D_N(t) \in \mathcal{L}^1(L^2((\mathbf{R}^d)^N))$, we already know that $D_N(t)$ is compact, so that its spectrum consists of eigenvalues only).

With the normalization condition $\text{trace}(D_N(t)) = 1$, one sees that $D_N(t)$ is of the form

$$D_N(t) = \sum_{n \geq 1} \lambda_n(t) |\psi_n(t, \cdot)\rangle\langle\psi_n(t, \cdot)|$$

where $(\psi_n(t, \cdot))_{n \geq 1}$ is a complete orthonormal system in $L^2(\mathbf{R}^d)^N$ and

$$\lambda_n(t) \geq 0, \quad \sum_{n \geq 1} \lambda_n(t) = 1.$$

In other words, $D_N(t)$ is a (possibly infinite) convex combination of the density matrices $|\psi_n(t, \cdot)\rangle\langle\psi_n(t, \cdot)|$ corresponding with pure states.

While the Schrödinger equation governs the evolution of quantum states described by wave functions, the von Neumann equation governs the evolution of mixed as well as pure states in quantum mechanics. If $D_N(t)$ satisfies the von Neumann equation

$$i\dot{D}_N(t) = [H_N, D_N(t)]$$

where

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l)$$

and V is such that iH_N is the generator of a unitary group on $L^2(\mathbf{R}^d)^N$ (as in Kato's theorem for instance), then the eigenvalues of $D_N(t)$ satisfy

$$\lambda_n(t) = \lambda_n(0), \quad \text{for each } n \geq 1.$$

The eigenfunctions of $D_N(t)$ are transformed as

$$\psi_n(t, \cdot) = e^{-itH_N} \psi_n(0, \cdot), \quad \text{for each } n \geq 1.$$

Throughout the following sections, we shall be dealing with pure states, although most of our arguments could easily be extended to mixed states.

The notion of partial trace discussed above leads to a very natural way of constructing mixed states, discussed in the exercise below.

Exercise. Let $\Psi_M \in L^2((\mathbf{R}^d)^M)$ be an M -particle wave function such that $\|\Psi_M\|_{L^2((\mathbf{R}^d)^M)} = 1$, and let $N \geq 1$ be such that $N < M$. Set $D_M := |\Psi_M\rangle\langle\Psi_M|$ and consider the operator $D_N := D_{M:N}$.

- 1) Check that $D_N = D_N^* \geq 0$, and that $\text{trace}(D_N) = 1$.
- 2) Assume that $D_N = |\psi\rangle\langle\psi|$ with $\psi \in L^2((\mathbf{R}^d)^N)$ such that $\|\psi\|_{L^2((\mathbf{R}^d)^N)} = 1$ and compute $\text{trace}(D_N|\psi\rangle\langle\psi|)$ in terms of Ψ_M .
- 3) Under which condition on Ψ_M does one have $D_N = D_N^2$? (Hint: use the result of question 2 and the equality case in the Cauchy-Schwarz inequality to find that Ψ_M is of the form $\Psi_M(x_1, \dots, x_M) = \psi(x_1, \dots, x_N)\phi(x_{N+1}, \dots, x_M)$.)

This exercise is inspired from the second paragraph in §14 of [64], where it is explained that mixed states arise for instance as quantum states for subsystems of a larger system in some pure state. The result obtained in the exercise above suggests that the state of such a subsystem (particles 1 to N) is pure if and only if the subsystem considered (the N first particles are independent from the $M-N$ remaining particles.)

1.10 The BBGKY hierarchy in quantum mechanics

In this section, we outline the BBGKY method presented above in the case of classical statistical mechanics, and explain how it leads to a rigorous derivation of the mean-field Hartree equation from the N -particle Schrödinger equation.

First we introduce some elements of notation.

For all $N \geq 1$, we set $X_N := (x_1, \dots, x_N)$ and $Y_N := (y_1, \dots, y_N)$; likewise for all $N \geq 1$ and $1 \leq k < N$, we adopt the notation $Z_N^k = (z_{k+1}, \dots, z_N)$.

Given an integral operator D_N acting on $L^2((\mathbf{R}^d)^N)$ with integral kernel $D_N(X_N, Y_N)$ we denote by $D_{N:k}$ the operator with integral kernel

$$D_{N:k}(X_k, Y_k) := \int_{(\mathbf{R}^d)^{N-k}} D_N(X_k, Z_N^k; Y_k, Z_N^k) dZ_N^k.$$

In terms of operators,

$$D_{N:k} = \text{trace}_k(D_N).$$

Here again, we use the same letter to designate an integral operator and its integral kernel. This obvious abuse of notation is deliberately chosen to avoid the unnecessary multiplication of mathematical symbols.

1.10.1 The quantum BBGKY hierarchy

First we explain how to deduce the BBGKY hierarchy from the N -particle Schrödinger equation.

Theorem 1.10.1 *Assume that V is a real-valued, even function belonging to $L^\infty(\mathbf{R}^d)$. Let $D_N^{\text{in}} = (D_N^{\text{in}})^* \geq 0$ be a trace-class operator with $\text{trace}(D_N^{\text{in}}) = 1$ on $\mathfrak{H}_N = \mathfrak{H}^{\otimes N} = L^2((\mathbf{R}^d)^N)$ with $\mathfrak{H} = L^2(\mathbf{R}^d)$, satisfying the indistinguishability symmetry, i.e.*

$$S_\sigma D_N^{\text{in}} = D_N^{\text{in}} \quad \text{for each } \sigma \in \mathfrak{S}_N.$$

Let

$$D_N(t) := e^{-itH_N} D_N^{\text{in}} e^{itH_N}, \quad t \in \mathbf{R},$$

where

$$H_N = -\frac{1}{2} \sum_{k=1}^N \Delta_k + \frac{1}{N} \sum_{1 \leq k < l \leq N} V_{kl}$$

is the N -particle Schrödinger operator. Here Δ_k designates the Laplacian acting on the k -th variable x_k , while V_{kl} designates the multiplication by $V(x_k - x_l)$.

Then the sequence of partial traces of D_N satisfies the BBGKY hierarchy of differential equations

$$\begin{aligned} i\dot{D}_{N:k} &= -\frac{1}{2} \sum_{j=1}^k [\Delta_j, D_{N:k}] + \frac{N-k}{N} \sum_{j=1}^k [V_{j,k+1}, D_{N:k+1}]_k \\ &\quad + \frac{1}{N} \sum_{1 \leq l < m \leq k} [V_{lm}, D_{N:k}] \end{aligned}$$

for all $k \geq 1$, with the convention

$$D_{N:N} = D_N, \quad \text{and } D_{N:k} = 0 \text{ whenever } k > N.$$

In terms of integral kernels, the BBGKY hierarchy reads

$$\begin{aligned} i\partial_t D_{N:k}(t, X_k, Y_k) &= -\frac{1}{2} \sum_{j=1}^k (\Delta_{x_j} - \Delta_{y_j}) D_{N:k}(t, X_k, Y_k) \\ &+ \frac{N-k}{N} \sum_{j=1}^k \int_{\mathbf{R}^d} (V(x_j - z) - V(y_j - z)) D_{N:k+1}(t, X_k, z, Y_k, z) dz \\ &+ \frac{1}{N} \sum_{1 \leq l < m \leq k} (V(x_l - x_m) - V(y_l - y_m)) D_{N:k}(t, X_k, Y_k) \end{aligned}$$

for all $k \geq 1$.

Proof. Consider the free N -body Schrödinger group

$$W_N(t) := \exp\left(-it\frac{1}{2}(\Delta_1 + \dots + \Delta_N)\right),$$

and set

$$F_N(t) := W_N(t)D_N(t)W_N(-t) = W_N(t)D_N(t)W_N(t)^*.$$

Starting from the von Neumann equation, one deduces that

$$i\dot{F}_N(t) = \frac{1}{N} \sum_{1 \leq l < m \leq N} [W_N(t)V_{lm}W_N(t)^*, F_N(t)].$$

Since $W_N(t)$ is a unitary operator on $L^2((\mathbf{R}^d)^N)$, the operator $F_N(t)$ is trace-class on $L^2((\mathbf{R}^d)^N)$. Since $V \in L^\infty(\mathbf{R}^d)$, all the operators V_{lm} are bounded on $L^2((\mathbf{R}^d)^N)$, so that $[W_N(t)V_{lm}W_N(t)^*, F_N(t)]$ is trace-class on $L^2((\mathbf{R}^d)^N)$. Taking partial traces of both sides of the equality above leads to

$$i\dot{F}_{N:k}(t) = \frac{1}{N} \sum_{1 \leq l < m \leq N} [W_N(t)V_{lm}W_N(t)^*, F_N(t)]_{:k}$$

for all $k \geq 1$.

Then we must distinguish three cases.

a) If $k < l < m \leq N$, then

$$[W_N(t)V_{lm}W_N(t)^*, F_N(t)]_{:k} = [\tilde{V}_{lm}(t), F_{N:m}(t)]_{:k} = 0,$$

with the notation

$$\tilde{V}_{lm}(t) := W_N(t)V_{lm}W_N(t)^* = e^{-it\frac{1}{2}(\Delta_l + \Delta_m)} V_{lm} e^{it\frac{1}{2}(\Delta_l + \Delta_m)}.$$

Indeed, let $A \in \mathcal{L}(L^2((\mathbf{R}^d)^k))$, and denote by I_p the identity in $\mathcal{L}(L^2((\mathbf{R}^d)^p))$. Then

$$[A \otimes I_{m-k}, \tilde{V}_{lm}(t)] = 0,$$

so that

$$\begin{aligned} \text{trace}_{\mathfrak{H}_k}([\tilde{V}_{lm}(t), F_{N:m}(t)]_{:k}A) &= \text{trace}_{\mathfrak{H}_m}([\tilde{V}_{lm}(t), F_{N:m}(t)]A \otimes I_{m-k}) \\ &= \text{trace}_{\mathfrak{H}_k}([A \otimes I_{m-k}, \tilde{V}_{lm}(t)]F_{N:m}(t)) = 0, \end{aligned}$$

with the notation $\mathfrak{H}_k := L^2((\mathbf{R}^d)^k)$.

b) If $1 \leq l < m \leq k \leq N$, then

$$[W_N(t)V_{lm}W_N(t)^*, F_N(t)]_{:k} = [W_k(t)V_{lm}W_k(t)^*, F_{N:k}(t)].$$

Indeed, with the same notation as above, for each $A \in \mathcal{L}(L^2((\mathbf{R}^d)^k))$,

$$\begin{aligned} &\text{trace}_{\mathfrak{H}_N}([W_N(t)V_{lm}W_N(t)^*, F_N(t)]A \otimes I_{N-k}) \\ &= \text{trace}_{\mathfrak{H}_N}([\tilde{V}_{lm}(t), F_N(t)]A \otimes I_{N-k}) \\ &= \text{trace}_{\mathfrak{H}_N}(\tilde{V}_{lm}(t)F_N(t)A \otimes I_{N-k}) \\ &\quad - \text{trace}_{\mathfrak{H}_N}(F_N(t)\tilde{V}_{lm}(t)A \otimes I_{N-k}) \\ &= \text{trace}_{\mathfrak{H}_N}(F_N(t)A \otimes I_{N-k}\tilde{V}_{lm}(t)) \\ &\quad - \text{trace}_{\mathfrak{H}_N}(F_N(t)\tilde{V}_{lm}(t)A \otimes I_{N-k}) \\ &= \text{trace}_{\mathfrak{H}_N}(F_N(t)(A\tilde{V}_{lm}(t)) \otimes I_{N-k}) \\ &\quad - \text{trace}_{\mathfrak{H}_N}(F_N(t)(\tilde{V}_{lm}(t)A) \otimes I_{N-k}) \\ &= \text{trace}_{\mathfrak{H}_k}(F_{N:k}(t)[A, \tilde{V}_{lm}(t)]) \\ &= \text{trace}_{\mathfrak{H}_k}([\tilde{V}_{lm}(t), F_{N:k}(t)]A) \\ &= \text{trace}_{\mathfrak{H}_k}([W_k(t)V_{lm}W_k(t)^*, F_{N:k}(t)]A). \end{aligned}$$

c) It remains to treat the case $1 \leq l \leq k < m \leq N$. Denote by $\sigma \in \mathfrak{S}_N$ the transposition exchanging $k+1$ and m . At this point we use the symmetry of both operators D_N and W_N , i.e. the fact that

$$S_\sigma D_N(t) = D_N(t) \quad \text{and} \quad S_\sigma W_N(t) = W_N(t)$$

for each $t \in \mathbf{R}$. First, one can check by direct inspection that

$$S_\sigma[\tilde{V}_{l,k+1}(t), F_N(t)] = [\tilde{V}_{l,m}(t), S_\sigma F_N(t)] = [\tilde{V}_{l,m}(t), F_N(t)].$$

Then, for each $A \in \mathcal{L}(L^2((\mathbf{R}^d)^k))$ and with the same notation as above,

$$\begin{aligned} \text{trace}_{\mathfrak{H}_k}([\tilde{V}_{l,m}(t), F_N(t)]_{:k}A) &= \text{trace}_{\mathfrak{H}_m}([\tilde{V}_{l,m}(t), F_N(t)]A \otimes I_{m-k}) \\ &= \text{trace}_{\mathfrak{H}_m}([\tilde{V}_{l,m}(t), F_N(t)]S_\sigma(A \otimes I_{m-k})) \\ &= \text{trace}_{\mathfrak{H}_m}(S_\sigma[\tilde{V}_{l,m}(t), F_N(t)]S_\sigma^2(A \otimes I_{m-k})) \\ &= \text{trace}_{\mathfrak{H}_m}(S_\sigma[\tilde{V}_{l,m}(t), F_N(t)](A \otimes I_{m-k})) \\ &= \text{trace}_{\mathfrak{H}_m}([\tilde{V}_{l,k+1}(t), F_N(t)](A \otimes I_{m-k})) \\ &= \text{trace}_{\mathfrak{H}_k}([\tilde{V}_{l,k+1}(t), F_N(t)]_{:k}A). \end{aligned}$$

(The second equality above follows from the fact that $S_\sigma(A \otimes I_{m-k}) = A \otimes I_{m-k}$ since σ acts as the identity on $\{1, \dots, k\}$; the third equality follows from the identities $\text{trace}(S_\sigma T) = \text{trace}(U_\sigma T U_\sigma^*) = \text{trace}(T)$ and $S_\sigma(BA) = U_\sigma B U_\sigma^* U_\sigma A U_\sigma = S_\sigma(B)S_\sigma(A)$, while the fourth equality is based on the relation $S_\sigma^2 = \text{Id}$.)

Thus

$$[\tilde{V}_{l,m}(t), F_N(t)]_{:k} = [\tilde{V}_{l,k+1}(t), F_N(t)]_{:k} = [\tilde{V}_{l,k+1}(t), F_{N:k+1}(t)]_{:k}$$

whenever $1 \leq l \leq k < m \leq N$ — the last equality being obvious.

Therefore

$$\begin{aligned} i\dot{F}_{N:k}(t) &= \frac{1}{N} \sum_{l=1}^k \sum_{m=k+1}^N [\tilde{V}_{l,m}(t), F_N(t)]_{:k} + \frac{1}{N} \sum_{1 \leq l < m \leq k} [\tilde{V}_{lm}(t), F_{N:k}(t)] \\ &= \frac{N-k}{N} \sum_{l=1}^k [\tilde{V}_{l,k+1}(t), F_{N:k+1}(t)]_{:k} + \frac{1}{N} \sum_{1 \leq l < m \leq k} [\tilde{V}_{lm}, F_{N:k}(t)], \end{aligned}$$

Undoing the conjugation with $W_k(t)$, we next arrive at the equality

$$\begin{aligned} i\dot{D}_{N:k} &= -\frac{1}{2} \sum_{j=1}^k [\Delta_j, D_{N:k}] + \frac{1}{N} \sum_{1 \leq l < m \leq k} [V_{lm}, D_{N:k}] \\ &\quad + \frac{N-k}{N} \sum_{j=1}^k \left(e^{-it\frac{1}{2}\Delta_{k+1}} [V_{j,k+1}, D_{N:k+1}] e^{it\frac{1}{2}\Delta_{k+1}} \right)_{:k}. \end{aligned}$$

It remains to check that

$$\left(e^{-it\frac{1}{2}\Delta_{k+1}} [V_{j,k+1}, D_{N:k+1}] e^{it\frac{1}{2}\Delta_{k+1}} \right)_{:k} = [V_{j,k+1}, D_{N:k+1}]_{:k}.$$

For each $A \in \mathcal{L}(L^2((\mathbf{R}^d)^k))$ and with the same notation as above, one has

$$\begin{aligned} &\text{trace} \left(\left(e^{-it\frac{1}{2}\Delta_{k+1}} [V_{j,k+1}, D_{N:k+1}] e^{it\frac{1}{2}\Delta_{k+1}} \right)_{:k} A \right) \\ &= \text{trace} \left(\left(e^{-it\frac{1}{2}\Delta_{k+1}} [V_{j,k+1}, D_{N:k+1}] e^{it\frac{1}{2}\Delta_{k+1}} \right) A \otimes I_1 \right) \\ &= \text{trace} \left([V_{j,k+1}, D_{N:k+1}] e^{it\frac{1}{2}\Delta_{k+1}} (A \otimes I_1) e^{-it\frac{1}{2}\Delta_{k+1}} \right) \\ &= \text{trace}([V_{j,k+1}, D_{N:k+1}] A \otimes I_1) \\ &= \text{trace}([V_{j,k+1}, D_{N:k+1}]_{:k} A) \end{aligned}$$

since

$$e^{it\frac{1}{2}\Delta_{k+1}} (A \otimes I_1) e^{-it\frac{1}{2}\Delta_{k+1}} = A \otimes I_1,$$

and this concludes the proof. ■

References for this section are [88, 7, 10].

1.10.2 The infinite quantum mean field hierarchy

From the quantum BBGKY hierarchy, we formally deduce an infinite hierarchy that is the quantum analogue of the infinite mean field hierarchy in classical statistical mechanics. The formal argument is as follows: assume that

$$D_{N:k}(t) \rightarrow D_k(t)$$

for each fixed $k \geq 1$ as $N \rightarrow \infty$ in some sense to be made precise, so that

$$[V_{lm}, D_{N:k}(t)] \rightarrow [V_{lm}, D_k(t)].$$

Then we pass to the limit as $N \rightarrow \infty$ in both terms

$$\frac{1}{N} \sum_{1 \leq l < m \leq k} [V_{lm}, D_{N:k}]$$

and

$$\frac{N-k}{N} \sum_{j=1}^k [V_{j,k+1}, D_{N:k+1}]_{:k}.$$

The first term vanishes as $N \rightarrow \infty$ since

$$\frac{1}{N} \sum_{1 \leq l < m \leq k} [V_{lm}, D_{N:k}] = O\left(\frac{k^2}{N}\right) \rightarrow 0,$$

while the second term satisfies

$$\frac{N-k}{N} \sum_{j=1}^k [V_{j,k+1}, D_{N:k+1}]_{:k} \rightarrow \sum_{j=1}^k [V_{j,k+1}, D_{k+1}]_{:k}$$

for each $k \geq 1$ as $N \rightarrow \infty$.

Therefore, we expect that the sequence of operators $(D_k(t))_{k \geq 1}$ should satisfy the infinite hierarchy of differential equations

$$i\dot{D}_k = -\frac{1}{2} \sum_{j=1}^k [\Delta_j, D_k] + \sum_{j=1}^k [V_{j,k+1}, D_{k+1}]_{:k}, \quad k \geq 1.$$

In terms of integral kernels

$$D_{N:k}(t, X_k, Y_k) \rightarrow D_k(t, X_k, Y_k),$$

for each $k \geq 1$ as $N \rightarrow \infty$, where $D_k(t, X_k, Y_k)$ is the integral kernel of the operator $D_k(t)$. Then, the sequence of functions $(D_k(t, X_k, Y_k))_{k \geq 1}$ satisfies the infinite hierarchy of integro-differential equations indexed by $k \geq 1$:

$$\begin{aligned} i\partial_t D_k(t, X_k, Y_k) &= -\frac{1}{2} \sum_{j=1}^k (\Delta_{x_j} - \Delta_{y_j}) D_k(t, X_k, Y_k) \\ &+ \sum_{j=1}^k \int_{\mathbf{R}^d} (V(x_j - z) - V(y_j - z)) D_{k+1}(t, X_k, z, Y_k, z) dz. \end{aligned}$$

Of course, the argument above is purely formal and remains to be justified rigorously. This is achieved by the following theorem.

Theorem 1.10.2 *Assume that the potential V is an even, real-valued function such that*

$$V \in C(\mathbf{R}^d \setminus \{0\}) \cap L^2_{loc}(\mathbf{R}^d), \quad V \rightarrow 0 \text{ at } \infty, \quad \text{and } V \geq -V_m$$

for some $V_m > 0$. Assume that the initial density matrix

$$D_N^{in} = |\Psi_N^{in}\rangle\langle\Psi_N^{in}| \quad \text{with } \int_{(\mathbf{R}^d)^N} |\Psi_N^{in}(X_N)|^2 dX_N = 1$$

satisfies the indistinguishability symmetry, i.e.

$$S_\sigma D_N^{in} = D_N^{in} \quad \text{for each } \sigma \in \mathfrak{S}_N,$$

and the energy bound

$$\begin{aligned} \mathcal{E}_N^{in} := & \frac{1}{2} \sum_{j=1}^N \int_{(\mathbf{R}^d)^N} |\nabla_{x_j} \Psi_N^{in}(X_N)|^2 dX_N \\ & + \frac{1}{N} \sum_{1 \leq l < m \leq N} \int_{(\mathbf{R}^d)^N} V(x_l - x_m) |\Psi_N^{in}(X_N)|^2 dX_N = O(N). \end{aligned}$$

Assume that, for each $k \geq 1$ and in the limit $N \rightarrow \infty$,

$$D_{N:k}^{in} \rightarrow D_k^{in} \text{ in } \mathcal{L}^1(L^2((\mathbf{R}^d)^k)) \text{ weak-}^*.$$

Then

(a) the sequence $(D_{N:k})_{k \geq 1}$ indexed by N is relatively compact in the infinite product space $\prod_{k \geq 1} L^\infty(\mathbf{R}; \mathcal{L}^1(L^2((\mathbf{R}^d)^k)))$, endowed with the product of weak- * topologies — $L^\infty(\mathbf{R}; \mathcal{L}^1(L^2((\mathbf{R}^d)^k)))$ being the dual of the Banach space $L^1(\mathbf{R}; \mathcal{K}(L^2((\mathbf{R}^d)^k)))$ equipped with the norm

$$\| \|K\| \| := \int_{\mathbf{R}} \|K(t)\|_1 dt;$$

(b) each limit point $(D_k)_{k \geq 1}$ of this sequence as $N \rightarrow \infty$ solves the infinite quantum mean field hierarchy written above in the sense of distributions, with initial data

$$D_k(0) = D_k^{in}, \quad k \geq 1.$$

Although the proof of this result relies on relatively soft functional analytic techniques, we shall not give it in detail. We just sketch the key arguments and refer the interested reader to [7] for the complete proof.

The general strategy is to use the uniform bounds on the operator $D_N(t)$ deduced from the condition $\text{trace}(D_N(t)) = 1$ and the conservation of energy to obtain the compactness property in statement (a) of the theorem above.

Next, one writes each equation in the BBGKY hierarchy²⁰ in the sense of distributions and passes to the limit as $N \rightarrow \infty$ for each $k \geq 1$ fixed. This strategy uses in particular various observations listed below.

A first important ingredient in the proof is the Cauchy-Schwarz inequality

$$|D_{N:k}(t, X_k, Y_k)|^2 \leq D_{N:k}(t, X_k, X_k)D_{N:k}(t, Y_k, Y_k)$$

since $D_N(t)$ is a nonnegative operator. It implies in particular the bound

$$\iint_{(\mathbf{R}^d)^k} |D_{N:k}(t, X_k, Y_k)|^2 dX_k dY_k \leq 1$$

that is uniform in $t \in \mathbf{R}$ and $N, k \geq 1$. We recall the convention $D_{N:k} = 0$ whenever $k > N$ and the equality

$$\int_{(\mathbf{R}^d)^k} D_{N:k}(t, Z_k, Z_k) dZ_k = 1,$$

since

$$\int_{(\mathbf{R}^d)^N} D_N(t, Z_N, Z_N) dZ_N = 1.$$

A second crucial ingredient in the proof is the H^1 bound

$$\frac{1}{2} \int_{(\mathbf{R}^d)^N} |\nabla_{x_l} \Psi_N(t, X_N)|^2 dX_N \leq \frac{\mathcal{E}_N^{in}}{N} + \frac{N-1}{2N} V_m$$

for each $l = 1, \dots, N$. This estimate is a consequence of the initial energy bound postulated on Ψ_N^{in} , together with the conservation of energy under the Schrödinger group, implying that

$$\begin{aligned} & \frac{1}{2} \sum_{l=1}^N \int_{(\mathbf{R}^d)^N} |\nabla_{x_l} \Psi_N(t, X_N)|^2 dX_N \\ &= \mathcal{E}_N - \frac{1}{N} \sum_{1 \leq k < l \leq N} \int_{(\mathbf{R}^d)^N} |V(x_k - x_l)| |\Psi_N(t, X_N)|^2 dX_N \\ &\leq \mathcal{E}_N + \frac{1}{2}(N-1)V_m \int_{(\mathbf{R}^d)^N} |\Psi_N(t, X_N)|^2 dX_N = \mathcal{E}_N + \frac{1}{2}(N-1)V_m \end{aligned}$$

and of the assumption of indistinguishable particles, so that one has, for each pair k, l such that $1 \leq k \neq l \leq N$,

$$\int_{(\mathbf{R}^d)^N} |\nabla_{x_k} \Psi_N(t, X_N)|^2 dX_N = \int_{(\mathbf{R}^d)^N} |\nabla_{x_l} \Psi_N(t, X_N)|^2 dX_N.$$

A third key step in the proof is based on the following result bearing on trace-class operators.

²⁰The BBGKY hierarchy has been derived from the N -particle Schrödinger equation in the case where the potential V belongs to $L^\infty(\mathbf{R}^d)$ — see Theorem 1.10.1. However its validity in the sense of distributions under the assumptions of Theorem 1.10.2 results from the same arguments as those used in the derivation of the infinite hierarchy and presented below.

Lemma 1.10.3 Consider a sequence of integral operators $A_n \in \mathcal{L}^1(L^2(\mathbf{R}^d))$ with integral kernels $a_n \equiv a_n(x, y)$ satisfying

$$A_n \rightarrow 0 \text{ in } \mathcal{L}^1(L^2(\mathbf{R}^d)) \text{ weak-}^*$$

as $n \rightarrow \infty$, and

$$\sup_{n \geq 1} \int_{\mathbf{R}^d} |a_n(z, z+h) - a_n(z, z)| dz \rightarrow 0 \text{ as } |h| \rightarrow 0.$$

Then, for each $\chi \in C_c(\mathbf{R}^d)$

$$\int_{\mathbf{R}^d} a_n(z, z) \chi(z) dz \rightarrow 0 \text{ as } n \rightarrow \infty.$$

See section 2 of [7] for the proof of this lemma.

This result is applied in the following context. For each $\Theta \in C_c((\mathbf{R}^d)^k)$, consider

$$a_{N,k}(t, z, w) := \iint_{(\mathbf{R}^d)^k \times (\mathbf{R}^d)^k} \Theta(X_k) \Theta(Y_k) D_{N:k+1}(t, X_n, z, Y_k, w) dX_k dY_k$$

Then by the Sobolev estimate above, one has

$$\int_{\mathbf{R}^d} |a_{N,k}(t, z, z+h) - a_{N,k}(t, z, z)| dz \leq |h| \|\Theta\|_{L^\infty}^2 \left(\frac{2\mathcal{E}_N^{in}}{N} + \frac{N-1}{N} V_m \right).$$

Thus

$$\int_{\mathbf{R}^d} a_{N,k}(z, z) \chi(z) dz \rightarrow \int_{\mathbf{R}^d} a_k(z, z) \chi(z) dz$$

as $N \rightarrow \infty$, where

$$a_k(t, z, w) := \iint_{(\mathbf{R}^d)^k \times (\mathbf{R}^d)^k} \Theta(X_k) \Theta(Y_k) D_{k+1}(t, X_n, z, Y_k, w) dX_k dY_k,$$

and where $\chi \in C^\infty(\mathbf{R})$ is such that $0 \leq \chi \leq 1$, with $\chi(z) = 1$ for $1/R \leq z \leq R$ and $\text{supp}(\chi) \subset [1/2R, R+1]$. This is the key step in obtaining the limit of the interaction term

$$\int_{\mathbf{R}^d} (V(x_k - z) - V(y_k - z)) D_{N:k+1}(t, X_k, z, Y_k, z) dz.$$

Some remarks are in order before going further.

Observe first that the assumptions on the potential V include the (repulsive) Coulomb potential in space dimension $d = 3$

$$V(z) = \frac{1}{4\pi} \frac{1}{|z|}$$

between identical charged particles. This case is obviously of fundamental importance in view of the (many) applications to atomic physics and quantum chemistry, in which the interacting particles are electrons.

Our second observation is of a more mathematical nature. Under the assumptions on the potential used in the theorem, the interaction integrand

$$(V(x_j - z) - V(y_j - z))D_{k+1}(t, X_k, z, Y_k, z)$$

may fail to belong to $L^1(\mathbf{R}_z^d)$ for each (or almost every) X_k, Y_k . Yet our analysis defines the interaction integral

$$\int_{\mathbf{R}^d} (V(x_j - z) - V(y_j - z))D_{k+1}(t, X_k, z, Y_k, z)dz$$

as a Radon *measure* in (X_n, Y_n) — instead of a *function* of these same variables.

A general reference for the material presented in this section is [7].

1.11 The mean field limit in quantum mechanics and and Hartree's equation

1.11.1 Mathematical statement of the mean field limit

The quantum analogue of the mean field limit obtained in classical statistical mechanics is the following result.

Theorem 1.11.1 *Let V be a real-valued, even, bounded measurable function defined on \mathbf{R}^d , such that $V \rightarrow 0$ at infinity. Let the initial single-particle wave function $\psi^{in} \in H^1(\mathbf{R}^d)$ satisfy $\|\psi^{in}\|_{L^2} = 1$, and let $\psi \equiv \psi(t, x)$ be the solution of the Cauchy problem for the Hartree equation*

$$\begin{cases} (i\partial_t + \frac{1}{2}\Delta_x)\psi(t, x) + \psi(t, x) \int_{\mathbf{R}^d} V(x-z)|\psi(t, z)|^2 dz = 0, \\ \psi(0, x) = \psi^{in}(x). \end{cases}$$

Let $\Psi_N^{in} = (\psi^{in})^{\otimes N}$ and let $\Psi_N(t) = e^{-itH_N}\Psi_N^{in}$ be the solution of N -particle Schrödinger equation in the mean field scaling, i.e. with

$$H_N = -\frac{1}{2} \sum_{j=1}^N \Delta_{x_j} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l).$$

Then, for each $k \geq 1$, one has

$$D_{N:k}(t) := |\Psi_N(t)\rangle\langle\Psi_N(t)|_{:k} \rightarrow D_k(t)$$

in $L^\infty(\mathbf{R}; \mathcal{L}^1(L^2((\mathbf{R}^d)^k)))$ weak- $$ as $N \rightarrow \infty$, where*

$$D_k(t) = |\psi(t)^{\otimes k}\rangle\langle\psi(t)^{\otimes k}|;$$

— *in other words*

$$D_k(t, X_k, Y_k) = \prod_{j=1}^k \psi(t, x_j) \overline{\psi(t, y_j)}.$$

As already observed in the case of the mean field limit in classical mechanics, using the hierarchy approach requires knowing that the mean field PDE is well-posed: see Proposition 1.8.2 above.

Here again, we only sketch the key arguments in the proof, and refer the interested reader to [88] or [7] for a complete account.

By Theorem 1.11.1, we know that the sequence $(D_{N:k})_{k \geq 1}$ indexed by N is relatively compact in

$$\prod_{k \geq 1} L^\infty(\mathbf{R}; \mathcal{L}^1(L^2((\mathbf{R}^d)^k)))$$

equipped with the product topology, where $L^\infty(\mathbf{R}; \mathcal{L}^1(L^2((\mathbf{R}^d)^k)))$ is endowed with the weak-* topology for each $k \geq 1$.

Besides, Theorem 1.11.1 implies that any limit point $(D_k)_{k \geq 1}$ of that sequence is a solution of the infinite quantum mean field hierarchy with initial data

$$D_k^{in} := |(\psi^{in})^{\otimes k}\rangle\langle(\psi^{in})^{\otimes k}|, \quad k \geq 1.$$

Proposition 1.11.2 *Let V be a real-valued, even, bounded measurable function defined on \mathbf{R}^d , such that $V \rightarrow 0$. Let the initial single-particle wave function $\psi^{in} \in H^1(\mathbf{R}^d)$ satisfy $\|\psi^{in}\|_{L^2} = 1$, and let $\psi \in C(\mathbf{R}; H^1(\mathbf{R}^d)) \cap C^1(\mathbf{R}; L^2(\mathbf{R}^d))$ be the solution of the Cauchy problem for the Hartree equation*

$$\begin{cases} (i\partial_t + \frac{1}{2}\Delta_x)\psi(t, x) + \psi(t, x) \int_{\mathbf{R}^d} V(x-z)|\psi(t, z)|^2 dz = 0, \\ \psi(0, x) = \psi^{in}(x). \end{cases}$$

Then the sequence

$$\rho_k(t) = |\psi(t, \cdot)^{\otimes k}\rangle\langle\psi(t, \cdot)^{\otimes k}|$$

is a particular solution of the Cauchy problem for the infinite quantum mean field hierarchy with initial data

$$\rho_k^{in} := |(\psi^{in})^{\otimes k}\rangle\langle(\psi^{in})^{\otimes k}|, \quad k \geq 1.$$

Proof. Since $\psi \in C(\mathbf{R}; H^1(\mathbf{R}^d)) \cap C^1(\mathbf{R}; L^2(\mathbf{R}^d))$ satisfies the Hartree equation, one has

$$\begin{aligned} i\partial_t(\psi(t, x)\overline{\psi(t, y)}) &= -\frac{1}{2}(\Delta_x - \Delta_y)\psi(t, x)\overline{\psi(t, y)} \\ &\quad + \psi(t, x)\overline{\psi(t, y)} \int_{\mathbf{R}^d} (V(x-z) - V(y-z))|\psi(t, z)|^2 dz \end{aligned}$$

in the sense of distributions on $\mathbf{R}_t \times \mathbf{R}_x^d \times \mathbf{R}_y^d$. Next, an elementary computation shows that, for each $k > 1$,

$$\begin{aligned}
i\partial_t \rho_k(t, X_k, Y_k) &= i \sum_{j=1}^k \prod_{\substack{l=1 \\ l \neq j}}^k \psi(t, x_l) \overline{\psi(t, y_l)} \partial_t (\psi(t, x_j) \overline{\psi(t, y_j)}) \\
&= -\frac{1}{2} \sum_{j=1}^k \prod_{\substack{l=1 \\ l \neq j}}^k \psi(t, x_l) \overline{\psi(t, y_l)} (\Delta_{x_j} - \Delta_{y_j}) \psi(t, x_j) \overline{\psi(t, y_j)} \\
&\quad + \sum_{j=1}^k \rho_k(t, X_k, Y_k) \int_{\mathbf{R}^d} (V(x_j - z) - V(y_j - z)) |\psi(t, z)|^2 dz \\
&= -\frac{1}{2} \sum_{j=1}^k (\Delta_{x_j} - \Delta_{y_j}) \prod_{l=1}^k \psi(t, x_l) \overline{\psi(t, y_l)} \\
&\quad + \sum_{j=1}^k \int_{\mathbf{R}^d} (V(x_j - z) - V(y_j - z)) \rho_k(t, X_k, Y_k) |\psi(t, z)|^2 dz \\
&= -\frac{1}{2} \sum_{j=1}^k (\Delta_{x_j} - \Delta_{y_j}) \rho_k(t, X_k, Y_k) \\
&\quad + \sum_{j=1}^k \int_{\mathbf{R}^d} (V(x_j - z) - V(y_j - z)) \rho_{k+1}(t, X_k, z, Y_k, z) dz.
\end{aligned}$$

Therefore, the sequence $(\rho_k(t, X_k, Y_k))_{k \geq 1}$ is a solution of the infinite quantum mean field hierarchy. ■

It remains to prove that all limit points $(D_k)_{k \geq 1}$ of the sequence $(D_{N:k})_{k \geq 1}$ as $N \rightarrow \infty$ fall in some uniqueness class for the infinite quantum mean field hierarchy. If this is the case, each limit point $(D_k)_{k \geq 1}$, being a solution of the infinite quantum mean field hierarchy with the same initial data as $(\rho_k)_{k \geq 1}$, must coincide with it for all $t \in \mathbf{R}$. By compactness and uniqueness of the limit point, one concludes that

$$D_{N:k}(t) \rightarrow \rho_k(t) := |\psi(t, \cdot)^{\otimes k}\rangle \langle \psi(t, \cdot)^{\otimes k}|, \quad \text{for each } k \geq 1$$

in the weak-* topology of $L^\infty(\mathbf{R}; \mathcal{L}^1(L^2((\mathbf{R}^d)^k)))$ as $N \rightarrow \infty$.

Since the integral kernels of the operators ρ_k are of factorized form, i.e.

$$\rho_k(t, X_k, Y_k) = \prod_{j=1}^k \psi(t, x_j) \overline{\psi(t, y_j)}, \quad k \geq 1,$$

this last statement is the quantum analogue of the propagation of chaos studied above in the context of the mean field limit in classical statistical mechanics.

In order to carry out this program, two things need to be checked:

a) one needs an estimate for the interaction terms

$$D_{k+1} \rightarrow [V_{j,k+1}, D_{k+1}]_{:k}$$

for $j = 1, \dots, k$, and

b) one needs an estimate for the growth of

$$D_k \quad \text{as } k \rightarrow \infty.$$

In the next section, we present an abstract framework explaining the role of each estimates.

1.11.2 A tool for studying infinite hierarchies

We first review a seemingly unrelated result, namely the Nirenberg-Ovcyannikov abstract analogue of the Cauchy-Kovalevska theorem. More precisely, we recall below a variant of this theorem due to Nishida.

The Nirenberg-Ovcyannikov abstract Cauchy-Kovalevska theorem

The Nirenberg-Ovcyannikov abstract Cauchy-Kovalevska theory bears on the Cauchy problem for differential equations of the form

$$\dot{u}(t) = F(t, u(t)),$$

in situations where one can apply neither the Cauchy-Lipschitz theorem nor the Peano existence theorem (see chapter 1 in [56]). Such situations arise typically when the solution $u(t)$ belongs to function spaces that are not invariant under the mapping $v \mapsto F(t, v)$. We first introduce the functional setting and present the main result obtained independently by Nirenberg [76] and Ovcyannikov [78].

The setting involves a family (a scale) of Banach spaces $(B_r)_{r>0}$ indexed by the positive real numbers. The norm in B_r is denoted by $\|\cdot\|_r$. This scale of Banach spaces is nonincreasing, in the sense that, for each $r, r' > 0$, one has

$$(HB_r) \quad r' \leq r \Rightarrow B_r \subset B_{r'} \quad \text{with} \quad \|v\|_{r'} \leq \|v\|_r \quad \text{for each } v \in B_r.$$

Next, we specify how the time-dependent “vector field” F behaves with respect to the scale of Banach spaces $(B_r)_{r>0}$.

Our first assumption bears on the joint dependence of F in both of its arguments:

(a) there exists $r_0 > 0$ s.t.

$$(HF_a) \quad 0 < r' < r < r_0 \Rightarrow F \in C(\mathbf{R} \times B_r, B_{r'}) \\ \text{and } B_r \ni v \mapsto F(t, v) \in B_{r'} \text{ is linear for all } t \in \mathbf{R}.$$

A second assumption bears on the dependence of F in its second argument, uniformly in the time variable t :

(b) there exists $C > 0$ s.t.

$$(HF_b) \quad 0 < r' < r < r_0 \Rightarrow \|F(t, v)\|_{r'} \leq C \frac{\|v\|_r}{r - r'}.$$

We state only the uniqueness part of the Nirenberg-Ovcyannikov theorem, and refer the interested reader to [77] for a the complete statement — that is an existence theorem as well, and moreover bears on possibly nonlinear “vector fields” F .

Theorem 1.11.3 *For all $r \in (0, r_0)$ and all $\alpha > 0$, the only solution u of the Cauchy problem*

$$\begin{cases} \dot{u}(t) = F(t, u(t)), \\ u(0) = 0, \end{cases}$$

such that $u \in C^1((-\alpha, \alpha), B_r)$ is $u = 0$.

In order to fully appreciate the meaning of assumption (HF_b) , we briefly explain how this theorem is related to the classical Cauchy-Kovalevska theorem.

Consider the PDE with unknown $u \equiv u(t, z) \in \mathbf{C}$,

$$\partial_t u(t, z) = P(t, z, \partial_z)u(t, z),$$

where $t \in \mathbf{R}$ and $z \in \mathbf{C}$. It is assumed that P is a 1st order linear differential operator of the form

$$P(t, z, \partial_z)u(t, z) := A(t, z)\partial_z u(t, z) + B(t, z)u(t, z),$$

with coefficients A and B bounded and analytic on $(-T, T) \times \Omega_{r_0}$, where $\Omega_r \subset \mathbf{C}$ is the open strip defined as follows:

$$\Omega_r := \{z \in \mathbf{C} \text{ s.t. } |\operatorname{Im}(z)| < r\}.$$

Denote by B_r the space of bounded holomorphic functions on Ω_r with

$$\|v\|_r := \sup_{z \in \Omega_r} |v(z)|.$$

We recall that, for each function f that is holomorphic and bounded in the strip Ω_r , one has

$$|f^{(k)}(z)| \leq \frac{\sup_{z \in \Omega_r} |f(z)|}{(r - r')^k} \quad \text{for all } z \in \Omega_{r'} \text{ and } k \geq 1,$$

because of Cauchy's estimates for holomorphic functions (see for instance chapter 4, section 2.3 in [3]).

Therefore, one has

$$\begin{aligned}
\|P(t, \cdot, \partial_z)u(t, \cdot)\|_{r'} &\leq \sup_{z \in \Omega_{r_0}} |A(t, z)| \sup_{z \in \Omega_{r'}} |\partial_z u(t, z)| \\
&\quad + \sup_{z \in \Omega_{r_0}} |B(t, z)| \sup_{z \in \Omega_{r'}} |u(t, z)| \\
&\leq \sup_{z \in \Omega_{r_0}} |A(t, z)| \frac{\sup_{z \in \Omega_r} |u(t, z)|}{r - r'} \\
&\quad + \sup_{z \in \Omega_{r_0}} |B(t, z)| \sup_{z \in \Omega_r} |u(t, z)| \\
&\leq C \frac{\sup_{z \in \Omega_r} |u(t, z)|}{r - r'}
\end{aligned}$$

with

$$C := \sup_{z \in \Omega_{r_0}} |A(t, z)| + r_0 \sup_{z \in \Omega_{r_0}} |B(t, z)|.$$

In other words, the 1st order differential operator $P(t, z, \partial_z)$ satisfies assumption (HF_b) as a consequence of the Cauchy inequalities for bounded holomorphic functions in the strip Ω_r .

Observe that differential operators $Q(t, z, \partial_z)$ of order higher than 1 do not satisfy assumption (HF_b) , but an inequality of the form

$$\|Q(t, \cdot, \partial_z)u(t, \cdot)\|_{r'} \leq C \frac{\sup_{z \in \Omega_r} |u(t, z)|}{(r - r')^k}, \quad \text{with } k = \text{order of } Q.$$

This is a weaker inequality than the one in (HF_b) , which follows again from Cauchy's estimates, this time on higher order derivatives of holomorphic functions.

In fact, this is not surprising: the Cauchy-Kovalevska theorem guarantees the local existence and uniqueness of a local analytic solution of the Cauchy problem for the PDE

$$\begin{cases} \partial_t u(t, z) = Q(t, z, \partial_z)u(t, z) \\ u|_{t=0} = u^{in} \end{cases}$$

defined for $|t| < T$ and $|\text{Im}(z)| < r^*$ for some $T > 0$ and some $r^* > 0$. This is obviously impossible in general if Q is of order higher than 1. Consider indeed the simplest possible example where $Q(t, z, \partial_z) = \partial_z^2$. It is well known that the Cauchy problem for the backward heat equation is not well-posed in any one of the class B_r . Indeed, for each $t > 0$, the semigroup $e^{t\partial_z^2}$ maps the set of distributions with compact support on \mathbf{R} into the set of functions that are entire holomorphic (i.e. holomorphic on \mathbf{C}).

Application of the abstract Cauchy-Kovalevska theorem to infinite hierarchies

In this section, we give an abstract theorem for proving the uniqueness of the solution of infinite hierarchies based on the abstract Cauchy-Kovalevska theorem presented above.

Our setting involves a sequence of Banach spaces $(E_n)_{n \geq 1}$. For each $n \geq 1$, the norm in E_n is denoted by $|\cdot|_n$.

Along with the Banach spaces E_n , our setting also involves

- a) a strongly continuous group of isometries $U_n(t)$ defined on E_n for each $n \geq 1$, and
- b) a sequence of bounded linear operators $L_{n,n+1} : E_{n+1} \rightarrow E_n$ defined for each $n \geq 1$.

It will be assumed that the sequence of operators $L_{n,n+1}$ satisfies the following bound: there exists $C > 0$ such that

$$(HL) \quad \|L_{n,n+1}\|_{\mathcal{L}(E_{n+1}, E_n)} \leq Cn, \quad \text{for each } n \geq 1.$$

In the setting so defined, we consider the infinite hierarchy of differential equations

$$\dot{u}_n(t) = U_n(t)L_{n,n+1}U_{n+1}(-t)u_{n+1}(t), \quad n \geq 1.$$

Theorem 1.11.4 *Let $t^* > 0$ and let $u_n \in C^1([0, t^*], E_n)$ for each $n \geq 1$ be a solution of*

$$\begin{cases} \dot{u}_n(t) = U_n(t)L_{n,n+1}U_{n+1}(-t)u_{n+1}(t), & n \geq 1, \\ u_n(0) = 0. \end{cases}$$

Assume there exists $R > 0$ such that

$$(Hu) \quad \sup_{0 \leq t \leq t^*} \|u_n(t)\|_n \leq R^n \quad \text{for all } n \geq 1.$$

Then

$$u_n(t) = 0 \quad \text{for all } t \in [0, t^*] \text{ and each } n \geq 1.$$

Proof. We apply the abstract Cauchy-Kovalevka theorem in the following setting. First we choose the scale of Banach spaces: for each $r > 0$, we set

$$B_r := \left\{ v = (v_n)_{n \geq 1} \in \prod_{n \geq 1} E_n \text{ s.t. } \|v\|_r := \sum_{n \geq 1} r^n |v_n|_n < \infty \right\}.$$

Obviously, if $0 < r' < r$, one has

$$B_r \subset B_{r'},$$

and

$$\|v\|_{r'} = \sum_{n \geq 1} r'^n |v_n|_n \leq \sum_{n \geq 1} r^n |v_n|_n = \|v\|_r$$

for each $v \in B_r$.

The mapping F is defined on sequences $v = (v_n)_{n \geq 1}$ as follows:

$$F(t, v) := (U_n(t)L_{n,n+1}U_{n+1}(-t)v_{n+1})_{n \geq 1}.$$

With this definition, observing that

$$nr'^n \leq r'^n + r^{n-1}r + \dots + r'r^{n-1} + r^n = \frac{r^{n+1} - r'^{n+1}}{r - r'},$$

assumption (HL) implies that

$$\begin{aligned} \|F(t, v)\|_{r'} &\leq C \sum_{n \geq 1} nr'^n |v_n|_n \leq C \sum_{n \geq 1} \frac{r^{n+1} - r'^{n+1}}{r - r'} |v_n|_n \\ &\leq \frac{C}{r - r'} \sum_{n \geq 1} r^{n+1} |v|_{n+1} \leq \frac{C \|v\|_r}{r - r'} \end{aligned}$$

for each $r, r' > 0$ such that $r' < r$, where C is the constant that appears in the control of the norm of $L_{n, n+1}$ in condition (HL).

This implies that F satisfies assumption (HF_b). As for assumption (HF_a), it follows from assumption (HF_b) and the fact that $U_n(t)$ is a linear group of isometries on E_n for each $n \geq 1$.

Thus, if a sequence $u(t) = (u(t)_n)_{n \geq 1}$ with $u(t)_n \in E_n$ for each $n \geq 1$ and each $t \in [0, t^*]$ satisfies the growth condition (Hu) and the infinite hierarchy, then $u(t) \in B_r$ for all $t \in [0, t^*]$ and for each $r \in (0, 1/R)$.

We deduce from the differential equation that $u \in C^1([0, t^*], B_r)$ for each $r \in (0, 1/R)$. By the abstract Cauchy-Kovalevskaja theorem, we conclude that $u(t) = 0$ for each $t \in [0, t^*]$, which means that

$$u_n(t) = 0 \quad \text{for each } t \in [0, t^*] \text{ and each } n \geq 1.$$

This is precisely the expected uniqueness property. ■

Notice that assumption (Hu) is essential for the uniqueness property above. Here is an easy counterexample, showing that this assumption cannot be dispensed with.

Consider the infinite hierarchy of ODEs

$$\begin{cases} \dot{y}_k(t) = ky_{k+1}(t), & k \geq 1, \\ y_k(0) = y_k^{in}, \end{cases}$$

This hierarchy has obvious factorized solutions: if x is the solution of the Riccati equation

$$\begin{cases} \dot{x}(t) = x(t)^2, \\ x(0) = x^{in}, \end{cases}$$

i.e.

$$x(t) = \frac{x^{in}}{1 - tx^{in}},$$

then

$$y_k(t) = x(t)^k, \quad k \geq 1$$

is a solution of the infinite hierarchy with initial data

$$y_k^{in} := (x^{in})^k, \quad k \geq 1.$$

The infinite hierarchy with $y_k^{in} = 0$ for all $k \geq 0$ has a unique solution satisfying the growth condition (Hu), which is $y_k(t) = 0$ for all $t \in \mathbf{R}$ and $k \geq 1$.

Consider now the function E defined by

$$E(t) = \begin{cases} e^{-1/t} & \text{if } t > 0 \\ 0 & \text{if } t \leq 0 \end{cases}$$

that is of class C^∞ on the real line and satisfies $E^{(n)}(0) = 0$ for all $n \geq 0$. Then the formula

$$y_k(t) = \frac{1}{(k-1)!} E^{(k-1)}(t), \quad t \in \mathbf{R} \text{ and } k \geq 1,$$

also defines a solution of the infinite hierarchy.

That this solution does not grows exponentially as $k \rightarrow \infty$ corresponds with the fact that E is not an analytic function on the line, since it vanishes on the half-line without being identically 0, which contradicts the principle of isolated zeros.

References for this section are [93, 6].

1.11.3 Application to the Hartree limit in the bounded potential case

Finally we explain how to prove Theorem 1.11.1 with the formalism discussed above.

Proof of Theorem 1.11.1.

Step 1: First we write the infinite quantum mean field hierarchy

$$i\dot{D}_j(t) = -\frac{1}{2} \sum_{k=1}^j [\Delta_j, D_j(t)] + \sum_{k=1}^j [V_{k,j+1}, D_{j+1}]_{:j}, \quad j \geq 1$$

in the form

$$\dot{u}_j(t) = U_j(t) L_{j,j+1} U_{j+1}(-t) u_{j+1}(t), \quad j \geq 1,$$

where

$$L_{j,j+1} D_{j+1} := \sum_{k=1}^j [V_{k,j+1}, D_{j+1}]_{:j}$$

while

$$U_j(t) D_j := e^{-\frac{1}{2}it(\Delta_1 + \dots + \Delta_j)} D_j e^{\frac{1}{2}it(\Delta_1 + \dots + \Delta_j)}.$$

As before, Δ_k designates the Laplacian acting on the k th variable in $L^2((\mathbf{R}^d)^j)$, for each $k = 1, \dots, j$, while

$$u_j(t) := U_j(t) D_j(t).$$

Step 2: Next we choose appropriate norms and function spaces so as to apply Theorem 1.11.4. Define $E_j := \mathcal{L}^1(L^2((\mathbf{R}^d)^j))$ with trace norm denoted by $\|\cdot\|_1$ (or $\|\cdot\|_{1,j}$ in cases where the previous notation would lead to ambiguities).

The operator $U_j(t)$ defined in Step 1 is an isometry of E_j for all $j \geq 1$ and all $t \in \mathbf{R}$, since it consists of conjugating elements of E_j with the unitary group associated to the j -particle free Schrödinger equation. Indeed, we recall the following elementary result.

Lemma 1.11.5 *Let \mathfrak{H} be a separable Hilbert space. For each $A \in L^1(\mathfrak{H})$ and each unitary operator U on \mathfrak{H} , then $UAU^* \in \mathcal{L}^1(\mathfrak{H})$ and one has*

$$\|UAU^*\|_1 = \|A\|_1.$$

Exercise: prove the lemma above. (Hint: use the definition of the trace-norm.)

Now we need to control the interaction term.

First, since $V \in L^\infty$, one has

$$\begin{aligned} \|[V_{k,j+1}, D_{j+1}]\|_1 &\leq \|V_{k,j+1}D_{j+1}\|_1 + \|D_{j+1}V_{k,j+1}\|_1 \\ &\leq 2\|V_{k,j+1}\| \|D_{j+1}\|_1 \leq 2\|V\|_{L^\infty} \|D_{j+1}\|_1 \end{aligned}$$

for each $(D_j)_{j \geq 1}$ with $D_j \in \mathcal{L}^1(L^2((\mathbf{R}^d)^j))$ for each $j \geq 1$.

Next, we use the following auxiliary result.

Lemma 1.11.6 *Set $\mathfrak{H} = L^2(\mathbf{R}^{m+n})$ and $\mathfrak{H}_1 = L^2(\mathbf{R}^m)$. Let $K \in \mathcal{L}^1(\mathfrak{H})$ be an integral operator of the form*

$$K\phi(x, z) = \int_{\mathbf{R}^{m+n}} k(x, z, y, w)\phi(y, w)dydw.$$

Let $K_{z,w}$ be the operator defined on \mathfrak{H}_1 by

$$K_{z,w}\psi(x) = \int_{\mathbf{R}^m} k(x, z, y, w)\psi(y)dy$$

for a.e. $z, w \in \mathbf{R}^n$. Then

- (1) the map $h \mapsto [z \mapsto K_{z,z+h}]$ belongs to $C(\mathbf{R}_h^n, L^1(\mathbf{R}_z^n, \mathcal{L}^1(\mathfrak{H}_1)))$;
- (2) for a.e. $z \in \mathbf{R}^n$ the operator $K_{z,z}$ is trace-class on $L^2(\mathbf{R}^m)$ and

$$\text{trace} \left| \int_{\mathbf{R}^n} K_{z,z} dz \right| \leq \int_{\mathbf{R}^n} \text{trace} |K_{z,z}| dz \leq \|K\|_1.$$

This result is an amplification of Lemma 1.9.1 — see Lemma 2.1 in [7].

We apply the lemma above to

$$K = [V_{k,j+1}, D_{j+1}],$$

which is an integral operator with integral kernel

$$\begin{aligned} & k(X_j, x_{j+1}, Y_j, y_{j+1}) \\ &= (V(x_k - x_{j+1}) - V(y_k - y_{j+1}))D_{j+1}(X_j, x_{j+1}, Y_j, y_{j+1}). \end{aligned}$$

This shows that

$$\begin{aligned} \|[V_{k,j+1}, D_{j+1}]_{:j}\|_1 &= \text{trace} \left| \int_{\mathbf{R}^d} K_{z_{j+1}, z_{j+1}} dz_{j+1} \right| \\ &\leq \|K\|_1 \leq 2\|V\|_{L^\infty} \|D_{j+1}\|_1. \end{aligned}$$

Therefore we conclude that

$$\|L_{j,j+1}\|_{\mathcal{L}(E_{j+1}, E_j)} \leq 2j\|V\|_{L^\infty},$$

which means that the infinite quantum mean field hierarchy with bounded potential satisfies assumption (HL) in Theorem 1.11.4.

Step 3: Finally we control the growth of D_j as $j \rightarrow \infty$, where D_j is a limit point of $D_{N:j}$ in $L^\infty(\mathbf{R}_+; \mathcal{L}^1(L^2((\mathbf{R}^d)^j)))$ weak-* as $N \rightarrow \infty$. First we recall that, for each $N \geq 1$ and each $t \geq 0$, one has

$$D_N(t) = D_N(t)^* \geq 0, \quad \text{and } \|D_N(t)\|_1 = \text{trace } D_N(t) = 1.$$

Applying the lemma above shows that

$$\|D_{N:j}(t)\|_1 \leq 1 \quad \text{for all } t \geq 0, \quad N, j \geq 1.$$

(We recall the convention $D_{N:j} = 0$ whenever $j > N$.) Since

$$D_{N:j} \rightarrow D_j(t) \text{ in } L^\infty(\mathbf{R}_+; \mathcal{L}^1(L^2((\mathbf{R}^d)^j))) \text{ weak-*},$$

we conclude that

$$\|D_j(t)\|_1 \leq 1 \quad \text{for all } t \geq 0, \quad j \geq 1.$$

Step 4: One can apply Theorem 1.11.4 since the infinite hierarchy under consideration satisfies the bound (HL) with $C = 2\|V\|_{L^\infty}$, while each limit point D_j of the sequence $D_{N:j}$ in $L^\infty(\mathbf{R}_+; \mathcal{L}^1(L^2((\mathbf{R}^d)^j)))$ as $N \rightarrow \infty$ satisfies the growth estimate (Hu) with $R = 1$.

Indeed, setting

$$v_j(t) := U_j(t)(D_j(t) - |\psi(t, \cdot)^{\otimes j}\rangle\langle\psi(t, \cdot)^{\otimes j}|)$$

we know that the sequence $(v_j)_{j \geq 1}$ is a solution of the infinite mean field hierarchy, which satisfies

$$\|v_j(t)\|_{1,j} \leq \|D_j(t)\|_{1,j} + \||\psi(t, \cdot)^{\otimes j}\rangle\langle\psi(t, \cdot)^{\otimes j}|\|_{1,j} \leq 1 + \|\psi(t, \cdot)\|_{L^2}^{2j} = 2.$$

Since $v_j(0) = 0$ for each $j \geq 1$, we conclude from Theorem 1.11.4 that $v_j(t) = 0$ for each $j \geq 1$ and each $t \geq 0$. In other words,

$$D_j(t) = |\psi(t, \cdot)^{\otimes j}\rangle\langle\psi(t, \cdot)^{\otimes j}|$$

for each $j \geq 1$, which is precisely the desired result. ■

Notice that the verification of the growth condition (Hu) on the sequence $(D_j)_{j \geq 1}$ is trivial in this problem. This is not always the case, and we shall see some examples below, where checking this crucial condition can be a serious difficulty.

References for this section are [88, 7].

1.12 Other mean field limits in quantum mechanics

1.12.1 Derivation of the Schrödinger-Poisson equation

The quantum analogue of the Vlasov-Poisson system is the following variant of the Hartree equation, where the interaction potential is the repulsive Coulomb potential (between particles of equal charges):

$$V(z) = \frac{1}{4\pi|z|}$$

in space dimension $d = 3$. It takes the form

$$\begin{cases} i\partial_t \psi(t, x) = -\frac{1}{2}\Delta_x \psi(t, x) + U(t, x)\psi(t, x), & x \in \mathbf{R}^3, \\ U(t, x) = \frac{1}{4\pi} \int_{\mathbf{R}^3} \frac{|\psi(t, y)|^2}{|x - y|} dy, \end{cases}$$

or equivalently

$$\begin{cases} i\partial_t \psi(t, x) = -\frac{1}{2}\Delta_x \psi(t, x) + U(t, x)\psi(t, x), & x \in \mathbf{R}^3, \\ -\Delta_x U(t, x) = |\psi(t, x)|^2. \end{cases}$$

This last form of the mean field equation explains why, as mentioned above, the Hartree equation in this case is also known as the ‘‘Schrödinger-Poisson’’ equation.

Although the Coulomb potential is unbounded near the origin, the Schrödinger-Poisson equation can be derived following the strategy described above: see [32] for this very interesting result. In that case, the right choice of spaces E_n is as follows. Define

$$S_j := \sqrt{I - \Delta_{x_j}}, \quad j = 1, \dots, N.$$

With the same notation as above, the sequence of Banach spaces in Theorem 1.11.4 is defined as follows:

$$E_n := \{D \in \mathcal{L}^1(L^2((\mathbf{R}^3)^n)) \mid S_1 \dots S_n D S_1 \dots S_n \in \mathcal{L}^1(L^2((\mathbf{R}^3)^n))\},$$

for all $n \geq 1$, with norm

$$\|D\|_{E_n} = \text{trace} |S_1 \dots S_n D S_1 \dots S_n|.$$

With this choice of spaces, the inequality in assumption (HL) in Theorem 1.11.4 follows from Hardy's inequality

$$\int_{\mathbf{R}^3} \frac{f(x)^2}{|x|^2} dx \leq C \int_{\mathbf{R}^3} |\nabla f(x)|^2 dx$$

(see Lemma 7.1 in [32]).

The estimate (Hu) is a follows from the conservation laws

$$\frac{d}{dt} \text{trace}(H_N^m D_N(t)) = 0 \quad \text{for all } m \geq 0,$$

where

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V_{kl}$$

(with V_{kl} denoting the multiplication by $V(x_k - x_l)$) and

$$D_N(t) = |e^{itH_N}(\psi^{in})^{\otimes N}\rangle \langle e^{itH_N}(\psi^{in})^{\otimes N}|.$$

A crucial step in the proof of the growth estimate (Hu) is to compare powers of the N -particle Hamiltonian H_N with powers of the N -particle free Schrödinger operator

$$L_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k}$$

— see Propositions 4.1 and 5.1 in [32]. Verifying the growth condition (Hu) is perhaps the most technical parts of [32].

A more direct proof, by a somewhat different argument, was proposed later in [80] — see section 1.12.4 below.

1.12.2 Derivation of the nonlinear Schrödinger equation

One can consider the mean field limit with even more singular interactions, viz. $V(z) = \delta_0(z)$. Equivalently, one can prove the mean field limit with a potential whose range shrinks to zero as the number of particles tends to infinity. Specifically, one can consider the N -particle Schrödinger operator in space dimension 1:

$$H_N := -\frac{1}{2} \sum_{k=1}^N \partial_{x_k}^2 + \frac{1}{N} \sum_{k,l=1}^N N^\gamma U(N^\gamma(x_k - x_l))$$

where $U \geq 0$ belongs to the Schwartz class $\mathcal{S}(\mathbf{R})$, and $\gamma \in (0, 1)$.

The corresponding mean-field equation is the cubic nonlinear Schrödinger equation

$$i\partial_t\psi(t, x) = -\frac{1}{2}\partial_x^2\psi(t, x) + a|\psi(t, x)|^2\psi(t, x), \quad x \in \mathbf{R},$$

where

$$a = \int_{\mathbf{R}} U(z) dz.$$

In this case again, the strategy outlined in Theorem 1.11.4 applies with some appropriate choice of norms. The right choice of Banach spaces in this case is as follows:

$$E_n := \{D \in \mathcal{L}^2(L^2(\mathbf{R}^n)) \mid S_1 \dots S_n D S_1 \dots S_n \in \mathcal{L}^2(L^2(\mathbf{R}^n))\},$$

with norm

$$\|D\|_{E_n} = (\text{trace}(|S_1 \dots S_n D S_1 \dots S_n|^2))^{1/2},$$

where, as in the previous example,

$$S_j := \sqrt{I - \partial_{x_j}^2}, \quad j = 1, \dots, N.$$

Controlling the interaction operator in the n -th equation of the infinite mean field hierarchy associated to the Schrödinger operator H_N is essentially equivalent to controlling n integral operators on $L^2(\mathbf{R}^n)$ with integral kernels of the form

$$D_{n+1}(x_1, \dots, x_n, x_1, y_1, \dots, y_n, x_1)$$

in terms of $\|D_{n+1}\|_n$.

If D_n is the density matrix associated to a factorized wave function, i.e. if

$$D_n(x_1, \dots, x_n, y_1, \dots, y_n) = \psi(x_1) \dots \psi(x_n) \overline{\psi(y_1)} \dots \overline{\psi(y_n)},$$

then $D_n \in E_n$ if and only if $\psi \in H^1(\mathbf{R})$ and $\|D_n\|_n = \|\psi\|_{H^1}^{2n}$. In this case,

$$\begin{aligned} D_{n+1}(x_1, \dots, x_n, x_1, y_1, \dots, y_n, x_1) \\ = \psi(x_1) |\psi(x_1)|^2 \psi(x_2) \dots \psi(x_n) \overline{\psi(y_1)} \dots \overline{\psi(y_n)} \end{aligned}$$

and the estimate in assumption (HL) reduces to the fact that the Sobolev space $H^1(\mathbf{R})$ is an algebra. (Indeed, we recall that

$$u, v \in H^1(\mathbf{R}) \Rightarrow uv \in H^1(\mathbf{R}),$$

with

$$\|uv\|_{H^1} \leq C \|u\|_{H^1} \|v\|_{H^1} \quad \text{for all } u, v \in H^1(\mathbf{R})$$

for some positive constant C . This elementary fact is most easily checked in terms of the Fourier transforms of u and v .)

Proving the bound in assumption (HL) for general density matrices (and not only in the factorized case) is a rather straightforward generalization of the (classical) proof that $H^1(\mathbf{R})$ is an algebra. Proving the bound in assumption (Hu) is somewhat more technical and will not be discussed here.

We refer the interested reader to [2] — see also [1] — for a detailed statement of the result and a complete proof thereof.

The analogous result in space dimension higher than 1 is considerably more involved — notice that $H^1(\mathbf{R}^d)$ is not an algebra whenever $d \geq 2$, so that the argument above for the bound in assumption (HL) is no longer valid. The proof of the mean field limit for interaction potentials shrinking to a Dirac measure can be found in [30, 33, 34, 81]. An interesting approach to the uniqueness problem in the corresponding infinite hierarchy can be found in [62].

A general reference for this and the previous section is [38]. However Gérard's survey in [38] predates Pickl's contributions to the subject, which are described in section 1.12.4 below.

1.12.3 The time-dependent Hartree-Fock equations

In the quantum mean field theories considered so far, the asymptotic N -particle wave function always approached a factorized state of the form

$$\Psi_N(t, x_1, \dots, x_N) \sim \prod_{k=1}^N \psi(t, x_k)$$

in the limit as $N \rightarrow \infty$. In fact, we have assumed that the initial state is already of this form, i.e.

$$\Psi_N(0, x_1, \dots, x_N) = \prod_{k=1}^N \psi^{in}(x_k)$$

in all the situations considered so far. In particular, Ψ_N is symmetric in its space variables, i.e.

$$\Psi_N(t, x_{\sigma(1)}, \dots, x_{\sigma(N)}) = \Psi_N(t, x_1, \dots, x_N)$$

for all $\sigma \in \mathfrak{S}_N$ and all $x_1, \dots, x_N \in \mathbf{R}^d$. In other words, all the mean field theories considered above apply to the case of bosons; the case of fermions requires a separate study.

In the case of fermions, one should replace the initial factorized state with

$$\Psi_N(0, x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \det(\psi_k^{in}(x_l))_{1 \leq k, l \leq N}$$

where (ψ_1, \dots, ψ_N) is an orthonormal system in $L^2(\mathbf{R}^d)$, i.e.

$$\int_{\mathbf{R}^d} \overline{\psi_k^{in}(x)} \psi_l^{in}(x) dx = \delta_{kl}, \quad k, l = 1, \dots, N.$$

This special form of N -particle wave function is referred to as a *Slater determinant*.

Elementary computations show that Slater determinants satisfy

$$\int_{(\mathbf{R}^d)^N} |\det(\psi_k^{in}(x_l))_{1 \leq k, l \leq N}|^2 dx_1 \dots dx_N = N!$$

so that $\Psi_N(0, \dots)$ is normalized in $L^2((\mathbf{R}^d)^N)$.

Moreover, one easily checks that the density matrix associated to a Slater determinant has its first marginal given by

$$D_{N:1}(0) := |\Psi_N(0, \dots)\rangle\langle\Psi_N(0, \dots)|_{:1} = \frac{1}{N} \sum_{k=1}^N |\psi_k^{in}\rangle\langle\psi_k^{in}|.$$

In other words, $ND_{N:1}(0)$ is the orthogonal projector on $\text{span}(\{\psi_1, \dots, \psi_N\})$, so that

$$D_{N:1}(0)^* = D_{N:1}(0) = ND_{N:1}(0)^2 \geq 0, \quad \text{and } \text{trace}(D_{N:1}(0)) = 1.$$

Higher order marginals of the density matrix associated with a Slater determinant are given in terms of the first marginal by the following expressions:

$$D_{N:n}(0) = \frac{N^n(N-n)!}{N!} D_{N:1}(0)^{\otimes n} \sum_{\sigma \in \mathfrak{S}_n} (-1)^{\text{sign}(\sigma)} U_\sigma$$

for all $n = 1, \dots, N$, where we recall that, for each permutation $\sigma \in \mathfrak{S}_n$, the operator U_σ is defined by

$$U_\sigma \Phi_n(x_1, \dots, x_n) = \Phi_n(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(n)})$$

for all $\Phi_n \in L^2((\mathbf{R}^d)^n)$.

Consider the N -particle Schrödinger operator in the mean field scaling, i.e.

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_k + \frac{1}{N-1} \sum_{1 \leq k < l \leq N} V_{kl}$$

for all $N > 1$, where we recall that V_{kl} designates the multiplication by $V(x_k - x_l)$ acting on $L^2((\mathbf{R}^d)^N)$.

The expected mean field equation in the case of fermions is the time-dependent Hartree-Fock (TDHF) equation, written below in the language of operators

:

$$i\dot{F}(t) = [-\frac{1}{2}\Delta, F(t)] + [V_{12}, F(t)]^{\otimes 2}(I - U_{12})_{:1}.$$

Assuming that $F(t)$ is an integral operator on $L^2(\mathbf{R}^d)$ with integral kernel $F(t, x, y)$, the equation above can be recast in terms of integral kernels as follows:

$$\begin{aligned} i\partial_t F(t, x, y) &= -\frac{1}{2}(\Delta_x - \Delta_y)F(t, x, y) \\ &+ \int_{\mathbf{R}^d} (V(x-z) - V(y-z))(F(t, x, y)F(t, z, z) - F(t, z, y)F(t, x, z))dz, \end{aligned}$$

or equivalently

$$\begin{aligned} i\partial_t F(t, x, y) &= -\frac{1}{2}(\Delta_x - \Delta_y)F(t, x, y) \\ &\quad + F(t, x, y) \int_{\mathbf{R}^d} (V(x-z) - V(y-z))F(t, z, z) dz \\ &\quad - \int_{\mathbf{R}^d} (V(x-z) - V(y-z))F(t, x, z)F(t, z, y) dz. \end{aligned}$$

The existence and uniqueness of the solution of the Cauchy problem for the TDHF equation is extensively studied in [18, 19, 27].

The mean field limit in the case of N fermions with 2-body bounded interaction is summarized in the following statement.

Theorem 1.12.1 *Assume that V is an even function belonging to $L^\infty(\mathbf{R}^d)$, and let (ψ_1, \dots, ψ_N) be an orthonormal system in $L^2(\mathbf{R}^d)$. Let*

$$\Psi_N(t, \cdot) = e^{-itH_N} \Psi_N^{in},$$

where

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l),$$

and

$$\Psi_N^{in}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \det(\psi_k(x_l))_{1 \leq k, l \leq N}.$$

is the Slater determinant built on the orthonormal system (ψ_1, \dots, ψ_N) .

Then the density operator $D_N(t) := |\Psi_N(t)\rangle\langle\Psi_N(t)|$ satisfies

$$D_{N:n}(t) - \frac{N^n(N-n)!}{N!} D_{N:1}(t)^{\otimes n} \sum_{\sigma \in \mathfrak{S}_n} (-1)^{\text{sign}(\sigma)} U_\sigma \rightarrow 0$$

in $\mathcal{L}^1(L^2((\mathbf{R}^d)^n))$ as $N \rightarrow \infty$ for each $n \geq 1$, and

$$D_{N:1}(t) - F_N(t) \rightarrow 0$$

in $\mathcal{L}^1(L^2(\mathbf{R}^d))$ as $N \rightarrow \infty$, where $F_N(t)$ is the solution of the Cauchy problem

$$\begin{cases} i\dot{F}_N(t) = [-\frac{1}{2}\Delta, F_N(t)] + [V_{12}, F_N(t)^{\otimes 2}(I - U_{12})]_{:1}, \\ F_N(0) = \frac{1}{N} \sum_{k=1}^N |\psi_k^{in}\rangle\langle\psi_k^{in}|. \end{cases}$$

See [8, 9] for proofs of this result and of more general theorems in the same direction.

There is another, more familiar formulation of the TDHF equation. Seek the operator $F(t)$ in the form

$$F(t) = \frac{1}{N} \sum_{k=1}^N |\psi_k(t, \cdot)\rangle\langle\psi_k(t, \cdot)|,$$

or equivalently its integral kernel in the form

$$F(t, x, y) = \frac{1}{N} \sum_{k=1}^N \psi_k(t, x) \overline{\psi_k(t, y)},$$

where $(\psi_1(t, \cdot), \dots, \psi_N(t, \cdot))$ is an orthonormal system in $L^2(\mathbf{R}^d)$. Then the functions $\psi_k(t, \cdot)$ should satisfy the system of PDEs

$$\begin{aligned} i\partial_t \psi_k(t, x) &= -\frac{1}{2} \Delta_x \psi(t, x) + \psi_k(t, x) \int_{\mathbf{R}^d} V(x-z) \frac{1}{N} \sum_{l=1}^N |\psi_l(t, z)|^2 dz \\ &\quad - \frac{1}{N} \sum_{k=1}^N \psi_l(x) \int_{\mathbf{R}^d} V(x-z) \overline{\psi_l(t, z)} \psi_k(t, z) dz, \quad 1 \leq k \leq N. \end{aligned}$$

In this formulation, the functions ψ_k indexed by $k = 1, \dots, N$ are referred to as “molecular orbitals” in the context of quantum chemistry.

These equations are to be compared with the Hartree equation discussed above, i.e.

$$i\partial_t \psi(t, x) = -\frac{1}{2} \Delta_x \psi(t, x) + \psi(t, x) \int_{\mathbf{R}^d} V(x-z) |\psi(t, z)|^2 dz.$$

Obviously the term

$$\psi_k(t, x) \int_{\mathbf{R}^d} V(x-z) \frac{1}{N} \sum_{l=1}^N |\psi_l(t, z)|^2 dz$$

is the analogue in the Hartree-Fock case of the term

$$\psi(t, x) \int_{\mathbf{R}^d} V(x-z) |\psi(t, z)|^2 dz$$

in Hartree’s equation. The additional term in the Hartree-Fock equation, i.e.

$$-\frac{1}{N} \sum_{k=1}^N \psi_l(x) \int_{\mathbf{R}^d} V(x-z) \overline{\psi_l(t, z)} \psi_k(t, z) dz$$

is called the “exchange interaction integral” and is special to the case of fermions: see for instance [64] (Problem 1 on p. 233).

Approaching the N -particle wave function of a system of fermions by a Slater determinant is obviously the most natural idea. However, other choices are also possible — and often made in practice, especially for the purpose of numerical computations in the context of quantum chemistry. One such method is the theory of multi-configuration time-dependent Hartree-Fock equations [11], where the N -particle functions is approximated by a linear combination of Slater determinants. For the first detailed analysis of the multi-configuration ansatz,

which has a very rich mathematical structure, we refer the interested reader to [4].

Hartree-Fock equations are used primarily in the context of quantum chemistry. Therefore, one has to take into account the following interactions

- (a) electron-electron,
- (b) electron-nuclei,
- (c) nuclei-nuclei.

In many situations, the nuclei are considered either as fixed (as in [66]), or as macroscopic objects governed by a system of ODEs (as in [24]), while the quantum description of the electron system involves the Hartree-Fock equations. In that case, the only part of the Hamiltonian that is approximated by a non-linear, self-consistent mean-field interaction is the repulsive force (a) between electrons.

All these interactions involve the Coulomb potential; the derivation of the time dependent Hartree-Fock theory from the N -particle Schrödinger equation with Coulomb interactions remains an open problem at the time of this writing.

1.12.4 Pickl's approach to quantum mean field limits

There are other approaches to the mean field limit in quantum mechanics — see for instance the work of Rodnianski and Schlein [85], which proposes an error estimate for the mean field limit, that uses the formalism of Fock spaces in second quantization, as well as the more recent references [35, 36].

In the present section, we give a brief presentation of yet another approach of the mean field limit that avoids the technicalities of BBGKY hierarchies as well as the formalism of Fock spaces. The discussion below is based on [80].

Pickl's idea is to consider some appropriate quantity that measures the distance between the first marginal $D_{N:1}(t)$ of the N -particle density matrix $D_N(t)$ and the single particle density matrix $|\psi(t, \cdot)\rangle\langle\psi(t, \cdot)|$ built on the solution ψ of the Hartree equation.

Let Ψ_N be the solution of the N -particle Schrödinger equation

$$\begin{cases} i\partial_t \Psi_N(t, x_1, \dots, x_N) = H_N \Psi_N(t, x_1, \dots, x_N), & x_1, \dots, x_N \in \mathbf{R}^d, \\ \Psi_N|_{t=0} = (\psi^{in})^{\otimes N}, \end{cases}$$

with

$$H_N := -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l).$$

Let ψ be the solution of Hartree's equation

$$\begin{cases} i\partial_t \psi(t, x) = -\frac{1}{2} \Delta_x \psi(t, x) + (V \star_x |\psi|^2) \psi(t, x), & x \in \mathbf{R}^d, \\ \psi|_{t=0} = \psi^{in}. \end{cases}$$

Consider the quantity

$$\mathcal{E}_N(t) := \text{trace}(D_{N:1}(t)(I - |\psi(t, \cdot)\rangle\langle\psi(t, \cdot)|)).$$

Pickl's derivation of the mean field limit is based on proving that

$$\mathcal{E}_N(t) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

This estimate implies that $D_{N:1}(t)$ converges to $|\psi(t, \cdot)\rangle\langle\psi(t, \cdot)|$ in operator norm, in view of the lemma below.

Henceforth we denote by \mathfrak{H}_N the N -particle Hilbert space $\mathfrak{H}_N := L^2((\mathbf{R}^d)^N)$ for each $N \geq 1$, and we set

$$\rho(t) := |\psi(t, \cdot)\rangle\langle\psi(t, \cdot)|.$$

Lemma 1.12.2 *Let $N \geq 1$ and Ψ_N be a symmetric element of \mathfrak{H}_N such that $\|\Psi_N\|_{\mathfrak{H}_N} = 1$. Let $D_N := |\Psi_N\rangle\langle\Psi_N|$ and let $\psi \in \mathfrak{H}_1$ satisfy $\|\psi\|_{\mathfrak{H}_1} = 1$. Then*

$$\text{trace}(D_{N:1}(I - |\psi\rangle\langle\psi|)) \rightarrow 0 \quad \text{as } N \rightarrow \infty$$

if and only if

$$D_{N:1} \rightarrow |\psi\rangle\langle\psi| \quad \text{in operator norm as } N \rightarrow \infty.$$

This elementary result is statement (a) in Lemma 2.3 of [80]. In some sense, it can be considered as a variant of the exercise at the end of section 1.9. Notice that $\Psi_N(t, \cdot)$ is a symmetric function of x_1, \dots, x_N for all $t \in \mathbf{R}$ by Lemma 1.8.5, and because of the choice of the initial data $\Psi_N|_{t=0} = (\psi^{in})^{\otimes N}$, which is itself a symmetric function of x_1, \dots, x_N .

Next we seek to control the evolution of $\mathcal{E}_N(t)$. We recall that, for $k, l = 1, \dots, N$, the notation V_{kl} designates the operator on \mathfrak{H}_N defined as

$$(V_{kl}\Phi_N)(x_1, \dots, x_N) := V(x_k - x_l)\Phi_N(x_1, \dots, x_N).$$

Since $\text{trace}(D_{N:1}(t)) = 1$, one has

$$\begin{aligned} \dot{\mathcal{E}}_N(t) &= -\frac{d}{dt} \text{trace}(D_{N:1}(t)\rho(t)) \\ &= -\text{trace}(\dot{D}_{N:1}(t)\rho(t)) - \text{trace}(D_{N:1}(t)\dot{\rho}(t)) \\ &= -\text{trace}(i[\frac{1}{2}\Delta, D_{N:1}(t)]\rho(t)) - \text{trace}(iD_{N:1}(t)[\frac{1}{2}\Delta, \rho(t)]) \\ &\quad + \frac{N-1}{N} \text{trace}(i[V_{12}, D_{N:2}(t)]_{:1}\rho(t)) + \text{trace}(iD_{N:1}(t)[V_{12}, \rho(t)]^{\otimes 2}_{:1}). \end{aligned}$$

First

$$[\frac{1}{2}\Delta, D_{N:1}(t)]\rho(t) + D_{N:1}(t)[\frac{1}{2}\Delta, \rho(t)] = [\frac{1}{2}\Delta, D_{N:1}(t)\rho(t)],$$

so that

$$\begin{aligned} \text{trace}([\frac{1}{2}\Delta, D_{N:1}(t)]\rho(t)) + \text{trace}(D_{N:1}(t)[\frac{1}{2}\Delta, \rho(t)]) \\ = \text{trace}([\frac{1}{2}\Delta, D_{N:1}(t)\rho(t)]) = 0. \end{aligned}$$

Next

$$\begin{aligned} \text{trace}([V_{12}, D_{N:2}(t)]_{:1} \rho(t)) &= \text{trace}([V_{12}, D_{N:2}(t)](\rho(t) \otimes I)), \\ \text{trace}(D_{N:1}(t)[V_{12}, \rho(t)^{\otimes 2}]_{:1}) &= \text{trace}(D_{N:2}(t)([V_{12}, \rho(t)^{\otimes 2}]_{:1} \otimes I)). \end{aligned}$$

Therefore

$$\begin{aligned} \dot{\mathcal{E}}_N(t) &= \frac{N-1}{N} \text{trace}(i[V_{12}, D_{N:2}(t)]\rho(t) \otimes I) + \text{trace}(iD_{N:2}(t)[V_{12}, \rho(t)^{\otimes 2}]_{:1}) \\ &= -i \text{trace}(D_{N:2}(t)[\frac{N-1}{N}V_{12} - (V \star |\psi(t, \cdot)|^2) \otimes I, \rho(t) \otimes I]). \end{aligned}$$

The result of this computation is summarized in the following lemma.

Lemma 1.12.3 *With the same notation as above, one has*

$$\dot{\mathcal{E}}_N(t) = \mathcal{F}_N(t)$$

where

$$\mathcal{F}_N(t) := 2 \text{Im} \text{trace}(D_{N:2}(t)(\rho(t) \otimes I)A((I - \rho(t)) \otimes I))$$

and

$$A := \frac{N-1}{N}V_{12} - (V \star |\psi(t, \cdot)|^2) \otimes I.$$

The core of Pickl's argument is the following estimate for $\mathcal{F}_N(t)$ in terms of $\mathcal{E}_N(t)$ and N .

Proposition 1.12.4 *Assuming that $r \geq 1$ and denoting by $r' = \frac{r}{r-1}$ the dual Hölder exponent of r , one has*

$$|\mathcal{F}_N(t)| \leq 10 \|V\|_{L^{2r}} \|\psi(t, \cdot)\|_{L^{2r'}} (\mathcal{E}_N(t) + \frac{1}{N}).$$

The proof of Proposition 1.12.4 is sketched below. The interested reader is referred to the original paper [80] for more details.

For the sake of notational simplicity, we set

$$p(t) := I - \rho(t).$$

Elementary computations show that

$$\begin{aligned} \mathcal{F}_N(t) &= 2 \text{Im} \text{trace}(D_{N:2}(t)\rho(t)^{\otimes 2} A(p(t) \otimes \rho(t))) \\ &\quad + 2 \text{Im} \text{trace}(D_{N:2}(t)\rho(t)^{\otimes 2} A p(t)^{\otimes 2}) \\ &\quad + 2 \text{Im} \text{trace}(D_{N:2}(t)(\rho(t) \otimes p(t)) A p(t)^{\otimes 2}). \end{aligned}$$

The term

$$\text{Im} \text{trace}(D_{N:2}(t)(\rho(t) \otimes p(t)) A(p(t) \otimes \rho(t)))$$

vanishes identically by symmetry of $\Psi_N(t, \cdot)$.

The first term on the right hand side is mastered as follows: observe that

$$(I \otimes \rho(t))A(I \otimes \rho(t)) = -\frac{1}{N}(V \star |\psi(t, \cdot)|^2) \otimes \rho(t)$$

— where $V \star |\psi(t, \cdot)|^2$ designates the operator on $\mathfrak{H}_1 = L^2(\mathbf{R}^d)$ defined by

$$\phi \mapsto (V \star |\psi(t, \cdot)|^2)\phi.$$

Therefore

$$\begin{aligned} & |\text{trace}(D_{N:2}(t)\rho(t)^{\otimes 2}A(p(t) \otimes \rho(t)))| \\ = & |\text{trace}(D_{N:2}(t)(\rho(t) \otimes I)(I \otimes \rho(t))A(I \otimes \rho(t))(p(t) \otimes I))| \\ & \leq \|(\rho(t) \otimes I)(I \otimes \rho(t))A(I \otimes \rho(t))(p(t) \otimes I)\| \|D_{N:2}\|_1 \\ & \leq \|(\rho(t) \otimes I)(I \otimes \rho(t))A(I \otimes \rho(t))\|. \end{aligned}$$

Then, observing that A is self-adjoint since V is a real-valued, even function, one has

$$\begin{aligned} & \|(\rho(t) \otimes I)(I \otimes \rho(t))A(I \otimes \rho(t))\|^2 \\ = & \|(\rho(t) \otimes I)((I \otimes \rho(t))A(I \otimes \rho(t)))^2(\rho(t) \otimes I)\| \\ = & \frac{1}{N^2} \|\langle \psi(t, \cdot) | (V \star |\psi(t, \cdot)|^2)^2 \psi(t, \cdot) \rangle \rho(t) \otimes \rho(t)\| \\ & \leq \frac{1}{N^2} \int_{\mathbf{R}^d} (V \star |\psi(t, \cdot)|^2)^2(x) |\psi(t, x)|^2 dx \\ & \leq \frac{1}{N^2} \| (V \star |\psi(t, \cdot)|^2)^2 \|_{L^r} \| \psi(t, \cdot)^2 \|_{L^{r'}} \\ & = \frac{1}{N^2} \| V \star |\psi(t, \cdot)|^2 \|_{L^{2r}}^2 \| \psi(t, \cdot) \|_{L^{2r'}}^2 \\ & \leq \frac{1}{N^2} \| V \|_{L^{2r}}^2 \| \psi(t, \cdot) \|_{L^{2r'}}^2. \end{aligned}$$

Indeed,

$$\|V \star |\psi(t, \cdot)|^2\|_{L^{2r}} \leq \|V\|_{L^{2r}} \| |\psi(t, \cdot)|^2 \|_{L^1} = \|V\|_{L^{2r}}$$

since the solution of Hartree's equation satisfies $\|\psi(t, \cdot)\|_{L^2} = 1$ for all $t \in \mathbf{R}$.

The third term satisfies

$$\begin{aligned} & |\text{trace}(D_{N:2}(t)(\rho(t) \otimes p(t))Ap(t)^{\otimes 2})| \\ & \leq \|(\rho(t) \otimes I)A(p(t) \otimes I)\| \| (I \otimes p(t))D_{N:2}(t)(I \otimes p(t)) \|_1 \\ = & \|(\rho(t) \otimes I)A(p(t) \otimes I)\| \text{trace}((I \otimes p(t))D_{N:2}(t)(I \otimes p(t))) \\ & \leq \|(\rho(t) \otimes I)A\| \text{trace}(D_{N:1}p(t)) \\ & = \|(\rho(t) \otimes I)A\| \mathcal{E}_N(t). \end{aligned}$$

Now

$$\begin{aligned} & \|(\rho(t) \otimes I)A\|^2 = \|(\rho(t) \otimes I)A^2(\rho(t) \otimes I)\| \\ & \leq (2\|V^2\|_{L^r} + 2\|(V \star |\psi(t, \cdot)|^2)^2\|_{L^r}) \| |\psi(t, \cdot)|^2 \|_{L^{r'}} \\ & = (2\|V\|_{L^{2r}}^2 + 2\|V \star |\psi(t, \cdot)|^2\|_{L^{2r}}^2) \| \psi(t, \cdot) \|_{L^{2r'}}^2 \\ & \leq 4\|V\|_{L^{2r}}^2 \| \psi(t, \cdot) \|_{L^{2r'}}^2, \end{aligned}$$

again because the solution ψ of Hartree's equation satisfies $\|\psi(t, \cdot)\|_{L^2} = 1$ for all $t \in \mathbf{R}$.

Controlling the second term in $\mathcal{F}_N(t)$ is slightly more complicated.

We shall need the following elements of notation. First we denote by $p(t)$ the projection $p(t) = I_1 - \rho(t) = I_1 - |\psi(t, \cdot)\rangle\langle\psi(t, \cdot)|$.

For each $j = 1, \dots, N$, we set $I_j := I_{\mathfrak{H}_j}$, and for each $T \in \mathcal{L}(\mathfrak{H}_1)$, we define $T_{j,N} \in \mathcal{L}(\mathfrak{H}_N)$ for $j = 1, \dots, N$ as

$$T_{j,N} := I_{j-1} \otimes T \otimes I_{N-j}.$$

For each $a \in \{0, 1\}^{\{1, \dots, N\}}$ and each $\pi \in \mathcal{L}(\mathfrak{H}_1)$ such that $\pi^* = \pi = \pi^2$, we define

$$P_N[a, \pi] := \prod_{j=1}^N \pi_{j,N}^{1-a(j)} (I - \pi_{j,N})^{a(j)}$$

Lemma 1.12.5 *Let*

$$M_N(t) = \frac{1}{N} \sum_{j=1}^N p_{j,N}(t)$$

Then

$$M_N(t) = \sum_{k=1}^N \frac{k}{N} \Pi_{k,N}[\rho(t)]$$

where

$$\Pi_{k,N}[\rho(t)] := \sum_{\substack{a \in \{0,1\}^{\{1,\dots,N\}} \\ a(1)+\dots+a(N)=k}} P_N[a, \rho(t)].$$

Besides

$$\Pi_{j,N}[\rho(t)]^* = \Pi_{j,N}[\rho(t)], \quad \text{and } \Pi_{j,N}[\rho(t)]\Pi_{k,N}[\rho(t)] = \delta_{jk}\Pi_{j,N}[\rho(t)]$$

for each $j, k = 1, \dots, N$, and

$$\sum_{k=0}^N \Pi_{k,N}[\rho(t)] = I_{\mathfrak{H}_N}.$$

In other words, the relation

$$M_N(t) = \sum_{k=0}^N \frac{k}{N} \Pi_{k,N}[\rho(t)]$$

is the spectral decomposition of the self-adjoint element $M_N(t)$ of $\mathcal{L}(\mathfrak{H}_N)$. These elementary computations are summarized in formula (6) of [80].

Define, for each $\alpha > 0$,

$$M_N^\alpha(t) = \sum_{k=1}^N \left(\frac{k}{N}\right)^\alpha \Pi_{k,N}[\rho(t)]$$

and

$$M_N^{-\alpha}(t) := \sum_{k=1}^N \left(\frac{k}{N} \right)^{-\alpha} \Pi_{k,N}[\rho(t)],$$

that is the pseudo-inverse of $M_N^\alpha(t)$ extended by 0 on $\text{Ker}(M_N(t))$. In other words

$$M_N^\alpha(t)M_N^{-\alpha}(t) = I_N - \Pi_{0,N}[\rho(t)]$$

In particular

$$M_N^\alpha(t)M_N^{-\alpha}(t)p_{j,N}(t) = p_{j,N}(t)$$

for each $j = 1, \dots, N$.

After this observation, the term that remains to be estimated, i.e.

$$\text{trace}(D_{N:2}(t)\rho(t)^{\otimes 2}A(I - \rho(t))^{\otimes 2})$$

is recast as

$$\text{trace}(D_N(t)\rho_{1,N}(t)\rho_{2,N}(t)AM_N^{1/2}(t)M_N^{-1/2}(t)p_{1,N}(t)p_{2,N}(t)).$$

Then

$$\begin{aligned} & |\text{trace}(D_N(t)\rho_{1,N}(t)\rho_{2,N}(t)AM_N^{1/2}(t)M_N^{-1/2}(t)p_{1,N}(t)p_{2,N}(t))| \\ & \leq \|M_N^{-1/2}(t)p_{1,N}(t)p_{2,N}(t)\Psi_N(t, \cdot)\|_{\mathfrak{H}_N} \\ & \quad \times \|M_N^{1/2}(t)A\rho_{1,N}(t)\rho_{2,N}(t)\Psi_N(t, \cdot)\|_{\mathfrak{H}_N}. \end{aligned}$$

The second factor on the right hand side is mastered by observing that

$$\begin{aligned} & \|M_N^{1/2}(t)A\rho_{1,N}(t)\rho_{2,N}(t)\Psi_N(t, \cdot)\|_{\mathfrak{H}_N}^2 \\ & = \langle \Psi_N(t, \cdot) | \rho_{1,N}(t)\rho_{2,N}(t)AM_N(t)A\rho_{1,N}(t)\rho_{2,N}(t)\Psi_N(t, \cdot) \rangle \\ & = \frac{N-2}{N} \langle \Psi_N(t, \cdot) | \rho_{1,N}(t)\rho_{2,N}(t)Ap_{3,N}(t)A\rho_{1,N}(t)\rho_{2,N}(t)\Psi_N(t, \cdot) \rangle \\ & \quad + \frac{2}{N} \langle \Psi_N(t, \cdot) | \rho_{1,N}(t)\rho_{2,N}(t)Ap_{1,N}(t)A\rho_{1,N}(t)\rho_{2,N}(t)\Psi_N(t, \cdot) \rangle \end{aligned}$$

since $\Psi_N(t, \cdot)$ is symmetric. The first summand is bounded by

$$\begin{aligned} & \frac{N-2}{N} \|\rho_{1,N}(t)A^2\rho_{1,N}(t)\|_{\mathcal{L}(\mathfrak{H}_N)} \|p_{3,N}(t)\Psi_N(t)\|_{\mathfrak{H}_N}^2 \\ & \leq \|\rho_{1,N}(t)A^2\rho_{1,N}(t)\|_{\mathcal{L}(\mathfrak{H}_N)} \mathcal{E}_N(t) \\ & \leq 4\|V\|_{L^{2r}}^2 \|\psi(t, \cdot)\|_{L^{2r'}}^2 \mathcal{E}_N(t), \end{aligned}$$

while the second is bounded by

$$\frac{2}{N} \|\rho_{1,N}(t)A^2\rho_{1,N}(t)\|_{\mathcal{L}(\mathfrak{H}_N)} \leq \frac{8}{N} \|V\|_{L^{2r}}^2 \|\psi(t, \cdot)\|_{L^{2r'}}^2.$$

Finally, we use again the fact that $\Psi_N(t, \cdot)$ is symmetric to conclude that

$$\begin{aligned}
 & N(N-1) \|M_N^{-1/2}(t) p_{1,N}(t) p_{2,N}(t) \Psi_N(t, \cdot)\|_{\mathfrak{H}_N}^2 \\
 &= N(N-1) \langle \Psi_N(t, \cdot), M_N^{-1}(t) p_{1,N}(t) p_{2,N}(t) \Psi_N(t, \cdot) \rangle \\
 &= 2 \sum_{1 \leq j < k \leq N} \langle \Psi_N(t, \cdot), M_N^{-1}(t) p_{j,N}(t) p_{k,N}(t) \Psi_N(t, \cdot) \rangle \\
 &\leq N^2 \langle \Psi_N(t, \cdot), M_N^{-1}(t) M_N^2(t) \Psi_N(t, \cdot) \rangle \\
 &= N^2 \langle \Psi_N(t, \cdot), M_N(t) \Psi_N(t, \cdot) \rangle \\
 &= N^2 \mathcal{E}_N(t).
 \end{aligned}$$

Putting all these estimates together establishes the bound in Proposition 1.12.4

Applying Gronwall's estimate, we deduce from Proposition 1.12.4 the following result, stated in space dimension 3 for the sake of simplicity. The assumptions on the potential V have been adapted to match those in Kato's Theorem 1.8.1.

Theorem 1.12.6 *Let V be a real-valued even function such that*

$$V \in L^{2r}(\mathbf{R}^3) \quad \text{and } V|_{\mathbf{R}^3 \setminus B(0,R)} \in L^\infty$$

for some $r \geq 1$ and some $R > 0$.

Let $\psi^{in} \in L^2(\mathbf{R}^3)$ be such that $\|\psi^{in}\|_{L^2} = 1$, and assume that the Cauchy problem for Hartree's equation with initial data ψ^{in} has a unique solution $\psi \in C(\mathbf{R}; L^{2r'}(\mathbf{R}^3))$, where $r' = \frac{r}{r-1}$ is the dual Hölder exponent of r . Let Ψ_N be the solution of the Cauchy problem for the N -particle Schrödinger equation with initial data $(\psi^{in})^{\otimes N}$, and $D_N(t) := |\Psi_N(t, \cdot)\rangle \langle \Psi_N(t, \cdot)|$.

Then, for each $t \in \mathbf{R}$, one has

$$D_{N;1}(t) \rightarrow |\psi(t, \cdot)\rangle \langle \psi(t, \cdot)| \text{ in operator norm as } N \rightarrow +\infty,$$

with the estimate

$$\begin{aligned}
 & \text{trace}(D_{N;1}(t)(I - |\psi(t, \cdot)\rangle \langle \psi(t, \cdot)|)) \\
 & \leq \frac{1}{N} \left(\exp \left| \int_0^t 10 \|V\|_{L^{2r}} \|\psi(s, \cdot)\|_{L^{2r'}} ds \right| - 1 \right).
 \end{aligned}$$

Some remarks are in order after this rather remarkable result.

The first obvious advantage of Pickl's argument is its simplicity. The proof of Proposition 1.12.4 and the resulting Theorem 1.12.6 provide a much simpler derivation of the mean field limit for potentials with a Coulomb singularity at the origin than the Erdős-Yau proof [32] based on the BBGKY hierarchy. According to Theorem 3.1 in [39], if $\psi^{in} \in H^k(\mathbf{R}^3)$, then the unique mild solution ψ of Hartree's equation belongs to $C(\mathbf{R}_+; H^k(\mathbf{R}^3))$ under the same assumption on V as in Theorem 1.12.6. Therefore $\psi \in C(\mathbf{R}; L^{2r'}(\mathbf{R}^3))$ by Sobolev's embedding theorem provided that k is chosen large enough. In fact, even stronger

singularities at the origin than Coulomb in the interaction potential can be handled with this method.

A second advantage of Pickl's method is its versatility. For instance, it can also be applied to the derivation of the Gross-Pitaevski: see [81]. In this latter reference, Pickl uses appropriate nonlinear functions of the operator $M_N(t)$, which are defined in terms of the spectral decomposition provided by Lemma 1.12.5. The same type of method also applies to study the convergence rate in the mean field limit [63] in a more general and systematic way than in Theorem 1.12.6 above.

On the other hand, unlike methods based on the BBGKY hierarchy, Pickl's argument [80] seems to be limited to pure states and to bosonic particles so far. Therefore, in spite of its appealing simplicity, Pickl's method does not really supersede all previous derivations of the mean field limits in quantum mechanics.

Besides, even if BBGKY hierarchies are a rather cumbersome mathematical object, they are ubiquitous in the field of nonequilibrium statistical physics, and appear in the treatment of quantum as well as classical mechanical models. This accounts for the importance of these hierarchies in these lectures.

1.13 Afterword

These notes are an updated and (much) expanded version of my earlier (2003) lectures [42]. I express my gratitude to my colleagues A. Muntean, J. Rademacher and A. Zagaris for their kind invitation to the NDNS+ 2012 Summer School at Universiteit Twente in Enschede. The first part of these notes (sections 1-6) were also presented in a joint course with L. Desvillettes at the 37th Summer School on Mathematical Physics in Ravello (2012). I am also very grateful to Profs. T. Ruggeri and S. Rionero, and to the participants for their positive feedback, as well as for the most enjoyable hospitality of the Ravello school.

As in [42], the core of the material presented here is the mean field limit of N -particle systems governed by the equations of classical mechanics in the case where the N -particle empirical measure is an exact weak solution of the mean field PDE, and the mean field limit of the N -particle Schrödinger equation.

Unlike in [42], I have chosen to introduce both the approach based on empirical measures and the method based on the BBGKY hierarchy on the mean field limit of the N -particle systems in classical mechanics with Lipschitz continuous interaction kernel K . The discussion of the propagation of chaos in section 1.6 is much more detailed here than in [42]. The connection between the empirical measure and the hierarchy approaches is hopefully clarified by the discussion in sections 1.6.2, 1.7.1 and 1.7.3.

The most recent developments — in particular results obtained since the publication of [42] — are surveyed in sections 1.7 and 1.12. However, I have chosen to give less many details on the derivation of the time-dependent Hartree-Fock equations from the N -particle Schrödinger equation. The discussion of the time-dependent Hartree-Fock equations in the present notes is limited to a

presentation of the equations and to the statement of the main result obtained on this problem. My earlier notes [42] contain a sketch of the proof of the mean field limit leading to the time-dependent Hartree-Fock equations; the interested reader is referred to [42] for more details in this direction.

I have limited myself to a discussion of evolution problems. Yet there are many important results bearing on steady problems: see for instance the work of Caglioti-Lions-Marchioro-Pulvirenti [23] and Kießling [61] on the Onsager statistical theory of vortices in incompressible fluids. I have also neglected to discuss the similarities and the differences between the mean field limit of large particles systems and the convergence of particle methods for mean field equations. The interested reader will find information on these issues in chapter 5 of [71] in the context of the vortex formulation of the Euler equations for two dimensional incompressible fluids. See also, in the context of Vlasov type equations, [13, 28, 97] and the references therein.

I have also deliberately chosen to avoid discussing results that would involve both the mean field limit (as the particle number N tends to infinity) and the classical limit of quantum mechanics (assuming that the typical action of an individual particle is large compared to Planck's constant \hbar). One of the reasons for this choice is that this part of the theory is technically more involved and perhaps not as complete as what has been presented above. Yet there are many important contributions of in this directions, and the interested reader should have a look at [51, 74], to quote only a few references exploring that topic.

Another conspicuous omission in the second part of these notes is the formalism of Fock spaces and quantum field theory. This mathematical setting allows considering data where the particle number can be infinite — more precisely, the particle number N is an unbounded operator in this formalism. The mean field limit can be formulated in this setting: see for instance [9, 35, 36], together with the papers [51, 40] already mentioned above, involving the classical limit in addition to the case of infinitely many particles. Interestingly, there is a striking analogy between the classical limit of quantum mechanics in formulated in terms of Egorov's theorem (Theorem 25.3.5 in [55]) and the point of view introduced in [35, 36] for the quantum mean field limit: see [35] on p. 1024.

I am indebted in various ways to several colleagues for the material presented in these notes. First I wish to thank my collaborators R. Adami, C. Bardos, B. Ducomet, L. Erdős, A. Gottlieb, N. Mauser, V. Ricci, A. Teta and H.-T. Yau, with whom I have worked on mean field limits on various occasions. Besides, the material presented here is in (many) places far from original, and the present notes owe much to earlier presentations of mean field limits — such as [92] or unpublished notes by C. Villani, as well as lectures by P.-L. Lions at the Collège de France. I also learned a lot from a series of lectures by C. Mouhot presenting his joint work with S. Mischler and B. Wennberg [72, 73] on quantitative estimates for the propagation of chaos. Most of what I know on the derivation of Vlasov type equations from classical particle dynamics comes from discussions with J. Batt, H. Neunzert, J. Wick on various occasions in the late 80s. I learned of Dobrushin's beautiful estimate [29] from a lecture given by M. Pulvirenti at Ecole Normale Supérieure in 1997.

Another key idea in these lectures is the use of the Nirenberg-Ovcyannikov abstract version of the Cauchy-Kovalevska theorem to handle BBGKY type hierarchies. I got acquainted with this idea in a seminar given by S. Ukai at the Sone seminar in 1998 in Kyoto. Ukai used this technique in a slightly different context (the derivation of the Boltzmann equation from the dynamics of a large number of hard spheres in the Boltzmann-Grad limit), and for a slightly different purpose (he wanted to simplify the uniform stability estimates in Lanford's argument). With his usual modesty, Ukai presented his result as a failed attempt at simplifying Lanford's notoriously intricate proof, and did not immediately published it — I came across his paper [93] only very recently. In the case of the infinite mean field hierarchies for quantum N -particle dynamics, I find the argument based on the abstract variant the Cauchy-Kovalevska theorem much more elegant and illuminating than the conventional argument based on the Duhamel series as in Lanford's proof, and thus I have chosen to present the former in these notes, as in [42]. The argument based on the Duhamel series can be found in many places — see for instance the proof of Theorem 5.7 on p. 610 in [88].

S. Ukai was at the origin of several fundamental results on the mathematical analysis of kinetic models — such as the existence and uniqueness of global solutions of the Boltzmann equation for all initial data near Maxwellian equilibrium, the existence and uniqueness of global solutions of the Vlasov-Poisson system [94] in space dimension 2, the hydrodynamic limit of the Boltzmann equation leading to the incompressible Navier-Stokes equations in the regime of “small” initial data. In view of his influence on some of the topics discussed above, these notes are dedicated to his memory.

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