Proceedings of the International Congress of Mathematicians
Vancouver, 1974

Time Evolution of Infinite Classical Systems

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I will discuss in this article some recent progress in the problem of proving existence and uniqueness of solutions to Newton's equations of motion for infinite systems of classical particles interacting by two-body forces which go to zero reasonably quickly as the particle separation goes to infinity. For technical simplicity, I will assume that the interparticle potential Φ has a Lipschitz continuous derivative and finite range, but the results I will describe have extensions which require neither finite range nor the absence of singularities in the potential.

To establish notation: We consider systems of infinitely many particles with positions (q_i) and momenta (p_i), moving in $\boldsymbol{R}^\nu$. The equations of motion are

$$(1) \qquad \frac{dq_i}{dt} = \frac{p_i}{m}, \qquad \frac{dp_i}{dt} = F_i = \sum_{j \neq i} F(q_i - q_j)$$

where m is the particle mass and $F = -\operatorname{grad} \Phi$ is the interparticle force. We assume that there are infinitely many particles, but that, initially at least, they are distributed so that there are only finitely many in each bounded region of space. Because of the infinite number of particles, these equations cannot be treated by the usual elementary techniques, and it is indeed not hard to imagine that some solutions may develop "singularities" in which, for example, infinitely many particles rush into a bounded region of space. What is needed is an existence result which assures us that such singularities are at least improbable.

The result to be described assumes, in addition to the regularity mentioned above, that the interparticle potential Φ has good thermodynamic properties. More specifically, we assume that Φ is *superstable* in the sense of Ruelle [**6**]. It is then possible to single out a class of probability measures on the phase space for the infinite system—the so-called Gibbs states—which represent thermodynamic equilibrium for the interaction in question. (See [1], [4], or [6].) What we show is that there exists a set of solutions to the equations of motion forming a set of probability one for each Gibbs state. We are, however, not able to describe in any very explicit way the set of phase points which lie on such solution curves, nor are we able to prove existence of solutions for initial phase points representing situations which are globally not in thermodynamic equilibrium. In this respect, the results described here are much weaker than previous work on one-dimensional systems [2] which proved existence and uniqueness of solutions for all initial phase points satisfying some reasonable regularity conditions.

Mathematically, the main novelty in the argument we will give is that it exploits the formal fact that Gibbs states ought to be invariant under the flow we are trying to construct. This leads to an a priori estimate which is shown to hold almost everywhere with respect to each Gibbs state. The idea is that Gibbs states are concentrated on very well-behaved phase points, and the invariance ought to imply good behavior at all times. The following result illustrates the argument:

PROPOSITION 1. *Let μ be a Gibbs state, and assume that the equations of motion can be solved almost everywhere to give a flow T^t leaving μ invariant. Then, for almost every phase point $\boldsymbol{x} = (q_i, p_i)$, there exists a constant M such that*

$$|q_i(t) - q_i| \leqq M \log_+(q_i) \quad \textit{for all } i \textit{ and } |t| \leqq 1. \tag{2}$$

(Here $\log_+(q)$ *denotes* $\log(|q|)$ *if* $|q| \geqq e$ *and* 1 *otherwise.)*

To prove this result, we define a function B on the infinite system phase space by

$$B(\boldsymbol{x}) = \sup_i \left\{ \frac{|p_i/m|}{\log_+(q_i)} \right\}. \tag{3}$$

To say that $B(\boldsymbol{x})$ is finite says that velocity fluctuations grow at most like the logarithm of the distance from the origin. A simple argument, using the Maxwellian (i.e., Gaussian) character of the momentum distribution, shows that B is integrable with respect to μ. Now define

$$\bar{B}(\boldsymbol{x}) = \int_{-1}^{1} dt\, B(T^t \boldsymbol{x}).$$

By Fubini's theorem and the assumed invariance of μ under T^t,

$$\int \bar{B}\, d\mu = \int_{-1}^{1} dt \int B \circ T^t \, d\mu = 2 \int B\, d\mu < \infty.$$

Hence, $\bar{B}$ is finite almost everywhere. We now claim that, where $\bar{B}(\boldsymbol{x})$ is finite, there exists a constant M (depending only on $\bar{B}(\boldsymbol{x})$) such that (2) holds. In fact, we have, for each i,

$$\left| \int_0^t dt_1 \frac{|dq_i(t_1)/dt|}{\log_+(q_i(t_1))} \right| \leqq \int_{-1}^{1} dt_1 \sup_i \left\{ \frac{|p_i(t_1)/m|}{\log_+(q_i(t_1))} \right\} = \bar{B}(\boldsymbol{x}).$$

It is now a matter of elementary calculus to show that, for any number b, there exists an $M(b)$ such that

$$\int_0^t dt_1 \frac{|dq_i(t_1)/dt|}{\log_+(q_i(t_1))} \leqq b \quad \text{implies} \quad |q_i(t) - q_i| \leqq M(b)\log_+(q_i).$$

This proves the proposition. Of course, the proposition is of little direct use, since it assumes what was to be proved, the existence of solutions to the equations. Its usefulness derives from the fact that we can find approximate solutions to the equations of motion which leave μ invariant and to which we can apply the above argument. One way to do this is as follows: For each positive integer s, let Λ_s denote the ball of radius s centered about the origin, and let $T^t_{(s)}$ denote the solution flow for the following dynamics:

(a) particles initially outside Λ_s are frozen where they are (i.e., both positions *and momenta* remain fixed);

(b) particles initially inside Λ_s move under their mutual interaction, with constant external forces exerted by the particles outside and with elastic reflection at the boundary of Λ_s.

The definition of Gibbs state readily implies that every Gibbs state is invariant under $T^t_{(s)}$ for all s. We are going to construct solutions to the equations of motion as limits, as $s \to \infty$, of $T^t_{(s)}$.

To do this, we introduce functions

$$\bar{B}_{(s)}(\boldsymbol{x}) = \frac{1}{\pi}\int_{-\infty}^{\infty} dt \frac{B(T^t_{(s)}\boldsymbol{x})}{1+t^2}$$

on the infinite system phase space. As before

$$\int \bar{B}_{(s)}\, d\mu = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{dt}{1+t^2} \int d\mu(\boldsymbol{x})\, B(T^t_{(s)}\boldsymbol{x}) = \int B\, d\mu \tag{4}$$

for all s, so $\bar{B}_{(s)} < \infty$ almost everywhere. Also, if $\bar{B}_{(s)}(\boldsymbol{x}) \leqq b < \infty$, then, for any i and $|t| \leqq \tau$,

$$\left|\int_0^t dt_1 \frac{dq_i^{(s)}(t_1)/dt}{\log_+(q_i^{(s)}(t_1))}\right| \leqq \left|\int_0^t dt_1\, B(T^{t_1}_{(s)}\boldsymbol{x})\right|$$
$$\leqq (1+\tau^2)\pi \frac{1}{\pi}\int_{-\tau}^{\tau} dt_1 \frac{B(T^{t_1}_{(s)}\boldsymbol{x})}{1+t_1^2} \leqq (1+\tau^2)\cdot\pi\cdot b,$$

and hence, in the notation of Proposition 1,

$$|q_i^{(s)}(t) - q_i| \leqq M((1+\tau^2)\cdot\pi\cdot b)\log_+(q_i)$$

for all i and all t with $|t| \leqq \tau$. This inequality is a kind of localization condition which says that particles stay relatively near their initial positions. We would like to have a bound like this which is uniform in s, for almost all $\boldsymbol{x}$. To get this bound, let

$$\bar{B}_\infty(\boldsymbol{x}) = \liminf_{s\to\infty} \bar{B}_{(s)}(\boldsymbol{x}).$$

By Fatou's lemma, $\bar{B}_\infty$ is integrable and hence is finite almost everywhere. We will show that, if $\bar{B}_\infty(\boldsymbol{x})$ is finite, then there is a solution of the equations of motion with initial data $\boldsymbol{x}$. If $\bar{B}_\infty(\boldsymbol{x})$ is finite, there is a real number b and a sequence (s_n) increasing to infinity such that $\bar{B}_{(s_n)}(\boldsymbol{x}) \leqq b$ for all n. By the argument just given, this means that, for any positive τ,

$$|q_i^{(s_n)}(t) - q_i| \leqq M((1 + \tau^2)\cdot\pi\cdot b) \log_+(q_i) \tag{5}$$

for all i and all t with $|t| \leqq \tau$.

It is now easy to finish the proof. The bound (5) together with the finite range of the interaction places a bound on the number of particles which can interact with the ith particle for times between $-\tau$ and τ. Since the potential has no singularities, the force which can be exerted by any single particle is bounded so this gives a bound on $|dp_i^{(s_n)}(t)/dt|$ for any fixed i which is uniform in t between $-\tau$ and τ and uniform in n provided s_n is large enough so the inequality (5) prevents the ith particle from colliding with the wall between time $-\tau$ and τ. The Arzelà-Ascoli theorem implies that a subsequence of the $p_i^{(s_n)}(t)$ converges uniformly for t between $-\tau$ and τ. But i and τ are arbitrary, so a diagonal procedure gives a subsequence along which each $p_i^{(s_n)}(t)$ converges uniformly on every bounded interval of times. Let us denote the limits by $(p_i(t))$. If we define

$$q_i(t) = q_i + \int_0^t dt_1\, p_i(t_1)/m \tag{6}$$

then a straightforward passage to the limit in the corresponding equation for the $p_i^{(s_n)}(t)$ gives

$$p_i(t) = p_i + \int_0^t dt_1 \sum_{j\neq i} F(q_i(t_1) - q_j(t_1)) \tag{7}$$

and equations (6) and (7) are simply the integral form of Newton's equations of motion. We have thus proved

THEOREM 2. *Let Φ be a finite-range superstable potential with Lipschitz continuous derivative, and let μ be a Gibbs state for Φ. Let $\bar{B}_\infty$ be defined as above. Then*

(i) *$\int \bar{B}_\infty\, d\mu < \infty$, and in particular $\bar{B}_\infty$ is finite almost everywhere.*

(ii) *If $\bar{B}_\infty(\boldsymbol{x})$ is finite, there exists a solution $\boldsymbol{x}(t) = (q_i(t), p_i(t))$ of the equations of motion with $\boldsymbol{x}(0) = \boldsymbol{x}$ which satisfies the localization condition*

$$\sup_{|t|\leqq\tau} \sup_i \frac{|q_i(t) - q_i|}{\log_+(q_i)} < \infty \tag{8}$$

for all finite τ.

An existence theorem like this one, without a corresponding uniqueness result, is of very little use. Furthermore, examples can be found in which solutions are nonunique, at least for systems of infinitely many hard spheres. Fortunately, the localization condition (8), together with some mild restrictions on the initial phase point $\boldsymbol{x}$ (which hold almost everywhere with respect to each Gibbs state), suffices to determine the solution uniquely. The proof of uniqueness is straightforward: The equations are rewritten as integral equations:

$$q_i(t) = q_i + t(p_i/m) + \int_0^t dt_1 \int_0^{t_1} dt_2\, F_i(t_2),$$

$$F_i(t) = \sum_{j \neq i} F(q_i(t) - q_j(t));$$

it is assumed that these equations have two solutions satisfying the same initial condition; the equations are subtracted and the localization condition (8) is inserted to obtain an integral inequality which is iterated to show that the two solutions must have been identical.

Once uniqueness has been established, the solution mappings give a flow T^t on the infinite system phase which is defined almost everywhere with respect to each Gibbs state. It may further be shown that T^t leaves each Gibbs state invariant, and that $T^t_{(s)}$ converges in measure to T^t as s approaches infinity.

The results described above are discussed in more detail in [3]; a slightly different proof is given in [5]. A manuscript giving the extension to long-range and singular interactions is in preparation. It should be mentioned that there is another approach to the problem of infinite system dynamics, due to Sinaĭ, in which it is shown that almost all initial phase points admit solutions in which, over any bounded interval of time, the particles break up into finite noninteracting clusters. This is proved for arbitrary densities in one dimension [7] and for small densities in more than one dimension [8]; it is surely not true at high densities in more than one dimension.

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