Derivation of Mean Field Equations for Classical Systems

Master Thesis

Niklas Boers

Derivation of Mean Field Equations for Classical Systems

Master Thesis

Niklas Boers

Fakultät für Mathematik, Informatik und Statistik

Ludwig-Maximilians-Universität München

München, January 2011

Supervisor: Prof. Dr. Detlef Dürr
Second Supervisor: Prof. Dr. Peter Pickl

Acknowledgements

This thesis would have never been possible without the great support of Detlef Dürr and Peter Pickl. Their ingenuity as well as their patience are deeply appreciated.

Contents

1 Introduction

Consider a Newtonian system of N identical particles interacting via a spherically symmetric pair potential $\phi \in \mathcal{C}_b^2(\mathbb{R}^d)$ in d dimensions, which might be either attractive or repulsive. Here, $\mathcal{C}_b^2(\mathbb{R}^d)$ shall denote the set of functions on $\mathbb{R}^d$ with bounded and continuous derivatives up to order 2. The Hamiltonian of such a system has the form

$$H_N(X) = \sum_{i=1}^{N} \frac{p_i^2}{2m_N} + \sum_{i<j} \phi(q_i - q_j) \tag{1}$$

with $X = (x_1, \dots, x_N) \in \mathbb{R}^{6N}$, $x_i = (q_i, p_i) \in \mathbb{R}^6$, leading to the equations of motion

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} = \frac{p_i}{m_N} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} = -\sum_{j=1}^{N} \nabla_{q_i} \phi(q_i - q_j). \end{aligned} \tag{2}$$

Note that, since ϕ is symmetric and thus $\nabla\phi(0) = 0$, we can omit the restriction $i \neq j$ in the sum. Substituting $\phi_N = \frac{1}{N}\phi$ for the potential and setting $m_N = 1$, one obtains

$$\begin{aligned} \frac{dq_i}{dt} &= p_i \\ \frac{dp_i}{dt} &= \frac{d^2 q_i}{dt^2} = -\frac{1}{N} \sum_{j=1}^{N} \nabla_{q_i} \phi(q_i - q_j). \end{aligned} \tag{3}$$

These are the equations of motion for N classical particles interacting through the potential $\frac{1}{N}\phi$. It is this dynamics from which the Vlasov equation can be derived. Note that the coupling becomes weaker with growing N.

In a more general setting the Hamiltonian looks like

$$H_N^\beta(X) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} \phi_N^\beta(q_i - q_j), \tag{4}$$

where

$$\phi_N^\beta(q) = N^{-1+\beta} \phi(N^{\beta/d} q) \tag{5}$$

in dimension d for spherically symmetric $\phi \in \mathcal{C}_b^2(\mathbb{R}^d)$. Hence the support of ϕ_N^β shrinks with N for positive β. The case described above obviously corresponds to $\beta = 0$ and $m = 1$. Usually the potential energy is expected to scale in the same way in N as the kinetic energy. This motivates the factor of N^{-1} in the expression for ϕ_N^β.

In general, the Newtonian equations of motion for N interacting particles are practically impossible to solve. One way to circumvent this problem and obtain at least some kind of solution is to change the level of description. Instead of the microscopic N-body problem, one considers an equation for a continuous mass density which *effectively* still describes the same situation but from a macroscopic point of view. It is intuitively clear that this coarse grained description gets more appropriate as the number of particles N increases, becoming exact in the limit $N \to \infty$. The crucial observation in the case where the potential scales with $1/N$, i.e. the $\beta = 0$ case, is that the force

$$\ddot{q}_i = -\frac{1}{N}\sum_{j=1}^{N} \nabla_{q_i}\phi(q_i - q_j) \quad , \quad i = 1, \ldots, N \tag{6}$$

looks like the empirical mean of the continuous function $\nabla\phi(q_i - \cdot)$ of the random variables q_j. In the limit $N \to \infty$, one might expect this to be equal to the expectation value of $\nabla\phi$, given by the convolution[1]

$$-f_t * \nabla\phi(q_i) = -\int \nabla_{q_i}\phi(q_i - q) f_t(q,p)dqdp, \tag{7}$$

where $f_t(q,p)$ for $q, p \in \mathbb{R}^3$ denotes the mass density at q with momentum p at time t. In replacing the empirical mean by its expectation value, we switch from the N-body problem to an *effective* external force problem: Instead of summing up all interaction terms, one expects a single particle to "feel" only the mean field produced by all particles together. But if there is only an external force $\dot{p}$ acting, then the time evolution of f_t is dictated by the continuity equation on $\mathbb{R}^6$:

$$\partial_t f_t + \nabla_q f_t \cdot \dot{q} + \nabla_p f_t \cdot \dot{p} = 0 \tag{8}$$

Inserting for $\dot{p}$ the expectation value (7) yields

$$\partial_t f_t + \nabla_q f_t \cdot \dot{q} - \nabla_p f_t \cdot f_t * \nabla\phi = 0. \tag{9}$$

[1] Young's inequality assures that the convolution $f * \nabla\phi$ exists for $f \in L^1(\mathbb{R}^6)$ if $\nabla\phi$ is bounded: $\|f_t * \nabla\phi\|_\infty \leq \|f_t\|_1 \|\nabla\phi\|_\infty$

This equation is known as the *Vlasov equation*, a partial non-linear differential equation which has a unique global solution in the space of probability densities if $\nabla\phi$ is bounded and Lipschitz continuous (see [3]). The question is how the replacement of (6) by (7) can be rigorously justified from microscopic dynamics. To put it differently, how well does a solution of the Vlasov equation approximate an actual configuration evolving in time according to Newton's equation of motion?

2 The Counting Measure

We can add to the Hamiltonian an external potential $V_t(q)$:

$$H_N^\beta(X) = \sum_{i=1}^N \frac{p_i^2}{2m_N} + \sum_{i<j} \phi_N^\beta(q_i - q_j) + \sum_{i=1}^N V_t(q_i) \tag{10}$$

Since an external force has the same effect on all particles, independently of their distribution, this should not affect the derivation of a hydrodynamic equation. Since we will in the following only consider differences between exact Newtonian and mean field dynamics, this external potential will not appear anymore.

For the mass density f_t, one has the continuity equation on 1-particle phase space $\Gamma^1 \cong \mathbb{R}^6$ containing points $x = (q, p)$

$$\partial_t f_t(x) + \nabla_q f_t(x) \cdot \frac{dq}{dt} + \nabla_p f_t(x) \cdot \frac{dp}{dt} = 0. \tag{11}$$

From this one obtains the approximating *mean field* equation by replacing the interaction part of the force with its expectation value. Hence, instead of summing up all interaction terms, one expects a single particle to "feel" only the mean field produced by all particles together. It is clear that, for different scaling parameters[2] β, this procedure leads to different hydrodynamic equations. In the next section we will investigate the case $\beta = 0$ as an example of the method that we shall present in the following.

If one looks at the mean field approximation from the perspective of a law of large numbers, one possibility to justify the replacement in the continuity equation would be to argue that the random variables $x_i \in \mathbb{R}^6$ are

[2]Recall:

$$\phi_N^\beta(q) = N^{-1+\beta}\phi(N^{\beta/d}q)$$

distributed identically and independently (*i.i.d.*). Formally, this means that the N-particle density[3] $\mathcal{F}$ is a product of the 1-particle densities:

$$\mathcal{F}(X) = \prod_{i=1}^{N} f(x_i) \tag{12}$$

for $X = (x_1, \ldots, x_N) \in \mathbb{R}^{6N}$ and $x_i = (q_i, p_i) \in \mathbb{R}^6$. This situation is called *molecular chaos*. The question of justifying the mean field approximation can now be reformulated: If, initially, the random variables $x_i \in \mathbb{R}^6$ were distributed according to

$$\mathcal{F}_0(X) = \prod_{i=1}^{N} f_0(x_i), \tag{13}$$

will this product structure survive the time-evolution? Moreover, in which sense will it survive, i.e. in which sense

$$\mathcal{F}_t(X) \approx \prod_{i=1}^{N} \tilde{f}_t(x_i) \tag{14}$$

for solutions $\tilde{f}_t$ of the effective equation?

Remark 2.1. It is crucial that the L^1-norm is not a suitable notion of distance in this context: Think of a situation in which some m out of N particles are not *i.i.d.*. Then the distributing function would be of the form

$$\mathcal{F}_t = g_t(x_1, \ldots, x_m) \prod_{i=m+1}^{N} \tilde{f}_t(x_i).$$

We would say that this is close to a product if m was small. The L^1-distance from a product distribution would be given by

$$\begin{aligned} &\int \Big| \mathcal{F}_t(x_1, \ldots, x_N) - \prod_{i=1}^{N} \tilde{f}_t(x_i) \Big| dx_1 \ldots dx_N \\ = &\int \Big| g_t(x_1, \ldots, x_m) - \prod_{i=1}^{m} \tilde{f}_t(x_i) \Big| dx_1 \ldots dx_m, \end{aligned}$$

[3]Here, we will exclusively deal with situations where the distributing measure is absolutely continuous.

which does not tell us anything about the value of m. The m "bad" particles might be distributed according to a function whose support is disjoint or has very little intersection with the support of $\tilde{f}_t^{\otimes m}$:

$$supp(g_t) \cap supp(\tilde{f}_t^{\otimes m}) \approx 0,$$

then

$$\int \left| \mathcal{F}_t(x_1, \dots, x_N) - \prod_{i=1}^{N} \tilde{f}_t(x_i) \right| dx_1 \dots dx_N = 2.$$

independently of m. Therefore the L^1-distance does not tell us what we want to know and we have to find a for our purposes more appropriate notion of distance.

The strategy for answering the above questions consists of two steps: First, look for a measure α that tells us how many particles are "nice", i.e. *i.i.d.*, in a way that $\alpha \approx 0$ if most particles are "nice" and $\alpha \approx 1$ if most of them are "bad". This will represent the desired notion of distance from product distribution. Then, secondly, try to prove a statement of the kind: If that measure was small in the beginning, then it will remain small for all times. This second step will most likely involve an application of Gronwall's lemma, which we will now state and prove:

Theorem 2.1. *(Gronwall's lemma) Let f and c denote real-valued functions defined on $[0, \infty)$ and let f be differentiable on $(0, \infty)$. If f satisfies*

$$\frac{d}{dt} f(t) \leq c(t) f(t),$$

then

$$f(t) \leq e^{\int_0^t c(s)ds} f(0).$$

Proof. Define a function g by

$$g(t) = e^{\int_0^t c(s)ds}$$

for $t \in [0, \infty)$. Then

$$\frac{d}{dt} g(t) = c(t) g(t).$$

It holds

$$\frac{d}{dt}\frac{f}{g} = \frac{f'g - fg'}{g^2} \leq \frac{cfg - cfg}{g^2} = 0$$

on $(0, \infty)$ and therefore

$$\frac{f(t)}{g(t)} \leq \frac{f(0)}{g(0)} = f(0)$$

since $g(0) = 1$ and $g(t) > 1$ for all $t \in (0, \infty)$. □

For finite particle numbers N, all our results will contain error terms depending on N. We therefore need the following

Corollary 2.1. *Let f denote a continuous real-valued function on $[0, \infty)$ and let f be differentiable on $(0, \infty)$. If f satisfies for positive constants c_1 and c_2*

$$\frac{d}{dt}f(t) \leq c_1 f(t) + c_2,$$

then

$$f(t) \leq e^{c_1 t} f(0) + \left(e^{c_1 t} - 1\right) \frac{c_2}{c_1}.$$

Proof. Define

$$g(t) := f(t) + \frac{c_2}{c_1},$$

then

$$\frac{d}{dt}g(t) = \frac{d}{dt}f(t) \leq c_1 f(t) + c_2 = c_1 g(t)$$

and thus by Gronwall's lemma

$$g(t) \leq e^{c_1 t} g(0),$$

which implies

$$f(t) = g(t) - \frac{c_2}{c_1} \leq e^{c_1 t} f(0) + \left(e^{c_1 t} - 1\right) \frac{c_2}{c_1}.$$

□

If a given physical system admits for a mean field approximation, then it is clear that a relation of the form

$$\dot{\alpha}_t \leq c\alpha_t + o(N) \tag{15}$$

must holds for a constant c: At a given time t, the growth of α_t will be caused by two different processes: There will be interactions within the *i.i.d.*-part of the particles *and* there will be interactions of not *i.i.d.* particles with ones that were *i.i.d.*, thereby "infecting" some of the "good" particles. Interactions among independently distributed particles occur statistically and are controllable by the law of large numbers. Interactions of "bad" particles with "good" ones on the other hand are what really causes the growth of α_t beyond statistical fluctuations. To control them we need an inequality like (15).

The measure α_t, if reasonably defined, shall tell us the amount of particles which are not *i.i.d.* at time t. Then the subsequent growth of this amount has to be bounded by a multiple of this amount, if a mean field description is to make any sense. By Gronwall's lemma, it follows from (15) that

$$\alpha_t \leq e^{ct}\alpha_0 + o(N).$$

This is intuitively clear, since the amount of particles which are not *i.i.d.* should grow exponentially in time.

Starting with a product distribution at time $t = 0$ corresponds to $\alpha_0 = 0$. Then the time-evolved measure will be $\alpha_t \sim o(N)$ and after carrying out the limit $N \to \infty$, it would hold $\alpha_t = 0$ for all times. Then we would say that the product structure of $\mathcal{F}$ survives the time-evolution. In other words, we would have shown the propagation of molecular chaos. Still, there remains the technical difficulty to find the right measure α such that the constant c is as small as possible. Note that it is one advantage of the method to be able to give an error estimate of the mean field approximation, depending on the particle number N.

Of course, due to the pair interaction, the independence will be destroyed through time-evolution. More precisely, during each small time interval Δt, because we consider only pair interactions, not more than two particles will fall out of molecular chaos.[4] Nonetheless, for appropriate scaling β one hopes for this effect to be weak compared to the mixing, such that molecular chaos survives the better the larger the number of particles is.

[4] The probability that two particles interact is of order Δt, thus the probability of having *two* interacting pairs is of order $(\Delta t)^2$ and is therefore negligible to first order in Δt

The proximity of $\mathcal{F}_t$ to a product density can, of course, only become exact in the limit $N \to \infty$. In fact, $\mathcal{F}_t$ itself cannot be expected to converge, since there will always be some few particles which fell out of the product distribution. Instead, one can hope that its s-particle correlation functions $\mathcal{F}_t^s$ will converge to an s-fold product of solutions of the mean field equation $\tilde{f}_t$. As will turn out, their L^1-distance will be bounded by a multiple of α, thus tending to zero as $N \to \infty$. To obtain this result, the symmetry of $\mathcal{F}_t$ under exchange of particles will be absolutely crucial.

Another way of formulating the desired result is that the following diagram commutes: For $f_0 \in L^1(\mathbb{R}^6)$, $\tilde{f}_t \in L^1(\mathbb{R}^6)$ and $\mathcal{F}_t \in L^1(\mathbb{R}^{6N})$

$$\begin{tikzcd}
 & f_0 \arrow[r, "MeanField"] \arrow[d, "\otimes^N"'] & \tilde{f}_t \arrow[r, "\otimes^s"] & \tilde{f}_t^{\otimes s} \\
f_0^{\otimes N} = & \mathcal{F}_0 \arrow[r, "Newton"'] & \mathcal{F}_t \arrow[r, "reducing"'] & \mathcal{F}_t^s \arrow[u, "L^1"']
\end{tikzcd} \tag{16}$$

2.1 Construction of the "Counting Measure"

At a given time t, the N-particle density $\mathcal{F}_t$ can be decomposed in the following way[5]:

Definition 2.1. For a solution $f_t : \mathbb{R}^6 \longrightarrow \mathbb{R}$ of the Vlasov equation, an N-particle density $\mathcal{F}_t : \mathbb{R}^{6N} \longrightarrow \mathbb{R}$ and $k \in \{0, \dots, N\}$, we define functions $g_t^k : \mathbb{R}^{6N} \longrightarrow \mathbb{R}$ by the following conditions (C):

$$g_t^k(X) = g_t^k(x_1, \dots, x_N) = \chi_t^k(x_1, \dots, x_N) \prod_{i=k+1}^{N} f_t(x_i)$$

and

$$\mathcal{F}_t = \left(\sum_{k=0}^{N} g_t^k \right)_{sym} := \frac{1}{N!} \sum_{\sigma \in S_n} \sum_{k=0}^{N} \chi_{t,\sigma}^k(x_1, \dots, x_N) \prod_{i=k+1}^{N} f_t(x_{\sigma(i)}), \tag{17}$$

and

[5]Such a decomposition always exists: Any function $\mathcal{F}$ can be written in such a way because the functions χ can be chosen to be such that (17) is true.

$$\int \chi^k_{t,\sigma}(x_1,\dots,x_N)dx_{\sigma(1)}\dots dx_{\sigma(k)} = c_k > 0 \quad \text{such that} \quad \sum_{k=0}^{N} c_k = 1$$

The sets

$$\mathcal{M}^k_{f_t} := \left\{ g^k_t : \mathbb{R}^{6N} \longrightarrow \mathbb{R} \middle| \text{conditions (C) are fulfilled} \right\}$$

we call different *sectors* for distinct k's.
Note that

$$\mathcal{M}^k_{f_t} \subset \mathcal{M}^l_{f_t}$$

for $k < l$, which shows that this decomposition of $\mathcal{F}_t$ is not unique.

Remark 2.2. In the following, we will make the symmetry property of $\mathcal{F}_t$ explicit only where it is needed and ignore it in the rest of the cases, writing

$$\mathcal{F}_t = \sum_{k=0}^{N} g^k_t \quad \text{with} \quad g^k_t = \chi^k_t(x_1,\dots,x_N) \prod_{i=k+1}^{N} f_t(x_i)$$

such that

$$\int \chi^k_t(x_1,\dots,x_N)dx_1\dots dx_k = c_k \quad \text{and} \quad \sum_{k=0}^{N} c_k = 1$$

Nevertheless, $\mathcal{F}_t$ will always be *understood* to be symmetric.

The c_k's are independent of $x_{k+1},\dots,x_N$ by definition and independent of time due to Liouville's theorem. The function χ^k_t itself depends on $x_{k+1},\dots,x_N$, which reflects the idea that those particles which are not *i.i.d.* depend on the positions and momenta of those particles which are, but in such a way that integrating over the non-*i.i.d.*-coordinates gives a constant.

The measure[6] α_t is supposed to tell us the relative amount of particles that are not distributed independently. For this purpose, we take a weighted sum of the integral over the functions g^k_t:

$$\alpha = \inf_{\mathcal{F}_t = \sum g^k_t} \sum_{k=0}^{N} \frac{k}{N} \int g^k_t dX \tag{18}$$

[6]Again we remark that we mean *measure* in the sense of a *counting device* and not in the sense of measure theory.

with the abbreviation $dX = dx_1 \dots dx_N$. The decomposition of the N-particle density $\mathcal{F}_t = \sum_{k=0}^{N} g_t^k$ is not unique, one could always put $\mathcal{F}_t = \chi_t^N$, yielding $\alpha = 1$ although it should possibly be much smaller. We want to give $\mathcal{F}_t$ as much product structure as possible. Therefore we have to put as much of its integral mass as possible into functions g_t^k with low k-values. To achieve this, we take for α the infimum of the weighted sum over all possible decompositions.

We take the integral over the g_t^k's because we want to benefit from the volume conservation of the Hamiltonian flow on phase space and from linearity of the integral in our derivation. This will become explicit when computing the time derivative of α below.

For technical reasons, we will have to allow for negative parts of the functions χ_t^k:

$$\chi_t^k = (\chi_t^k)^+ + (\chi_t^k)^-$$

in such a way that still $c_k = \int \chi_t^k dX > 0$. This is possible since we can always put $\mathcal{F}_t = \chi_t^N$ with $\int \chi_t^N dX = c_N = 1 > 0$. But it is crucial that all functions over which we integrate in (18) are positive, otherwise we could get $\alpha = 0$ for a non-product state: e.g.

$$\mathcal{F}_t = \underbrace{\prod f_t}_{g^0} + \underbrace{\mathcal{F}_t - \prod f_t}_{g^N},$$

then we would find

$$\alpha = \frac{0}{N} + \frac{N}{N} \int (\mathcal{F}_t - \prod f_t) dX = 0,$$

the positive and negative parts of $(\mathcal{F}_t - \prod f_t)$ exactly compensate due to Liouville's theorem.

Obviously $\int (g_t^k)^+ dX \geq \int g_t^k dX = c_k$. But, since we are dealing with probability densities, we want to have just the integral mass of the g_t^k's, given by the c_k's, in the positive parts of the g_t^k's. Therefore we shift some integral mass of $(g_t^k)^+$ over to the negative part, thereby constructing new functions:

Definition 2.2. Let $(g_t^k)^g$ be defined in such a way that it fulfills

$$(g_t^k)^g \geq 0 \quad \text{and} \quad \int (g_t^k)^g dx_1 \dots dx_N = c_k$$

In addition

$$(g_t^k)^n := g_t^k - (g_t^k)^g \tag{19}$$

such that

$$\int (g_t^k)^n dx_1 \dots dx_N = \int \left(g_t^k - (g_t^k)^g\right) dX = 0. \tag{20}$$

These conditions are realized by[7]

$$(\chi_t^k)^g := (\chi_t^k)^+ \frac{c_k}{\int (\chi_t^k)^+ dx_1 \dots dx_k}, \tag{21}$$

where the coordinates $x_{k+1}, \dots, x_N$ are kept fixed. From this we get

$$(g_t^k)^g := (g_t^k)^+ \frac{c_k}{\int (\chi_t^k)^+ dx_1 \dots dx_k}, \tag{22}$$

which is obviously positive.

We are now in a position to define the counting device which shall tell us how good $\mathcal{F}_t$ can be approximated by a product $f_t^{\otimes N}$:

Definition 2.3. Let $\mathcal{F}_t \in L^1(\mathbb{R}^{6N})$ be the N-particle density and let $f_t \in L^1(\mathbb{R}^6)$ be a solution of the mean field equation in question. Then we define

$$\alpha(\mathcal{F}_t, f_t) := \inf_{\mathcal{F}_t = \sum g_t^k, g_t^k \in \mathcal{M}_{f_t}^k} \left[\sum_{k=0}^{N} \frac{k}{N} \underbrace{\int (g_t^k)^g dX}_{=: c_k} + \sum_{k=0}^{N} \|(g_t^k)^n\|_1 \right] \tag{23}$$

Suppose that at some time t the N-particle density is given by

$$\mathcal{F}_t = \sum g_t^k = \sum (g_t^k)^g + \sum (g_t^k)^n. \tag{24}$$

Then, developing these g_t^k's a time interval Δt further, we get

$$\mathcal{F}_{t+\Delta t} = \mathcal{F}_t \circ \Phi_{-\Delta t} = \sum (g_t^k)^g \circ \Phi_{-\Delta t} + \sum (g_t^k)^n \circ \Phi_{-\Delta t}. \tag{25}$$

The whole construction is such that one has to find a new decomposition at each time t. We will construct a decomposition of $\mathcal{F}_{t+\Delta t}$ by time-evolving the single g_t^k's and decomposing in such a way that the corresponding α is not too large:

[7] We could have started with this, but we wanted to keep the definition as general as possible and what we really need is that $\int (g_t^k)^g = c_k$.

Let Φ and $\tilde{\Phi}$ denote the Hamiltonian flows of the microscopic and the mean field dynamics. The exact dynamics develops $(g_t^k)^g \in \mathcal{M}_{f_t}^k$ into $(g_t^k)^g \circ \Phi_{-\Delta t} \in \mathcal{M}_{f_t}^{k+2}$ to first order in Δt:

$$(g_t^k)^g \circ \Phi_{-\Delta t} = (g_t^k)^g + \sum_{i=1}^N \nabla_{q_i}(g_t^k)^g \cdot \dot{q}_i \Delta t + \sum_{i=1}^N \nabla_{p_i}(g_t^k)^g \cdot \dot{p}_i \Delta t \tag{26}$$

and with

$$\dot{p}_i = -\frac{1}{N} \sum_{j=1}^N \nabla_{q_i}\phi(q_i - q_j)$$

we see that $\nabla_{p_i}(g_t^k)^g$ is multiplied with $\nabla_{q_i}\phi(q_i - q_j)$, resulting in a loss of two *i.i.d.* particles for $i, j \in \{k+1, \ldots, N\}$. But giving $(g_t^k)^g \circ \Phi_{-\Delta t}$ a prefactor of $\frac{k+2}{N}$ in the counting device would be too coarse since there still remain parts for which only k coordinates are not *i.i.d.*. If we look at the exact time evolution as mean field evolution plus a perturbation, i.e.

$$(g_t^k)^g \circ \Phi_{-\Delta t} = (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} + \Delta\left((g_t^k)^g \circ \Phi_{-\Delta t}\right),$$

where the perturbation is defined by this equation, then it is clear that all parts of $(g_t^k)^g \circ \Phi_{-\Delta t}$ for which $k+2$ particles are "bad" are in the perturbation $\Delta\left((g_t^k)^g \circ \Phi_{-\Delta t}\right)$. Liouville's theorem implies that

$$\int (g_t^k)^g \circ \Phi_{-\Delta t} dX = \int (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} dX = \int (g_t^k)^g dX = c_k \tag{27}$$

and hence

$$\int \Delta\left((g_t^k)^g \circ \Phi_{-\Delta t}\right) dX = 0.$$

This means that $\Delta(g_t^k)^g \circ \Phi_{-\Delta t}$ has as much negative as positive integral mass. But in the definition of α we demand positivity of each term. Therefore we put for $0 < \theta_k < 1$

$$(g_t^k)^g \circ \Phi_{-\Delta t} = \underbrace{\Delta\left((g_t^k)^g \circ \Phi_{-\Delta t}\right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t}}_{\in \mathcal{M}_{f_t}^{k+2}} + \underbrace{(1-\theta_k)(g_t^k)^g \circ \tilde{\Phi}_{-\Delta t}}_{\in \mathcal{M}_{f_t}^{k}} \tag{28}$$

with θ_k such that the first term, which will get a prefactor of $\frac{k+2}{N}$ in α, is positive for typical fluctuations of the exact dynamics around the mean field orbit. For stronger fluctuations this term can still be negative, which will be dealt with by writing

$$\begin{aligned}\Delta\left((g_t^k)^g\circ\Phi_{-\Delta t}\right)+\theta_k(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t} &= \left(\Delta\left((g_t^k)^g\circ\Phi_{-\Delta t}\right)+\theta_k(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}\right)^g\\ &+\left(\Delta\left((g_t^k)^g\circ\Phi_{-\Delta t}\right)+\theta_k(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}\right)^n\end{aligned}$$

and absorbing the $(\cdot)^n$-part into the second sum in α (together with $(g_t^k)^n\circ\Phi_{-\Delta t}$). We could have shifted all the negative parts of the perturbation over to the second sum in α by writing $\Delta\left((g_t^k)^g\circ\Phi_{-\Delta t}\right)=\Delta\left((g_t^k)^g\circ\Phi_{-\Delta t}\right)^g+\Delta\left((g_t^k)^g\circ\Phi_{-\Delta t}\right)^n$, but then the estimates for this term would become too bad. Heuristically, the introduction of θ_k allows us to draw a line between typical and untypical fluctuations.

Remark 2.3. At this point we can already identify a constraint of the new strategy: If $(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}=0$ on some set, we cannot "take anything from it" by writing a convex combination as in (28) and the procedure fails. Eventually, this will translate into the condition that $\nabla_p f_t\leq c(t)f_t$ for some function $c(t)$ which is bounded on compact time intervals, as will become more explicit in due course.

At time t, α is given by

$$\alpha(\mathcal{F}_t,f_t)=\inf_{\mathcal{F}_t=\sum g_t^k,g_t^k\in\mathcal{M}_{f_t}^k}\sum\frac{k}{N}\int(g_t^k)^g dX+\sum\|(g_t^k)^n\|_1 \tag{29}$$

Suppose the decomposition is such that[8]

$$(\Delta t)^2+\alpha(\mathcal{F}_t,f_t)=\sum\frac{k}{N}\int(g_t^k)^g dX+\sum\|(g_t^k)^n\|_1 \tag{30}$$

for some (small) Δt. At time $t+\Delta t$, because it includes the infimum over the decompositions at this time, $\alpha(\mathcal{F}_{t+\Delta t},\tilde{f}_{t+\Delta t})$ will be smaller than the α we constructed by time-evolving and suitably decomposing the right hand side of (30), which is given by

[8]We do not know if the infimum is actually attained. The decomposition here is chosen to be such that its corresponding α (without an infimum in front) is by $(\Delta t)^2$ larger than the infimum of it over all decompositions.

$$\begin{aligned}
\tilde{\alpha}(\mathcal{F}_{t+\Delta t}, \tilde{f}_{t+\Delta t}) &:= \sum_{k=0}^{N} \frac{k+2}{N} \int \left(\Delta \left((g_t^k)^g \circ \Phi_{-\Delta t} \right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \right)^g dX \\
&+ \sum_{k=0}^{N} \frac{k}{N} \int (1-\theta_k)(g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} dX \\
&+ \sum_{k=0}^{N} \left\| \left(\Delta \left((g_t^k)^g \circ \Phi_{-\Delta t} \right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \right)^n + (g_t^k)^n \circ \Phi_{-\Delta t} \right\|_1 \\
&= \sum_{k=0}^{N} \left(\frac{k+2}{N} \theta_k c_k + \frac{k}{N}(1-\theta_k) c_k \right) \qquad (31) \\
&+ \sum_{k=0}^{N} \left\| \left(\Delta \left((g_t^k)^g \circ \Phi_{-\Delta t} \right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \right)^n + (g_t^k)^n \circ \Phi_{-\Delta t} \right\|_1 \\
&\leq \sum_{k=0}^{N} \frac{k}{N} c_k + \sum_{k=0}^{N} \|(g_t^k)^n\|_1 + \frac{2}{N} \sum_{k=0}^{N} \theta_k c_k \\
&+ \sum_{k=0}^{N} \left\| \left(\Delta \left((g_t^k)^g \circ \Phi_{-\Delta t} \right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \right)^n + (g_t^k)^n \circ \Phi_{-\Delta t} \right\|_1
\end{aligned}$$

It follows that

$$\begin{aligned}
&\frac{\tilde{\alpha}(\mathcal{F}_{t+\Delta t}, \tilde{f}_{t+\Delta t}) - \alpha(\mathcal{F}_t, f_t)}{\Delta t} \leq \qquad (32) \\
&\leq \Delta t + \frac{1}{\Delta t} \left[\frac{2}{N} \sum_{k=0}^{N} \theta_k c_k + \right. \\
&\left. + \sum_{k=0}^{N} \left\| \left(\Delta \left((g_t^k)^g \circ \Phi_{-\Delta t} \right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \right)^n \right\|_1 \right]
\end{aligned}$$

and hence we have

$$\begin{aligned}
&\dot{\alpha}(t) \leq \lim_{\Delta t \to 0} \frac{\tilde{\alpha}(t+\Delta t) - \alpha(t)}{\Delta t} \leq \qquad (33) \\
&\leq \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left[\frac{2}{N} \sum_{k=0}^{N} \theta_k c_k + \right. \\
&\left. + \sum_{k=0}^{N} \left\| \left(\Delta \left((g_t^k)^g \circ \Phi_{-\Delta t} \right) + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \right)^n \right\|_1 \right].
\end{aligned}$$

Remark 2.4. Observe that this derivation heavily relies on volume conservation: Throughout the computation we use line (27), implying the time-independence of the c_k's. In a way, also the introduction of θ reflects the idea that volume is preserved by the Hamiltonian flow: $\int \theta_k (g_t^k)^g dX = \theta_k c_k$ stands for that amount of integral mass which *typically* moves from a sector $\mathcal{M}_{f_t}^k$ to $\mathcal{M}_{f_t}^{k+2}$, see line (31) above.

This is as far as we can get without specifying θ_k which depends on the scaling behavior of the interaction. Later we will give the right expression for θ_k for an interaction potential with scaling property $\phi_N = \frac{1}{N}\phi$ and then derive the Vlasov equation. But first we will show that propagation of molecular chaos implies convergence of the marginals of the N-particle density towards products of solutions of the mean field equation. From that, we will also derive convergence of empirical densities towards solutions of the mean field equation.

But for the sake of argument, assume ϵ_k was such that for $N \to \infty$

$$\dot{\alpha}(t) \leq c_1 \alpha(t) + c_2, \tag{34}$$

where c_2 stands for the error term that should go to zero as N goes to infinity. Then an application of Gronwall's lemma would imply

$$\alpha(t) \leq e^{c_1 t}\alpha(0) + (e^{c_1 t} - 1)\frac{c_2}{c_1} \tag{35}$$

and since $\alpha(0) = 0$ if we assume all particles to be *i.i.d.* initially, it would follow $\alpha(t) \leq o(N)$ for all t, leading to $\alpha(t) = 0$ in the limit $N \to \infty$.

For finite N, the estimation for α will include an error term decreasing with N. One advantage of the presented method is thus that the result is not just a statement for the limit $N \to \infty$, but it is actually possible to establish the speed of convergence in the particle number N.

If one succeeds in proving an equation of the type (15), one can show that the *s-marginal* of the symmetric N-particle density $\mathcal{F}_t$, defined as

$$\mathcal{F}_t^s := \int \mathcal{F}_t dx_{s+1} \dots dx_N \tag{36}$$

converges in L^1-norm to an s-fold product of solutions f_t of the mean field equation:

Theorem 2.2. *Let $\mathcal{F}_t \colon \mathbb{R}^{6N} \longrightarrow \mathbb{R}_+$ denote the time-dependent probability density of N particles evolving according to Newton's equations of motion with interaction potential ϕ_N^β as above and let $f_t \colon \mathbb{R}^6 \longrightarrow \mathbb{R}_+$ be a solution of the mean field equation in question. If for α as defined above holds*

$$\alpha(\mathcal{F}_t, f_t) \overset{N\to\infty}{\longrightarrow} 0, \tag{37}$$

then the marginals of $\mathcal{F}_t$ *converge:*

$$\mathcal{F}_t^s \overset{L_1}{\longrightarrow} \prod_{i=1}^{s} f_t(x_i) \quad \forall t \in \mathbb{R}_+ \quad \forall s \in \mathbb{N} \tag{38}$$

as $N \to \infty$.

Remark 2.5. By definition it is possible to choose for each N a decomposition of $\mathcal{F}_t$ such that

$$\alpha(\mathcal{F}_t, f_t) + \frac{1}{N} = \sum_{k=0}^{N} \frac{k}{N} c_k + \|(g_t^k)^n\|_1.$$

To see this, observe that the integral mass of $\mathcal{F}_t$ can be freely distributed over the g_t^k's (yielding the values of the c_k's) as long as the right hand side stays larger than α, which carries the infimum over all decompositions of $\mathcal{F}_t$. Since $\lim_{N\to\infty} \alpha = 0$, sending $N \to \infty$ on both sides yields

$$\lim_{N\to\infty} \left(\sum_{k=0}^{N} \frac{k}{N} c_k + \|(g_t^k)^n\|_1 \right) = 0.$$

This means that in the limit there exists a decomposition of $\mathcal{F}_t$ which minimizes $\sum \frac{k}{N} c_k + \|(g_t^k)^n\|_1$ if the counting measure vanishes. We will need this for the following proof.

Proof. Pick a decomposition of $\mathcal{F}_t$ such that

$$\alpha(\mathcal{F}_t, f_t) + \frac{1}{N} = \sum \frac{k}{N} c_k + \|(g_t^k)^n\|_1.$$

We make use of the symmetry of $\mathcal{F}_t$ and reorder the permutations σ into permutations σ' for which the first s particles are distributed according to f_t and permutations σ'' for which this is not the case:

$$
\begin{aligned}
\mathcal{F}_t^s &:= \int \mathcal{F}_t dx_{s+1}\dots dx_N \\
&= \sum_{k=0}^{N-s}\left[\frac{1}{N!}\sum_{\sigma'} f_t(x_1)\cdots f_t(x_s)\int \chi^k_{t,\sigma'}(x_1,\dots,x_N)\times\right. \\
&\times \prod_{i=k+1,\sigma'(i)\neq 1,\dots,s} \tilde{f}(x_{\sigma'(i)})dx_{s+1}\dots dx_N \\
&+ \left.\frac{1}{N!}\sum_{\sigma''}\int \chi^k_{t,\sigma''}(x_1,\dots,x_N)\prod_{i=k+1}^N f_t(x_i)dx_{s+1}\dots dx_N\right] \\
&+ \sum_{k=N-s+1}^{N}\frac{1}{N!}\sum_{\sigma}\int \chi^k_{t,\sigma}(x_1,\dots,x_N)\prod_{i=k+1}^N f_t(x_i)dx_{s+1}\dots dx_N.
\end{aligned}
$$

The relative frequency for the permutations σ' is

$$\frac{N-k}{N}\cdots\frac{N-k-s+1}{N-s+1} = \frac{(N-s)!}{N!}\frac{(N-k)!}{(N-k-s)!} < 1,$$

whereas for the permutations σ'' the relative frequency can be estimated from above as[9]

$$
\begin{aligned}
\frac{(N-s)!}{N!}\sum_{i=0}^{s-1}\binom{s}{i}\frac{k!}{(k-s+i)!}\frac{(N-k)!}{(N-k-i)!} &\leq \sum_{i=0}^{s-1}\binom{s}{i}\left(\frac{k}{N}\right)^{s-i}\left(\frac{N-k}{N-s}\right)^i \\
&\leq c(s)\left(\frac{N}{N-s}\right)^s\frac{k}{N}
\end{aligned}
$$

for $c(s)=\sum_{i=0}^{s-1}\binom{s}{i}$. We therefore have

$$
\begin{aligned}
\mathcal{F}_t^s &\leq f_t(x_1)\cdots f_t(x_s) \qquad (40)\\
&+ \left(\frac{N}{N-s}\right)^s c(s)\sum_{k=0}^N\frac{k}{N}\int \chi^k_{t,\sigma''}(x_1,\dots,x_N)\prod_{i=k+1}^N f_t(x_i)dx_{s+1}\dots dx_N \\
&+ \sum_{k=N-s+1}^N\frac{1}{N!}\sum_\sigma\int \chi^k_{t,\sigma}(x_1,\dots,x_N)\prod_{i=k+1}^N f_t(x_i)dx_{s+1}\dots dx_N
\end{aligned}
$$

[9]Note that they sum up to one:

$$\frac{(N-s)!}{N!}\sum_{i=0}^{s}\binom{s}{i}\frac{k!}{(k-s+i)!}\frac{(N-k)!}{(N-k-i)!} = 1 \qquad (39)$$

With

$$\sum_{k=N-s+1}^{N} \frac{N}{k} \frac{k}{N} \frac{1}{N!} \sum_{\sigma} \int \chi_{t,\sigma}^{k}(x_1, \ldots, x_N) \prod_{i=k+1}^{N} f_t(x_i) dx_{s+1} \ldots dx_N$$
$$\leq \frac{N}{N-s+1} \sum_{k=0}^{N} \frac{k}{N} \frac{1}{N!} \sum_{\sigma} \int \chi_{t,\sigma}^{k}(x_1, \ldots, x_N) \prod_{i=k+1}^{N} f_t(x_i) dx_{s+1} \ldots dx_N \quad (41)$$

in the last line above it follows that

$$\begin{aligned} \|\mathcal{F}_t^s - f_t(x_1) \cdots f_t(x_s)\|_1 &\leq \left(\frac{N}{N-s}\right)^s c(s) \sum_{k=0}^{N} \frac{k}{N} c_k + \frac{N}{N-s+1} \sum_{k=0}^{N} \frac{k}{N} c_k \\ &\leq \underbrace{\left[\left(\frac{N}{N-s}\right)^s c(s) + \frac{N}{N-s+1}\right]}_{\overset{N\to\infty}{\longrightarrow} c(s)+1} \left(\alpha(\mathcal{F}_t, f_t) + \frac{1}{N}\right) \\ &\overset{N\to\infty}{\longrightarrow} 0 \end{aligned}$$

by assumption and hence

$$\mathcal{F}_t^s \xrightarrow{L^1} f_t(x_1) \cdots f_t(x_s).$$

□

Remark 2.6. Under the conditions of the theorem, the L^1-convergence

$$\mathcal{F}_t^s \xrightarrow{L^1} f_t(x_1) \cdots f_t(x_s) \quad (42)$$

for all t and s implies w^*-convergence of the corresponding measures:

$$\mathcal{F}_t^s dX \xrightarrow{w^*} \prod_{i=1}^{s} f_t(x_i) dx_i \quad (43)$$

Weak convergence of the empirical density

$$\mu_N^{X(t)} := \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i(t)}$$

towards weak solutions of the Vlasov equation $\mu(t)$ was shown, among others, by Neunzert and Braun and Hepp (see [1],[2],[3]). The key equation in Neunzert's proof is

$$d_{BL}(\mu_N^{X(t)}, \mu(t)) \leq e^{ct} d_{BL}(\mu_N^{X(0)}, \mu(0)) \quad (44)$$

for the bounded Lipschitz distance d_{BL} (see e.g. [3]). We will show that for absolutely continuous measures, this result follows from the L^1-convergence of the marginals towards products of solutions of the Vlasov equation:

Corollary 2.2. *Let $\mu_N^{X(t)}$ describe the positions and momenta of N particles and let $\mu^{f_t}(dx) = f_t(x)dx$ for $f : \mathbb{R} \times \mathbb{R}^6 \to \mathbb{R}$. Then the L^1-convergence*

$$\mathcal{F}_t^1 \longrightarrow f_t \quad and \quad \mathcal{F}_t^2 \longrightarrow f_t \otimes f_t \tag{45}$$

implies

$$\mu_N^{X(t)} \stackrel{d_{BL}}{\longrightarrow} \mu^{f_t} \tag{46}$$

in mean with respect to $\mathbb{P}^{\mathcal{F}_t}$.

Proof. The crucial observation is that the metric d_{BL} is defined for functions g which are Lipschitz continuous with constant 1:

$$\mathcal{D} := \{g \colon \mathbb{R} \to [0,1], |g(x) - g(y)| \leq |x - y|\}.$$

A partition of phase space $\Gamma^1 \cong \mathbb{R}^6$ into cells Δ_i of sidelength δ is very useful, because the test functions g vary at most by δ on such a cell:

$$\begin{aligned} d_{BL}(\mu_N^{X(t)}, \mu^{f_t}) &:= \sup_{g\in\mathcal{D}} \Big| \int \mu_N^{X(t)}(dx)g(x) - \int f_t(x)g(x)dx \Big| \\ &= \sup_{g\in\mathcal{D}} \Big| \sum_i \int_{\Delta_i} \mu_N^{X(t)}(dx)g(x) - \int_{\Delta_i} f_t(x)g(x)dx \Big| \\ &\leq \sum_i \sup_{g\in\mathcal{D}} \Big| \int_{\Delta_i} \mu_N^{X(t)}(dx)g(x) - \int_{\Delta_i} f_t(x)g(x)dx \Big| \end{aligned}$$

Now $g \in \mathcal{D}$ and hence, as already explained, there exists $\delta > 0$ such that $|g(x) - g(y)| \leq \delta$ for all $x, y \in \Delta_i$ and, in addition, $g(x) \leq 1$ for all x:

$$\begin{aligned} d_{BL}(\mu_N^{X(t)}, \mu^{f_t}) &\leq \sum_i (1+\delta) \Big| \int_{\Delta_i} \mu_N^{X(t)}(dx) - \int_{\Delta_i} f_t(x)dx \Big| \\ &\leq 2\delta + \sum_i \Big| \mu_N^{X(t)}(\Delta_i) - \mu^{f_t}(\Delta_i) \Big| \end{aligned}$$

Integrating this with respect to $\mathbb{P}^{\mathcal{F}}$ and noting that

$$\int \mathcal{F}(X) d_{BL}(\mu_N^{X(t)}, \mu^{f_t}) dX = \int \mathcal{F}_t(X) d_{BL}(\mu_N^X, \mu^{f_t}) dX$$

since $\mathcal{F}(X) = \mathcal{F}_t(X(t))$ by definition, we obtain by dominated convergence

$$\int \mathcal{F}_t(X) d_{BL}(\mu_N^X, \mu^{f_t}) dX \le \sum_i \underbrace{\int \mathcal{F}_t(X) \left| \mu_N^X(\Delta_i) - \mu^{f_t}(\Delta_i) \right| dX}_{=:\lambda} + 2\delta. \quad (47)$$

Using Cauchy-Schwarz's inequality, we get

$$\begin{aligned}
\lambda &\le \left(\int \mathcal{F}_t(X) dX \left(\mu_N^X(\Delta_i) - \mu^{f_t}(\Delta_i) \right)^2 \right)^{1/2} \\
&= \left(\int \mathcal{F}_t(X) dX \left(\left(\mu_N^X(\Delta_i) \right)^2 - 2\mu_N^X(\Delta_i) \mu^{f_t}(\Delta_i) + \left(\mu^{f_t}(\Delta_i) \right)^2 \right) \right)^{1/2} \\
&= \left(\frac{1}{N} \int_{\Delta_i} \mathcal{F}_t^1(x) dx + \frac{N(N-1)}{N^2} \int_{\Delta_i} \int_{\Delta_i} \mathcal{F}_t^2(x,y) dx dy \right. \qquad (48) \\
&- \left. 2 \int_{\Delta_i} \mathcal{F}_t^1(x) dx \int_{\Delta_i} f_t(x) dx + \left(\int_{\Delta_i} f_t(x) dx \right)^2 \right)^{1/2} \\
&\le \left(\frac{1}{N} \int_{\Delta_i} \mathcal{F}_t^1(x) dx - \frac{1}{N} \int_{\Delta_i} \int_{\Delta_i} \mathcal{F}_t^2(x,y) dx dy \right. \\
&+ \int_{\Delta_i} \int_{\Delta_i} \left| \mathcal{F}_t^2(x,y) - f_t(x) f_t(y) \right| dx dy \\
&+ \left. 2 \int_{\Delta_i} \left| \mathcal{F}_t^1(x) - f_t(x) \right| dx \int_{\Delta_i} f_t(x) dx \right)^{1/2} \stackrel{N\to\infty}{\longrightarrow} 0
\end{aligned}$$

and since the left hand side of (47) is independent of δ, sending δ to zero implies

$$\lim_{N\to\infty} \int \mathcal{F}_t(X) d_{BL}(\mu_N^X, \mu^{f_t}) dX = 0. \quad (49)$$

Note that to get line (48), we used the symmetry of $\mathcal{F}_t$ under particle exchange. $\square$

Remark 2.7. This obviously implies for all $\kappa > 0$

$$\mathbb{P}^N\left(\left\{X=(x_1,\ldots,x_N)\middle| d_{BL}(\mu_N^{X(t)},\mu^{f_t})>\kappa\right\}\right)\overset{N\to\infty}{\longrightarrow}0 \tag{50}$$

since

$$\int \mathcal{F}_t\chi_{\left\{\frac{d_{BL}(\mu_N^{X(t)},\mu^{f_t})}{\kappa}>1\right\}}dx_1\ldots dx_N \leq \frac{1}{\kappa}\int \mathcal{F}_t d_{BL}(\mu_N^{X(t)},\mu^{f_t})dx_1\ldots dx_N, \tag{51}$$

which tends to zero for all κ.

3 Derivation of the Vlasov equation

In the last section we explained how one can in principle derive an effective mean field equation from microscopic dynamics using the "counting measure" α. However, we did this in very general terms and stopped at the point where a specification of the parameters θ_k was inevitable. θ_k was introduced to compensate for the negative parts in the difference $(g_t^k)^g\circ\Phi_{-\Delta t}-(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}$ at least as long as the dynamics stays within typical fluctuations. At this stage it is quite clear that we expect these typical fluctuations to be of order $\sqrt{N}$ in total, i.e. $1/\sqrt{N}$ per particle, since we have the law of large numbers at our disposal and the fluctuations from the mean field orbit are the deviations from the expectation value.

Hence, $\theta_k(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}$ should be of the typical size of the difference between[10]

$$(g_t^k)^g\circ\Phi_{-\Delta t}=(g_t^k)^g+\sum_{i=1}^N\nabla_{q_i}(g_t^k)^g\cdot\Delta q_i+\sum_{i=1}^N\nabla_{p_i}(g_t^k)^g\cdot\Delta p_i \tag{52}$$

and

$$(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}=(g_t^k)^g+\sum_{i=1}^N\nabla_{q_i}(g_t^k)^g\cdot\Delta q_i+\sum_{i=1}^N\nabla_{p_i}(g_t^k)^g\cdot\Delta\pi_i, \tag{53}$$

where we defined

[10]Note that the following equations are only true to first order in Δt.

$$\Delta p_i = -\frac{1}{N}\sum_{j=1}^{N} \nabla_{q_i}\phi(q_i - q_j)\Delta t \quad \text{for } i = 1, \dots, N \tag{54}$$

and

$$\Delta \pi_i = \begin{cases} -\frac{1}{N}\sum_{j=1}^{N} \nabla_{q_i}\phi(q_i - q_j)\Delta t, & \text{for } i = 1, \dots, k \\ -\int f_t(q,p)\nabla_{q_i}\phi(q_i - q)dqdp\Delta t, & \text{for } i = k+1, \dots, N \end{cases} \tag{55}$$

for a solution f_t of the Vlasov equation. Note that we ignored the part of the force coming from an external potential, namely $-\nabla_{q_i}V_t(q_i)$, because it appears in both Δp_i and $\Delta\pi_i$ and we only consider the difference $\Delta p - \Delta\pi$. The splitting of the "mean field momenta" $\Delta\pi_i$ is for technical reasons. We could have let the k "bad" particles evolve according to the expectation value of the force, but it doesn't matter so much since they are not *i.i.d.* and can thus not be expected to act according to mean field dynamics.

We will in the following use the abbreviation

$$\delta K(q_i - q_j) := \nabla_{q_i}\phi(q_i - q_j) - \int \nabla_{q_i}\phi(q_i - q)f_t(q,p)dqdp. \tag{56}$$

For the difference between the two time evolutions we then have

$$\begin{aligned} \nabla_p (g_t^k)^g \cdot (\Delta p - \Delta\pi) = \sum_{i=k+1}^{N} \nabla_{p_i}(g_t^k)^g \frac{1}{N}\Bigg[\sum_{j=1}^{k} (-\delta K(q_i - q_j)) \\ + \sum_{j=k+1}^{N} (-\delta K(q_i - q_j)) \Bigg]\Delta t, \end{aligned} \tag{57}$$

where one should keep in mind that the first k particles are not distributed according to a product, whereas the last $N-k$ particles are, therefore the splitting into two sums. We need a bound for the set in N-particle phase space Γ^N on which $(g_t^k)^g \circ \Phi_{-\Delta t} - (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t}$ is still negative. We will now define θ_k and then show that this set is in fact exponentially small in N.

Definition 3.1. For an interaction potential scaling as $\phi_N(q) = \frac{1}{N}\phi(q)$ with ϕ such that $\nabla\phi$ is bounded, the parameter θ_k shall be defined for $k \in \{0, \dots, N\}$ and $0 < \kappa < \frac{1}{2}$ as

$$\theta_k := \left\| \frac{\nabla_p f_t}{f_t} \right\|_\infty \|\nabla\phi\|_\infty k\Delta t + \left\| \frac{\nabla_p f_t}{f_t} \right\|_\infty (N-k)^{1/2+\kappa}\Delta t \tag{58}$$

Remark 3.1. 1. The first term will, together with the prefactor $1/N$, produce a new α in (32). The second term is, again with a prefactor $1/N$, of order $N^{-1/2+\kappa}$ and will thus tend to zero for $N \to \infty$.

2. For the k "bad" particles, the law of large numbers is of no use to derive a bound for δK, the difference between the actual force and its mean field approximation. In order to get a finite θ_k, we will therefore need this to be bounded by assumption: $\sup \delta K < \infty$, which translates to a bounded $\nabla\phi$.

3. The term $\nabla_{p_i}(g_t^k)^g$ in (57) will in the following be divided pointwise by $(g_t^k)^g$, and since $i = k+1, \ldots, N$ here, the p-differentiation is only with respect to "nice" coordinates. We can therefore divide the whole fraction by $(\chi_t^k)^g$. This yields $\frac{\nabla_p f_t}{f_t}$ in the expression for θ_k. This was the reason for the maybe unexpected definition of $\Delta\pi$, namely to let the k "bad" particles evolve according to the exact dynamics. The condition that $\frac{\nabla_p f_t}{f_t}$ is bounded is not as strong as it might seem at first glance. We can show that those initial conditions f_0 for which pointwise $\nabla_p f_t \le c(t) f_t$ on compact time intervals lie dense in $L^1(\mathbb{R}^6) \cap \mathcal{C}^1(\mathbb{R}^6)$.

4. Note that, since θ_k carries a Δt itself, it holds $\theta_k(g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} = \theta_k(g_t^k)^g$ to first order in Δt.

For the set in question, we thus find to first order in Δt[11]:

$$\begin{aligned}
&\left\{X = (x_1, \ldots, x_N) \middle| (g_t^k)^g \circ \Phi_{-\Delta t} - (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} < 0 \right\} \\
= &\left\{X = (x_1, \ldots, x_N) \middle| \frac{N-k}{N} \nabla_{p_i}(g_t^k)^g \sum_{j=1}^{k} \delta K(q_i - q_j)\Delta t \right. \\
+ &\left. \frac{N-k}{N} \nabla_{p_i}(g_t^k)^g \sum_{j=k+1}^{N} \delta K(q_i - q_j)\Delta t > \theta_k (g_t^k)^g \right\} \\
\subset &\left\{X = (x_1, \ldots, x_N) \middle| \frac{1}{N} \sum_{j=k+1}^{N} \delta K(q_i - q_j) > N^{-1/2+\kappa} \right\} =: \Omega^k.
\end{aligned}$$

For the second term in (32), we thus get (again to first order in Δt):

[11] Keep in mind that coordinates q_i for $i = k+1, \ldots, N$ are *i.i.d.*, while the others are not.

$$\begin{aligned}
&\left\| \Big((g_t^k)^g \circ \Phi_{-\Delta t} - (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} + \theta_k (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} \Big)^n \right\|_1 \qquad (59)\\
=\ & 2 \int_{\mathbb{R}^{6N}} \left| \Big((g_t^k)^g \circ \Phi_{-\Delta t} - (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t} + \theta_k (g_t^k)^g \Big)^- \right| dX \\
\leq\ & 2 \int_{\Omega^k} (g_t^k)^g \left| \frac{(g_t^k)^g \circ \Phi_{-\Delta t} - (g_t^k)^g \circ \tilde{\Phi}_{-\Delta t}}{(g_t^k)^g} + \theta_k \right| dX \\
\leq\ & 2 \Big[(N-k) \Big\| \frac{\nabla_p f_t}{f_t} \Big\|_\infty \|\nabla \phi\|_\infty \Delta t + \theta_k \Big] \int_{\Omega^k} (g_t^k)^g dX.
\end{aligned}$$

The set Ω^k contains those parts of phase space for which large deviations from the mean field orbit occur. If the estimation above is not too coarse, such a set should be small:

Lemma 3.1. *Let the functions $(g_t^k)^g$ be defined as above and let $\nabla \phi$ be bounded. For Ω^k as above holds*

$$\int_{\Omega^k} (g_t^k)^g dX \leq c_k e^{-\frac{N^{2\kappa}}{2\mathbb{E}[\delta K^2]}} r(\delta K, N) \quad for \quad 0 < \kappa < \frac{1}{2}, \qquad (60)$$

where $r(\delta K, N) \to 1$ as $N \to \infty$.

Proof. Let χ_M denote the characteristic function of the set M. For $i \in \{k+1, \dots, N\}$ it holds for all $s > 0$

$$\begin{aligned}
\int_{\Omega^k} (g_t^k)^g dx_1 \dots dx_N &= \int_{\mathbb{R}^{6N}} (g_t^k)^g \chi_{\left\{ \frac{1}{N} \sum_{j=k+1}^N \delta K(q_i - q_j) > N^{-1/2+\kappa} \right\}} dx_1 \dots dx_N \\
&\leq \int_{\mathbb{R}^{6N}} (g_t^k)^g \frac{\exp(s \sum_{j=k+1}^N \delta K(q_i - q_j))}{\exp(s N^{1/2+\kappa})} dx_1 \dots dx_N \\
&= e^{-sN^{1/2+\kappa}} \int_{\mathbb{R}^{6N}} e^{s \sum_{j=k+1}^N \delta K(q_i - q_j)} \\
&\times \ \left(\chi_t^k\right)^g (x_1, \dots, x_N) dx_1 \dots dx_k \prod_{l=k+1}^N f_t(x_l) dx_l \\
&= c_k e^{-sN^{1/2+\kappa}} \int_{\mathbb{R}^{6N}} \prod_{j=k+1}^N e^{s\delta K(q_i - q_j)} f_t(x_j) dx_j \\
&= c_k e^{-sN^{1/2+\kappa}} \mathbb{E}^{f_t} \big[e^{s\delta K} \big]^{N-k} \\
&= c_k e^{-sN^{1/2+\kappa}} e^{(N-k) \ln \mathbb{E}^{f_t} [e^{s\delta K}]}
\end{aligned}$$

Using Taylor's theorem and the mean value theorem, we obtain

$$\begin{aligned} e^{s\delta K} &= 1 + s\delta K + \frac{s^2}{2}\delta K^2 + \int_0^s \frac{(s-\xi)^2}{2}(\delta K)^3 e^{\xi\delta K} d\xi \\ &= 1 + s\delta K + \frac{s^2}{2}\delta K^2 + s\frac{(s-\bar{\xi})^2}{2}(\delta K)^3 e^{\bar{\xi}\delta K} \end{aligned}$$

for some $\bar{\xi} \in [0, s]$. Since $\mathbb{E}[\delta K] = 0$[12],

$$\mathbb{E}[e^{s\delta K}] \;=\; 1 + \frac{s^2}{2}\mathbb{E}[\delta K^2] + s\frac{(s-\bar{\xi})^2}{2}\mathbb{E}[(\delta K)^3 e^{\bar{\xi}\delta K}]$$

and thus

$$\ln \mathbb{E}[e^{s\delta K}] \;\leq\; \frac{s^2}{2}\mathbb{E}[\delta K^2] + s\frac{(s-\bar{\xi})^2}{2}\mathbb{E}[(\delta K)^3 e^{\bar{\xi}\delta K}].$$

It therefore holds

$$\begin{aligned} \int_{\Omega^k} (g_t^k)^g dX &\leq c_k \exp\left(- sN^{1/2+\kappa} + (N-k)\frac{s^2}{2}\mathbb{E}[\delta K^2]\right) \times \\ &\times \exp\left((N-k)s\frac{(s-\bar{\xi})^2}{2}\mathbb{E}\Big[(\delta K)^3 e^{\bar{\xi}\delta K}\Big]\right) \\ &\leq c_k \exp\left(- sN^{1/2+\kappa} + N\frac{s^2}{2}\mathbb{E}[\delta K^2] + N\frac{s^3}{2}\mathbb{E}\Big[|\delta K|^3 e^{s|\delta K|}\Big]\right). \end{aligned} \tag{61}$$

Since this is true for all s, it also holds for the special choice

$$s = \frac{N^{-1/2+\kappa}}{\mathbb{E}[\delta K^2]} \tag{62}$$

We therefore get

$$\int_{\Omega^k} (g_t^k)^g dX \;\leq\; c_k e^{-\frac{N^{2\kappa}}{2\mathbb{E}[\delta K^2]}} \underbrace{\exp\left(\frac{N^{-1/2+3\kappa}}{2\mathbb{E}[\delta K^2]^3}\mathbb{E}\Big[\delta K^2 e^{\frac{N^{-1/2+\kappa}|\delta K|}{\mathbb{E}[|\delta K|^3]}}\Big]\right)}_{=:r(\delta K, N)} \tag{63}$$

This proves the lemma. □

[12] In the following, $\mathbb{E}$ will alway denote the expectation value with respect to f_t.

The above leads to

$$\begin{aligned}
&\sum_{k=0}^{N}\Big\|\Big((g_t^k)^g\circ\Phi_{-\Delta t}-(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}+\theta_k(g_t^k)^g\circ\tilde{\Phi}_{-\Delta t}\Big)^n\Big\|_1 && (64)\\
\leq\ &\sum_{k=0}^{N}2\Big[(N-k)\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty\|\nabla\phi\|_\infty\Delta t+\theta_k\Big]c_k r(\delta K,N)e^{-\frac{N^{2\kappa}}{2\mathbb{E}[\delta K^2]}}\\
\leq\ &\underbrace{\sum_{k=0}^{N}c_k}_{=1}\cdot const.\cdot N\cdot\Delta t\cdot r(\delta K,N)e^{-\frac{N^{2\kappa}}{2\mathbb{E}[\delta K^2]}}\overset{N\to\infty}{\longrightarrow}0
\end{aligned}$$

and we have thus proven the

Lemma 3.2. *Let the measure α be defined as above and let the interaction potential be given by $\phi_N(q)=\frac{1}{N}\phi(q)$ for symmetric ϕ such that $\nabla\phi$ is bounded. Furthermore let the N-particle density be given by $\mathcal{F}_t\in L^1(\mathbb{R}^{6N})$ and let $f_t\in L^1(\mathbb{R}^6)\cap\mathcal{C}^1(\mathbb{R}^6)$ be a probability density which solves the Vlasov equation with initial condition f_0. In addition, let f_t be such that the pointwise fraction $\frac{\nabla_p f_t}{f_t}$ is bounded. Then for $0<\kappa<\frac{1}{2}$*

$$\begin{aligned}
\dot{\alpha}_t\ &\leq\ 2\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty\|\nabla\phi\|_\infty\alpha_t && (65)\\
&+\ 2\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty N^{-1/2+\kappa}\\
&+\ 2\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty\left(2N\|\nabla\phi\|_\infty+N^{1/2+\kappa}\right)r(\delta K,N)e^{-\frac{N^{2\kappa}}{2\mathbb{E}[\delta K^2]}}.
\end{aligned}$$

We make the abbreviations

$$\lambda_1:=2\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty\|\nabla\phi\|_\infty$$

and

$$\lambda_2:=2\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty N^{-1/2+\kappa}+2\Big\|\frac{\nabla_p f_t}{f_t}\Big\|_\infty\left(2N\|\nabla\phi\|_\infty+N^{1/2+\kappa}\right)r(\delta K,N)e^{-\frac{N^{2\kappa}}{2\mathbb{E}[\delta K^2]}}.$$

Keep in mind that λ_1 does not depend on the particle number N, whereas λ_2 is of order $N^{-1/2+\kappa}$. An application of Gronwall's lemma yields:

Theorem 3.1. *Under the conditions of the lemma, it holds*

$$\alpha_t \leq e^{\lambda_1 t}\alpha_0 + \left(e^{\lambda_1 t} - 1\right)\frac{\lambda_2}{\lambda_1},$$

and thus in fact: If the particles are distributed independently at $t = 0$, i.e. $\alpha_0 = 0$, then

$$\alpha_t \leq \mathcal{O}\left(\frac{1}{\sqrt{N}}\right).$$

We will now investigate the requirement that $\|\nabla_p \tilde{f}_t\| \leq c(t)\tilde{f}_t$ for some positive $c(t)$ which is bounded for finite t.[13] First, we will show that those initial conditions for which this requirement is fulfilled are dense in $L^1(\mathbb{R}^6) \cap \mathcal{C}(\mathbb{R}^6)$. Secondly, we will show that the corresponding solutions of the Vlasov equation still fulfill that requirement on compact time intervals.

Lemma 3.3. *For $f \in L^1(\mathbb{R}^6) \cap \mathcal{C}(\mathbb{R}^6)$ define*

$$f^\delta := \frac{1}{n(\delta)} f{*}\exp\left(-\frac{\|\cdot\|^2}{(1+\|\cdot\|)\delta}\right) = \frac{1}{n(\delta)}\int f(y)\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right) d^3y, \tag{66}$$

where

$$n(\delta) = \int \exp\left(-\frac{\|x\|^2}{(1+\|x\|)\delta}\right) d^3x.$$

Then f^δ fulfills[14]

$$\|\nabla_x f^\delta\| \leq \frac{3\sqrt{6}}{\delta} f^\delta \quad \forall \delta > 0. \tag{67}$$

Proof. We calculate

$$\begin{aligned} \frac{\partial}{\partial x_i}\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right) &= (x_i - y_i)\left(\frac{\|x-y\|^2}{\delta(1+\|x-y\|)} - \frac{2}{\delta(1+\|x-y\|)}\right)\times \\ &\quad \exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right) \\ &\leq \frac{3}{\delta}\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right) \end{aligned}$$

[13] Here, $\|\cdot\|$ denotes the euclidean norm.

[14] Since $\|\nabla_p f^\delta\| \leq \|\nabla_x f^\delta\|$, we can focus on the x-gradient to estimate the p-gradient. This will be essential when proving that the boundedness is preserved during time evolution.

and conclude

$$\|\nabla_x f^\delta(x)\| = \left(\sum_{i=1}^{6}\left(\int f(y)\frac{\partial}{\partial x_i}\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right)d^3y\right)^2\right)^{1/2} \leq \sqrt{6}\frac{3}{\delta}f^\delta(x).$$

□

Lemma 3.4. *The functions f^δ as defined in (66) are dense in $L^1(\mathbb{R}^6)\cap\mathcal{C}(\mathbb{R}^6)$.*

Proof. Since f is continuous, we have $\forall\epsilon>0\exists\xi>0:|f(x)-f(y)|<\epsilon\forall y\in U_\xi(x)$. We split the integration in f^δ into an integral over $U_\xi(x)$ and one over its complement $U_\xi^c(x)$ and estimate from above using the continuity of f:

$$\begin{aligned} f^\delta(x) &= \frac{1}{n(\delta)}\int_{U_\xi(x)} f(y)\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right)d^3y \\ &+ \frac{1}{n(\delta)}\int_{U_\xi^c(x)} f(y)\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right)d^3y \\ &\leq (f(x)+\epsilon)\underbrace{\frac{1}{n(\delta)}\int_{U_\xi(x)}\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right)d^3y}_{A} \\ &+ \underbrace{\frac{1}{n(\delta)}\int_{U_\xi^c(x)} f(y)\exp\left(-\frac{\|x-y\|^2}{(1+\|x-y\|)\delta}\right)d^3y}_{B} \end{aligned} \tag{68}$$

For δ small enough, we have that $A=1-\epsilon$ and $B\leq\epsilon\sup(f)$ and thus

$$f^\delta(x)\leq f(x)-\epsilon f(x)+\epsilon-\epsilon^2+\epsilon\sup(f).$$

Similarly, we find that

$$f^\delta(x)\geq(f(x)-\epsilon f(x))(1-\epsilon)$$

and therefore

$$-\epsilon\leq f^\delta(x)-f(x)\leq\epsilon+\epsilon\sup(f),$$

implying pointwise convergence of f^δ to f for $\delta\to 0$. Since this implies L^1-convergence, the lemma is proven. □

Next, we will show that the boundedness of the pointwise fraction $\frac{\nabla_x f_0}{f_0}$ for an initial condition f_0 is preserved by the Vlasov dynamics:

Lemma 3.5. *Let $f_t^\delta \in L^1(\mathbb{R}^6) \cap \mathcal{C}^1(\mathbb{R}^6)$ denote a solution of the Vlasov equation with initial condition f_0^δ.*[15] *Let $K = f_t^\delta * \nabla\phi$, the force term in the Vlasov equation, be such that its Jacobian DK is bounded in operator norm. Then there exists $M > 0$ such that*

$$\frac{d}{dt}\Big\|\frac{\nabla_x f_t^\delta}{f_t^\delta}\Big\| \leq M\Big\|\frac{\nabla_x f_t^\delta}{f_t^\delta}\Big\| \tag{69}$$

and therefore, by Gronwall and the lemma above,

$$\Big\|\frac{\nabla_x f_t^\delta}{f_t^\delta}\Big\| \leq e^{Mt}\Big\|\frac{\nabla_x f_0^\delta}{f_0^\delta}\Big\| \leq e^{Mt}\frac{3\sqrt{6}}{\delta}. \tag{70}$$

Proof. At a given time t and a point (q_0, p_0), we look at a small displacement h in p-direction, make use of the time evolution of the probability density f_t and expand in a suitable manner:

$$\begin{aligned}
f_t(q_0,p_0) - f_t(q_0,p_0+h) &= f_{t+\Delta t}(q_0 + p_0\Delta t, p_0 + K(q_0)\Delta t) \\
&- f_{t+\Delta t}(q_0 + (p_0+h)\Delta t, p_0 + h + K(q_0)\Delta t) \\
&= f_{t+\Delta t}(q_0 + p_0\Delta t, p_0 + K(q_0)\Delta t) \\
&- f_{t+\Delta t}(q_0 + (p_0+h)\Delta t, p_0 + K(q_0)\Delta t) \\
&+ f_{t+\Delta t}(q_0 + (p_0+h)\Delta t, p_0 + K(q_0)\Delta t) \\
&- f_{t+\Delta t}(q_0 + (p_0+h)\Delta t, p_0 + h + K(q_0)\Delta t)
\end{aligned}$$

It follows with the chain rule that

$$\begin{aligned}
\nabla_p f_t(q_0,p_0) &= \nabla_q f_{t+\Delta t}(q_0 + p_0\Delta t, p_0 + K(q_0)\Delta t)\Delta t \\
&+ \nabla_p f_{t+\Delta t}(q_0 + p_0\Delta t, p_0 + K(q_0)\Delta t)
\end{aligned}$$

and thus

$$\frac{d}{dt}\nabla_p f_t(q_0,p_0) = -\nabla_q f_t(q_0,p_0).$$

Similarly, for a small displacement in q-direction, we find

[15] It is clear that the solution originating from the convolution $f_0^\delta = f * \exp\left(-\frac{\|\cdot\|^2}{(1+\|\cdot\|)\delta}\right)$ will not have the form of a convolution anymore.

$$\begin{aligned}
f_t(q_0,p_0) - f_t(q_0+h,p_0) &= f_{t+\Delta t}(q_0+p_0\Delta t, p_0+K(q_0)\Delta t) \\
&- f_{t+\Delta t}(q_0+h+p_0\Delta t, p_0+K(q_0+h)\Delta t) \\
&= f_{t+\Delta t}(q_0+p_0\Delta t, p_0+K(q_0)\Delta t) \\
&- f_{t+\Delta t}(q_0+h+p_0\Delta t, p_0+K(q_0)\Delta t) \\
&+ f_{t+\Delta t}(q_0+h+p_0\Delta t, p_0+K(q_0)\Delta t) \\
&- f_{t+\Delta t}(q_0+h+p_0\Delta t, p_0+K(q_0+h)\Delta t)
\end{aligned}$$

and since $K(q_0+h)\Delta t \approx K(q_0)\Delta t + DK(q_0)h\Delta t$, the chain rule this time yields

$$\begin{aligned}
\nabla_q f_t(q_0,p_0) &= \nabla_q f_{t+\Delta t}(q_0+p_0\Delta t, p_0+K(q_0)\Delta t) \\
&+ DK(q_0)\nabla_p f_{t+\Delta t}(q_0+p_0\Delta t, p_0+K(q_0)\Delta t)\Delta t,
\end{aligned}$$

and hence

$$\frac{d}{dt}\nabla_q f_t(q_0,p_0) = -DK(q_0)\nabla_p f_t(q_0,p_0).$$

Putting both time-derivatives together, we obtain

$$\frac{d}{dt}\nabla_x f_t(q_0,p_0) = -\begin{pmatrix} 0 & \mathbb{I}_3 \\ DK(q_0) & 0 \end{pmatrix} \nabla_x f_t(q_0,p_0)$$

and because the matrix is bounded in operator norm by assumption, we get (reintroducing the superscript δ)

$$\frac{d}{dt}\left\|\nabla_x f_t^\delta\right\| \leq M \left\|\nabla_x f_t^\delta\right\|$$

Since the Vlasov equation reads $\frac{d}{dt} f_t^\delta = 0$, we can pointwise divide by f_t^δ to obtain the desired result:

$$\frac{d}{dt}\left\|\frac{\nabla_x f_t^\delta}{f_t^\delta}\right\| \leq M \left\|\frac{\nabla_x f_t^\delta}{f_t^\delta}\right\|$$

□

Corollary 3.1. *With the foregoing, we can rephrase the theorem for solutions of the Vlasov equation with initial condition f_0^δ as defined in (66): Under the conditions of the theorem, together with the additional requirement that*

$K = f_t^\delta * \nabla\phi$ be such that its Jacobian DK is bounded in operator norm, it holds for all $\delta > 0$ in the limit $N \to \infty$

$$\dot{\alpha}(\mathcal{F}_t, \tilde{f}_t^\delta) \leq e^{Mt} \frac{6\sqrt{6}}{\delta} \|\delta K\|_\infty \alpha(\mathcal{F}_t, \tilde{f}_t^\delta) \tag{71}$$

and therefore

$$\alpha(\mathcal{F}_t, \tilde{f}_t^\delta) \leq \exp\left(\frac{6\sqrt{6}}{\delta} \|\delta K\|_\infty \int_0^t e^{Ms} ds \right) \alpha(\mathcal{F}_0, f_0^\delta). \tag{72}$$

Since $\alpha(\mathcal{F}_0, f_0^\delta) = 0$ only if $\mathcal{F}_0(X) = \prod_{i=1}^N f_0^\delta(x_i)$, we have hereby proven the propagation of molecular chaos for all initial distributions of the form $\mathcal{F}_0(X) = \prod_{i=1}^N f_0^\delta(x_i)$.

4 Conclusion

The method using a "counting measure" in order to derive mean field equations from microscopic dynamics has proven very successful for quantum mechanical systems. The Hartree equation (see [4]), which might be seen as the quantum mechanical analogue of the Vlasov equation, as well as - more importantly - the Gross-Pitaevskii equation (see [5]) have been derived using a measure which tells us "how much" an N-particle density has product form. The purpose of this thesis was to test if this method could be modified in such a way as to be applicable to classical systems. The major new technical difficulty showing up in the transition from L^2 to L^1 was (little surprisingly) the loss of a scalar product and thereby of a notion of orthogonality. Nevertheless, we succeeded in translating the method and were able to derive the Vlasov equation, which might be called the simplest example provided to us by physics. There already exist various rigorous derivations of the Vlasov equation in the literature. With slightly stronger conditions on the initial values of solutions of the Vlasov equation, these results could be reproduced although we started from a very different perspective. Whereas all derivations that are known to us concentrate on proving convergence of discrete point distributions towards solutions of the Vlasov equation with a suitable notion of distance, we focussed on the product structure of the distributing function. In order to assess the distance of that N-particle density from a product, we constructed a measure which in the simplest cases just counts the number of particles which fell out of the initial identical and independent distribution. In proving that this measure remains small if it was small in the beginning, we derived the Vlasov equation in a - we think - more intuitive way than has been done so far. Most surprisingly, it was possible to show that the L^1-distance of the s-marginal of the N-particle density from an s-fold product of solutions of the Vlasov equation is bounded by a multiple of that measure.

References

[1] H. Neunzert: *An Introduction to the Nonlinear Boltzmann-Vlasov Equation*, 1984

[2] W. Braun and K. Hepp: *The Vlasov Dynamics and Its Fluctuations in the 1/N Limit of Interacting Classical Particles*, Commun. math. Phys. 56, 125-146, 1977

[3] H. Spohn: *Large Scale Dynamics of Interacting Particles*, Springer, Heidelberg, 1991

[4] P. Pickl: *A simple derivation of mean field limits for quantum systems*, preprint

[5] P. Pickl: *Derivation of the time dependent Gross Pitaevskii equation with external fields*, preprint

Selbstständigkeitserklärung

Hiermit erkläre ich, die vorliegende Arbeit selbstständig verfaßt und keine anderen als die genannten Quellen und Hilfsmittel verwendet zu haben.

München, den 30. Januar 2011

Niklas Boers