

The Mean-Field Limit for the Dynamics of Large Particle Systems

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Abstract

This short course explains how the usual mean-field evolution PDEs in Statistical Physics — such as the Vlasov-Poisson, Schrödinger-Poisson or time-dependent Hartree-Fock equations — are rigorously derived from first principles, i.e. from the fundamental microscopic models that govern the evolution of large, interacting particle systems.

Mon cher Athos, je veux bien, puisque votre santé l'exige absolument, que vous vous reposiez quinze jours. Allez donc prendre les eaux de Forges ou telles autres qui vous conviendront, et rétablissez-vous promptement. Votre affectionné

TRÉVILLE

ALEXANDRE DUMAS *Les Trois Mousquetaires*

1. A review of physical models

The subject matter of these lectures is the relation between “exact” microscopic models that govern the evolution of large particle systems and a certain type of approximate models known in Statistical Mechanics as “mean-field equations”. This notion of mean-field equation is best understood by getting acquainted with the most famous examples of such equations, described below.

MSC 2000 : 82C05, 82C10, 82C22, 35A10, 35Q40, 35Q55.

Keywords : mean-field limit, Vlasov equation, Hartree approximation, Hartree-Fock equations, BBGKY hierarchy, propagation of chaos, Slater determinant.

1.1. Examples of mean-field equations

Roughly speaking, a mean-field equation is a model that describes the evolution of a typical particle subject to the collective interaction created by a large number N of other, like particles. The state of the typical particle is given by its phase space density; the force field exerted by the N other particles on this typical particle is approximated by the average with respect to the phase space density of the force field exerted on that particle from each point in the phase space.

Here are the most famous examples of mean-field equations.

1.1.1. The Vlasov equation

The Vlasov equation is the kinetic model for collisionless gases or plasmas. Let $f \equiv f(t, x, \xi)$ be the phase space density of point particles that occupy position $x \in \mathbf{R}^D$ and have momentum $\xi \in \mathbf{R}^D$ at time $t \geq 0$. Let $V \equiv V(x, y)$ be the potential describing the pairwise interaction exerted by a particle located at position y on a particle located at position x . Vlasov's equation reads

$$\begin{aligned} \partial_t f + \frac{1}{m} \xi \cdot \nabla_x f + F(t, x) \cdot \nabla_\xi f &= 0, \quad x, \xi \in \mathbf{R}^D, \\ F(t, x) &= -\nabla_x \iint_{\mathbf{R}^D \times \mathbf{R}^D} V(x, y) f(t, y, \xi) d\xi dy. \end{aligned} \quad (1.1)$$

The parameter m in the PDE above is the particle mass; below, we shall set it to be 1 without further apology, along with other physical constants.

In other words, Vlasov's equation can be put in the form of a Liouville equation

$$\partial_t f + \{H_{f(t, \cdot, \cdot)}, f\} = 0$$

with a time-dependent Hamiltonian given by the formula

$$H_{f(t, \cdot, \cdot)}(x, \xi) = \frac{1}{2m} |\xi|^2 + \iint_{\mathbf{R}^D \times \mathbf{R}^D} V(x, y) f(t, y, \xi) d\xi dy. \quad (1.2)$$

This formulation may be the best justification for the term “mean-field”: the field exerted on the typical particle at time t and position x is created by the potential

$$\int_{\mathbf{R}^D} V(x, y) \left(\int_{\mathbf{R}^D} f(t, x, \xi) d\xi \right) dy$$

which is the sum of the elementary potentials created at position x by one particle located at position y distributed according to the macroscopic density

$$\rho_f(t, x) = \int_{\mathbf{R}^D} f(t, x, \xi) d\xi. \quad (1.3)$$

The best known physical example of (1.1) (in space dimension $D = 3$) is the case where

$$V(x, y) = \frac{q}{4\pi} \frac{1}{|x - y|} \quad \text{electrostatic potential created by a charge } q$$

that is used to model collisionless plasmas with negligible magnetic effects. In truth, plasmas are made of several species of charged particles (electrons and ions); thus in reality the description of a plasma would involve as many transport equations in (1.1) as there are particle species to be considered, while the total electric force would be computed in terms of the sum of macroscopic densities of all particles weighted by the charge number of each particle species (e.g., if q is minus the charge of one electron, $Z = -1$ for electrons, $Z = 1, 2, \dots$ for positively charged ions...)

Another physical example of (1.1) is the case where

$$V(x, y) = -\frac{Gm}{|x - y|} \quad \text{gravitational potential created by a mass } m$$

where G is Newton's constant. This model is used in Astronomy, in very specific contexts. Its mathematical theory is harder than that of the electrostatic case because the interaction between like particles in the present case is attractive (unlike in the previous case, where particle of like charges are repelled by the electrostatic force), which may lead to buildup of concentrations in the density.

Both models go by the name of “Vlasov-Poisson” equation, since V is, up to a sign, the fundamental solution of Poisson's equation

$$-\Delta_x U = \rho$$

in $\mathbf{R}^3$.

There are many more physical examples of mean field equations of the Vlasov type than these two. For instance, one can replace the electrostatic interaction with the full electromagnetic interaction between charged, relativistic particles. The analogue of the Vlasov-Poisson equation in this case (in the somewhat unphysical situation where only one species of charged particles is involved) is

$$\partial_t f + \frac{1}{m} \xi \cdot \nabla_x f + \frac{q}{m} \left(E + \frac{1}{c} v(\xi) \times B(t, x) \right) \cdot \nabla_\xi f = 0 \quad (1.4)$$

coupled to the system of Maxwell's equations

$$\begin{aligned} \partial_t E - c \operatorname{curl}_x B &= -j_f, & \operatorname{div}_x E &= \rho_f, \\ \partial_t B + c \operatorname{curl}_x E &= 0, & \operatorname{div}_x B &= 0, \end{aligned} \quad (1.5)$$

where

$$v(\xi) = \frac{\xi}{\sqrt{m^2 + \frac{|\xi|^2}{c^2}}}, \quad j_f(t, x) = \int_{\mathbf{R}^3} v(\xi) f(t, x, \xi) d\xi.$$

The system (1.4)-(1.5) is called “the relativistic Vlasov-Maxwell system”. It is a good exercise to find its Hamiltonian formulation.

There are many more examples of Vlasov type equations, such as the Vlasov-Einstein equation which is the relativistic analogue of the gravitational Vlasov-Poisson equation above. There also exists a Vlasov-Yang-Mills equation for the quark-gluon plasma.

1.1.2. The mean-field Schrödinger equation

Vlasov-type equations are classical, instead of quantum, models. There exist non-relativistic, quantum analogues of Vlasov's equation (1.1). We shall be mainly concerned with two such models, the mean-field Schrödinger equation that is presented in this section, and the time-dependent Hartree-Fock equation, to be described in the next section.

The recipe for building the mean-field Schrödinger equation is to start from the time-dependent, classical mean-field Hamiltonian (1.2) in the form

$$H_{\rho(t,\cdot)}(x, \xi) = \frac{1}{2m}|\xi|^2 + \int_{\mathbf{R}^D} V(x, y)\rho(t, y)dy$$

and to *quantize* it by the usual rule $\xi \mapsto \frac{\hbar}{i}\nabla_x$, leading to the operator

$$\mathcal{H}_{\rho(t,\cdot)} = -\frac{\hbar^2}{2m}\Delta_x + \int_{\mathbf{R}^D} V(x, y)\rho(t, y)dy.$$

If one considers a large number of undistinguishable quantum particles in the same "pure" state, the whole system of such particles is described by one wave function $\psi \equiv \psi(t, x) \in \mathbf{C}$, and the density ρ is given by

$$\rho(t, x) = |\psi(t, x)|^2.$$

The evolution of the wave function ψ is governed by the mean-field Schrödinger equation

$$\begin{aligned} i\hbar\partial_t\psi &= \mathcal{H}_{|\psi(t,\cdot)|^2}\psi \\ &= -\frac{\hbar^2}{2m}\Delta_x\psi + \left(\int_{\mathbf{R}^D} V(x, y)|\psi(t, y)|^2dy \right) \psi \end{aligned} \quad (1.6)$$

It may also happen that the N particles are in distinct quantum states, defined by a family of N wave functions, $\psi_k \equiv \psi_k(t, x)$, $k = 1, \dots, N$, that are orthonormal in L^2 , i.e. $\langle \psi_k | \psi_l \rangle = \delta_{kl}$. In this case, the density ρ is

$$\rho(t, x) = \frac{1}{N} \sum_{k=1}^N |\psi_k(t, x)|^2,$$

and each wave function is governed by the Schrödinger equation defined by the Hamiltonian $\mathcal{H}_{\rho(t,\cdot)}$, i.e. the system

$$\begin{aligned} i\hbar\partial_t\psi_k &= -\frac{\hbar^2}{2m}\Delta_x\psi_k + \left(\frac{1}{N} \sum_{k=1}^N \int_{\mathbf{R}^D} V(x, y)|\psi_k(t, y)|^2dy \right) \psi_k, \\ &k = 1, \dots, N. \end{aligned} \quad (1.7)$$

One might think that the mean-field Schrödinger equation is a less universal object than its classical counterpart (the Vlasov equation) since there are so many variants of it — (1.6) and (1.7) for instance.

In fact, (1.6) and (1.7) (and all the other variants of the mean-field Schrödinger equation) are unified by considering instead the formulation of Quantum Mechanics

in terms of operators. In this formulation, the state of this system is described by a time-dependent, integral operator $D(t) \in \mathcal{L}(L^2(\mathbf{R}^D))$ — with integral kernel denoted by $D(t, x, y)$ — that satisfies the von Neumann equation

$$i\hbar\partial_t D = [\mathcal{H}_{\rho(t, \cdot)}, D], \quad \text{where } \rho(t, x) = D(t, x, x). \quad (1.8)$$

The operator $D(t)$ is usually referred to as the density operator, while its integral kernel $D(t, x, y)$ is called the density matrix. A more explicit form of (1.8) is

$$\begin{aligned} i\hbar\partial_t D(t, x, y) = & -\frac{\hbar^2}{2m}(\Delta_x - \Delta_y)D(t, x, y) \\ & + D(t, x, y) \int (V(x - z) - V(y - z))D(t, z, z)dz. \end{aligned} \quad (1.9)$$

In the case corresponding to the single mean-field Schrödinger equation (1.6), the density matrix is given by

$$D(t, x, y) = \psi(t, x)\overline{\psi(t, y)}, \quad (1.10)$$

and the density operator it defines is usually denoted

$$D(t) = |\psi(t, \cdot)\rangle\langle\psi(t, \cdot)|.$$

In the case corresponding to the system of N coupled mean-field Schrödinger equations (1.7), the density matrix is given by

$$D(t, x, y) = \frac{1}{N} \sum_{k=1}^N \psi_k(t, x)\overline{\psi_k(t, y)}, \quad (1.11)$$

while the density operator it defines is

$$D(t) = \frac{1}{N} \sum_{k=1}^N |\psi_k(t, \cdot)\rangle\langle\psi_k(t, \cdot)|.$$

Of course, in either case, the mean-field von Neumann equation (1.8) is equivalent to (1.6) or (1.7) — up to some unessential phase factor that may depend on t , the wave functions are recovered as the eigenfunctions of the density operator.

However, the mean-field von Neumann equation (1.8) does not take into account a purely quantum effect, the “exchange interaction”, that is described in the next section.

1.1.3. The (time-dependent) Hartree-Fock equation

It is a well-known fact that the electrical interaction of (non-relativistic) charged particles is independent of their spins. However, the effect of the spin of non-relativistic particles is seen on their statistics. Indeed, one deduces from Relativistic Quantum Mechanics that particles with integer spin are bosons, meaning that the wave function of a system consisting of N such particles is a symmetric function of their positions (see [20], §11). A similar argument shows that the wave function of a

system of N particles with half-integer spin is a skew-symmetric function of their positions (see [20], §25); in other words, such particles are fermions. For instance photons, α particles, hydrogen atoms, or π mesons are bosons, while electrons, positrons, protons, neutrons etc... are fermions. That the wave function of a system of N fermions is skew-symmetric implies *Pauli's exclusion principle*: two (or more) fermions cannot find themselves in the same quantum state. This apparently innocuous statement has far-reaching physical consequences — for instance on the structure of atoms, where successive electronic layers are filled with electrons of opposite spins.

Returning to the discussion in the previous section, one immediately sees that the mean-field Schrödinger equation (1.6), applies to bosons only, since it is a model based on the assumption that the N particles are in the same quantum state characterized by the wave function ϕ . This particular situation is referred to as “Bose condensation”, and is typical for bosons at zero temperature.

Consider next a system consisting of 2 fermions: its wave function takes the form

$$\frac{1}{\sqrt{2}} (\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)) ,$$

where (ψ_1, ψ_2) is an orthonormal system of $L^2(\mathbf{R}^D)$. If $V \equiv V(|x_1 - x_2|)$ is a pairwise interaction potential, the interaction energy of this system is

$$\begin{aligned} & \iint V(x_1 - x_2) |\psi_1(x_1)|^2 |\psi_2(x_2)|^2 dx_1 dx_2 \\ & - \iint V(x_1 - x_2) \psi_1(x_1) \overline{\psi_1(x_2)} \psi_2(x_2) \overline{\psi_2(x_1)} dx_1 dx_2 . \end{aligned} \quad (1.12)$$

In the expression above, the second integral is the “exchange interaction” (see [19], §62, problem 1).

From this elementary computation, one easily arrives at the mean-field equation for N fermions: the k -th particle is subject to the sum of all interactions of the form (1.12) exerted by the $N - 1$ other particles:

$$\begin{aligned} i\hbar\partial_t\psi_k(t, x) &= -\frac{\hbar^2}{2m}\Delta\psi_k(t, x) \\ &+ \frac{1}{N} \sum_{l=1}^N \psi_k(t, x) \int V(|x - y|) |\psi_l(t, y)|^2 dy \\ &- \frac{1}{N} \sum_{l=1}^N \psi_l(t, x) \int V(|x - y|) \psi_k(t, y) \overline{\psi_l(t, y)} dy , \quad 1 \leq k \leq N . \end{aligned} \quad (1.13)$$

This system of equations is known as the “time dependent Hartree-Fock equations” (abbreviated as TDHF); the wave functions ψ_k go by the name of “orbitals” of the system — we recall that the term “orbital” applies to that part of the wave function that does not depend on the spin variables.

Perhaps the simplest method for obtaining this system consists in writing the Hamiltonian as the sum of the kinetic energies of each particle, i.e.

$$\sum_{k=1}^N \frac{\hbar^2}{2m} \int |\nabla_x \psi_k(t, x)|^2 dx ,$$

and of all the terms of the form (1.12) corresponding to each pair of particles. Then the evolution equation associated to the resulting Hamiltonian, say $\mathcal{H}$, is

$$i\hbar\partial_t\psi_k = \frac{\delta\mathcal{H}}{\delta\psi_k(t,x)}.$$

The constant $1/N$ on the right-hand side of (1.13) scales the interaction so that in the total energy (Hamiltonian $\mathcal{H}$), both the kinetic and interaction energies are of the same order of magnitude.

To emphasize the similarity between the TDHF equations and (1.9) — which may not seem that obvious on the formulation involving orbitals — let us write the operator form of (1.13). Let $D \equiv D(t, x, y)$ be the density matrix defined as in (1.11); assuming that the orbitals ψ_k satisfy (1.13), $D(t, x, y)$ must satisfy

$$\begin{aligned} i\hbar\partial_t D(t, x, y) = & -\frac{\hbar^2}{2m}(\Delta_x - \Delta_y)D(t, x, y) \\ & + \int (V(x-z) - V(y-z))D(t, x, y)D(t, z, z)dz \\ & - \int (V(x-z) - V(y-z))D(t, x, z)D(t, z, y)dz. \end{aligned} \quad (1.14)$$

In fact there are several variants of the TDHF equations presented here. In many applications (to Chemistry, for instance), they govern the evolution of electrons. In this case, the interaction potential V involved in equations (1.13) is the Coulomb repulsive potential between negatively charged particles; it is also necessary to include other terms modelling the effect of the positively charged particles (nuclei, ions...). In most cases, including these terms does not result in additional mathematical difficulties, since they lead to linear perturbations of (1.13) in the electronic orbitals. For this reason, we shall restrict our attention to the simplified model (1.13) or (1.14) in this course.

1.2. First principle equations

Next we turn our attention to the fundamental equations describing the dynamics of a system of N particles. In this course, we only consider non-relativistic particles. We are mainly concerned with quantum models; however, we also discuss the derivation of Vlasov's equation from the classical N -body problem, in the limit as $N \rightarrow +\infty$.

1.2.1. The classical N -body problem

Consider a system of N point particles of mass m . In the absence of external forces (such as gravity), these particles are subject only to binary interactions corresponding to a potential $V \equiv V(x_1, x_2)$. (Obviously, V is symmetric: $V(x_1, x_2) = V(x_2, x_1)$). If $x_k \equiv x_k(t)$ denotes the position of the k -th particle, Newton's second law of motion for each particle is expressed in the form of the system of N second-order differential equations:

$$m\ddot{x}_k = - \sum_{1 \leq l \neq k \leq N} \nabla_{x_k} V(x_k, x_l), \quad 1 \leq k \leq N. \quad (1.15)$$

Equivalently, one can write the Hamiltonian of this system of N particles as the total energy = kinetic energy + potential energy, i.e.

$$H_N(x_1, \dots, x_N, \xi_1, \dots, \xi_N) = \sum_{k=1}^N \frac{|\xi_k|^2}{2m} + \sum_{1 \leq l < k \leq N} V(x_k, x_l). \quad (1.16)$$

The system of second order differential equations (1.15) is equivalent to the system of Hamilton's equations

$$\dot{x}_k = \nabla_{\xi_k} H_N, \quad \dot{\xi}_k = -\nabla_{x_k} H_N. \quad (1.17)$$

The integral curves of this system of first-order differential equations are the characteristic curves of the Liouville equation

$$\begin{aligned} \partial_t F_N + \{H_N, F_N\} := \\ \partial_t F_N + \sum_{k=1}^N \nabla_{\xi_k} H_N \cdot \nabla_{x_k} F_N - \sum_{k=1}^N \nabla_{x_k} H_N \cdot \nabla_{\xi_k} F_N = 0 \end{aligned} \quad (1.18)$$

In (1.18), $F_N \equiv F_N(t, x_1, \dots, x_N, \xi_1, \dots, \xi_N)$ can be seen as the joint probability density of the system of N particles in the N -body phase space, i.e.

$$F_N(t, x_1, \dots, x_N, \xi_1, \dots, \xi_N) dx_1 \dots dx_N d\xi_1 \dots d\xi_N$$

is the probability that the particle 1 is to be found in a volume $dx_1 d\xi_1$ of the 1-particle phase space $\mathbf{R}^D \times \mathbf{R}^D$ around (x_1, ξ_1) , that the particle 2 is to be found in a volume $dx_2 d\xi_2$ of the 1-particle phase space $\mathbf{R}^D \times \mathbf{R}^D$ around (x_2, ξ_2) , and so on. (In truth, the system of characteristics (1.17) can be used to propagate just *any* function F_N on the N -body phase space, but the only such function that is physically meaningful is the joint probability density described above).

1.2.2. The quantum N -body problem

Next we describe the quantum analogue of (1.15). The quickest route to this model is to *quantize* the Hamiltonian H_N in (1.16), as we already did for the mean-field Hamiltonian. Here, *quantization* means associating to a *function* defined on the N -body *phase space* $(\mathbf{R}_x^D \times \mathbf{R}_\xi^D)^N$ an *operator* acting on the Hilbert space $L^2((\mathbf{R}_x^D)^N)$ — here, $(\mathbf{R}_x^D)^N$ is usually called the *configuration space*. For an arbitrary function, there is more than one way of doing this; but for a function such as H_N , quantization means replacing the momentum *variable* ξ_k with the momentum *operator* $\frac{\hbar}{i} \nabla_{x_k}$. Therefore, the Hamiltonian function H_N is transformed into the Hamiltonian operator

$$\mathcal{H}_N = \sum_{k=1}^N -\frac{\hbar^2}{2m} \Delta_{x_k} + \sum_{1 \leq k < l \leq N} V(x_k, x_l). \quad (1.19)$$

With the Hamiltonian (1.19), one writes the N -body Schrödinger equation

$$\begin{aligned} i\hbar \partial_t \Psi_N &= \mathcal{H}_N \Psi_N \\ &= \sum_{k=1}^N -\frac{\hbar^2}{2m} \Delta_{x_k} \Psi_N + \sum_{1 \leq k < l \leq N} V(x_k, x_l) \Psi_N. \end{aligned} \quad (1.20)$$

Here $\Psi_N \equiv \Psi_N(t, x_1, \dots, x_N)$ is the wave-function of the system of N particles.

The analogue of the classical, N -body Liouville equation (1.18) is the N -body von Neumann equation

$$\begin{aligned} i\hbar\partial_t D_N(t, X_N, Y_N) &= [\mathcal{H}_N, D_N](t, X_N, Y_N) \\ &= \sum_{k=1}^N -\frac{\hbar^2}{2m}(\Delta_{x_k} - \Delta_{y_k})D_N(t, X_N, Y_N) \\ &\quad + \sum_{1 \leq k < l \leq N} (V(x_k, x_l) - V(y_k, y_l))D_N(t, X_N, Y_N), \end{aligned} \quad (1.21)$$

with the notation $X_N = (x_1, \dots, x_N)$, $Y_N = (y_1, \dots, y_N)$, where the density matrix is defined in terms of the wave-function by the formula

$$D_N(t, X_N, Y_N) = \Psi_N(t, X_N) \overline{\Psi_N(t, Y_N)}.$$

It is left as an easy exercise to check that, if Ψ_N is a solution of the Schrödinger equation (1.20), then the density matrix defined by the formula above is a solution of the von Neumann equation (1.21).

1.3. Another example of mean-field limit

There is another classical example of mean-field limit, namely the vorticity formulation of the two-dimensional Euler equation of perfect, incompressible fluids. Let $u(t, x) = (u_1(t, x_1, x_2), u_2(t, x_1, x_2))$ be the velocity field and $\omega = (\partial_{x_1} u_2 - \partial_{x_2} u_1)$. The Euler equation is

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

Taking the curl of the equation above leads to

$$\partial_t \omega + \operatorname{div}_x(u\omega) = 0, \quad u = \nabla_x^\perp \Delta^{-1} \omega$$

where the orthogonal gradient is defined as $\nabla^\perp = (-\partial_{x_2}, \partial_{x_1})$. The operator $\nabla_x^\perp \Delta^{-1}$ — say, on $\mathbf{T}^2$ — is an integral operator of the form

$$u(t, x) = (K \star \omega(t, \cdot))(x),$$

where K is the orthogonal gradient of the fundamental solution of Δ , so that the vorticity formulation above of the Euler equation is recast as

$$\partial_t \omega + \operatorname{div}_x((K \star \omega(t, \cdot))\omega) = 0. \quad (1.22)$$

This is another example of mean-field PDE, very similar to the Vlasov-Poisson equation. In his famous article [28], Onsager got the idea of explaining two-dimensional turbulence by the methods of Statistical Mechanics applied to (1.22), viewed as the mean-field limit of a system of point vortices of equal strengths located at the positions $z_1(t), \dots, z_N(t)$ satisfying the system of ODEs

$$\dot{z}_k = \frac{1}{N} \sum_{1 \leq l \neq k \leq N} K(Z_k(t) - z_l(t)), \quad 1 \leq k \leq N. \quad (1.23)$$

We refer to [9] and to [17] for a mathematical treatment of some of the main ideas in Onsager's paper.

This description is also used to design numerical methods for the two-dimensional Euler equations (the so-called vortex method): we refer the interested reader to the book by Marchioro-Pulvirenti [23] and to the references therein.

However, we shall not insist too much on this theme in these lectures, since the N -vortex system (1.23) is not a fundamental principle of physics, but rather an approximation of the physical model (1.22). Yet, in view of the simplicity of this model, we shall use it instead of Vlasov's equation in Appendices A-B to part I of these lectures, to show Dobrushin's stability estimate in terms of the Wasserstein distance, with its application to the propagation of chaos.

1.4. The Boltzmann equation is not a mean-field equation

Vlasov's equation belongs to the kinetic theory of plasmas. Indeed, it governs the 1-particle phase space density of a system consisting of a large number of like point particles, which is precisely the fundamental notion that appeared in the founding papers by Maxwell and Boltzmann.

However, not every kinetic model is a mean-field equation. The most famous of such models, the Boltzmann equation itself, is not. It reads

$$(\partial_t + v \cdot \nabla_x) f = \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (f' f'_1 - f f_1) |v \cdot \omega| dv_1 d\omega \quad (1.24)$$

where $f \equiv f(t, x, v)$ is the probability density of particles which, at time t , are at position x with velocity v . The notations f_1 , f' and f'_1 designate respectively $f(t, x, v_1)$, $f(t, x, v')$, and $f(t, x, v'_1)$, where

$$v' = v - (v - v_1) \cdot \omega \omega, \quad v'_1 = v_1 + (v - v_1) \cdot \omega \omega.$$

It is interesting to compare the Vlasov equation (1.1) with (1.24). Since the momentum $\xi = mv$ where m is the particle mass, this amounts to comparing

$$-F \cdot \nabla_\xi f \quad \text{with} \quad \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (f' f'_1 - f f_1) |v \cdot \omega| dv_1 d\omega.$$

The latter term, which is Boltzmann's collision integral, describes the loss of particles with velocity v due to binary collisions with particles located at the same position x with an arbitrary velocity v_1 , and the creation of particles with that velocity v due to binary collisions involving one particle with velocity v' and another particle with velocity v'_1 , both located at that same position x . Here, particles are viewed as hard spheres with radius 0 and the collisions are assumed to be perfectly elastic. Hence, each particle is unaffected by all the other particles, unless it touches another particle, in which case a collision of the type described above occurs. Because the radius of these particles is negligible — or 0 — collisions involving more than two particles are infinitely rare events and are discarded in Boltzmann's equation.

By contrast, the former term, i.e. the mean-field term in Vlasov's equation, takes into account the effect on any given particle of all the other particles, and not

only the effect of its closest neighbor. In this sense, one could think that Vlasov's equation is better adapted at describing long-range interactions, while Boltzmann's equation is better suited for short-range interactions. There is some truth in such a statement, which however fails to capture the essential differences between both models.

In fact, Boltzmann's equation for hard spheres was rigorously derived by Lanford [22] from the model analogous to (1.15) where the potential V is replaced with hard sphere collisions, under some scaling assumption known as *the Boltzmann-Grad scaling*. There is an unpublished proof by King [18] that does the same for some class of short-range potentials. Vlasov's equation is also derived from (1.15), but under a very different scaling assumption.

Rather strikingly, both limits lead to very different qualitative behaviors. For instance, it is believed (and indeed proved in a variety of cases by Desvillettes and Villani [13]) that the long time limit of the Boltzmann equation in a compact domain (e.g. on a flat 3-torus) leads to uniform Maxwellian distributions (i.e. Gaussian distributions in the v variable with moments that are constant in the variable x). Boltzmann's H-Theorem states that, if f is a solution to the Boltzmann equation, the quantity

$$- \iint f(t, x, v) \ln f(t, x, v) dx dv \quad (1.25)$$

(which represents some form of entropy) increases until f reaches a Maxwellian equilibrium. This is related to the notion of *irreversibility* in Statistical Mechanics, however in a way that was very misleading in Boltzmann's time, thereby leading to bitter controversy.

On the contrary, this quantity is a constant if f is a solution to the Vlasov equation — this is left as an easy exercise, whose solution is reminiscent of the proof of Liouville's theorem on Hamilton's equation (i.e. the invariance of the measure $dx d\xi$ under the Hamiltonian flow). Moreover, the long time limit of the solution of Vlasov's equation on a compact domain, say on a flat torus, is not yet understood, and seems a rather formidable open problem. By the way, it is interesting to note that the quantum analogue of (1.25) is

$$\text{trace}(D(t) \ln D(t))$$

where $D \equiv D(t)$ is the density operator — notice that $D(t) \ln D(t)$ is well defined by the continuous functional calculus, since $D(t)$ is a positive self-adjoint operator and $z \mapsto z \ln z$ a continuous function on $\mathbf{R}_+$.

OUTLINE

PART I: FROM THE CLASSICAL N -BODY PROBLEM TO VLASOV'S EQUATION

PART II: FROM THE QUANTUM N -BODY PROBLEM TO HARTREE'S EQUATION

PART III: FROM THE QUANTUM N -BODY PROBLEM TO THE TDHF EQUATIONS

Part I. From the classical N -body problem to Vlasov's equation

In this section, we start from the classical N -body problem in Hamiltonian form:

$$\begin{aligned}\dot{x}_k &= \xi_k, \\ \dot{\xi}_k &= -\frac{1}{N} \sum_{1 \leq l \leq N} \nabla_x V(x_k, x_l)\end{aligned}\tag{I.1}$$

which is equivalent to (1.17) with a Hamiltonian

$$H_N(x_1, \dots, x_N, \xi_1, \dots, \xi_N) = \sum_{k=1}^N \frac{1}{2} |\xi_k|^2 + \frac{1}{N} \sum_{1 \leq l < k \leq N} V(x_k, x_l)\tag{I.2}$$

where the interaction potential $V \equiv V(x, y)$ is scaled by the $1/N$ factor.

This situation is known as “the weak coupling scaling”; it naturally leads to mean-field equations, since the force exerted on each particle is of order one as $N \rightarrow +\infty$.

Perhaps the most convincing argument in favor of this scaling is as follows: since the total kinetic energy is a sum of N terms and the total potential energy is a sum of $\frac{1}{2}N(N-1)$ terms, the $1/N$ factor in multiplying the potential scales the kinetic and potential energy in the Hamiltonian to be of the same order of magnitude as $N \rightarrow +\infty$.

For notational simplicity, we set $z_k = (x_k, \xi_k) \in \mathbf{R}^D \times \mathbf{R}^D$, with $k = 1, \dots, N$. The potential $V : \mathbf{R}^D \times \mathbf{R}^D \rightarrow \mathbf{R}$ is assumed to satisfy

$$V \in C_b^2(\mathbf{R}^D \times \mathbf{R}^D), \quad V(x, y) = V(y, x) \text{ for all } x, y \in \mathbf{R}^D.\tag{I.3}$$

Under this assumption, the Hamiltonian vector field

$$Z \mapsto (\nabla_{x_k} H_N(Z), -\nabla_{\xi_k} H_N(Z))_{1 \leq k \leq N}^T$$

belongs to $C_b^1((\mathbf{R}^D \times \mathbf{R}^D)^N, (\mathbf{R}^D \times \mathbf{R}^D)^N)$.

By the Cauchy-Lipschitz theorem, for each $Z_N^0 \in (\mathbf{R}^D \times \mathbf{R}^D)^N$, there exists a unique solution $Z_N(t) = (x_k(t), \xi_k(t))_{1 \leq k \leq N}$ to the system of ODEs (1.17) such that $Z_N(0) = Z_N^0$. This solution is denoted by $Z_N \equiv Z_N(t, Z_N^0)$ and is defined for all times. Finally, Z_N belongs to $C^1(\mathbf{R} \times (\mathbf{R}^D \times \mathbf{R}^D)^N; (\mathbf{R}^D \times \mathbf{R}^D)^N)$.

Definition I.1. *The empirical distribution of the system of N particles is the probability measure on $\mathbf{R}^D \times \mathbf{R}^D$ defined as*

$$f_{N, Z_N^0}(t, \cdot) = \frac{1}{N} \sum_{k=1}^N \delta_{z_k(t, Z_N^0)}.$$

This is a probability measure *on the 1-particle phase space*, and yet, it is equivalent to know f_{N, Z_N^0} or to know the trajectory of each of the particles considered. This probability measure is not to be confused with the unknown in the Liouville equation (1.18), the latter being a probability measure *on the N -particle phase space*.

We shall discuss the relation between these two probability measures in Appendix B below.

For the time being, let us point at a nice feature of the empirical distribution: like the solution f of the Vlasov's equation — the target equation to be derived from (1.17) — it is already defined on the 1-particle phase space, unlike the solution of the Liouville equation (1.18), that lives in a different, bigger space.

In fact, f_{N,Z_N^0} is a solution — in fact an approximate solution — to (1.1) in the sense of distributions, and this statement is equivalent to the fact that (x_k, ξ_k) is a solution to (1.17).

Lemma I.2. *Let $Z_N \equiv Z_N(t, Z_N^0)$ be the solution of (I.1) with initial data $Z_N(0, Z_N^0) = Z_N^0$. Then the empirical distribution f_{N,Z_N^0} satisfies*

$$\begin{aligned} \partial_t f_{N,Z_N^0} + \xi \cdot \nabla_x f_{N,Z_N^0} + \operatorname{div}_\xi (F_{N,Z_N^0}(t, x) f_{N,Z_N^0}) \\ = \frac{1}{N^2} \sum_{k=1}^N \operatorname{div}_\xi (\nabla_x V(x_k, x_k) \delta_{z_k(t, Z_N^0)}) \end{aligned} \quad (\text{I.4})$$

in the sense of distributions, where

$$F_{N,Z_N^0}(t, x) = -\nabla_x \iint V(x, y) f_{N,Z_N^0}(t, dy, d\xi).$$

(In (I.4), $\nabla_x V$ designates the derivative with respect to the first group of variables in the product space $\mathbf{R}^D \times \mathbf{R}^D$).

Proof. Let $\phi \equiv \phi(x, \xi) \in C_c^\infty(\mathbf{R}^D \times \mathbf{R}^D)$. Then

$$\begin{aligned} \partial_t \langle f_{N,Z_N^0}(t), \phi \rangle &= \frac{1}{N} \sum_{k=1}^N \dot{x}_k(t) \cdot \nabla_x \phi(x_k(t), \xi_k(t)) \\ &\quad + \frac{1}{N} \sum_{k=1}^N \dot{\xi}_k(t) \cdot \nabla_\xi \phi(x_k(t), \xi_k(t)) \\ &= \frac{1}{N} \sum_{k=1}^N \xi_k(t) \cdot \nabla_x \phi(x_k(t), \xi_k(t)) \\ &\quad + \frac{1}{N} \sum_{k=1}^N F_{N,Z_N^0}(t, x_k(t)) \cdot \nabla_\xi \phi(x_k(t), \xi_k(t)) \\ &\quad - \frac{1}{N^2} \sum_{k=1}^N \nabla_x V(x_k(t), x_k(t)) \cdot \nabla_\xi \phi(x_k(t), \xi_k(t)) \end{aligned}$$

which gives the announced equality. $\square$

Next we study the limiting behavior of f_{N,Z_N^0} as $N \rightarrow +\infty$; some uniform estimates are needed for this. In fact we need only the conservation of Hamilton's function under the Hamiltonian flow (1.17), expressed in the following manner:

Lemma I.3. Let $Z_N^0 = (x_k^0, \xi_k^0)_{1 \leq k \leq N}$. Assume that

$$\sup_{\substack{1 \leq k \leq N \\ N \geq 1}} |\xi_k^0| < +\infty.$$

Then

$$\sup_{\substack{N \geq 1 \\ t \in \mathbf{R}}} \iint |\xi|^2 f_{N, Z_N^0}(t, x, \xi) dx d\xi < +\infty.$$

Proof. The Hamiltonian H_N is constant on the integral curves of the associated Hamiltonian vector field; hence

$$\frac{1}{N} H_N(Z_N(t, Z_N^0)) = \frac{1}{N} H_N(Z_N^0) \leq \frac{1}{2} \sup_{1 \leq k \leq N, N \geq 1} |\xi_k^0|^2 + \frac{1}{2} \|V\|_{L^\infty}.$$

On the other hand, one has

$$\begin{aligned} \iint |\xi|^2 f_{N, Z_N^0}(t, x, \xi) dx d\xi &= \frac{1}{N} \sum_{k=1}^N |\xi_k(t)|^2 \\ &\leq \frac{2}{N} H_N(Z_N(t, Z_N^0)) + \|V\|_{L^\infty}, \end{aligned}$$

which implies the announced result. $\square$

Lemma I.4. Let $V \in C_r^2(\mathbf{R}^D \times \mathbf{R}^D)^1$. Let Z_N^0 be such that

$$f_{N, Z_N^0}(0) = \frac{1}{N} \sum_{k=1}^N \delta_{(Z_N^0)_k} \rightarrow f^0$$

weakly- $*$ in $\mathcal{M}(\mathbf{R}^D \times \mathbf{R}^D)^2$ and

$$H_N(Z_N^0) = O(N)$$

as $N \rightarrow +\infty$. Then, the sequence f_{N, Z_N^0} is relatively compact in $C(\mathbf{R}_+; w^* - \mathcal{M}(\mathbf{R}^D \times \mathbf{R}^D))$ (for the topology of uniform convergence on compact subsets of $\mathbf{R}_+$) and each of its limit points as $N \rightarrow +\infty$ is a solution f to the Vlasov equation

$$\begin{aligned} \partial_t f + \xi \cdot \nabla_x f + F(t, x) \cdot \nabla_\xi f &= 0, \quad x, \xi \in \mathbf{R}^D, \\ F(t, x) &= -\nabla_x \iint_{\mathbf{R}^D \times \mathbf{R}^D} V(x, y) f(t, y, \xi) d\xi dy. \end{aligned} \tag{I.5}$$

in the sense of distributions, with initial data

$$f|_{t=0} = f^0.$$

¹We denote by $C_r^k(\mathbf{R}^N)$ the space of C^k functions f on $\mathbf{R}^D$ such that, for all $n \geq 0$ and all $p = 1, \dots, k$, $|D^p f(x)| = O(|x|^{-n})$ as $|x| \rightarrow +\infty$.

²We denote by $\mathcal{M}(X)$ the space of Radon measures on a locally compact space X ; its weak- $*$ topology is the one defined by duality with test functions in $C_c(X)$.

Proof. For each $t \geq 0$, $f_{N, Z_N^0}(t)$ is a sequence of probability measures on $\mathbf{R}^D \times \mathbf{R}^D$. Hence f_{N, Z_N^0} is weakly-* relatively compact in $\mathcal{M}(\mathbf{R}_+ \times \mathbf{R}^D \times \mathbf{R}^D)$. Denote by $f_{N', Z_{N'}^0}$ be a subsequence of f_{N, Z_N^0} weakly-* converging to f . Because of Lemma I.3,

$$\int f_{N', Z_{N'}^0}(t, x, \xi) d\xi \rightarrow \int f(t, x, \xi) d\xi$$

weakly-* in $\mathcal{M}(\mathbf{R}_+ \times \mathbf{R}^D)$ as $N' \rightarrow +\infty$.

On the other hand, any solution to the Hamiltonian system (I.1) satisfies the bound

$$\sup_{\substack{t \geq 0 \\ 1 \leq k \leq N}} |\ddot{x}_k(t)| \leq \|\nabla_x V\|_{L^\infty}.$$

From this bound, an easy argument shows that, for each $\phi \in C_c(\mathbf{R}^D \times \mathbf{R}^D)$, the sequence of functions

$$t \mapsto \langle f_{N', Z_{N'}^0}(t), \phi \rangle \quad (\text{I.6})$$

is equicontinuous on compact subsets of $\mathbf{R}_+$. By Ascoli's theorem

$$F_{N', Z_{N'}^0} \rightarrow \iint -\nabla_x V(x, y) f(t, y, \eta) d\eta dy$$

uniformly on compact subsets of $\mathbf{R}_+ \times \mathbf{R}^D$ as $N' \rightarrow +\infty$. Thus

$$F_{N', Z_{N'}^0} f_{N', Z_{N'}^0} \rightarrow f(t, x, \xi) \iint -\nabla_x V(x, y) f(t, y, \eta) d\eta dy$$

in the sense of distributions on $\mathbf{R}_+ \times \mathbf{R}^D \times \mathbf{R}^D$. Hence f solves Vlasov's equation (I.1) in the sense of distributions. Also, $f|_{t=0} = f^0$ because of the equicontinuity of (I.6). $\square$

Notice that classical solutions to the Vlasov equation (I.5) are uniquely defined by their initial data, as shown by the following

Lemma I.5. *Let $V \in C_r^2(\mathbf{R}^D \times \mathbf{R}^D)$, and let $f^0 \in C^1(\mathbf{R}^D \times \mathbf{R}^D)$ be such that*

$$f^0 \geq 0, \quad \iint (1 + |\xi|)^2 f^0(x, \xi) dx d\xi < +\infty.$$

Then the Vlasov equation (I.5) has a unique classical solution $f \in C^1(\mathbf{R}_+ \times \mathbf{R}^D \times \mathbf{R}^D)$ with initial data

$$f|_{t=0} = f^0.$$

Any $g \in C(\mathbf{R}_+, w^* - \mathcal{M}(\mathbf{R}^D \times \mathbf{R}^D))$ that solves (I.1) in the sense of distributions on $\mathbf{R}_+^* \times \mathbf{R}^D \times \mathbf{R}^D$ and satisfies $g|_{t=0} = f^0$ must coincide with f on all of $\mathbf{R}_+^* \times \mathbf{R}^D \times \mathbf{R}^D$.

The (easy) proof of this Lemma is left to the reader (we shall prove a slightly more general result later).

Collecting the results in Lemmas I.4 and I.5, we arrive at the following Theorem, proved by several authors (Neunzert [26], Braun-Hepp [8], Dobrushin [14] and Maslov [24]).

Theorem I.6. *Let $V \in C_r^2(\mathbf{R}^D \times \mathbf{R}^D)$. Start from a sequence $Z_N^{0,N}$ of initial configurations of N particles such that*

$$\frac{1}{N} \sum_{k=1}^N \delta_{(Z_N^{0,N})_k} \rightarrow f^0 \text{ in } w^* - \mathcal{M}(\mathbf{R}^D \times \mathbf{R}^D)$$

and

$$H_N(Z_N^{0,N}) = O(N).$$

Then

$$\frac{1}{N} \sum_{k=1}^N \delta_{z_k(t, Z_N^{0,N})} \rightarrow f(t, \cdot, \cdot) \text{ in } w^* - \mathcal{M}(\mathbf{R}^D \times \mathbf{R}^D)$$

uniformly on compact subsets of $\mathbf{R}_+$, where f is the solution to the Vlasov equation (1.1) with initial data f^0 .

Hence, Vlasov's equation (1.1) is shown to be the mean-field limit of the N -body Hamiltonian system (1.17) as $N \rightarrow +\infty$.

In fact the proof given here reduces to the continuous dependence on initial data of the solution to Vlasov's equation.

I.A. Mean-field PDEs and Wasserstein distance

In this first appendix to Part I, we present Dobrushin's beautiful idea of proving stability of first order mean-field PDEs in the Wasserstein distance.

Definition I.7. *Let μ and ν be two probability measures on $\mathbf{R}^D$. The Wasserstein distance between μ and ν is*

$$W(\mu, \nu) = \inf\{\mathbf{E}|X - Y| \mid X \text{ (resp. } Y) \text{ has distribution } \mu \text{ (resp. } \nu)\}$$

In other words, let $E(\mu, \nu)$ be the set of probability measures P on $\mathbf{R}^D \times \mathbf{R}^D$ such that the image of P under the projection on the first factor (resp. on the second factor) is μ (resp. ν). Then

$$W(\mu, \nu) = \inf_{P \in E(\mu, \nu)} \iint |x - y| P(dxdy).$$

Consider next the mean-field, 1st order PDE, for the unknown $\rho \equiv \rho(t, z)$,

$$\partial_t \rho + \operatorname{div}_z((K \star_z \rho) \rho) = 0, \quad \rho|_{t=0} = \rho^0. \quad (\text{I.7})$$

where K is a Lipschitz continuous vector-field on $\mathbf{R}^D$ and $\star_z$ denotes the convolution in z . This model is analogous to the vorticity formulation of the two-dimensional Euler equation (see section 1 above), except that the function K in that case is singular at the origin. In the context of vortex method for the Euler equation, it is customary to replace the original kernel K by a truncation of it near the origin — this is called the “vortex blob” method, since it amounts to assign a positive thickness to each vortex center in the system considered: see [23].

The associated system of characteristics is

$$\begin{aligned}\dot{z}(t, a, \rho^0) &= (K \star_z \rho(t))(z(t, a, \rho^0)), \\ z(0, a, \rho^0) &= a, \quad \rho(t) = z(t, \cdot, \rho^0)_* \rho^0.\end{aligned}\tag{I.8}$$

(We recall the following usual notation for transportation of measure: given two measurable spaces $(X, \mathcal{M})$ and $(Y, \mathcal{N})$, a measurable map $f : X \rightarrow Y$ and a measure μ on $(X, \mathcal{M})$, one defines a measure ν on $(Y, \mathcal{N})$ called the “image of μ by f ” and denoted by $\nu = f_* \mu$, by the formula $\nu(B) = \mu(f^{-1}(B))$ for $B \in \mathcal{N}$. In other words

$$\dot{z}(t, a, \rho^0) = \int K(z(t, a, \rho^0) - z(t, a', \rho^0)) \rho^0(da'). \tag{I.9}$$

Let $\mu \equiv \mu(t, dz)$ and $\nu \equiv \nu(t, dz)$ be two solutions to the mean-field PDE (I.7) in $C(\mathbf{R}_+, w^* - \mathcal{M}^1(\mathbf{R}^D))^3$. Then

DOBRUSHIN’S INEQUALITY

$$W(\mu(t), \nu(t)) \leq W(\mu^0, \nu^0) e^{2t\|K\|_{Lip}}, \quad t \geq 0.$$

Proof. Let $P^0 \in E(\mu^0, \nu^0)$; define $P(t)$ to be the image of P^0 under the map $(a, b) \mapsto (z(t, a, \mu^0), z(t, b, \nu^0))$. Then $P(t) \in E(\mu(t), \nu(t))$. Set

$$\Phi(t) = \iint |a - b| P(t, dadb) = \iint |z(t, a, \mu^0) - z(t, b, \nu^0)| P^0(dadb).$$

Observe that

$$\begin{aligned}z(t, a, \mu^0) &= a + \int_0^t \int K(z(s, a, \mu^0) - z(s, a', \mu^0)) \mu^0(da') ds \\ &= a + \int_0^t \iint K(z(s, a, \mu^0) - z(s, a', \mu^0)) P^0(da' db') ds\end{aligned}$$

and similarly

$$\begin{aligned}z(t, b, \nu^0) &= b + \int_0^t \int K(z(s, b, \nu^0) - z(s, b', \nu^0)) \nu^0(db') ds \\ &= b + \int_0^t \iint K(z(s, b, \nu^0) - z(s, b', \nu^0)) P^0(da' db') ds,\end{aligned}$$

so that

$$\begin{aligned}|z(t, a, \mu^0) - z(t, b, \nu^0)| &\leq |a - b| \\ &\quad + \int_0^t \iint \|K\|_{Lip} |(z(s, a, \mu^0) - z(s, a', \mu^0)) \\ &\quad \quad - (z(s, b, \nu^0) - z(s, b', \nu^0))| P^0(da' db') ds \\ &\leq |a - b| + \|K\|_{Lip} \int_0^t |z(s, a, \mu^0) - z(s, b, \nu^0)| ds \\ &\quad + \|K\|_{Lip} \int_0^t \iint |z(s, a', \mu^0) - z(s, a', \nu^0)| P^0(da' db') ds.\end{aligned}$$

³ $\mathcal{M}^1(X)$ denotes the set of probability measures on X .

Integrating both sides of this inequality with respect to $P^0(dadb)$ leads to

$$\begin{aligned} \iint |z(t, a, \mu^0) - z(t, b, \nu^0)| P^0(dadb) &\leq \iint |a - b| P^0(dadb) \\ &+ \|K\|_{Lip} \int_0^t \iint |z(s, a, \mu^0) - z(s, b, \nu^0)| P^0(dadb) ds \\ &+ \|K\|_{Lip} \int_0^t \iiint |z(s, a', \mu^0) - z(s, b', \nu^0)| P^0(da'db') P^0(dadb) ds \end{aligned}$$

which implies that

$$\begin{aligned} \iint |z(t, a, \mu^0) - z(t, b, \nu^0)| P^0(dadb) &\leq \iint |a - b| P^0(dadb) \\ &+ 2\|K\|_{Lip} \int_0^t \iint |z(s, a, \mu^0) - z(s, b, \nu^0)| P^0(dadb) ds \end{aligned}$$

or in other words

$$\Phi(t) \leq \Phi(0) + 2\|K\|_{Lip} \int_0^t \Phi(s) ds.$$

By Gronwall's inequality

$$\Phi(t) \leq \Phi(0) e^{2t\|K\|_{Lip}}$$

and taking the infimum of both sides of this inequality over $E(\mu^0, \nu^0)$ leads to Dobrushin's inequality. $\square$

At this point, Dobrushin's inequality can be used in two different ways in the proof of the mean-field limit:

- it proves in particular the uniqueness of the solution to (I.7) within the class $C(\mathbf{R}_+, w^* - \mathcal{M}^1(\mathbf{R}^D))$;
- if one takes $\nu^{0,N}$ to be of the form

$$\nu^{0,N} = \frac{1}{N} \sum_{k=1}^N \delta_{z_k^{0,N}},$$

then for each $k \geq 1$, $z_k^N(t, z_k^{0,N}, \nu^{0,N})$ is the solution to the system of ODE

$$\begin{aligned} \dot{z}_k^N(t, z_k^{0,N}, \nu^{0,N}) &= \frac{1}{N} \sum_{l=1}^N K(z_k^N(t, z_k^{0,N}, \nu^{0,N}) - z_l^N(t, z_l^{0,N}, \nu^{0,N})) \\ z_k^N(0, z_k^{0,N}, \nu^{0,N}) &= z_k^{0,N}; \end{aligned}$$

then, by setting

$$\nu^N(t) = \frac{1}{N} \sum_{k=1}^N \delta_{z_k^N(t, z_k^{0,N}, \nu^{0,N})},$$

a direct application of Dobrushin's inequality shows that

$$W(\mu(t), \nu^N(t)) \rightarrow 0 \text{ for each } t > 0 \text{ as } N \rightarrow +\infty$$

if $W(\mu^0, \nu^{0,N}) \rightarrow 0$. Since the Wasserstein distance metricizes the weak-* topology of $\mathcal{M}^1(\mathbf{R}^D)$, this gives another proof of the mean-field limit as in Theorem I.6

I.B. Chaotic sequences

In Theorem I.6, we proved the convergence of the empirical distribution of particles to the solution of Vlasov's equation in the large N limit and for the weak coupling scaling.

Even if the empirical distribution is a natural object encoding the motion of N particles under the Hamiltonian flow of (I.1), it is a probability measure on the 1-particle phase space. Another, equally natural object to consider is the joint distribution of the same system of N undistinguishable particles which is a probability measure on the N -particle phase space.

The next Lemma explains how both objects are related.

More generally, this Appendix is aimed at explaining in detail the respective roles of the N -particle and the 1-particle phase spaces in the mean-field limit.

Lemma I.8. *Let $f \in \mathcal{M}^1(\mathbf{R}^D)$ and, for all $N \geq 1$, $F_N \in \mathcal{M}^1((\mathbf{R}^D)^N)$ symmetric in all variables — i.e. F_N is invariant under the transformation*

$$(x_1, \dots, x_N) \mapsto (x_{\sigma(1)}, \dots, x_{\sigma(N)})$$

for each $\sigma \in \mathfrak{S}_N$. The two following statements are equivalent
(1) for each $\epsilon > 0$ and each $\phi \in C_c(\mathbf{R}^D)$,

$$F_N(\{(x_1, \dots, x_N) \in (\mathbf{R}^D)^N \mid |\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \rangle| \geq \epsilon\}) \rightarrow 0$$

as $N \rightarrow +\infty$;

(2) the sequence $F_{N:j}$ of marginal distributions of F_N — i.e. $F_{N:j}$ is the image of F_N under the projection $(x_1, \dots, x_N) \mapsto (x_1, \dots, x_j)$ — satisfies

$$F_{N:j} \rightarrow f^{\otimes j} \text{ weakly-}^*, \quad \text{as } N \rightarrow +\infty.$$

Proof. Let us show how (1) implies (2). First, (1) clearly implies that

$$\mathbf{E}^{F_N} \left| \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \right\rangle \right|^j \rightarrow 0 \text{ for all } j \geq 1$$

as $N \rightarrow +\infty$. For $j = 1$, observe that, by symmetry of F_N ,

$$\begin{aligned} \mathbf{E}^{F_N} \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \right\rangle &= \mathbf{E}^{F_N} \left(\frac{1}{N} \sum_{k=1}^N \phi(x_k) \right) - \langle f, \phi \rangle \\ &= \mathbf{E}^{F_{N:1}} \phi - \langle f, \phi \rangle \end{aligned}$$

and hence

$$F_{N:1} \rightarrow f \text{ weakly-}^* \text{ as } N \rightarrow +\infty.$$

For $j = 2$

$$\begin{aligned} \mathbf{E}^{F_N} \left(\left\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \right\rangle \right)^2 &= \mathbf{E}^{F_N} \left(\frac{1}{N} \sum_{k=1}^N \phi(x_k) \right)^2 \\ &\quad - 2\langle f, \phi \rangle \mathbf{E}^{F_N} \left(\frac{1}{N} \sum_{k=1}^N \phi(x_k) \right) + \langle f, \phi \rangle^2. \end{aligned}$$

On the other hand

$$\begin{aligned}
\mathbf{E}^{F_N} \left(\frac{1}{N} \sum_{k=1}^N \phi(x_k) \right)^2 &= \frac{1}{N^2} \mathbf{E}^{F_N} \sum_{k=1}^N \phi(x_k)^2 \\
&\quad + \frac{1}{N^2} \mathbf{E}^{F_N} \sum_{1 \leq k \neq l \leq N} \phi(x_k) \phi(x_l) \\
&= \frac{1}{N} \mathbf{E}^{F_{N:1}} \phi^2 + \frac{N(N-1)}{N^2} \mathbf{E}^{F_{N:2}} \phi^{\otimes 2}
\end{aligned}$$

so that, by using again the symmetry of F_N ,

$$\begin{aligned}
\mathbf{E}^{F_N} \left(\left\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \right\rangle \right)^2 &= \frac{N(N-1)}{N^2} \mathbf{E}^{F_{N:2}} \phi^{\otimes 2} \\
&\quad - 2 \langle f, \phi \rangle \mathbf{E}^{F_{N:1}} \phi + \langle f, \phi \rangle^2 + \frac{1}{N} \mathbf{E}^{F_{N:1}} \phi^2
\end{aligned} \tag{I.10}$$

Hence, if

$$\mathbf{E}^{F_N} \left(\left\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \right\rangle \right)^2 \rightarrow 0$$

as $N \rightarrow +\infty$, one has

$$F_{N:2} \rightarrow f^{\otimes 2} \text{ weakly-}^* \text{ as } N \rightarrow +\infty.$$

The extension to j s larger than 2 is done in the same manner.

Conversely, assume that (2) holds for $j = 1, 2$. By the Bienayme-Chebyshev inequality

$$\begin{aligned}
F_N(\{(x_1, \dots, x_N) \in (\mathbf{R}^D)^N \mid |\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \rangle| \geq \epsilon\}) \\
\leq \frac{1}{\epsilon^2} \mathbf{E}^{F_N} \left\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \right\rangle^2
\end{aligned}$$

so that, because of (I.10)

$$\begin{aligned}
F_N(\{(x_1, \dots, x_N) \in (\mathbf{R}^D)^N \mid |\langle \frac{1}{N} \sum_{k=1}^N \delta_{x_k} - f, \phi \rangle| \geq \epsilon\}) \\
= \frac{1}{\epsilon^2} \left(\frac{N(N-1)}{N^2} \mathbf{E}^{F_{N:2}} \phi^{\otimes 2} - 2 \langle f, \phi \rangle \mathbf{E}^{F_{N:1}} \phi + \langle f, \phi \rangle^2 + \frac{1}{N} \mathbf{E}^{F_{N:1}} \phi^2 \right).
\end{aligned}$$

Keeping $\epsilon > 0$ fixed and letting $N \rightarrow +\infty$ leads to (1) because of the limits

$$\mathbf{E}^{F_{N:1}} \phi \rightarrow \langle f, \phi \rangle, \quad \mathbf{E}^{F_{N:2}} \phi^{\otimes 2} \rightarrow \langle f, \phi \rangle^2$$

as $N \rightarrow +\infty$. □

Definition I.9. A sequence $F_N \in \mathcal{M}^1(X^N)$ that satisfies either one of the equivalent statements in Lemma I.8 is called “chaotic”.

An obvious example of chaotic sequence is $F_N = f^{\otimes N}$. In this case, and for $X = \mathbf{R}^D$, the condition (1) in Lemma I.8 can be improved as follows.

Define $\Omega = (\mathbf{R}^D)^{\mathbf{N}^*}$ to be the space of $\mathbf{R}^D$ -valued sequences $(a_n)_{n \geq 1}$, endowed with the σ -algebra generated by cylinders⁴. The infinite tensor product $F_\infty = f^{\otimes \mathbf{N}^*}$ defines a probability measure on Ω with that σ -algebra.

Lemma I.10. For F_∞ -a.e. $a = (a_1, a_2, a_3, \dots) \in \Omega$, the empirical measure

$$f_{N,a} = \frac{1}{N} \sum_{k=1}^N \delta_{a_k} \rightarrow f \text{ weakly-}^* \text{ on } \mathbf{R}^D.$$

In the particular case of $F_\infty = f^{\otimes \mathbf{N}^*}$ considered here, condition (1) in Lemma I.8 can be recast as

$$\lim_{N \rightarrow +\infty} F_\infty(\{a \in \Omega \mid |\langle f_{N,a} - f, \phi \rangle| > \epsilon\}) = 0$$

for each $\epsilon > 0$; in other words, it expresses that, for all $\phi \in C_c(\mathbf{R}^D)$

$$\langle f_{N,a}, \phi \rangle \rightarrow \langle f, \phi \rangle \text{ in } F_\infty\text{-probability as } N \rightarrow +\infty,$$

while Lemma I.10 says that

$$\langle f_{N,a}, \phi \rangle \rightarrow \langle f, \phi \rangle \text{ } F_\infty\text{-a.e. as } N \rightarrow +\infty,$$

which is a stronger statement (we recall that a.e.- convergence is a stronger notion of convergence than convergence in probability — more precisely, a.e.-convergence implies convergence in probability, while convergence in probability implies only the a.e.-convergence modulo extraction of subsequences).

Proof. Pick $\phi \in C_c(\mathbf{R}^D)$ and set $Y_n(a) = \phi(a_n)$. Clearly, the random variables $(Y_n)_{n \geq 1}$ are independent on Ω and identically distributed (under f). By the strong law of large numbers,

$$\frac{1}{N} \sum_{n=1}^N Y_n(a) \rightarrow \mathbf{E}^{F_\infty}(Y_n) = \langle f, \phi \rangle \text{ } F_\infty\text{-a.e. on } \Omega \text{ as } N \rightarrow +\infty.$$

By a classical separability argument, one can choose the F_∞ -negligible set in the statement above to be independent of ϕ , which gives the announced statement. $\square$

Let us go back to our original problem, namely the mean-field limit of a system of N particles. Our aim is to apply the notion of chaotic sequence to that problem. We shall do so for the first-order mean-field PDE on which we explained Dobrushin’s

⁴i.e. sets of the form $\prod_{n \geq 1} B_n$, with B_n a Borel set in $\mathbf{R}^D$ for each $n \geq 1$ and $B_n = \mathbf{R}^D$ for all but a finite number of ns .

inequality, rather than on the Vlasov equation itself, the extension of arguments to this latter case being obvious.

Given $Z_N^0 = (z_1^0, \dots, z_N^0)$, let $Z_N(t, Z_N^0) = (z_1(t, Z_N^0), \dots, z_N(t, Z_N^0))$ be the solution of the system of ODEs

$$\begin{aligned}\dot{z}_k(t, Z_N^0) &= \frac{1}{N} \sum_{l=1}^N K(z_k(t, Z_N^0) - z_l(t, Z_N^0)) \\ z_k(0, Z_N^0) &= z_k^0, \quad k = 1, \dots, N.\end{aligned}\tag{I.11}$$

We designate by $f_{N, Z_N^0}(t)$ the empirical measure

$$f_{N, Z_N^0}(t) = \frac{1}{N} \sum_{k=1}^N \delta_{z_k(t, Z_N^0)}.$$

Given $f^0 \in \mathcal{M}^1(\mathbf{R}^D)$, we denote by $F_N(t)$ the image of $(f^0)^{\otimes N}$ under the map $Z_N^0 \mapsto Z_N(t, Z_N^0)$, i.e.

$$F_N(t) = Z_N(t, \cdot)_*(f^0)^{\otimes N}.$$

Theorem I.11. *Assume that K is Lipschitz continuous on $\mathbf{R}^D$, and let $f^0 \in \mathcal{M}^1(\mathbf{R}^D)$. Then, for each $n \geq 1$ and each $t > 0$,*

$$F_{N:n}(t) \rightarrow f(t)^{\otimes n} \text{ weak-}^* \text{ as } N \rightarrow +\infty$$

where $f(t)$ is the solution to the mean-field PDE

$$\partial_t f + \operatorname{div}_z((K \star_z f)f) = 0, \quad f|_{t=0} = f^0.\tag{I.12}$$

Proof. Let $h \in C_c((\mathbf{R}^D)^m)$; one has

$$\mathbf{E}^{F_N(t)} \langle (f_{N, Z_N^0}^0)^{\otimes m}, h \rangle = \mathbf{E}^{F_N(0)} \langle (f_{N, Z_N^0}(t))^{\otimes m}, h \rangle = \mathbf{E}^{F_\infty} \langle (f_{N, \bullet}(t))^{\otimes m}, h \rangle$$

in the notation of Lemma I.10.

For F_∞ -a.e. $a \in \Omega$, Lemma I.10 implies that

$$f_{N,a}(0) \rightarrow f^0 \text{ weakly-}^* \text{ as } N \rightarrow +\infty.$$

By the analogue of Theorem I.6 adapted to the mean-field limit of (I.11) — which follows directly from Dobrushin's inequality — one has

$$f_{N,a}(t) \rightarrow f(t) \text{ weakly-}^* \text{ as } N \rightarrow +\infty$$

for F_∞ -a.e. $a \in \Omega$ and each $t > 0$.

Hence, given any $h \in C_c((\mathbf{R}^D)^m)$,

$$\langle (f_{N,a}(t))^{\otimes m}, h \rangle \rightarrow \langle f(t)^{\otimes m}, h \rangle \text{ weakly-}^* \text{ as } N \rightarrow +\infty$$

for F_∞ -a.e. $a \in \Omega$ and each $t > 0$. On the other hand, one has

$$|\langle (f_{N,a}(t))^{\otimes m}, h \rangle| \leq \|h\|_{L^\infty}$$

so that, by dominated convergence

$$\mathbf{E}^{F_N(t)} \langle (f_{N,Z_N^0}^0)^{\otimes m}, h \rangle = \mathbf{E}^{F_\infty} \langle (f_{N,\bullet}(t))^{\otimes m}, h \rangle \rightarrow \langle f(t)^{\otimes m}, h \rangle$$

as $N \rightarrow +\infty$, for each $t > 0$.

Using the Bienayme-Chebyshev inequality as in the proof of Lemma I.8 shows that, for each $t > 0$, $F_N(t)$ satisfies condition (1) in that Lemma. Hence it must also satisfy condition (2) there, which is precisely our claim. $\square$

In other words, if $F_N(t)$ is the solution to the Liouville equation

$$\begin{aligned} \partial_t F_N + \sum_{1 \leq k, l \leq N} \operatorname{div}_{z_k} (K(z_k - z_l) F_N) &= 0, \\ F_N(0) &= (f^0)^{\otimes N}, \end{aligned}$$

with $f^0 \in \mathcal{M}^1(\mathbf{R}^D)$, then, for each $t > 0$, $F_N(t)$ is a chaotic sequence and its marginal distributions satisfy

$$F_{N:n}(t) \rightarrow f(t)^{\otimes n} \text{ weakly-}^* \text{ as } N \rightarrow +\infty$$

for each $t > 0$, where f is the solution to (I.12). Thus, the fact that $F_N(0) = (f^0)^{\otimes N}$, i.e. that $F_N(0)$ is the simplest chaotic sequence imaginable, implies that $F_N(t)$ is chaotic for all $t > 0$. This property is called *propagation of chaos* and is of paramount importance in Statistical Mechanics.

Part II. From the quantum N -body problem to Hartree's equation

In this section, we explain how the nonlinear, mean-field Schrödinger equation (1.6) can be derived from the linear N -body Schrödinger equation (1.20). One way of doing this is through the weak-coupling scaling similar to (I.2) in the classical case. Hence the potential V is replaced by V/N in (1.19), leading to

$$\mathcal{H}_N = \sum_{k=1}^N -\frac{1}{2} \Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k, x_l). \quad (\text{II.1})$$

(Here, for simplicity, we switch to dimensionless variables, so that $\hbar = m = 1$). We assume that the potential V in (II.1) satisfies

$$V \in L^\infty(\mathbf{R}^D \times \mathbf{R}^D), \quad V(x, y) = V(y, x) \in \mathbf{R} \text{ for a.e. } x, y \in \mathbf{R}^D. \quad (\text{II.2})$$

The quantum, N -body Hamiltonian $\mathcal{H}_N$ in (II.1) is an unbounded self-adjoint operator on $L^2((\mathbf{R}^D)^N)$ with domain $H^2((\mathbf{R}^D)^N)$. By Stone's theorem, $-\frac{i}{\hbar} \mathcal{H}_N$ generates a unitary group on $L^2((\mathbf{R}^D)^N)$. Thus, given any $\Psi_N^0 \in H^2((\mathbf{R}^D)^N)$, $e^{-it\mathcal{H}_N/\hbar} \Psi_N^0$ defines the only classical solution Ψ_N to the linear N -body Schrödinger equation

$$\begin{aligned} i\partial_t \Psi_N &= \mathcal{H}_N \Psi_N = -\frac{1}{2} \sum_{k=1}^N \Delta_{x_k} \Psi_N \\ &\quad + \frac{1}{N} \sum_{1 \leq k < l \leq N} V(x_k - x_l) \Psi_N(t, X_N, Y_N) \\ \Psi_N|_{t=0} &= \Psi_N^0. \end{aligned} \quad (\text{II.3})$$